NEW CHEMICAL

ENVIRONMENTAL FATE AND EFFECTS SCIENCE CHAPTER

Environmental Fate and Ecological Risk Assessment

For

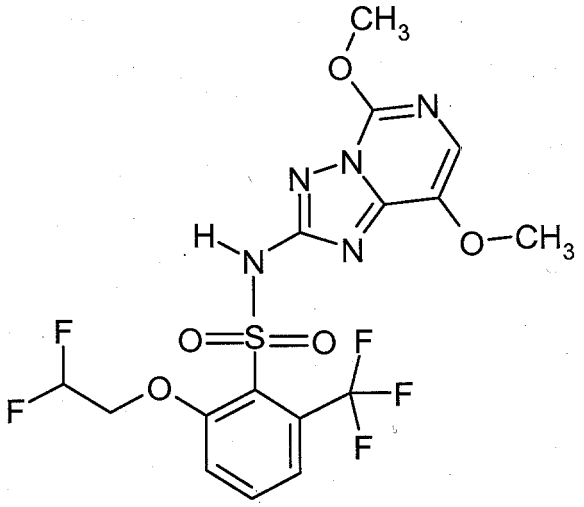
PENOXSULAM
(CAS No. 219714-96-2, Company Code: XDE-638)

IUPAC Name

3-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-α,α,α-trifluorotoluene-2-sulfonamide

CAS Name

2-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide



P.C. Code 119031

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I. EXECUTIVE SUMMARY

A. Predicted Environmental Exposure

1. Nature of Chemical Stressor

Penoxsulam is a new post-emergence, acetolactate synthase (ALS) inhibitor herbicide developed by Dow AgroSciences to be used as a foliar spray on dry-seeded rice crops, or as either a foliar spray or a granular formulation on water-seeded rice crops in order to control broadleaf weeds, aquatic plants, and certain grasses.

This report focused on the proposed agronomic practices associated with the use of penoxsulam on rice crops in the main rice growing regions of the United States – the Gulf Coast, the lower Mississippi Valley, and central California. Penoxsulam comes in liquid and granular formulations. Foliar application is recommended for use of the liquid formulation of penoxsulam on both dry- and water-seeded crops. For water-seeded rice, the application practice is to lower the paddy water depth sufficiently to expose at least 50% of the target plant before spraying. The granular formulation of penoxsulam is only recommended for use on flooded paddies. In its application, the water depth is raised sufficiently to completely submerge the target plants. Although rice paddies are typically constructed to limit the amount of water escaping into the open environment, penoxsulam can reach surface waters through spray drift and particulate drift during application, or by subsequent release of paddy water.

2. Environmental Fate

Screening level environmental fate assessments of pesticides being applied directly to water typically assume a water body depth and use the application rate to estimate potential environmental concentrations. A similar approach was taken in this risk assessment. For assessing the risk to aquatic plants and terrestrial plants in semi-aquatic settings, an approved interim modeling approach for rice was used to estimate both peak concentrations and holding periods which would ensure released paddy water would not exceed levels of concern.

The major route of dissipation for penoxsulam is through direct aqueous photolysis in clear and shallow surface water under favorable light conditions, a common condition in rice paddies where the crop canopy has not yet fully developed. Penoxsulam is somewhat persistent in aerobic soil environments. Although Penoxsulam is very mobile, the design of paddies to maintain a permanent flood and the lack of persistence in paddy water limit the ability to leach to ground water. Considering its low vapor pressure and Henry's Law constant, volatilization from soil and water is not expected to contribute significantly to the dissipation of penoxsulam into the environment. Penoxsulam has low potential to bioaccumulate in fish.

Eleven major degradation products have been identified[1] [BSTCA, 2-amino-TCA, 5-OH-penoxsulam, SFA, sulfonamide, 5,8-di-OH-penoxsulam, BSA, 2-amino-TP, TPSA, BSTCA methyl, and 5-OH 2 amino TP]. Data are not available to fully characterize these degradates and their respective degradation pathways. The uncertainty introduced by this absence of information

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[1]see **Table A6** in **Appendix A** for the structures and full Chemical Abstract Service Names of the penoxsulam transformation products.

was addressed in the screening assessment by using the acute penoxsulam concentration as the chronic concentration for risk quotient determination. This approach ensures that the assessment addresses the potential threat posed by degradates as long as they are not significantly more toxic or persistent than the parent. Based on a limited analysis using the Office of Toxic Substance's ECOSAR program (described in greater detail in Chapter IV under uncertainties), it is believed that this is a valid assumption. Additional information on the toxicity of all major degradates to terrestrial plants and to Duckweed would improve confidence in this risk assessment. The latter would be especially useful for assessing the paddy holding times that would provide greater confidence that levels of concern (LOCs) were not exceeded upon water release.

B. Potential Risks to Non-Target Organisms in the Rice Use Pattern

As an acetolactate synthase (ALS) inhibitor, the expected potential direct risks to be posed by penoxsulam would be to aquatic and terrestrial plants. Indirect effects due to habitat loss or alteration were not addressed.

Terrestrial plants

Tests of terrestrial plants were not conducted with the end use product. Rather, studies were done on a number of plants using only the technical grade active ingredient in a crop oil concentrate. Data should be provided based on testing of the end use product. Penoxsulam use poses potential acute risk to non-target terrestrial and aquatic plants. Tier 1 screening level risk quotients (RQs) for terrestrial plants exceeded levels of concern (LOCs) for four out of ten crops tested[2] for seedling emergence with peak RQs of 44 for non-endangered and 120 for endangered terrestrial plants based on testing of onions. Vegetative vigor testing resulted in exceedances for eight out of ten crops tested with peak RQs of 13 for non-endangered plants based on testing of soybean and 120 for endangered plants based on testing of ryegrass. Shoot weight was the sensitive endpoint for each of these risk quotients. Because potential levels of concern for terrestrial plants were exceeded, AgDrift modeling was conducted to provide estimates of required buffer zones to reduce drift below levels of concern. The results of these analyses are detailed in Chapter IV. Chapter IV also details threatened and endangered species potentially at risk if they are present inside of the indicated buffer zones.

For exposure of terrestrial plants in semi-aquatic settings, seedling emergence is one of two endpoints to be addressed by a risk assessment. Release and run off to these areas of paddy water could pose residual phytotoxicity concerns if paddy water was released too soon after treatment or if degradates have analogous toxicity to the parent. No degradate seedling emergence data were provided. ECOSAR does not provide estimates of relative terrestrial plant phytotoxicity, so this remains an uncertainty in the risk assessement. As a minimum, Tier 1 seedling emergence and vegetative vigor tests should be completed for all major degradates, with Tier 2 testing conducted as needed.

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[2]Four out of ten seedling emergence tests were not conducted at sufficiently high concentrations to unequivocally rule out exceedances for non-threatened or endangered plants.

Aquatic plants

Test data on aquatic plants were provided with some tests utilizing the technical and other tests using the end-use product or selected degradates. The technical grade product produced screening level exceedances for endangered vascular plants (RQ of 45) and non-endangered aquatic vascular plants (RQ of 15). RQs for endangered nonvascular aquatic plants using the technical grade product and the end-use product were 9 and 5, respectively.

Based on evaluation of penoxsulam fate data, computations were made to estimate the paddy water holding time which would provide sufficient penoxsulam degradation to not pose a potential threat to aquatic plants upon release. Computations detailed later in the report suggest this would take 13 to 23 days to address all Level of Concern issues.

It is important to note, however, that this estimate does not consider the potential impacts of non-tested degradates. In particular, BSTCA methyl,5,8-di-OH-penoxsulam, and SFA are untested degradates for which ECOSAR projects analogous toxicity to the parent. These degradates should be tested on Duckweed.

Terrestrial and aquatic animals

Penoxsulam is practically nontoxic to terrestrial and aquatic vertebrates and practically nontoxic to moderately toxic to aquatic invertebrates. No RQ for liquid penoxsulam exceeded a LOC for an animal. The results of screening-level risk assessments are interpreted to mean that liquid penoxsulam has little potential to cause direct effects to these animals at proposed application rates. However, data were not provided to EFED on the effects of degradates on mammals and birds. Without this information, it is impossible to establish the potential of the degradates, some of which are more persistent than the parent, to pose a risk through contaminated foliage or small insect consumption.

II. PROBLEM FORMULATION

This environmental fate and effects risk assessment is intended to support the Registration Division risk management decision for both the liquid and the granular formulations of a new post-emergence chemical herbicide, penoxsulam. This first-time use of penoxsulam is being proposed for the food crop, rice. In this document, EFED has characterized the potential risk of ecological effects from use on rice grown under both dry- and water-seeded conditions. The new chemical screen package requesting review of the supporting data was submitted under DP barcode #288160. Proposed product labels have been submitted under the following DP barcodes:

#298227 for the Granite SC-SL (21.7%) label,

#298401 for the GRASP or GF-443-SC (21.7%) label,

#298489 for the Technical (98%) label,

#298490 for the Granite - granule/waterseeded rice-G (0.24%) label,

#298491 for the GF-947- granule/waterseeded rice-G (0.24%) label, and

#298492 for the manufacturing use product (50%) label.

A. Stressor Source and Distribution

1. Chemical Properties

Penoxsulam's chemical names or other designations and a table of selected physicochemical properties are given below in Table 1.

2. Mode of Action

Penoxsulam is a systemic, post-emergence herbicide belonging to the triazolopyrimidine sulfonamides chemistry family. The mode of action upon susceptible weeds is by inhibition of acetolactate synthase (ALS), the first enzyme in the biosynthetic pathway for the amino acids leucine, valine, and isoleucine.

3. Use Characterization

End-Use Products

Dow AgroSciences is petitioning for the registration of the post-emergence herbicide penoxsulam for use on rice when formulated into the end-use products:

GF-443 SC SF and Grasp SC, (liquid products containing 21.7% active ingredient); GF-947 Granule SF and Grasp GR (granular products containing 0.24% active ingredient); and

Granite GR and Granule CA (granular products formulated for use in California containing 0.24% active ingredient).

The proposed label recommends application rates for the end-use products of 2.8 fl. oz./acre for the liquid formulations, and 18.5 lbs./acre for the granular formulations. The one seasonal application allowed for the formulated product on each of these labels is equivalent to an annual application rate for the active ingredient of 0.044 lb./acre (49 g/ha).

Table 1. Physical-Chemical Properties of Penoxsulam

PARAMETER	VALUE
Chemical name	2-(2,2-difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide
Chemical Abstract Service number	219714-96-2
Molecular weight	483.4
Solubility in water	5.7 mg/L (pH 5), 410 mg/L (pH 7), 1500 mg/L (pH 9)
pK_a	5.1
Vapor pressure at 25°C	9.55×10^{-14} Pa
Octanol-water partition coefficient (log K_{ow})	1.1 (pH 5), -0.60 (pH 7), -1.4 (pH 9)
Hydrolysis half-life (pH 5, pH 7, pH 9)	stable
Aqueous photolysis half-life	$t_{1/2}$ = 1.5 - 14 days
Soil photolysis half-life	$t_{1/2}$ = 19 - 109 days
Aerobic metabolism half-lives	$t_{1/2}$ = 12 - 118 days
Anaerobic metabolism half-lives	$t_{1/2}$ = 6.6 - 11 days
Soil-water distribution coefficient (K_d)	13 - 305 (1130 sediment) mL/g

Application Methods

The proposed label for penoxsulam would allow both ground and aerial application from the one leaf stage of the rice up to 60 days prior to harvest, the specific timing of the application dependant upon the type of weeds requiring treatment. It is recommended not to apply penoxsulam through any type of irrigation system.

In the United States, rice is grown primarily in two regions. The Southern region consists of the Gulf Coast of Texas and Louisiana and the Mississippi River Valley in Louisiana, Mississippi, Arkansas, and Missouri. The remainder of domestic rice production is located in the Sacramento Valley and San Joaquin Valley in California.

The irrigation of rice paddies in association with rice cultivation follows a variety of practices. At the one extreme, there is dry seeding wherein seeds are grown in dry beds several weeks before establishing a permanent flood in the paddy. Small amounts of water are used to assist seed germination, but the field is left dry until the rice has sprouted and begun to grow. This is the most common practice in the Southern region of the United States.

There also is "pin point" flood culture, where sprouted rice is aerially applied to flooded fields. The fields are drained a few days after seeding, and then flooded several days later. Water is released from the paddy then re-flooded primarily to inhibit red rice growth by draining after pre-spouted rice has become established but before the red rice has pegged (put down roots) and to reduce arsenic concentrations which can affect grain formation through a condition known as"straight-heading". When rice is water seeded in the Southern region, the "pin-point flood" culture is the preferred method. Applying pre-sprouted rice to a field is known as wet seeding.

At the other end of the continuum are practices such as continuous flood, where there is a steady flow of aerobic water through the paddy. In California, the majority of rice production is water seeded with a continuous flood. [3] Further discussion in this risk assessment will refer to the first practice as "dry seeding", the second practice as "wet seeding", and the latter practice as "water seeding".

When a liquid formulation (either GF-443 SC SF or Grasp SC) is applied preflood to dryseeded rice crops, it is recommended to flush the field first if moisture stressed, then drain to expose at least 50% of weed. When applied postflood, it is also recommended to drain enough water to expose at least 50% of weed. It is specified that either a surfactant or a crop oil concentrate other than organosilicone must be added to liquid formulated penoxsulam.

When a granular formulation (GF-947 Granule SF, Grasp GR, Granite GR, Granule CA) is applied, paddies are pre-flooded to a depth of 2 to 4 inches, completely submerging the weeds prior to application. The 2 to 4 inch water depth is maintained for 10 days post application for optimum weed control, but may be increased to provide coverage of the target plants. Treated land should not be rotated with crops other than rice for three months following application. The

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[3]Breithaupt, James; February 2001 RED Science Chapter for Molinate; Appendix A - Use Profile; edited for generic rice crops

labels for the granular formulations indicate that penoxsulam provides some residual weed control to susceptible weed species.

The label indicates penoxsulam can be applied to fields used for crayfish production. However, the label advises not to fish, or commercially grow fish, shellfish or other crustaceans on treated acres during the year of treatment. There is no indication on the label that a safener is present in the formulated products.

Target Crops and Pests

The proposed label for penoxsulam would allow only one application (ground or aerial) between the one leaf stage of rice crops and 60 days prior to rice harvest, depending on the type of weeds requiring treatment. This herbicide is intended to control broadleaf weeds, aquatic plants and certain grasses, all at differing developmental stages depending upon the specific target weed.

As indicated earlier in the use characterization portion of this chapter, rice may be dry seeded, water seeded, or wet seeded. In any case, there are scenarios under which penoxsulam and its transformation products will eventually have the potential for release to non-target aquatic environments. The amount which will be released will be dependent on a variety of factors, most significantly whether there is a period between pesticide application and field flooding and the time between pesticide contact with the water and its subsequent release[4]. For the purposes of acute aquatic exposure assessment to the liquid form of the pesticide, it has been assumed that the pesticide is directly applied to paddy water and immediately released. This assumption most closely tracks the principal agronomic practice used in California. Terrestrial plants in terrestrial settings are assumed to be exposed only to spray drift while terrestrial plants in semi-aquatic settings are assumed to be exposed to both aqueous runoff (release) and spray drift.

To better quantify the uncertainty introduced by this approach in other application scenarios, modeling is conducted to assess the relative reduction in released penoxsulam concentration that might be anticipated with various holding times in the paddy prior to release. This second approach will enable the risk assessment to bracket the range of expected concentrations which might be observed as a result of coupling water holding times with typical agronomic practices.

4. Environmental Fate

Penoxsulam is expected to be very mobile, but not persistent, in both aqueous and terrestrial environments. Penoxsulam exists almost exclusively in a disassociated state at pH values normally found in rice paddy water, but not in terrestrial environments where lower pH values may be found. Penoxsulam degrades by two different transformation mechanisms,

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[4]The continuous flow of water normally maintained through rice paddies to ensure aerobic conditions is interrupted when holding times are required. Release of the paddy water after a holding time means that the continuous flow is reinstated, allowing paddy water from adjacent fields to mix. Paddies are not drained after holding times unless otherwise indicated by normal agronomic practices.

producing thirteen different identified transformation products, for photolytic and biotic degradation.

Persistence

Penoxsulam is not expected to be persistent in the environment. In aqueous environments, penoxsulam is expected to be stable to hydrolysis, but to dissipate rapidly through aqueous photolysis in clear shallow waters, and somewhat more slowly through biotic degradation when sunlight has a limited ability to penetrate turbid waters, or when waters are shaded by trees, riparian vegetation, and/or crop canopies. In terrestrial environments, penoxsulam is expected to dissipate through soil photolysis and aerobic soil degradation.

Transport

Penoxsulam is expected to be very mobile in both aqueous and terrestrial environments, not binding strongly to either soil or sediment. Submitted mobility data for three penoxsulam degradation products (BSTCA, 5-OH-penoxsulam, and BST) indicate environmental mobility roughly equivalent to the parent compound. However, there are no data regarding the mobility of the remaining transformation products nor of combined parent/degradate residues. Penoxsulam has low volatility indicating that atmospheric transport is, at best, a very minor route of transportation.

Transformation

Data are not available to fully characterize the complex, potential degradation pathways of penoxsulam. Submitted laboratory studies demonstrate that penoxsulam transforms by competing mechanisms, through several generations of degradation products. Examination of the specific transformation products formed in the submitted laboratory studies suggests that the more rapid photolytic transformation proceeds primarily through cleavage of the parent molecule on, or adjacent to, the sulfonamide bridge. The slower biotic degradation pathway proceeds primarily through fragmentation of the pyrimidine ring or its residues. This complex degradation pathway of penoxsulam produces a large number of degradation products.

Only limited fate data are available for the penoxsulam transformation products. Six of the thirteen identified transformation products failed to reach peak concentrations at study termination: 2-amino-TP, BSTCA, 2-amino-TCA, SFA, sulfonamide and 5,8-di-OH penoxsulam. These six compounds are potentially more persistent than the parent compound, and would probably have reached even greater concentrations with time. Eleven of the thirteen penoxsulam transformation products reported in laboratory studies are considered major degradates: BSA, 2-amino-TP, TPSA, BSTCA methyl, BSTCA, 2-amino-TCA, 5-OH-penoxsulam, SFA, sulfonamide, 5,8-di-OH and 5-OH 2 amino TP. Two of the thirteen penoxsulam transformation products are considered minor degradates: di-FESA and BST.(see **Table 6A** in **Appendix A** for the structure and full Chemical Abstract Service Names of the penoxsulam transformation products).

Bioaccumulation

Bioconcentration in fish data are not available for either parent or degradates, but submitted supplemental data do not suggest that penoxsulam will bioconcentration. Further, what

accumulation that was observed in testing of crayfish was followed by rapid depuration. Given penoxsulam's proposed single annual application, this is unlikely to be an issue.

B. Assessment Endpoints

Assessment endpoints are defined as "explicit expressions of the actual environmental value that is to be protected". Defining an assessment endpoint involves two steps: 1) identifying the valued attributes of the environment that are considered to be at risk, and 2) operationally defining the assessment endpoint in terms of an ecological entity (*i.e.*, a community of fish and aquatic invertebrates) and its attributes (*i.e.*, survival and reproduction). Therefore, selection of the assessment endpoints is based on valued entities (*i.e.*, ecological receptors), the ecosystems potentially at risk, the migration pathways of pesticides, and the routes by which ecological receptors are exposed to pesticide-related contamination. The selection of clearly defined assessment endpoints is important because they provide direction and boundaries in the risk assessment for addressing risk management issues of concern.

1. Ecosystem(s) Potentially At Risk

Ecosystems potentially at risk are expressed in terms of the selected assessment endpoints. The typical assessment endpoints for screening-level pesticide ecological risks are reduced survival, and reproductive and growth impairment for both aquatic and terrestrial animal species. Aquatic animal species of potential concern include freshwater fish and invertebrates, estuarine/marine fish and invertebrates, and amphibians. Terrestrial animal species of potential concern include birds, mammals, beneficial insects, and earthworms. For both aquatic and terrestrial animal species, direct acute and direct chronic exposures are considered. Although these endpoints are measured at the individual level, they provide insight about risks at higher levels of biological organization (*e.g.* populations and communities). For example, pesticide effects on individual survivorship have important implications for both population rates of increase and habitat carrying capacity.

For terrestrial and semi-aquatic plants, the screening assessment endpoint is the perpetuation of populations of non-target species (crops and non-crop plant species). Existing testing requirements have the capacity to evaluate emergence of seedlings and vegetative vigor. Although it is recognized that the endpoints of seedling emergence and vegetative vigor may not address all terrestrial and semi-aquatic plant life cycle components, it is assumed that impacts at emergence and in active growth have the potential to impact individual competitive ability and reproductive success.

For aquatic plants, the assessment endpoint is the maintenance and growth of standing crop or biomass. Measurement endpoints for this assessment endpoint focus on algal and vascular plant (*i.e.*, duckweed) growth rates and biomass measurements.

The ecological relevance of selecting the above mentioned assessment endpoints is as follows: 1) complete exposure pathways exist for these receptors; 2) the receptors may be potentially sensitive to pesticides in affected media and in residues on plants, seeds, and insects;

and 3) the receptors could potentially inhabit areas where pesticides are applied, or areas where runoff and/or spray drift may impact the sites because suitable habitat is available.

2. Ecological Effects

Each assessment endpoint requires one or more "measures of ecological effect," which are defined as changes in the attributes of an assessment endpoint itself or changes in a surrogate entity or attribute in response to exposure to a pesticide. Ecological measurement endpoints for the screening-level risk assessment are based on a suite of registrant-submitted toxicity studies performed on a limited number of organisms in the following broad groupings:

- Birds (mallard duck and bobwhite quail) used as surrogate species for terrestrial-phase amphibians and reptiles,
- Mammals (laboratory rat),
- Freshwater fish (bluegill sunfish and rainbow trout) used as a surrogate for aquatic phase amphibians,
- Freshwater invertebrates (*Daphnia magna*),
- Estuarine/marine fish (Silverside),
- Estuarine/marine invertebrates (*Crassostrea virginica* and *Americamysis bahia*),
- Terrestrial plants (corn, onion, ryegrass, wheat, cucumber, soybean, tomato, sugar beets, cotton, and kale), and
- Algae and aquatic plants (*Selenastrum capricornutum* and *Lemna gibba*).

Within each of these very broad taxonomic groups, an acute and chronic endpoint is selected from the available test data, as the data sets allow. Additional ecological effects data were available for other taxa and have been incorporated into the risk characterization as other lines of evidence. These data include:

- Acute laboratory toxicity data on non-guideline freshwater invertebrates including midges, and amphipods and
- Acute laboratory contact and oral toxicity on honeybees.

A complete discussion of all toxicity data available for this risk assessment and the resulting measurement endpoints selected for each taxonomic group are included in Section III.B of this document. A summary of the assessment and measurement endpoints selected to characterize potential ecological risks associated with exposure to penoxsulam and its degradates is provided in Table 2.

Table 2. Summary of Assessment and Measurement Endpoints

Assessment Endpoint	Measurement Endpoint
1. Abundance (*i.e.*, survival, reproduction, and growth) of bird populations	1a. Bobwhite quail acute oral LD_{50} 1b. Bobwhite quail and mallard duck subacute dietary LD_{50} 1c. Bobwhite quail and mallard duck chronic reproduction NOAEC and LOAEC
2. Abundance (*i.e.*, survival, reproduction, and growth) of mammal populations	2a. Laboratory rat acute oral LD_{50} 2b. Laboratory rat developmental and chronic NOAEC and LOAEC
3. Survival and reproduction of freshwater fish and invertebrate communities	3a. Rainbow trout and bluegill sunfish acute LC_{50} 3b. Rainbow trout chronic (early-life) NOAEC and LOAEC 3c. Water flea (and other freshwater invertebrates) acute EC_{50} 3d. Water flea chronic (life-cycle) NOAEC and LOAEC
4. Survival and reproduction of estuarine/marine fish and invertebrate communities	4a. Sheepshead minnow acute LC_{50} 4b. Estimated chronic NOAEC and LOAEC values based on the acute-to-chronic ratio for freshwater fish 4c. Eastern oyster and mysid acute LC_{50} 4d. Mysid chronic (life-cycle) NOAEC and LOAEC
5. Perpetuation of populations of non-target terrestrial and semi-aquatic species (crops and non-crop plant species)	5a. Monocot and dicot seedling emergence and vegetative vigor EC_{25} values
6. Survival of beneficial insect populations	6a. Honeybee acute contact LD_{50}
7. Maintenance and growth of standing crop or biomass of aquatic plant populations	7a. Algal and vascular plant (*i.e.*, duckweed) EC_{50} values for growth rate and biomass measurements

LD_{50} = Lethal dose to 50% of the population.

NOAEC = No observed adverse effect level.

LOAEC = Lowest observed adverse effect level.

LC_{50} = Lethal concentration to 50% of the population.

EC_{50}/EC_{25} = Effect concentration to 50%/25% of the population.

C. Conceptual Model

In order for a chemical to pose an ecological risk, it must reach ecological receptors in biologically significant concentrations. An exposure pathway is the means by which a contaminant moves in the environment from a source to an ecological receptor. For an ecological exposure pathway to be complete, it must have a source, a release mechanism, an environmental transport medium, a point of exposure for ecological receptors, and a feasible route of exposure. In addition, the potential mechanisms of transformation (*i.e.*, which degradates may form in the environment, in which media, and how much) must be known, especially for a chemical whose metabolites/degradates are of greater toxicological concern. The assessment of ecological exposure pathways, therefore, includes an examination of the source and potential migration pathways for constituents, and the determination of potential exposure routes (*e.g.*, ingestion, inhalation, dermal absorption).

Ecological receptors that may potentially be exposed to penoxsulam and its degradates include terrestrial and semi-aquatic wildlife (*i.e.*, mammals, birds, and reptiles), terrestrial and semi-aquatic plants, and soil invertebrates. In addition to terrestrial ecological receptors, aquatic receptors (*e.g.*, freshwater and estuarine/marine fish and invertebrates, amphibians) may be exposed to potential migration of pesticides from the site of application to various watersheds and other aquatic environments via release or granular/spray drift. However, because penoxsulam is an ALS inhibitor, it is not anticipated to be very toxic to aquatic or terrestrial animals.

The main sources in the environment for the stressor, the post-emergence herbicide penoxsulam, are through direct application to either wet- or dry-seeded rice crops, and through spray drift. Unlike terrestrial row crops, the major growth and development phases for a rice crop take place in a flooded field, or paddy. A paddy is typically designed to capture and maintain a uniform depth of irrigation (flood) water. This design minimizes aquatic transport via levee overflow, breaching, and leaching (also known as deep percolation).

Surface water contamination by penoxsulam is assumed to occur through drift or designed release to a stream or pond. Potential emission of volatile compounds is not considered as a viable release mechanism, since volatilization is not expected to be a significant route of dissipation for this chemical. Likewise, because paddies are generally designed to effectively retain water, the potential for ground water contamination is considered low. Exposure to terrestrial animals could occur through consumption of drift-contaminated vegetation on berms and adjoining fields or direct consumption of the granular.

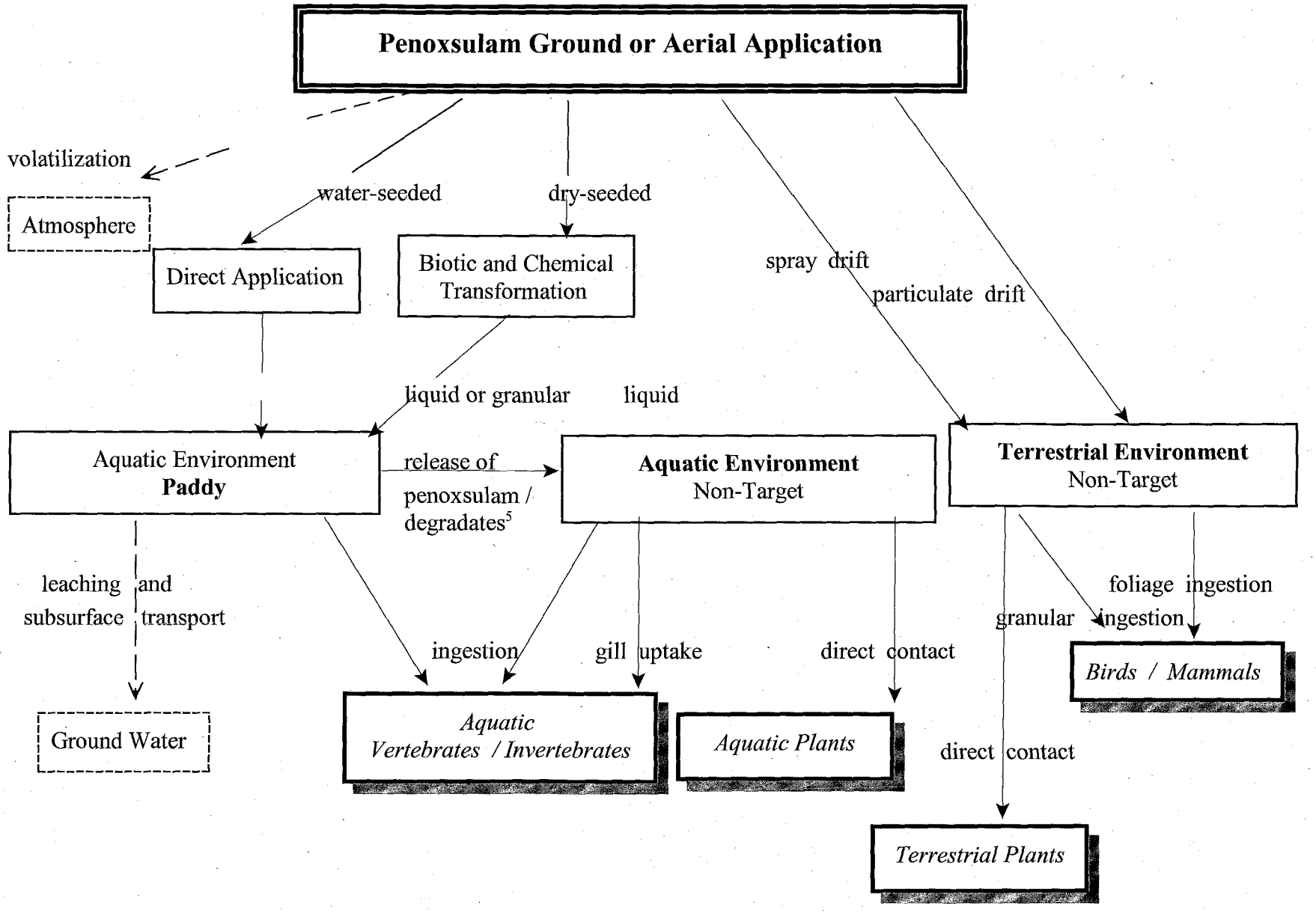
For terrestrial plants in terrestrial settings, exposure is assumed to occur through direct spraying or drift. The assessment endpoints considered are vegetative vigor and seedling emergence. For terrestrial plants in semi-aquatic settings, the possibility of exposure from release of paddy water to low lying areas cannot be ruled out. This release is modeled based on the presumption that one acre of paddy water is released onto one acre of non-target plants. The endpoint evaluated is seedling emergence. Spray drift is modeled as for terrestrial settings.

For aquatic plants, exposure is assessed as a consequence of immediate release of paddy water because at least some cultivation practices involve continuous flow through and the label does not specify a minimum holding time post treatment. From an efficacy standpoint, some holding interval is likely. Modeling is also conducted to ascertain the holding period which would drop paddy water concentrations beneath levels of concern.

A cursory review of the physical and chemical properties of penoxsulam, as outlined in Table 1, indicates that fairly rapid transformation can be expected for penoxsulam in the environment. These properties, coupled with the extremely low application rate of penoxsulam suggest limited need to consider long term or indirect effects. In addition, food chain accumulation is not expected.

The conceptual site model is shown in Figure 1.

Figure 1: Transport Pathway for Combined Penoxsulam and Transformation Product Residues



[5] **Biotic Degradates** - BSTCA, BSTCA methyl, 5-OH penoxsulam, BST, SFA, sulfonamide, 5,8-di OH
Chemical Transformation Products - BSTCA, BSTCA methyl, BSA, 2-amino TP, TPSA, 5-OH 2-amino TP, TCA, di-FESA

D. Key Uncertainties and Information Gaps

There is currently no peer-reviewed modeling approach within EFED that takes into account transformation and/or degradation processes while estimating chronic pesticide concentrations in rice paddy water. Dow AgroSciences has submitted a document (MRID 458308-11) that addressed the modeling of chronic surface water concentrations of penoxsulam from the proposed use on rice. With some modification, Dow used an approach similar to modeling methods used for the propanil RED and cyhalofop butyl Section 3 documents. EFED also used the interim rice model with appropriate modification of input parameters, as is discussed later in the document.

A potentially major gap in this risk assessment is a lack of fate and ecological effects information on many of the degradates. On the one hand, only one treatment per season was proposed and it is recommended on the label that other crops not be grown in a field for at least three months after application of penoxsulam. On the other, there are eleven major degradates and the parent is expected to be relatively short lived in the paddy environment. The combination of these two pieces of information would suggest at least some of the degradates may provide some of the needed phytotoxicity. Studies were not submitted for many of the degradates.

From a fate perspective, six penoxsulam transformation products (BSTCA, BST, 2-amino-TP, 2-amino TCA, 5,8-diOH , and sulfonamide) reached peak concentrations at study termination. Laboratory data are not available to quantitatively determine degradation rates, and therefore the degree of persistence, for these transformation products under environmental conditions. Furthermore, mobility data submitted for three penoxsulam transformation products (BSTCA, BST, and 5-OH-penoxsulam) indicated mobility roughly equivalent to that of the parent compound, penoxsulam. However, laboratory data are not available to quantitatively determine the degree of mobility for seven identified transformation products under environmental conditions.

III. Analysis (*Selection and Evaluation of Data For Risk Characterization*)

A. Exposure Characterization

1. Evaluation of Aquatic and Terrestrial Fate Studies

Identification of Endpoints

A reported vapor pressure of 9.55×10^{-14} Pa at 25°C indicates that volatilization is not expected to be significant for penoxsulam in the environment.

In aqueous environments, penoxsulam is stable to hydrolysis at pH 5, pH 7 and pH 9. Penoxsulam is expected to dissipate in clear shallow waters through aqueous photolysis. Laboratory data indicate that the four photolytic half-lives reported for penoxsulam in water range from 1.5 to 3.1 days between pH 7 and pH 8, and 14 days at pH 5.8. A reported pK_a value of 5.1 suggests that pH may have an effect upon the photolytic half-life. However, the paddy

water in a cropped plot is known to rapidly equilibrate to at or above a pH 7 within a few hours of flooding, so pH should not significantly impact photolysis. Penoxsulam is expected to dissipate more slowly through biotic degradation when sunlight has a limited ability to penetrate colored or turbid waters, or when waters are shaded by trees, riparian vegetation, and/or crop canopies.

In terrestrial environments, penoxsulam is expected to dissipate through soil photolysis and biotic degradation. Penoxsulam has photolytic half-lives of 19 and 109 days, on the two soils studied at pH 6 ± 0.2. Aerobic soil metabolism was studied in three soils. The resulting three half-lives calculated through linear regression of log transformed data were 34 days, 43 days, and 118 days. Aerobic aquatic metabolism, the principal biotic degradation mechanism in rice paddies, was studied in six soil/water test systems. The six total system half-lives calculated through linear regression of log transformed data ranged from 16 to 38 days. Anaerobic aquatic metabolism, a degradation mechanism only anticipated in non-target environmental compartments, was studied in three soil/water test systems. The three total system half-lives calculated through linear regression of log transformed data were 5 days, 7 days, and 11 days.

Penoxsulam is expected to be very mobile in the environment. The soil to water partitioning coefficients (K_d) derived from the seventeen soils and one sediment studied ranged from 0.13 to 4.69, with an average value of 0.92 and a standard deviation of 1.07. However, if one excludes sand, volcanic, and Canadian soils which are not typical of rice growing regions, K_d values range from 0.13 to 1.96, with an average value of 0.62 and a standard deviation of 0.53.

Submitted mobility data for three penoxsulam degradation products, BSTCA, 5-OH-penoxsulam, and BST, indicate environmental mobility roughly equivalent to that of the parent compound. The soil to water partitioning coefficients (K_d) for BSTCA derived from the six soils studied ranged from 0.085 to 4.4. The soil to water partitioning coefficients (K_d) for 5-OH-penoxsulam, derived from the eight soils studied ranged from 0.14 to 1.4. The soil to water partitioning coefficients (K_d) for BST derived from the eight soils studied ranged from 0.075 to 0.61. However, there are no data regarding the degradation rates of other penoxsulam degradation products or the mobility of the remaining transformation products or of combined parent/degradate residues. Table 3 summarizes the environmental fate properties of penoxsulam. Information regarding the environmental fate studies used in this report is detailed in Appendix A. Table 4 summarizes the penoxsulam transformation products identified in the submitted data.

Table 3 - Summary of Environmental Fate Properties of Penoxsulam Used in Assessment

Study Type	Value	Test System	Study MRID	Study Status
Hydrolysis -- $t_{1/2}$	stable	pH 5, 7, 9 buffers / natural waters	45830721	acceptable
Photodegradation in Water -- $t_{1/2}$	1.5 days, 1.5 days, 3.1 days, 14 days	pH 7 buffer, pH 7.8 natural waters, pH 7 AR pond water, pH 5.8 flooded soil	45834801, 45830722	supplemental, supplemental
Photodegradation on Soil -- $t_{1/2}$	19 days, 109 days	flooded silt loam, silty clay loam	45830723	supplemental
Aerobic Soil Metabolism -- $t_{1/2}$	34 days, 43 days, 118 days	AR silt loam CA clay loam, ND loam	45830724	acceptable
Anaerobic Aquatic Metabolism -- $t_{1/2}$ (total system)	5 days, 11 days, 7 days	AR pond water / silt loam clay sediment, AR pond water / silt loam soil, distilled water / silty loam soil (Italy)	45830725	acceptable
Aerobic Aquatic Metabolism -- $t_{1/2}$ (total system)	16 days, 29 days, 12 days, 38 days, 30 days, 31 days	AR pond water / silt loam clay sediment, AR pond water / silt loam soil, Italian channel water / loam sediment, French lake water / sand sed., HPLC water / volcanic loam soil (Japan), HPLC water / loam soil (Japan)	45830726	acceptable
Adsorption/Desorption – K_d	0.37, 0.56, 0.49, 0.45, 1.96, 0.48, 0.16, 0.32, 1.4, 0.51, 0.64, 0.13	AR Silt loam Sandy clay loam (Japan), CA Clay loam ND Loam, (ND, USA) Silty clay loam (Italy), Silty clay loam (France), Sandy clay loam (UK), Sandy loam (Italy), AR Silty clay sediment Sandy loam (Brazil), Clay loam (Brazil), Sandy clay loam (Brazil)	45830801, 45834802, 45830802	acceptable, supplemental, (aged column mobility study of limited value) supplemental (BSTCA, BST, 5-OH-penoxsulam)
Bioconcentration in Aquatic, Non-Target Organisms - BCF	0.02 mL/g	crayfish (*Procambarus clarkii*), 14 days, at 0.5 ppm under flow-through conditions	45830001	acceptable
Aquatic Field Dissipation -- $t_{1/2}$ (total system)	16 days, 16 days, 5 days, 10 days, 4 days	AR bareground plot, dry seeded (liquid), AR cropped plot, dry seeded (liquid), CA bareground plot, water seeded (liquid), CA cropped plot, water seeded (liquid), CA cropped plot, water seeded (granular)	45830804, 45830805	supplemental, acceptable

Table 4 - Summary of Penoxsulam Transformation Products from Environmental Fate Data

Study Type	Degradates	Maximum % Applied	Major / Minor	Maximum at Study Termination*	Study MRID
Photodegradation in Water	BSA,	36%,	major,	no,	45834801,
	2-amino TP,	18%,	major,	no,	
	TPSA,	56%,	major,	no,	45830722
	2-amino-TCA,	85%,	major,	yes,	
	5-OH, 2-amino TP,	32%,	major,	no,	
	BSTCA methyl,	12%,	minor,	no,	
	BSTCA,	7.2%,	minor,	no,	
	di-FESA	7.6%	minor	no	
Photodegradation on Soil	BSTCA,	11%,	major,	no,	45830723
	2-amino TP,	10%,	major,	yes,	
	BSA,	8.1%,	minor,	no,	
	$^{14}CO_2$	3.2%	minor	yes	
Aerobic Soil Metabolism	BSTCA,	37%,	major,	yes,	45830724
	5-OH-penoxsulam,	63%,	major,	no,	
	SFA,	15%,	major,	yes,	
	sulfonamide,	33%,	major,	yes,	
	$^{14}CO_2$,	16%,	major,	yes,	
	BSTCA methyl,	1.4%,	minor,	no,	
	BST	6.3%	minor	no	
Anaerobic Aquatic Metabolism	BSTCA,	25%,	major,	no,	45830725
	BSTCA methyl,	13%,	major,	no,	
	5-OH-penoxsulam,	42%,	major,	no,	
	5,8-di OH,	11%,	major,	yes,	
	BST,	4.8%,	minor,	no,	
	$^{14}CO_2$	1.2%	minor	yes	
Aerobic Aquatic Metabolism	5-OH-penoxsulam,	40%,	major,	no,	45830726
	BSTCA,	39%,	major,	yes,	
	$^{14}CO_2$	2.4%	minor	yes	

*Maximum % of applied reported at study termination indicates that amounts may have continued to increased with time

Study Classification

All three of the submitted photodegradation studies, the aged soil column leaching study, and one of the two aquatic field dissipation studies have been classified as supplemental. In the soil photolysis studies, the mass balance was not acceptable, the temperature and the soil moisture were not adequately maintained. In the supplemental aqueous photolysis studies, either the test systems were not sterile, the study author had not adequately identified or described all

degradates >10% of applied, the mass balance for each test system was not adequate, and/or the CO_2 data were contradictory. In the aged soil column leaching study, only two soils and one label were used in one portion of the study, and insufficient water was used. In the aquatic field dissipation study, it could not determine whether the penoxsulam degradation products of toxicological concern which formed in the paddy water partitioned into the sediment or degraded. However, in spite of these deficiencies, no additional environmental fate data are required at this time.

Study Variability

The four photolytic half-lives reported for penoxsulam in water had R squared values for the regressed data points from each test system that ranged from 0.95 to 0.99. The two photolytic half-lives for penoxsulam on soil had R squared values for the regressed data points from each test system that ranged from 0.7 to 0.9. The three aerobic degradation half-lives for penoxsulam had R squared values for the regressed data points from each test system that ranged from 0.81 to 0.93, with an average value of 0.89. The six total system, aerobic aquatic degradation half-lives for penoxsulam had R squared values for the regressed data points from each test system that ranged from 0.80 to 0.99, with an average value of 0.91. The three total system, anaerobic aquatic degradation half-lives for penoxsulam had R squared values for the regressed data points from each test system of 0.98.

In some cases, use of non-linear regression to calculate half-lives would have produced a shorter half-life and an overall better fit for the values in that particular data set than linear regression of log transformed data. However, while linear regression of the log transformed data generally underestimates the initial degree of biotic degradation of pesticides in soil systems, non-linear regression generally underestimates the amount of parent material still present after several weeks/months of degradation. Additionally, for the purposes of generating an overall half-life value from multiple data sets, decrease in half-life would generally be offset by an increase in the standard deviation for the data sets.

2. Aquatic Organism Exposure Modeling

General Approach

EFED does not have a peer reviewed model for the assessment of releases from rice paddies. As an interim approach for the evaluation of registration actions, EFED has developed a screening model for calculating EECs and required holding times to provide a reasonable degree of confidence that levels of concern will not be exceeded. This model is identical to the one which has been used for previous rice pesticide evaluations.

Aquatic concentrations are estimated by applying the total annual application to the paddy[6], partitioning the pesticide between the water and the paddy sediment, then calculating the

[6]Since penoxsulam is a single application pesticide, the maximum single application is the annual application rate.

dissolved concentration occurring in the water column. This concentration represents the maximum concentration expected to be found in water released from the paddy. Degradation processes, dilution with uncontaminated water outside the paddy, and movement of pesticide on suspended sediment are not considered in this calculation.

While this approach is extremely conservative for estimating chronic environmental concentrations for quickly degrading compounds with short half lives, it also helps prevent underestimation in cases where little is known about major degradates and when labels do not contain explicit holding times for treated paddy water. It also provides some margin of safety in acute exposure assessments to reflect the paucity of information relating to the amount of paddy water that could reasonably be expected to impact any given acre of adjoining semi-aquatic areas[7]. It is less conservative than the approach taken to modeling aquatic pesticides where there is direct application to waterways.

The model paddy considered in estimating EECs with the interim method is assumed to have a four inch depth with the pore space in a 1 cm thick sediment interaction zone. A standard assumption is made for the bulk density of surface horizons of mineral soils. K_d and K_{oc} are estimated according to the methods recommended for other surface water models in EFED's Input Parameter Guidance (USEPA, 2002). The equation **(EQ1)** to use for this calculation is:

$$EEC = \frac{10^9 M_T}{V_T + m_{sed} K_d} \qquad \textbf{(EQ 1)}$$

where M_T is the total mass of pesticide in kg applied per ha of paddy, V_T is 1.067×10^6 L ha^{-1} which is the volume of water in a paddy 4 inches (10.16 cm) deep, and includes the pore space in a 1 cm sediment interaction zone. The mass of sediment, m_{sed}, is the amount found in the top 1 cm interaction zone and is 130,000 kg ha^{-1} when the sediment bulk density was assumed to be 1.3 kg L^{-1}, a standard assumption for the bulk density of surface horizons of mineral soils (Brady, 1984; Hillel, 1982). The 10^9 constant converts the units of mass from kg to μg.

When the level of concern in a risk assessment is not exceeded using an EEC calculated by this screening method, there is high confidence that there will be little or no risk above the level of concern from exposure through water resources. The size of the area and the length of time for which the estimate is reasonable depends upon how fast the pesticide degrades, the rate of removal onto uncontaminated bed sediments, the nature of the local stream network, and all of the previously mentioned factors.

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[7]This lack of information is in marked contrast to the conventional PRZM/EXAMS scenarios where one or ten acres of runoff are projected to impinge upon a one acre pond.

As a further refinement to calculating surface water environmental concentrations, the modeling approach used for the refined assessment associated with the propanil RED [8] was utilized. The refinement introduced in the propanil assessment partitions the pesticide between the paddy water and the soil, degrades the pesticide using the rate constant from the dominant mechanism for the environmental compartment, and calculates concentrations which can be useful for suggesting potential holding times of paddy water.

The dominant route of dissipation for penoxsulam in paddy water is expected to be through aqueous photolysis. However, photolysis can be strongly influenced by turbidity, clouds and canopy cover can also contribute to slower degradation rates. Dow, in a study submission (MRID 458308-11), proposed use of total system aquatic field dissipation rates to estimate suggested holding times. Because these rates were generally consistent with laboratory data, EFED also modeled decay using these rates[9].

Criteria For Scenario Selection

The interim approach described in this assessment is substantially independent of the location of US rice production. Consequently, no additional scenario development is required.

Model Results

Applying the method outlined in the current EFED interim policy for calculating estimated environmental concentrations (EECs) and estimated drinking water concentrations (EDWCs) resulting from the use of pesticides on rice crops produced an ***upper bound screening estimation***, using the lowest K_d value (0.13) for a non-sand soil, of ***45 ppb*** (ug/L) ***in paddy waters***. This estimated EEC is used for both acute and chronic EECs, as well as for both aquatic ecological risk assessments and for drinking water exposure (EDWCs) in human health risk assessments. This value changes to 43 ppb (ug/L) if calculated from the average K_d value typical of rice growing regions. EECs for individual penoxsulam transformation products can not exceed the values estimated for the parent, penoxsulam, using the interim method. Individual EECs were not calculated for any transformation product.

Modeling aquatic concentrations using the standard Tier 1 model, SCI-GROW, estimated parent-only ground water concentrations of 0.67 ppb (ug/L). Even so, EFED does not regard ground water contamination from a pesticide applied to rice to be a significant route of dissipation.

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[8]EFED Response to Registrant Request for a Seven (7) Day Holding Period for Propanil Use in Rice Paddies; DP Barcode: D290202; PC Code: 028201; 9/11/03.

[9]Dow estimates for EECs differed significantly from EFEDs due to the use of inappropriate values for both degradation and partitioning, and incorporation of a holding period which is not supported by the current labels.

Estimated Holding Times Necessary to Reduce Aquatic Concentrations of Penoxsulam in Rice Paddy Water to Levels Below Ecological Effects LOCs

Estimated values of residual penoxsulam in paddy water are plotted below considering degradation due to aqueous photolysis only (Figure 2), degradation following the rate reported for the 90% confidence interval in the paddy water phase of submitted aquatic field dissipation studies (Figure 3), and the degradation following the rate reported the total system of submitted aquatic field dissipation studies (Figure 4). Total system aqueous field dissipation rate differs from the aqueous phase dissipation in that the total system dissipation half-lives are calculated from combined percent of applied radiation identified as penoxsulam in both the soil and in the paddy water at each sampling interval. Aqueous phase dissipation rates are calculated from the percent of applied radiation identified as penoxsulam in the paddy water alone. While aqueous photolysis is expected to be the most dominant route of degradation for penoxsulam in rice paddies, environmental factors such as turbidity, canopy cover and atmospheric conditions will reduce the degradation rate by limiting the amount of solar energy impinging upon the aquatic phase of the system. Use of the total system half-lives combines concentrations temperately residing in sediment with concentrations present in paddy water. The most realistic approach is to use the aquatic field dissipation rates in paddy water alone for estimating suggested holding times. The results from the three separate approaches are provided to generate a sense of the potential variability which might be seen under actual conditions.

Figure 2: Estimated Concentrations for Paddy Water for Dry-Seeded Rice Using Photolysis Degradation Rate

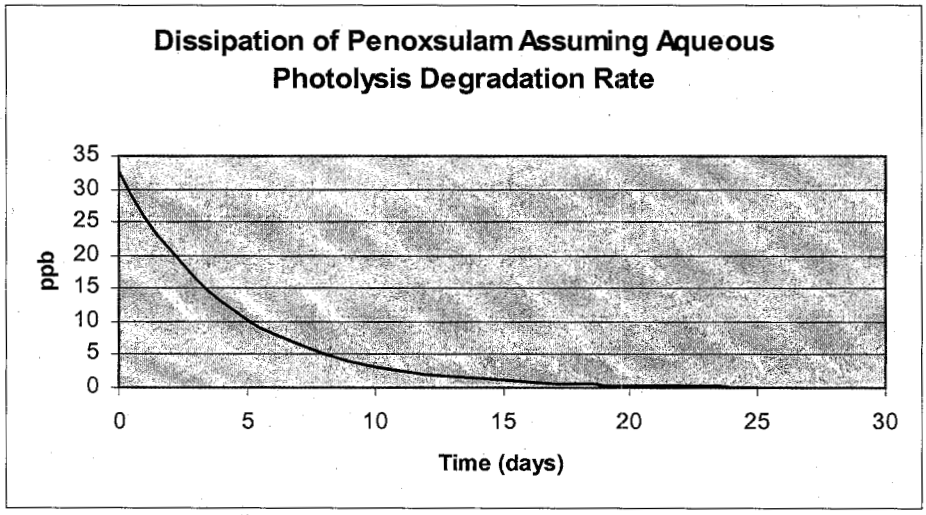


Figure 3: Estimated Concentrations for Paddy Water for Dry-Seeded Rice Using Aquatic Field Dissipation Paddy Water Degradation Rate

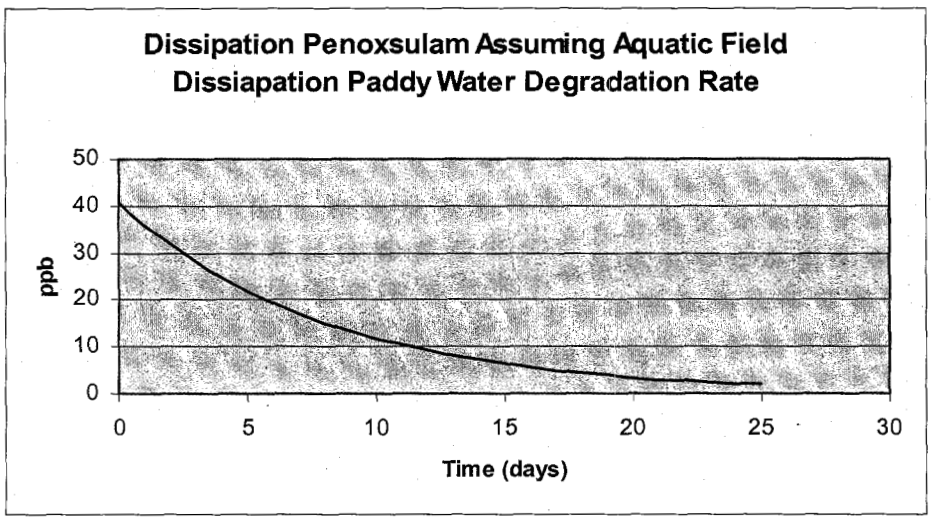
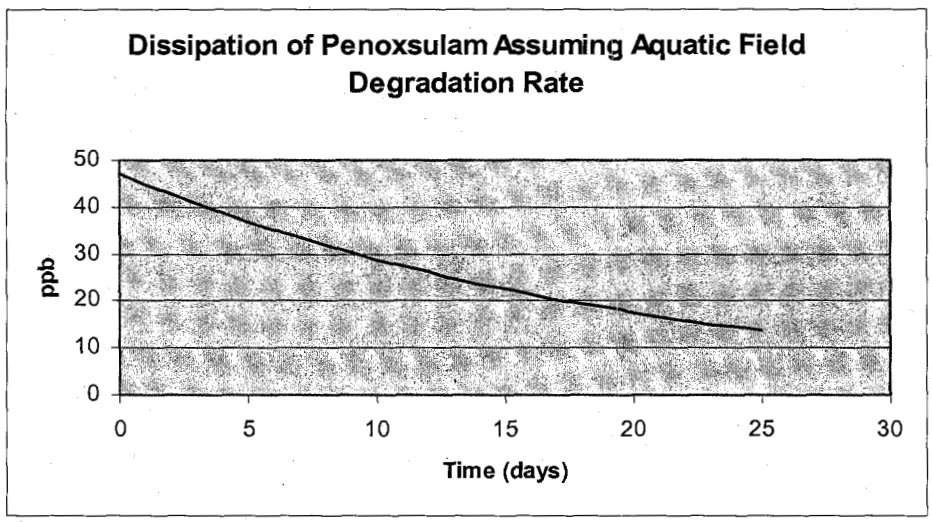


Figure 4: Estimated Concentrations for Paddy Water for Dry-Seeded Rice Using Aquatic Field Dissipation Total System Degradation Rate



Monitoring Information

Penoxsulam is a new chemical being proposed for registration. Therefore, no surface water monitoring data are currently available. Nevertheless, aquatic field dissipation half-lives were generally consistent with submitted laboratory data. Penoxsulam dissipated from dry seeded rice

paddies with calculated, total system half-lives of 16 days for each of the two test sites. Penoxsulam dissipated from the three water-seeded test sites where abiotic transformation would be expected to have a more dominant influence with calculated half-lives of 4 days, 5 days and 10 days.

3. Terrestrial Organism Exposure Modeling

General Approach

Terrestrial wildlife exposure estimates are typically calculated for bird and mammals, emphasizing a dietary exposure route for uptake of pesticide active ingredients. These exposures are considered as surrogates for terrestrial-phase amphibians as well as reptiles. For exposure to terrestrial organisms, such as birds and small mammals, pesticide residues on food items are estimated, based on the assumption that organisms are exposed to a single pesticide residue in a given exposure scenario.

For penoxsulam spray applications, estimation of pesticide concentrations in wildlife food items focuses on quantifying possible dietary ingestion of residues on vegetative matter and insects. The residue estimates are based on a nomogram that relates residues to pesticide application rate. The estimated environmental concentrations (EECs) are generated from a spreadsheet model (EL-FATE) that calculates the decay of a chemical applied to plant surfaces for single or multiple applications.

The terrestrial exposure assessment for liquid-based applications is based on the methods of Hoerger and Kenaga (1972) as modified by Fletcher *et al.* (1994). Terrestrial EECs for nongranular formulations (Table 5) were derived using the maximum application rate. Uncertainties in the terrestrial EECs are primarily associated with a lack of data on interception and subsequent dissipation from foliar surfaces. When data are absent, EFED assumes a 35-day dissipation half-life, based on the work of Willis and McDowell (1987). For penoxsulam, it can not be determined whether this is a conservative assumption due to lack of information on degradate toxicity.

The EECs on food items may be compared directly with dietary toxicity data or converted to an oral dose. The screening-level risk assessment for penoxsulam uses upper bound predicted residues as the measure of exposure. The predicted maximum and mean residues of penoxsulam are those which may be expected to occur on selected avian or mammalian food items immediately following application (at the maximum annual or seasonal label rate). For mammals, the residue concentration is converted to daily oral dose based on the fraction of body weight consumed daily as estimated through mammalian allometric relationships.

Model Results

Table 5. Estimated Environmental Concentrations (EECs) on avian and mammalian food items (ppm) immediately following an application of 0.044 lbs a.i./A. [1]

Food Items	EEC (ppm) Predicted Maximum Residue	EEC (ppm) Predicted mean Residue
Short grass	11	3.7
Tall grass	4.8	1.6
Broadleaf plants / Insects[2]	5.9	2.0
Seeds	0.66	0.31

[1] Predicted maximum and mean residues are based on Hoerger and Kenaga (1972) as modified by Fletcher *et al.* (1994).

[2] The surface to volume ratios of broadleaf plants and insects are similar, therefore, the residues may be similar.

Granular applications

Birds and mammals in the field may be exposed to seed treated with pesticides by ingesting granular pesticide directly with the diet. They also may be exposed by other routes, such as incidental ingestion of contaminated soil, dermal contact with treated seed surfaces and soil during activities in the treated areas, preening activities, and ingestion of drinking water contaminated with pesticide. Traditionally, EFED has only considered ingestion of pesticide granules as a route of exposure. There are two reasons such an analysis was not undertaken for penoxsulam. First, penoxsulam is not being proposed for a seed treatment, nor is it being formulated with a grain or other material attractive to birds or small mammals. Consequently, the chances of more than incidental consumption of the granular are limited. Secondly, acute toxicity was not demonstrated, nor expected, for penoxsulam and its degradates.

B. Ecological Effects Characterization

In screening-level ecological risk assessments, effects characterization describes the types of effects a pesticide can produce in an organism or plant. This characterization is based on registrant-submitted studies that describe acute and chronic toxicity effects for various aquatic and terrestrial animals and plants. In addition, other sources of information, including reviews of the open literature and the Ecological Incident Information System (EIIS), may be used to further refine the characterization of potential ecological effects.

Appendix D summarizes the results of the registrant-submitted toxicity studies used to characterize effects for this risk assessment. Toxicity studies reported in this section do not represent all species of birds, mammals, or aquatic organisms. Only a few surrogate species for both freshwater fish and birds are used to represent all freshwater fish (2000+) and bird (680+) species in the United States. For mammals, acute studies are usually limited to Norway rat. Estuarine/marine studies are usually limited to a crustacean, a mollusk, and a fish. Neither

reptiles nor amphibians are studied. The risk assessment assumes that avian and reptilian toxicities are similar. The same assumption is used for fish and amphibians.

1. Evaluation of Aquatic and Terrestrial Ecotoxicity Studies

Testing of the active ingredient suggest that penoxsulam is practically nontoxic to freshwater fish, birds, mammals, and honeybees on an acute basis. In many tests, no adverse effects were seen at highest tested levels. Consequently, toxicity category labels reflect the highest possible risk nomenclature, rather than a clear demonstration of toxicity at that level. For instance, the degradate TPSA was only tested on the bluegill to a level of 1.4 ppm. An LC50 for the bluegill of 1.4 ppm would result in the toxicity category of "Moderately toxic". In actuality, the LC50 could be much higher and justify a classification of anything up to "Practically nontoxic".

Because penoxsulam is an ALS inhibitor, it does have an effect on plants. For these cases, there is a greater liklihood that indicated classifications are the proper ones. There also is some potential for greater concern with respect to invertebrates. In both of these cases, lack of information on the degradates limits the evaluation of the ecotoxicity of penoxsulam.

Acute Toxicity to Freshwater Fish

Studies using the rainbow trout, carp, and the bluegill sunfish were used to evaluate acute toxicity. The rainbow trout and bluegill sunfish acute studies are consistent with Guideline §72-1(a) and §72-1(c) requirements and are classified as core. The acute study using the common carp is classified as supplemental because this species is not recognized as acceptable for use in acute toxicity studies of freshwater fish. No adverse effects were noted in any of these studies. Information on degradates was not provided. The results are tabulated below in Table 6.

Chronic Toxicity to Freshwater Fish

A freshwater fish early life stage study using the fathead minnow (*Pimephales promelas)* was submitted. No treatment-related effects on hatchability, survival, and/or terminal growth parameters were observed. The NOAEC was 10.2 ppm, the highest level tested. Although this study is scientifically sound, it is classified as supplemental because a LOAEC value was not determined.

Toxicity to Freshwater Invertebrates

The *Daphnia magna*, as well as a midge *(Chironomus sp.*), and an amphipod (*Gammarus* sp.) were used to study the toxicity of technical penoxsulam to freshwater invertebrates. The toxicities of an end-use product and several degradates were studied with the water flea. The 48-hr EC_{50} value for *D. magna* with the technical grade product is >98 ppm. This study fulfills the §72-2 guideline.

Table 6. Freshwater Fish - Acute and Chronic Aquatic Toxicity Data.

Species and Chemical	Acute Toxicity		Chronic Toxicity	
	96-hr LC_{50} (ppm)	Toxic Category (MRID)	NOAEC (mg/L)	Endpoints (MRID)
Rainbow Trout ***Oncorhynchus mykiss***				
Technical grade	>102	Practically Nontoxic (45834804)	None	
Degradates and End-use products	None			
Bluegill sunfish ***Lepomis macrochirus***				
Technical grade	>103	Practically Nontoxic (45831010)	None	
GF-443[1]	>147	Practically Nontoxic (45831011)		
Degradate	None			
Common Carp ***Cyprinus carpio***				
Technical grade	>101	Practically Nontoxic (45831009)	None	
Degradates and End-use products	None		None	
Fathead minnow ***Pimephales promelas***				
Technical grade	None	None	10.2	None (45831027)

[1]GF-443 is the liquid formulation containing 21.7% penoxsulam

Several studies were submitted on the acute toxicity of the degradates of penoxsulam to *D. magna*. Seven of them, the studies on BSTCA, BST, 5-hydroxy-XDE-638[10], 2-amino-TP, TPSA, (5-OH, 2-amino-TP), and BSA, were acceptable for risk analysis. Their 48-hour EC_{50} values ranged from >1.0 ppm to >100 ppm. Supplemental data on the acute toxicity of penoxsulam to other non-guideline freshwater invertebrates showed that when studied with the amphipod, *Gammarus* sp., penoxsulam had a 48-hr EC_{50} >126 ppm.. The results are tabulated below in Table 7.

Acute Toxicity to Estuarine/Marine Fish

Acute toxicity studies were performed on an estuarine/marine fish, a mollusk and a crustacean. The estuarine/marine fish acute toxicity study on the Silverside (*Menidia beryllina*) was done using the active ingredient. No impacts were observed. The results are tabulated below in Table 8.

Acute Toxicity to Estuarine/Marine Invertebrates

Acute penoxsulam toxicity data are available for the mysid (*Americamysis bahia*) and the Eastern oyster (*Crassostrea virginica*), and are summarized in Table 8. The 96-hour mysid LC_{50} is 114 ppm; therefore, penoxsulam is classified as practically nontoxic to estuarine/marine crustaceans on an acute exposure basis. The acute mysid study is scientifically sound and is consistent with Guideline §72-3(c) requirements.

A study with the eastern oyster found that penoxsulam is practically nontoxic to mollusks, with an LC_{50} of >127 ppm, a NOAEC of 127 ppm. After 96 hours of exposure, there was one mortality in the control and no mortalities in the treatment groups. No statistically significant reductions in shell deposition were observed at any level.

Chronic Toxicity to Estuarine/Marine Fish

No data were submitted. Requirements are reserved.

[10]Also referred to by its common name, 5-OH-penoxsulam.

Table 7. Freshwater Invertebrates - Acute and Chronic Aquatic Toxicity Data.

Species and Chemical	Acute Toxicity		Chronic Toxicity	
	48-hr EC_{50} (ppm)	Toxicity Category (MRID)	NOAEC (ppm)	Endpoints (MRID)
Water flea *Daphnia magna*				
Technical grade	>98	Slightly Toxic (45831012)	3.0	Live young (45831026)
BSTCA	>100	Practically Nontoxic (45831014)		
BST	>96	Slightly Toxic (45831018)		
5-hydroxy-XDE-638	>1	Moderately Toxic (45831013)		
2-amino-TP	>1	Moderately Toxic (45831014)		
TPSA	>1.4	Moderately Toxic (45831018)		
5-OH,2amino-TP	>1	Moderately Toxic (45831016)		
BSA	>1.6	Moderately Toxic (45831017)		
Midge *Chironomus* sp.				
Technical grade	> 140	Practically Nontoxic (45831102)	7.1	Development (45831102)
Amphipod *Gammarus* sp.				
Technical grade	>126	Practically Nontoxic (45831021)		

Chronic Toxicity to Estuarine/Marine Invertebrates

Chronic toxicity testing was performed on the mysid (*Americamysis bahia).* Statistically significant effects were seen at all tested levels for male dry weight. At the lowest tested level of 8.1 mg/L, there was a 20% reduction in male body weight versus the controls. At 59 mg/L and higher levels much higher male weight loss was seen and statistically significant reductions in number of young/female/day were also observed. At 119 mg/L, effects were seen on the length of both sexes. Data were not provided on male survival, nor on sex distribution of offspring. Because no NOAEC was identified, the study is classified as supplemental.

Table 8. Estuarine and Marine Animals - Acute and Chronic Toxicity Data.

	Acute Toxicity		Chronic Toxicity	
Species and Chemical	**96-hr LC_{50} (ppm)**	**Toxicity Category (MRID)**	**NOAEC (mg/L)**	**Endpoints (MRID)**
Silverside *Menidia beryllina*				
Technical grade	>129	Practically Nontoxic (45831022)		
Eastern oyster *Crassostrea virginica*				
Technical grade	>127	Practically Nontoxic (45831023)		
Mysid *Americamysis bahia*				
Technical grade	114	Practically Nontoxic (45831024)	<8.1	Male dry weight

Chronic Toxicity to Freshwater Invertebrates

A freshwater aquatic invertebrate life-cycle study using the TGAI was submitted for penoxsulam using the preferred species *Daphnia magna* and summarized in Table 7. Mortality and immobilization data were not analyzed because less than 50% mortality and immobilization occurred during the test. However, a statistically-significant reduction in the number of live offspring produced was observed at the 9.8 ppm a.i. level. Based on the number of live offspring (the only endpoint affected), the NOAEC and LOAEC values were 3.0 and 9.8 ppm a.i., respectively. The study is scientifically sound, consistent with Guideline §72-4(b), and is classified as core. A chronic study with a midge found an EC_{50} (development rate) of >140 mg a.i./L and a NOAEC of 7.1 mg a.i./L.

Toxicity to Aquatic Plants

Acute plant toxicity data are presented in Table 9 below. Studies using the technical grade product, end-use products, and degradates were submitted for vascular and nonvascular plants. As shall be discussed in greater detail in the uncertainties section, data were not provided on the sulfonamide and SFA degradates.

Table 9. Aquatic Plants - Acute Toxicity Data

Species and Chemical	MRID	Acute EC_{50} (mg/L)	NOAEC (mg/L)	EC_{05} (mg/L)	Affected Endpoint
Vascular plants- Duckweed *Lemna gibba*					
Technical grade	45831120	0.003	0.001	0.0007	Number of fronds
BSTCA	45831106	>10	10	ND	None
5-hydroxy-XDE-638	45831104	>11	0.22	0.095	Number of fronds
BST	45831105	>6.2	<0.1	ND[1]	Number of fronds Growth rate
2-amino-8-methoxy Tier 1	45831108	>1.25	1.25	ND	None
2-amino-TP Tier 1	45831111	>1.0	1.0	ND	None
BSA Tier 1	45831110	>1.6	1.6	ND	None
TPSA Tier 1	45831109	>1.4	1.4	ND	None
Nonvascular plants- Green algae *Selenastrum capricornutum*					
Technical grade	45834805	0.092	0.005	0.007	Cell density
GF-443	45831107	0.094	0.009	0.005	Biomass
BSTCA	45831119	>10	10	ND	None
BST	45831117	>9.6	3.9	ND	Growth rate Biomass
5-hydroxy-XDE-638	45831118	>10	10	ND	None
TPSA	45831113	>1.4	1.4	ND	None
5-OH,2-amino-TP	45831114	>1.0	1.0	ND	None
BSA	45831112	>1.6	1.6	ND	None
2-Amino TP	45831115	>1.0	1.0	ND	None
Nonvascular plants- Freshwater diatom *Navicula pelliculosa*					
Technical grade	45831121	>49.6	49.6	ND	None
Nonvascular plants- Freshwater alga *Anabaena flos-aquae*					
Technical grade	45831122	0.27	0.194	0.027	Cell density Biomass
Nonvascular plants Tier I Saltwater diatom *Skeletonema costatum*					
Technical grade	45831123	>46.7	2.33	0.43	Cell Density Biomass
TPSA	45831113	>1.4	1.4	ND	None
5-OH, 2-amino-TP	45831114	>1.0	1.0	ND	None
2-Amino TP	45831115	>1.0	1.0	ND	None
BSA	45831112	>1.6	1.6	ND	None

[1]Not determined because non-monotonic response.

Acute Toxicity to Aquatic Plants

Vascular plants

The vascular plant used was duckweed (*Lemna gibba).* The technical's acute EC_{50} and EC_{05} were 0.003 mg/L and 0.0007 mg/L, respectively. Its NOAEC was 0.001 mg/L. The most sensitive effect for duckweed was the number of fronds. No studies of the effect of the end-use product, GF-443, on a vascular plant were submitted. The toxicities of the degradates BSTCA, 5-hydroxy-XDE-638, BST, 2-amino-8-methoxy , 2-amino-TP, BSA, and TPSA were studied. A NOAEC was not obtained for BST at 0.1 mg/L, but all other toxicities were demonstrated to be less than that of the technical. It is not expected that BST would be more toxic than the technical based on the level of response.

Nonvascular plants

The active ingredient affected the green algae *Selenastrum capricornutum* by reducing its cell density. The EC_{50} was 0.092 mg/L, NOAEC was 0.005 mg/L, and the EC_{05} was 0.007 mg/L. The most sensitive end point was cell density. The end use product, GF-443, had essentially the same toxicity. Its EC_{50}, NOAEC, and EC_{05} values were 0.094, 0.009, and 0.005 mg/L, respectively and the most sensitive end point was biomass. The penoxsulam degradates BSTCA; BST; 5-hydroxy-XDE-638; TPSA; 5-OH,2-amino-TP; BSA; and 2-Amino TP were not as toxic as the parent material.

The effect of the technical grade product was also studied on the diatom *Navicula pelliculosa*, the freshwater alga *Anabaena flos-aquae*, and the saltwater diatom *Skeletonema costatum*. The most sensitive was *Anabaena flos-aquae*, which had a NOAEC of 0.194 mg a.i./L, an EC_{50} of 0.27 mg a.i./L, and an EC_{05} of 0.027 mg/L and affected cell density. Of these species, only *Skeletonema costatum* had study reports for degradates, none of which exhibited a toxic response.

Toxicity to Terrestrial Animals

Eight studies on the toxicity of penoxsulam were submitted and are being used for risk characterization. The results are presented below in Table 10. The registrant submitted two acute and dietary toxicity studies with the technical grade product and one with the end use product GF-443. All found that the stressors were practically nontoxic to birds. The only observed effect in any of the studies was a statistically significant reduction of feed consumption on the first three days of the testing of acute oral toxicity of GF-443 to the bobwhite quail.

Chronic toxicity of the technical grade was tested on both the quail and the duck. An avian dietary study on the bobwhite quail found a NOAEC of 231 ppm. Effects were observed for food consumption and body weight gain. A study on the mallard duck found a NOAEC of 501 mg/kg. The endpoint of concern was male body weight gain. No reproductive effects were observed.

Acute oral toxicity of the technical grade was tested at a dose level of 5000 mg/kg. Five male and 5 female Fischer 344 rats were used in the study. No animals died during the study. Clinical abnormalities were transient and only observed in a few animals. Chronic mammalian

testing of the technical grade in a two generation reproductive test of the Norway rat found a NOAEC of 600 ppm. The effect observed was delay of preputial separation in F_1 males. This is a developmental delay effect.

Table 10. Acute and Chronic Toxicity for Terrestrial Animals.

	Acute Toxicity		Dietary Toxicity		Chronic Toxicity	
Species and Chemical	LD_{50} (ppm)	Category (MRID)	LC_{50} (mg/kg)	Category (MRID)	NOAEC (ppm) (MRID)	Endpoints
Northern bobwhite quail *Colinus virginianus*						
Technical grade	>2,025	Practically Nontoxic (45830928)	>4,411	Slightly Toxic (45831002)	231 (45831006)	Food consumption, Male & female body weight gain
GF-443	>2,190	Practically Nontoxic (45831001)				
Mallard duck *Anas platyrhynchos*						
Technical grade	>1,900	Practically Nontoxic (45830929)	>4310	Slightly Toxic (45831003)	501 (46276401)	Adult male body weight
GF-443	None					
Norway Rat *Rattus norvegicus*						
Technical Grade	>5000 mg/kg bw	(45830812)			600 (45830920)	
Honey bee *Apis meliferus*						
Species Chemical	Acute Contact (µg/bee contact)	MRID				
Technical grade	>100	45831124				
GF-443	>22	45831127				

Toxicity to Terrestrial Plants

Studies (MRID 45831116) on the toxicity of penoxsulam to terrestrial plants were submitted. The data are presented in Tables 11a and 11b for seedling emergence and vegetative vigor, respectively. Testing was not provided on the end use product. Rather, testing was conducted on a 16% crop oil concentrate of penoxsulam. Both studies were scientifically sound and fulfilled the guideline requirements for seedling emergence and vegetative vigor studies (Guidelines 123-1 (a & b; TIER II)).

Table 11a. Terrestrial Plants- Tier II Data, Seedling Emergence.

Species	Shoot length (g ai/ha)			Shoot weight (g ai/ha)			Most Sensitive Parameter	Slope
	NOAEC	EC_{05}	EC_{25}	NOAEC	EC_{05}	EC_{25}		
Dicots								
Sugarbeet	1.2	2.5	5.5	1.2***	1.1	3.2*	Weight	2.2
Cotton	33	ND	>33	33	ND	>33	None	n/a
Soybean	33	ND	>33	33	ND	>33	None	n/a
Cucumber	33	ND	>33	33	ND	>33	None	n/a
Kale	3.7	3.9	11	3.7	2.3	6.7	Weight	2.1
Tomato	3.7	4.9	18	3.7	3.2	11	Weight	1.8
Monocots								
Onion	3.7	0.28	6.2	0.41****	0.066	1.1**	Weight	0.79
Wheat	100	ND	>100	100	ND	>100	None	n/a
Corn	100	ND	>100	100	ND	>100	None	n/a
Ryegrass	33	ND	>100	33	ND	>33	None	n/a

* Most sensitive EC25 dicot ** Most sensitive EC25 monocot *** Most sensitive NOAEC dicot
**** Most sensitive NOAEC monocot

Table 11b. Terrestrial Plants- Tier II, Vegetative Vigor

Species	Shoot length (g ai/ha)			Shoot weight (g ai/ha)			Most Sensitive Parameter	Slope
	NOAEC	EC_{05}	EC_{25}	NOAEC	EC_{05}	EC_{25}		
Dicots								
Soybean	3.7	1.9	4.4	1.2***	2.1	3.9*	Weight	3.7
Sugarbeet	11.1	6.4	20	1.2***	1.7	4.6	Weight	2.3
Tomato	3.7	1.5	8.0	1.2***	3.0	8.1	Length	1.3
Cotton	3.7	11	73	33	35	>100	Length	1.2
Cucumber	33	32	63	33	21	49	Weight	n.d.
Kale	3.7	3.2	10	3.7	3.6	8.6	Weight	2.6
Monocots								
Ryegrass	33	ND	>100	0.41****	0.08	17**	Weight	0.42
Corn	100	ND	>100	100	ND	>100	None	n/a
Wheat	100	ND	>100	100	ND	>100	None	n/a
Onion	3.7	7.8	36	11	20	31	Length Weight	n.d.

* Most sensitive EC25 dicot ** Most sensitive EC25 monocot *** Most sensitive NOAEC dicot
**** Most sensitive NOAEC monocot

Seedling emergence

Based on the results of the Tier II terrestrial plant toxicity studies, it appears that both monocot and dicot species of non-target plants are very selective with respect to sensitivity to penoxsulam, particularly for the seedling emergence test. In the seedling emergence test, six out of the ten test species showed no effect at the highest concentration of penoxsulam tested. With the exception of corn and wheat, which were tested at maximum penoxsulam concentrations of 100 g a.i./ ha, the highest test concentration for the other species was 33 g a.i./ha (less than the proposed maximum application rate of 49 g a.i./ha). Out of the six plant species showing no sensitivity to penoxsulam, three were dicots (i.e., cotton, soybean, and cucumber) and three were monocots (wheat, corn, and ryegrass). The most sensitive endpoint for plants that exhibited seedling emergence sensitivity to penoxsulam (onion, sugarbeet, kale, and tomato), as defined by $\geq$ 25% inhibition, was shoot weight.

Vegetative vigor

In the vegetative vigor test, two monocot species (corn and wheat) showed no sensitivity to penoxsulam at maximum concentrations of 100 g a.i./ha. Of the species that were sensitive to treatment, EC_{25} values for the most sensitive dicot (soybean) and monocot (ryegrass) were 3.9 and 17 g a.i./ha. Both vegetative vigor endpoints were based on shoot weight.

2. Open Literature Review

Because penoxsulam is a new active ingredient, which has not yet been produced, no evaluation of the open literature was conducted.

3. Incident Data Review

Since penoxsulam has never been registered, a search of the incident data base was not performed.

IV. Risk Characterization

Risk characterization is the integration of exposure and effects characterizations to determine the ecological risk from the use of the pesticide and the likelihood of effects on aquatic life, wildlife, and plants based on varying pesticide use scenarios. The risk characterization provides an estimation and a description of the risk; articulates risk assessment assumptions, limitations, and uncertainties; synthesizes an overall conclusion; and provides the risk managers with information to make regulatory decisions regarding a pesticide.

A. Integration of Exposure and Effects Data

Results of the exposure and toxicity effects data are used to evaluate the likelihood of adverse ecological effects on non-target species. For the assessment of penoxsulam risks, the risk quotient (RQ) method is used to compare exposure and measured toxicity values. Estimated environmental concentrations (EECs) are divided by acute and chronic toxicity values. The RQs are compared to the Agency's levels of concern (LOCs). These LOCs are the Agency's interpretive policy and are used to analyze potential risk to non-target organisms and the need to consider regulatory action. These criteria are used to indicate when a pesticide's use as directed on the label has the potential to cause adverse effects on non-target organisms. Appendix E of

this document summarizes the LOCs used in this risk assessment. Appendix F provides detailed spreadsheets of all derived RQs for non-target species.

1. Risk Quotient

Nontarget Aquatic Animals and Plants

Surface water concentrations resulting from penoxsulam application to selected crops were predicted with the previously described preliminary rice exposure model. Because of the manner in which rice is grown all EECs were determined to be 0.045 ppm. The peak EEC was 0.045 ppm. The peak EEC was then compared to acute toxicity endpoints to derive acute RQs. This EEC was also compared to chronic toxicity endpoints (NOAEC values) to derive chronic RQs for freshwater and for estuarine/marine organisms. Acute and chronic RQs for freshwater and estuarine/marine organisms are summarized in Tables 12 through 14, respectively.

For aquatic vascular and non-vascular plants, peak EECs were compared to acute EC_{50} and NOAEC toxicity endpoints to derive acute non-endangered and endangered species RQs, respectively. Acute non-endangered and endangered species RQs for aquatic vascular and non-vascular plants are summarized in Table 15.

For the current application rates of penoxsulam to rice, acute LOCs are exceeded only by the technical grade product and the end use product GF-443 on the vascular plant, duckweed (*Lemna gibba*), and the green alga *Selenastrum capricornutum*.

Risk to Freshwater Fish

The acute and chronic risk quotients were determined for freshwater fish. A chronic risk quotient was also determined for one species. The RQs are tabulated below. No freshwater fish acute or chronic LOCs were exceeded. No studies were submitted using a degradate.

Risk to Freshwater Invertebrates

Three species of freshwater invertebrates were studied. The calculated acute and chronic risk quotients are tabulated below. No acute or chronic Levels of Concern were exceeded in the studies on freshwater invertebrates. Studies were done on *Daphnia magna*, the preferred species, but studies were also submitted using an amphipod (*Gammarus* sp.) and a midge (*Chironomus* sp.). Studies using the technical grade product were done for all three species. Several degradates were also assessed using the Daphnid. None of the RQs from these studies exceeded the Level of Concern.

Table 12. Freshwater Fish - Risk Quotients

Species and Chemical	Acute LC_{50} (ppm)	Chronic NOAEC (ppm)	EEC Peak (ppm)	EEC 21-Day Average (ppm)	Acute RQ (ppm) EEC/EC_{50}	Chronic RQ (ppm) EEC/NOAEC
Rainbow trout *Oncorhynchus mykiss*						
Technical grade	>102		0.045	0.045	<0.001	
GF-443	None					
Degradates	None					
Bluegill Sunfish *Lepomis macrochirus*						
Technical grade	>103		0.045	0.045	<0.001	
GF-443	>147		0.045	0.045	<0.001	
Degradates	None					
Fathead Minnow *Pimephales promelas*						
Technical grade		10.2	0.045	0.045		0.004
GF-443	None					
Degradates	None					

Table 13. Freshwater Invertebrates - Acute and Chronic Risk Quotients.

Species and Chemical	Acute EC_{50} (ppm)	Chronic NOAEC (ppm)	EEC Peak (ppm)	EEC 21-Day Average (ppm)	Acute RQ EEC/EC_{50}	Chronic RQ EEC/NOAEC
Daphnia magna						
Technical grade	>98.3	3.0	0.045	0.045	<0.001	0.0015
BSTCA	>100		0.045	0.045	<0.001	
BST	>96		0.045	0.045	<0.001	
5-hydroxy-XDE-638	>1		0.045	0.045	<0.045	
2-amino-TP	>1		0.045	0.045	<0.045	
TPSA	>1.4		0.045	0.045	<0.032	
5-OH,2-amino-TP	>1		0.045	0.045	<0.045	
BSA	>1.6		0.045	0.045	<0.028	
Midge *Chironomus* sp.						
Technical grade	>140	7.1	0.045	0.045	<0.001	0.006
Amphipod *Gammarus* sp.						
Technical grade	>126		0.045		<0.001	

Risk to Estuarine and Marine Animals

Three acute and one chronic study on the toxicity of technical grade penoxsulam were submitted. It is not possible to ascertain from the chronic test that the LOC would not be exceeded, however, there is an order of magnitude factor of safety even based on an acute EEC. Given that there was no mortality in the tests and the magnitude of the weight loss endpoint at tested levels, it is viewed as unlikely that the level would be exceeded in repeat testing. No studies on degradates were submitted.

Table 14. Estuarine and Marine Animals - Risk Quotients

Species and Chemical	Acute EC_{50} (ppm)	Chronic NOAEC (ppm)	EEC Peak (ppm)	EEC 21-Day Average (ppm)	Acute RQ EEC/EC_{50}	Chronic RQ EEC/NOAEC
Silverside *Menidia beryllina*						
Technical grade	>129		0.045	0.045	<0.001	
Eastern oyster *Crassostrea virginica*						
Technical grade	>127		0.045	0.045	<0.001	
Mysid *Americamysis bahia*						
Technical grade	114	<8.1	0.045	0.045	<0.001	>.006

Risk to Aquatic Plants

The risk quotients for vascular and nonvascular plants were calculated from the Estimated Environmental Concentration (0.045 ppm) and the EC_{50} for acute risk, and the NOAEC when one exists, or the EC_{05} . The sole exception is in the case of an endangered endpoint for BST where it was not felt the assessment endpoint was reliable enough to estimate an endpoint. The results are tabulated below.

The duckweed study with the technical grade product found an exceedance for both non-endangered and endangered species Levels of Concern (RQs of 15 and >45, respectively). The green alga studies with the technical grade product and an end-use product found RQs of 9 and 4.1, respectively. These RQs exceed endangered species Levels of Concern.

While there were no other LOC exceedances, several major degradates were not tested.

Table 15. Risk Quotients for Aquatic Plants.

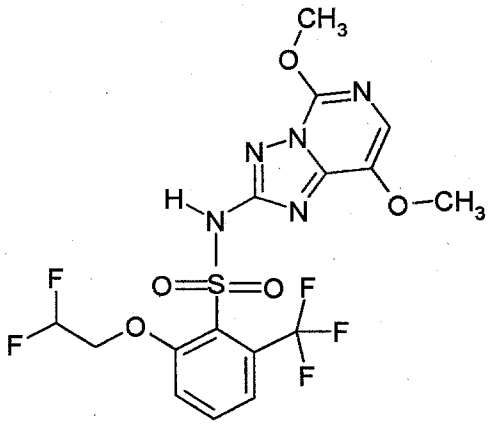
Species Chemical	MRID	EEC- PEAK (ppm)	EC_{50} (mg/L)	NOAEC or EC_{05}[1] (ppm)	Risk Quotients: Non-endangered Species EEC/EC_{50}	Risk Quotients: Endangered Species EEC/NOAEC or EC_{05}
Vascular plants- Duckweed *Lemna gibba*						
Technical grade	45831120	0.045	0.003	0.001	15*	>45*
BSTCA	45831106	0.045	>10	10	<0.005	<0.005
5-hydroxy-XDE-638	45831104	0.045	>11	0.22	<0.004	0.49
BST	45831105	0.045	>6.2	<0.1	<0.007	ND[2]
2-amino-8-methoxy Tier 1	45831108	0.045	>1.25	1.25	<0.036	0.036
2-amino-TP Tier 1	45831111	0.045	>1.0	1.0	<0.045	0.045
BSA Tier 1	45831110	0.045	>1.6	1.6	<0.028	0.028
TPSA Tier 1	45831109	0.045	>1.4	1.4	<0.032	0.032
Nonvascular plants- Green algae *Selenastrum capricornutum*						
Technical grade	45834805	0.045	0.092	0.005	0.49	9.0*
GF-443	45831107	0.045	0.094	0.009	0.48	5.0*
BSTCA	45831119	0.045	>10	10	<0.005	0.005
BST	45831117	0.045	>9.6	3.9	<0.005	0.013
5-hydroxy-XDE-638	45831118	0.045	>10	10	<0.005	0.005
TPSA	45831113	0.045	>1.4	1.4	<0.032	0.032
5-OH,2-amino-TP	45831114	0.045	>1.0	1.0	<0.045	0.045
BSA	45831112	0.045	>1.6	1.6	<0.028	0.028
2-Amino TP	45831115	0.045	>1.0	1.0	<0.045	0.045
Nonvascular plants- Freshwater diatom *Navicula pelliculosa*						
Technical grade	45831121	0.045	>49.6	49.6	<0.001	0.001
Nonvascular plants- Freshwater alga *Anabaena flos-aquae*						
Technical grade	45831122	0.045	0.27	0.194	0.17	0.23
Nonvascular plants Tier I Saltwater diatom *Skeletonema costatum*						
Technical grade	45831123	0.045	>46.7	2.33	0.001	0.019
TPSA	45831113	0.045	>1.4	1.4	≤0.032	0.032
5-OH, 2-amino-TP	45831114	0.045	>1.0	1.0	≤0.045	0.045
2-Amino TP	45831115	0.045	>1.0	1.0	≤0.045	0.045
BSA	45831112	0.045	>1.6	1.6	≤0.028	0.028

[1] NOAEC or, if NOAEC isn't available, the EC_{50} *Exceeds LOC

[2]Could not reliably estimate

Appendix A - Detailed Environmental Fate Evaluation and Submitted Data

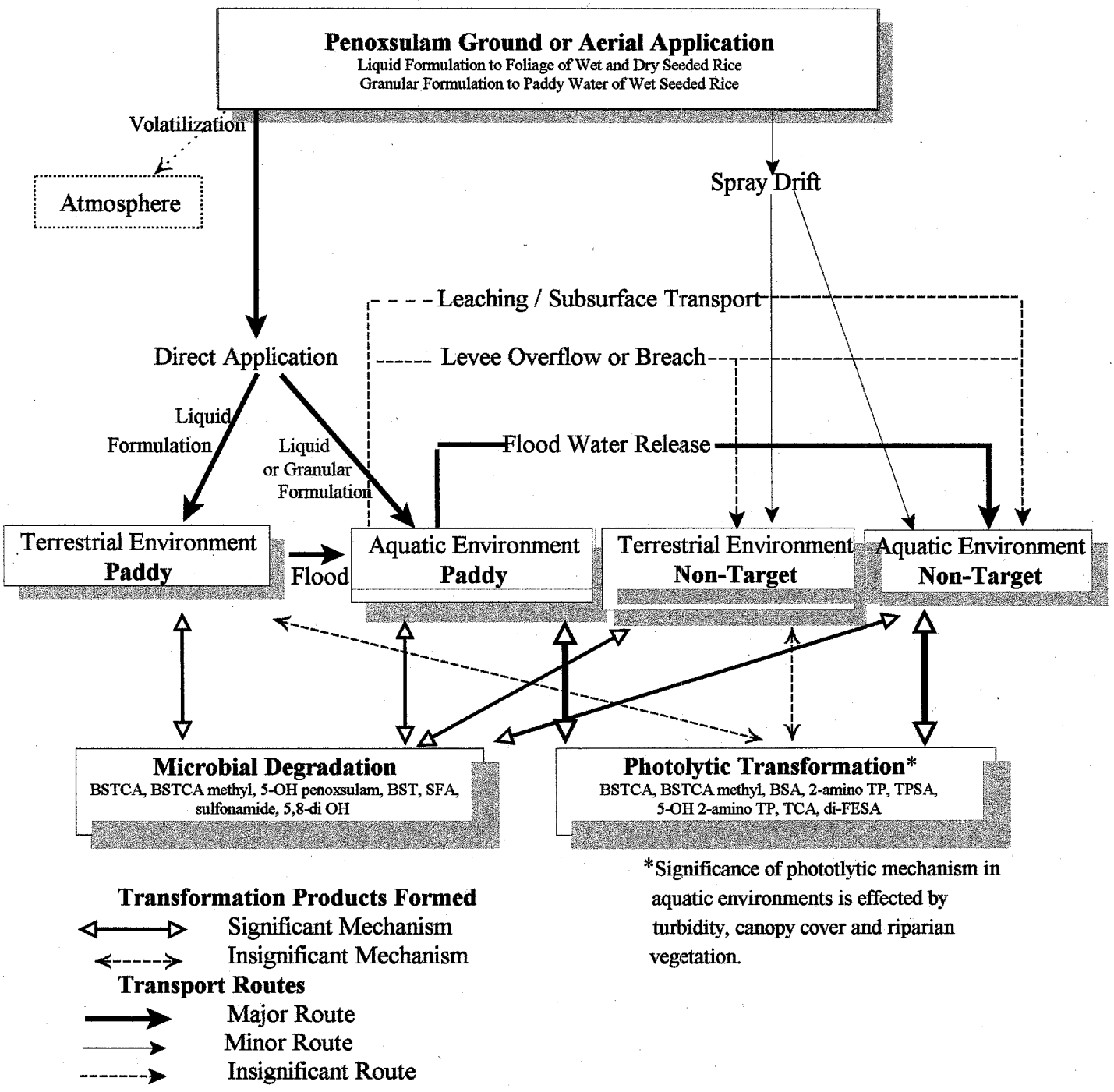
Based on submitted laboratory data (a more detailed description of the individual study reports data appears below), penoxsulam dissipates quickly in aqueous environments, and is not expected to be persistent in terrestrial environments.



Penoxsulam degrades by competing mechanisms in the environment (see **Figure A1** below). The major routes of dissipation in aqueous environments are expected to be aqueous photolysis (half-lives of 1.5 to 14 days, with the longer half-life reported at the lowest pH) and anaerobic degradation (half-lives of 5 to 11 days). However, it should be remembered that anaerobic conditions are not normally found in flooded rice paddies, and the slower aerobic degradation processes (half-lives of 12 to 118 days) would dominate.

The aqueous photolysis study author (MRID 458307-22) suggested that the longer, 14 day photolytic half-life in the flooded soil was due to the turbidity of the samples. It was proposed that the suspended soil reduced the amount of light available for photodegradation. However, it is also plausible that the pH of the test system effected the photolytic half-life. At a pH at or above 7, as reported in the three remaining photolytic test systems, ≥99% penoxsulam exists in an ionized form, as calculated with the Henderson-Hasselbalch equation from a reported pK_a of 5.1. At the flooded soil system pH of 5.8, only 83% of the penoxsulam exists in an ionized form. The remaining 17% exists as the associated species. Because the most labile proton in penoxsulam is located near both of the sulfonamide bridge cleavage sites observed for photolytic transformation, it is possible that this change in speciation, from the ionized to the associated form, could influenced phototransformation. Additionally, trees, riparian vegetation and crop canopies shading environments waters would reduce the significance of photolysis as a degradation route for penoxsulam.

Figure A1: Transport Pathway for Combined Penoxsulam and Transformation Products



Photolysis on soil is expected to be an important route of dissipation in terrestrial environments (half-lives of 19 to 109 days). However, photolysis is limited to the shallow depth of soil that can be penetrated by sunlight. Once penoxsulam moves from the upper soil layer, aerobic degradation will become the dominate route of environmental dissipation (half-lives of 12 to 117 days). It was noted in the submitted aquatic field dissipation studies that the total system half-lives for penoxsulam applied to the water of the simulated wet seeded rice crop (half-lives of 4 to 10 days) was similar to the half-lives in the water alone. In the submitted aquatic field dissipation studies, the total system half-lives for penoxsulam applied to the soil of the simulated dry seeded rice crop (half-lives of 13 to 16 days) were longer, as expected in the soil alone. Penoxsulam is stable to hydrolysis at all environmental pH's. Mineralization is not a major route of dissipation for penoxsulam.

Characterization of the transformation products reported in the submitted laboratory studies indicates that the degradation of penoxsulam proceeds through two competing pathways. Photolysis proceeds through a mechanism that initiates cleavage of the sulfonamide bridge of the parent molecule. Biotic degradation proceeds through the degradation of the pyrimidine ring and its substitutes. This complex degradation pathway of penoxsulam produces a large number of degradation products. Environmental fate data are not available to fully characterize either these degradation products or their respective potential degradation pathways.

Only limited fate data are available for the penoxsulam transformation products. Six of the thirteen identified transformation products (see **Table A6** for the structure and full Chemical Abstract Service Name of the penoxsulam transformation products) reached peak concentrations at study termination: 2-amino-TP, BSTCA, 2-amino-TCA, SFA, sulfonamide and 5,8-di-OH penoxsulam. These six compounds are potentially more persistent than the parent compound, and would probably have reached even greater concentrations with time. Eleven of the thirteen penoxsulam transformation products reported in laboratory studies are considered major degradates: BSA, 2-amino-TP, TPSA, BSTCA methyl, BSTCA, 2-amino-TCA, 5-OH-penoxsulam, SFA, sulfonamide, 5,8-di-OH and 5-OH 2 amino TP. Two of the thirteen penoxsulam transformation products are considered minor degradates: di-FESA and BST.(see **Table A6**).

Three degradation products were determined to be of potential ecological concern. An examination of chemical structure of identified degradation products revealed a sulfonamide residue which was not hindered by stearic factors in three degradates (SFA, Sullfonamide, BSA). Ecological endpoints were calculated for these three degradation products, along with the parent compound, with the EPA structural analysis program, Estimation Program Interface (EPI) Suite[1]. Comparison of the predicted ECOSAR class endpoints for the three degradation products with those of penoxsulam indicate these thee degradation products are not expected to be of toxicological concern.

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[1]

Six of the penoxsulam degradation products have been identified by the Health Effects Division as residues of concern for the water assessment.

Based on submitted laboratory data, penoxsulam is expected to have a high degree of mobility in the environment. However, penoxsulam susceptibility to both photolytic and biotic degradation limits the potential for the parent compound to accumulate in the environment. Based upon a reported (MRID #458307-05) vapor pressure of 9.55×10^{-14} Pa at 25°C, penoxsulam is expected to have low volatility under environmental conditions. A pK_a value of 5.1 indicates that penoxsulam will exist predominately in its anionic form in all but strongly acidic soils[2], making it susceptible to the repulsive interactions responsible for the tendency of anions to be weakly sorbed to most soils. Reported soil to water partitioning coefficients between 0.13 and 4.7, with a median K_d value of 0.54, indicates a substantial potential for off-site movement. Reported K_{oc} values were generally between 13 and 305, with one K_{oc} value reported as 1130, and a median K_{oc} value of 40. No strong correlation was demonstrated between mobility and clay content, organic matter content, or pH for the soils tested. The possibility of transport exists through runoff, leaching, sediment erosion during a rainfall event, and through the windblown movement of soil in terrestrial environments. In rice paddies, a potential for off-site movement exists through breaching or overspill of levees, through the 0.5 to 2 acre-feet of water typically lost annually from most rice soils through deep percolation[3], through channels dug through levee walls by crayfish, and through movement through cracks in dry soils with high clay contents into more permeable soil layers beneath "puddled" paddies when rice is dry seeded[4]. Mobility data has been submitted for three penoxsulam degradates (BSTCA, 5-OH-penoxsulam, and BST) indicating that each is expected to display mobility roughly equal to that of the parent compound.

Results from submitted aquatic field dissipation studies were consistent with submitted laboratory data. It was interested to note that the dissipation of penoxsulam application to bareground and dry-seeded rice plots was dominated by soil kinetics, while the dissipation of penoxsulam application to flooded bareground and wet-seeded rice plots was dominated by water kinetics.

Summarys of the individual Data Evaluation Reports (DER) for the submitted environmental fate studies supporting the proposed registration of penoxsulam for rice crops follow the tabulated data below.

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[2] Http://www.esf.edu/pubprog/brochure/soilph/soilph.htm

[3] http://agronomy.ucdavis.edu/uccerice/PRODUCT/rpic05.htm

[4] http://www.knowledgebank.irri.org/oryza2000/Oryza_User_Manual/6_-_Soil_-_water_balance...

Table A1. Degradation and Metabolism of Penoxsulam (see Table B6 for full Chemical Abstract Service Names of Transformation Products)

Study MRID	Study Type	System	Parent half-life	Maximum transformation products (% of applied)												
				BSTCA	BSA	2-amino TP	TPSA	5-OH 2-amino TP	2-amino-TCA	BSTCA methyl	di-FESA	5-OH-penoxsulam	BST	SFA	Sulfonamide	5,8-diOH
45830721	Hydrolysis (161-1)	Sterile aqueous buffers / natural waters	stable	--	--	--	--	--	--	--	--	--	--	--	--	--
45834801	Photodegradation in Water (161-2)	Sterile aqueous buffers (pH 7)	1.5 days	7.0	36.1	18.2	56	--	85	1.2	5.1	--	--	--	--	--
		Natural waters (pH 7.8)	1.5 days	7.2	33.5	17.8	53	--	81.7	4.4	7.6	--	--	--	--	--
45830722	Photodegradation in Water (161-2)	AR pond water (pH 7)	3.1 days	--	--	17	--	--	--	3.7	--	--	--	--	--	--
		Flooded silt loam soil (pH 5.8)	14 days	--	--	9.4	--	--	--	12	--	--	--	--	--	--
45830723	Photodegradation on Soil (161-3)	Flooded silt loam	19 days	11.1	80.1	10.4	--	--	--	--	--	--	--	--	--	--
		Silty clay loam	109 days	nr	nr	nr	nr	nr	nr	nr	nr	nr	nr	nr	nr	nr
45830724	Aerobic Soil Metabolism (162-1)	AR silt loam	34 days	37.2	--	--	--	--	--	1.3	--	62.6	6.3	14.7	33.0	--
		CA clay loam	43 days	32.4	--	--	--	--	--	1.4	--	40.9	4.5	3.3	1.4	--
		ND loam	118 days	20.6	--	--	--	--	--	--	--	25.0	1.8	--	--	--
45830725	Anaerobic Aquatic Metabolism (162-3) (total system)	AR pond water / silt loam clay sediment	5 days	25.4	--	--	--	--	--	12.8	--	38.6	4.8	--	--	11.0
		AR pond water / silt loam soil	11 days	20.5	--	--	--	--	--	--	--	41.6	2.9	--	--	--
		distilled water / silty loam soil (Italy)	7 days	18.7	--	--	--	--	--	4.6	--	32.6	3.0	--	--	--

Study MRID	Study Type	System	Parent half-life	Maximum transformation products (% of applied)												
				BSTCA	BSA	2-amino TP	TPSA	5-OH 2-amino TP	2-amino-TCA	BSTCA methyl	di-FESA	5-OH-penoxsulam	BST	SFA	Sulfonamide	5,8-diOH
45830726	Aerobic Aquatic Metabolism (162-4)	AR pond water / silt loam clay sediment	16 days	39.4	--	--	--	--	--	--	--	32.3	--	--	--	--
	(total system)	AR pond water / silt loam soil	29 days	29.7	--	--	--	--	--	--	--	22.7	--	--	--	--
		Italian channel water / loam sediment	12 days	24.0	--	--	--	--	--	--	--	22.0	--	--	--	--
		French lake water / sand sed.	38 days	12.8	--	--	--	--	--	--	--	29.7	--	--	--	--
		HPLC water / volcanic loam soil (Japan)	30 days	10.4	--	--	--	--	--	--	--	32.2	--	--	--	--
		HPLC water / loam soil (Japan)	31 days	25.7	--	--	--	--	--	--	--	40.3	--	--	--	--

nr = not reported

Table A2. Mobility Properties of Penoxsulam (MRID # 458308-01)

Soil	% Organic Carbon	K_d (mL/g)	K_{oc} (mL/g)
NC Sand	0.40	0.27	76
AR Silt loam	0.97	0.37	40
Volcanic Loam (Japan)	3.7	0.59	22
Sandy clay loam (Japan)	2.2	0.56	40
Volcanic Loam (Japan)	3.4	4.69	305
Volcanic Loam (Japan)	1.3	1.55	194
CA Clay loam	2.5	0.49	20
ND Loam	2.8	0.45	21
Silty clay loam (Italy)	0.99	1.96	253
Silty clay loam (France)	0.97	0.48	66
Sandy clay loam (UK)	1.6	0.16	13
Sandy loam (Italy)	0.85	0.32	46
AR Silty clay sediment	0.12	1.4	1130
Sandy loam (Brazil)	1.5	0.51	35
Clay loam (Brazil)	4.8	0.64	14
Sandy clay loam (Brazil)	1.0	**0.13**	13
Clay loam (Canada)	2.0	1.4	73
Clay loam (Canada)	3.6	0.67	19
Median Value		**0.54**	**40**

Table A3. Mobility Properties of BSTCA (Penoxsulam Metabolite) (MRID 458308-02)

Soil	% Organic Carbon	K_d (mL/g)	K_{oc} (mL/g)
Silty clay loam (France)	0.97	0.72	74
NC Sand	0.4	0.19	46
AR Silt loam	0.97	1.5	156
CA Clay loam	2.5	0.61	25
Silty clay loam (Italy)	0.99	4.4	444
Sandy clay loam (UK)	1.6	0.085	5
Median Value		**0.67**	**60**

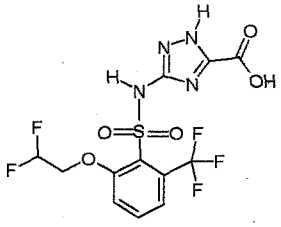
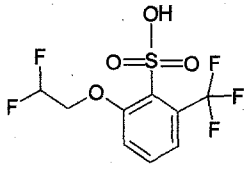
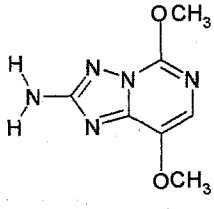
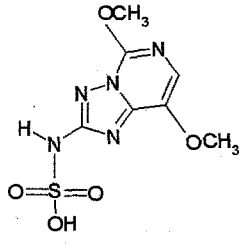
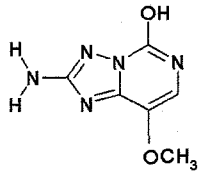
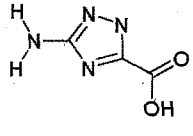
Table A4. Mobility Properties of BST (Penoxsulam Metabolite) (MRID 458308-02)

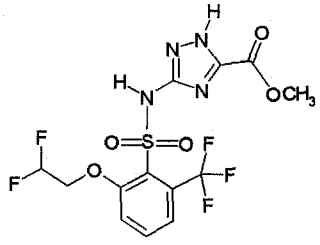
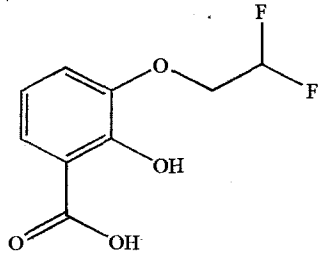
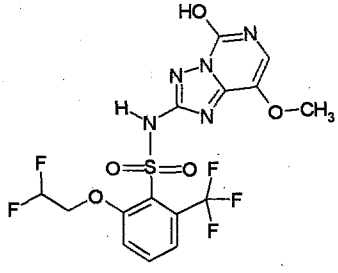
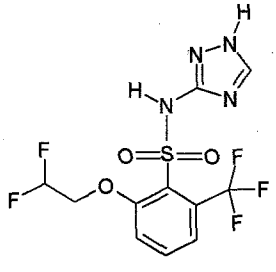
Soil	% Organic Carbon	K_d (mL/g)	K_{oc} (mL/g)
NC Sand	0.4	0.14	34
AR Silt loam	0.97	0.59	61
CA Clay loam	2.5	0.42	18
ND Loam	2.7	0.5	21
Silty clay loam (Italy)	0.99	0.84	85
Silty clay loam (France)	0.97	0.47	48
Sandy clay loam (UK)	1.6	0.075	5
Sandy loam (Italy)	0.86	0.61	71
Median Value		**0.49**	**41**

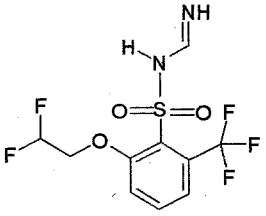
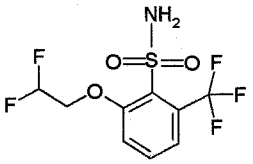
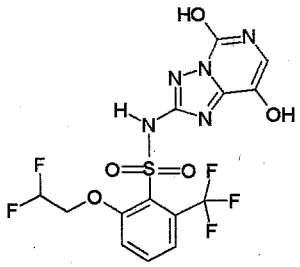
Table A5. Mobility Properties of 5-OH-penoxsulam (Penoxsulam Metabolite) (MRID 458308-02)

Soil	% Organic Carbon	K_d (mL/g)	K_{oc} (mL/g)
NC Sand	0.4	0.14	34
AR Silt loam	0.97	0.33	34
CA Clay loam	2.5	0.46	18
ND Loam	2.7	1	38
Silty clay loam (Italy)	0.99	1.4	144
Silty clay loam (France)	0.97	0.4	42
Sandy clay loam (UK)	1.6	0.28	18
Sandy loam (Italy)	0.86	0.3	34
Median Value		**0.37**	**34**

Table A6. Maximum Reported Amounts of Specific Degradation Products

Degradate Name	Structure	Maximum % Applied	Study Type
BSTCA 3-[[[2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)phenyl]-sulfonyl]amino]-1H-1,2,4-triazole-5-carboxylic acid		11.1% 7.2% 39.4%* 37.2%* 25.4%	soil photolysis aqueous photolysis aerobic aquatic metabolism aerobic soil metabolism anaerobic aquatic metabolism
BSA 2-(2,2-difluoroethoxy)-6-(trifluoromethyl) benzenesulfonic acid		8.1% 36.1%	soil photolysis aqueous photolysis
2-amino-TP 5,8-dimethoxy [1,2,4]triazolo[1,5-c] pyrimidin-2-amine		10.4%* 18.2%	soil photolysis aqueous photolysis
TPSA (5,8-dimethoxy [1,2,4]triazolo-[1,5-c]pyrimidin-2-yl-sulfamic acid)		56%	aqueous photolysis
5-OH, 2-Amino TP 8-methoxy-[1,2,4]triazolo[1,5-c]pyrimidin-5-ol-2-amine		32%	aqueous photolysis
2-Amino TCA 2-amino-1,2,4-triazole carboxylic acid		85%*	aqueous photolysis

Degradate Name	Structure	Maximum % Applied	Study Type
BSTCA methyl Methyl 5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphonyl]amino], 1H-1,2,4-triazole-3-carboxylic acid)		12% 1.4% 12.8%	aqueous photolysis aerobic soil metabolism anaerobic aquatic metabolism
Di-FESA 3-(2,2-Difluoroethoxy)-2-hydroxybenzoic acid		7.6%	aqueous photolysis
5-OH-penoxsulam 2-(2,2-Difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl) benzenesulfonamide		40.3% 62.6% 41.6%	aerobic aquatic metabolism aerobic soil metabolism anaerobic aquatic metabolism
BST 2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazole-3-yl-6-(trifluoromethyl) benzenesulfonamide		6.3% 4.8%	aerobic soil metabolism anaerobic aquatic metabolism

Degradate Name	Structure	Maximum % Applied	Study Type
SFA 2-2,2-Difluoroethoxy)-N-(iminomethyl-6-(trifluoromethyl)-benzenesulfonamide		14.7%*	aerobic soil metabolism
Sulfonamide 2-(2,2-Difluoroethoxy) -6-(trifluoromethyl)-benzenesulfonamide		33.0%*	aerobic soil metabolism
5,8-diOH 2-(2,2-Difluoroethoxy) -6-trifluoromethyl-N-(5,8-dihydroxy-[1,2,4] triazolo[1,5-c] pyrimidin-2-yl) benzenesulfonamide		11.0%*	anaerobic aquatic metabolism
$^{14}CO_2$		not reported	aqueous photolysis
		3.2%*	soil photolysis
		16.1%*	aerobic soil metabolism
		1.2%*	anaerobic aquatic metabolism
		2.4%*	aerobic aquatic metabolism
Non-extractable Residues		30.1%*	aqueous photolysis (over sediment)
		30.9%*	soil photolysis
		55.5%	aerobic soil metabolism
		57.9%*	aerobic aquatic metabolism
		55.5%	anaerobic soil metabolism

*Maximum % of applied reported at study termination indicating that amounts may have continued to increased with time

Summary of Reviewed Study Reports

161-1 ***Hydrolysis*** **MRID #458307-21**

Penoxsulam (1 mg a.i./L) was stable to hydrolysis in the dark, at 25°C in sterile aqueous buffered solutions at pH 5 (acetate), pH 7 (piperazineethanesulfonic acid), pH 9 (borate), and in natural water from White River, ID (ph 8.0). No major or minor transformation products were identified in any of the test systems. Volatiles were not measured. Hydrolysis is expected to be an insignificant route of dissipation in the environment. This study is *acceptable* and satisfies the hydrolysis data requirement.

161-2 ***Aqueous Photolysis*** **MRID #45830722**

The photo degradation of penoxsulam was studied at 23°C for 28 days, in nonsterile AR pond water at pH 7 at a concentration of 0.1 mg a.i./L, and for 59 days in flooded AR silt loam soil at pH 5.8 at a concentration of 0.1 mg a.i./g. Penoxsulam degraded when irradiated outdoors under natural light in a neutral pH solution, with a half-life of 3.1 days, and in a flooded, aerobic soil system with a half-life of 14.2 days. The study author suggested that the longer half-life in the flooded soil was due to the turbidity of the samples. However, it is also plausible that the pH of the test system effected the photolytic half-life. Volatiles were not measured. Samples were analyzed by HPLC, with further analysis using MS.

The major transformation products in natural water were 5-OH 2-Amino TP, and 2-amino TP (see Table B6 for full Chemical Abstract Service names of transformation products). The major transformation products in flooded soil were 5-OH 2-amino TP, BST, and BSTCA. The minor transformation products in natural water were BSTCA, BSTCA-methyl, 5-OH 2-Amino TP, and di-FESA. An unidentified peak believed to consist of multiple polar compounds was a maximum 64% of the applied at study termination. The minor transformation product in flooded soil was 2-amino TP.

In a supplementary study conducted under similar conditions using [^{14}C-phenyl]penoxsulam, it was demonstrated that 20.5% of the applied was evolved as $^{14}CO_2$ from the buffer solution and 11.7% was evolved from the natural water by 14 days posttreatment. Two proposed major routes of degradation involved the cleavage of the sulfonamide group at different sites. The proposed minor route of degradation involved the opening of the pyrimidine ring. All transformation pathways end with the formation of more than 15 polar photodegradation products.

This study is classified *supplemental* because the study was conducted using either nonsterile unbuffered pond water or flooded soil. Additionally, environmental conditions during outdoor incubation were not adequately described (i.e., cloud cover, hours of sunlight). However, no additional date is required at this time.

161-2 ***Aqueous Photolysis*** **MRID #45834801**

Penoxsulam degraded rapidly when irradiated in neutral pH solutions, with environmental phototransformation half-lives of 1.5 days in both test systems. The photo degradation of

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penoxsulam was studied for the equivalent of 28 days of 12 hour light/12 hour dark cycles under a Xenon lamp, at 25 ± 2°C in sterile pH 7 aqueous phosphate buffer and in pH 7.8 natural water (Letcombe, England) at a nominal concentration of 0.15 µg a.i./mL under continuous irradiation, using a UV-filtered xenon lamp. Volatiles were not measured. Samples were analyzed directly by LSC and HPLC.

The major transformation products were BSA, TPSA, 2-amino TP, BSA, 5-OH 2-amino TP, and 2-amino TCA (see Table B6 for full Chemical Abstract Service names of transformation products). Minor transformation products were BSTCA, BSTCA-methyl, 5-OH, 2-amino TP, and di-FESA. Polar compounds totaled a maximum of 74% of the applied at 28 days posttreatment. In a supplementary study conducted under similar conditions using [^{14}C-phenyl]penoxsulam, it was demonstrated that 21% of the applied was evolved as $^{14}CO_2$ from the buffer solution and 12% was evolved from the natural water by 14 days posttreatment. Two proposed major routes of degradation involved the cleavage of the sulfonamide group at different sites. The proposed minor route of degradation involved the opening of the pyrimidine ring. All transformation pathways end with the formation of more than 15 polar photodegradation products.

This study is classified *supplemental* because material balances in the phenyl-labeled experiment was incomplete. Additionally, the portion of this study using natural water does not fulfill requirements because the CO_2 data are contradictory. However, no additional date is required at this time.

161-3 *Soil Photolysis* MRID #458307-23

Penoxsulam degraded photolytically with a calculated environmental phototransformation half-lives of 31 days on Italian silty clay loam soil, and 19.1 days on AR silt loam soil. The photodegradation of penoxsulam was studied for 20 days under a 12 hour light/12 hour dark cycle at 18.9 ± 1.6 °C on silty clay loam soil from Italy, and for 37 days under continuous irradiation at 24.1 ± 2.0 °C on silt loam soil from Arkansas at approximately 50 g a.i./ha under a UV-filtered Xenon arc lamp. The soil extracts, extracted soils, and volatile traps were analyzed for total radioactivity using LSC. The soil extracts were also analyzed for penoxsulam and its transformation products using HPLC by comparison to unlabeled reference standards that were cochromatographed with the samples. Further identification of isolated compounds was done with LC-MS.

The major transformation products in AR silt loam soil were 2-amino TP and BSTCA (see Table B6 for full Chemical Abstract Service names of transformation products). There were no minor transformation products identified in AR silt loam soil.. No major or minor transformation products were identified in the Italian silty clay loam soil. A maximum of 3.2% of the applied was evolved as $^{14}CO_2$ in the AR test systems. Volatiles were not measured in the Italian test system.

This study is classified supplemental, and does not satisfy the soil photolysis data requirement. The study is scientifically valid, but the mass balance for one test system dropped to <90% of the applied, the temperature was not maintained at 25 ± 1°C either of the soil studies, the moisture content was not maintained or adjusted in one soil study, and transformation products were

identified in the Italian silty clay loam soil. However, no additional date is required at this time.

162-1 ***Aerobic Soil Metabolism*** **MRID #458307-24**

Penoxsulam degraded aerobically with a calculated half-lives of 33.8 days in an pH 5.8 Arkansas silt loam soil, 43.4 days in a pH 6.5 California clay loam soil, and 117.5 days in a pH 6.9 North Dakota loam soil. The biotransformation of [phenyl-U-^{14}C]- and [triazolopyrimidine-2-^{14}C]-labeled penoxsulam was studied in three United States soils for 365 days, at an application rate equivalent to 150 g a.i./ha, under aerobic conditions in darkness at 25 ± 1°C and soil moisture 75% at 1/3 bar. Soil extracts, extracted soil and volatile trapping solutions were analyzed for total radioactivity using LSC. Extracts were analyzed for [^{14}C]penoxsulam and its transformation products by reverse-phase HPLC. [^{14}C]Compounds were identified by comparison to reference standards. Identifications of penoxsulam degradates were confirmed using LC/MS.

Among the three soil systems, major transformation products include: 5-OH-penoxsulam, BSTCA, SFA, and CO_2. Minor transformation products include: BST, sulfonamide, BSTCA methyl, and CO_2.

In a supplementary study to provide degradation information for future residue studies to carried out in Japan, an additional two Japanese loam soils (pH 5.5 and pH 5.3) were studied for 120 days at 25 ± 1°C and soil moisture 40% of moisture holding capacity. Based on first-order linear regression analysis, the half-lives are reported to be 50.2 and 41.0 days..

A possible transformation pathway for the degradation of penoxsulam (see Table B6 for full Chemical Abstract Service names of transformation products) in aerobic soil was proposed by the study author. Penoxsulam could degrade via demethylation of the methoxy group in the 5-position of the triazolopyrimdine ring to 5-OH-penoxsulam. 5-OH-penoxsulam could then degrade via the BSTCA methyl transformation product to BSTCA. BSTCA could, in turn, degrade to BST, and then to SFA. This proposed transformation pathway is consistent with submitted laboratory studies. This study is classified *acceptable* and can be used to fulfill the aerobic soil metabolism data requirement for penoxsulam.

162-4 ***Aerobic Aquatic Metabolism*** **MRID #458307-26**

Penoxsulam degraded aerobically under aquatic conditions with calculated, total system half-lives of: 16 days (13 to 23 days at the 90% confidence interval) in AR pond water- silty clay sediment (pH 6.3), 29 days (23 to 38 days at the 90% confidence interval) in AR pond water- silt loam soil (pH 5.8), 12 days (11 to 15 days at the 90% confidence interval) in Italian channel water-loam sediment (pH 7.7), 38 days (27 to 64 days at the 90% confidence interval) in French lake water-sand sediment (pH 6.6), 30 days (28 to 32 days at the 90% confidence interval) in HPLC water-Japanese volcanic loam soil (pH 6.9), and 31 days (28 to 35 days at the 90% confidence interval in HPLC water-Japanese nonvolcanic loam soil (pH 5.3).

All incubations were conducted for 99 days under aerobic conditions in darkness either at 25°C (Arkansas and Japan systems) or 20°C (Italy and France systems). Based on the water

volume, [^{14}C]penoxsulam was applied at a nominal rate of either 0.1 mg a.i./L (Arkansas, Italy and France systems) or 0.04 mg a.i./L (Japan systems), with a sediment/soil:water ratio of 1:4. Sodium hydroxide solution in a sidearm flask was used for the passive collection of CO_2, but volatile organic compounds were not trapped. The water-sediment/soil systems were pre-incubated 14 days, except for the 0-day Arkansas soil, France sediment and Japan soil (volcanic and nonvolcanic) systems which were prepared and treated the same day.

[^{14}C]Residues partitioned from the water layer to the sediment/soil with distribution ratios (water:sediment/soil) between 1:3 and 1:1 at 3 months. Major nonvolatile transformation products for both labels in all six systems were identified via LC/MS as 5-OH-penoxsulam and BSTCA (see Table B6 for full Chemical Abstract Service names of transformation products). With the exception of CO_2, no minor transformation products were positively identified. A possible transformation pathway was proposed by the study authors. Under aerobic aquatic conditions, the 5-methoxy group on the triazolopyrimdine ring could be converted to a hydroxy group to yield 5-OH-penoxsulam. 5-OH-penoxsulam could then degrade to BSTCA. This proposed transformation pathway is consistent with submitted laboratory studies.

This study is classified *acceptable*, and can be used toward the fulfillment of the aerobic aquatic metabolism guideline data requirements for penoxsulam.

162-3 *Anaerobic Aquatic Metabolism* MRID #458307-25

Penoxsulam degraded anaerobically under aquatic conditions with calculated, total system half-lives of: 4.8 days (4.3 to 5.4 days at the 90% confidence interval) in AR pond water- silty clay sediment (pH 6.3 water, pH 5.1 sediment), 11 days (9.6 to 12 days at the 90% confidence interval) in AR pond water- silt loam soil (soil pH 5.8), and for 6.6 days (6.0 to 7.3 days at the 90% confidence interval) distilled water- Italian silty clay loam soil (soil pH 6.2).

The biotransformation of penoxsulam was studied in darkness, for one year in AR pond water- silty clay sediment at 25°C, and for 120 days in AR pond water- silt loam soil at 25°C, and distilled water- Italian silty clay loam soil at 20°C, all at an application rate based on water volume of 0.1 mg a.i./L. The sediment:water ratio used was 1:3 and the soil:water ratio was 1:2. The water-sediment/soil systems were pre-incubated 29 days. Sodium hydroxide solution in a sidearm flask was used for the passive collection of CO_2, but volatile organic compounds were not trapped.

Water layers, sediment/soil extracts, extracted sediment/soil and trapping solutions were analyzed for total radioactivity using LSC. Water layers and sediment/soil extracts were analyzed for [^{14}C]penoxsulam and its transformation products by reverse-phase HPLC. [^{14}C]Compounds were identified by comparison to unlabeled reference standards. Identifications were confirmed using LC/MS.

[^{14}C]Residues partitioned from the water layer to the sediment/soil with distribution ratios (water:sediment/soil) between 1:2 after 3 months. Major nonvolatile transformation products for both labels in any test system were identified as 5-OH-penoxsulam, BSTCA, BSTCA-methyl and

5,8-di-OH (see Table B6 for full Chemical Abstract Service names of transformation products). Minor transformation products were BSTCA-methyl, BST, and CO_2.

A transformation pathway was proposed by the study authors. Under anaerobic conditions, the 5-methoxy group on the triazolopyrimdine ring is converted to a hydroxy group to yield 5-OH-penoxsulam (see Table B6 for full Chemical Abstract Service names of transformation products). 5-OH-penoxsulam can yield either 5,8-di-OH or BSTCA-methyl. BSTCA-methyl then degrades to BSTCA which then yields BST. This proposed transformation pathway is consistent with submitted laboratory studies. In a supplemental experiment, the presence of penoxsulam, at 0.1 µg/L, had no impact on the microbial viability of the water-sediment/soil systems.

The portions of this study conducted using the Arkansas pond water-silty clay sediment system and the Arkansas pond water-silt loam soil system are classified *acceptable* and can be used towards fulfillment of the anaerobic aquatic metabolism guideline data requirements for penoxsulam. The portion of this study conducted using the Italian distilled water-silty clay loam soil system is classified as *supplemental.* That portion of the study is scientifically valid, but cannot be used towards fulfillment of the anaerobic aquatic metabolism guideline data requirements for penoxsulam because an inappropriate test water was used for the distilled water-silty clay loam soil system.

163-1 *Adsorption/Desorption* MRID #458308-01

The adsorption/desorption characteristics of [triazolopyrimidine-2-^{14}C]-labeled penoxsulam were studied in a batch equilibrium experiment in a sand soil from North Carolina (pH 5.6), a silt loam soil from Arkansas (pH 5.8), a clay loam soil from California (pH 6.5), a loam soil from North Dakota (pH 6.9), a silty clay sediment from Arkansas (pH 5.1), a loam soil from Japan (pH 6.9), a sandy clay loam soil from Japan (pH 6.3), two loam soils from Japan (pH 5.5 and pH 5.3), a sandy loam soil from Brazil (pH 6.0), a clay loam soil from Brazil (pH 6.7), a sandy clay loam soil from Brazil (pH 7.3), two clay loam soils from Canada (pH 6.0 and pH 8.1), a silty clay loam from Italy (pH 6.2), a sandy loam soil from Italy (pH 6.3), a silty clay loam soil from France (pH 6.2) and a sandy clay loam soil from the UK (pH 8.0). The adsorption phase of the study was carried out in 12 of the 18 soils by equilibrating moist soil with [triazolopyrimidine-2-^{14}C]penoxsulam at nominal concentrations of 0.08, 0.4, 2.0, and 10.0 mg a.i/kg soil at 20°C for 24 hours. The adsorption phase of the study was carried out for the remaining 5 foreign soils and one domestic sediment by equilibrating moist soil with [triazolopyrimidine-2-^{14}C]penoxsulam at a nominal concentration of 2.0 mg a.i/kg soil at 20°C for 24 hours.

The desorption phase of the study was carried out by twice replacing the adsorption solution with an equivalent volume of pesticide-free 0.01M $CaCl_2$ solution and equilibrating for 24 hours 20°C. After adsorption and desorption, the supernatant solution was separated by centrifugation, decanted, and were analyzed for total radioactivity using LSC. Following desorption, the soils were extracted two or three time, centrifuged, and analyzed using LSC. [^{14}C]Residues remaining in the extracted soil were quantified by LSC following combustion..

[^{14}C]Penoxsulam was stable in the adsorption supernatants and first desorption solutions, based on HPLC analyses. Greater than 90% was unchanged parent compound. Several second desorption and extraction samples showed 85-90% unchanged penoxsulam. After 24 hours of equilibration, between 11 and 86% of the applied [^{14}C]penoxsulam was adsorbed.

Simple adsorption K_d values were 0.33, 0.34, 0.95, 0.80, 9.4, 2.4, 0.63, 0.60, 2.5, 0.60, 0.19, 0.37, 1.4, 0.51, 0.636, 0.13, 1.4, and 0.67 for the NC sand, AR silt loam, Japanese loam, Japanese sandy clay loam, Japanese loam, Japanese loam, CA clay loam, ND loam, Italian silty clay loam, French silty clay loam, sandy clay loam from the UK, Italian sandy loam soils, AR silty clay sediment, Brazilian sandy loam, Brazilian clay loam, Brazilian sandy clay loam, Canadian clay loam, and Canadian clay loam soils, respectively. Freundlich K_{ads} values were 0.27, 3.71, 0.59, 0.56, 4.69, 1.55, 0.49, 0.45, 1.96, 0.48, 0.16, and 0.32 for the same 12 soils, for the NC sand, AR silt loam, Japanese loam, Japanese sandy clay loam, Japanese loam, Japanese loam, CA clay loam, ND loam, Italian silty clay loam, French silty clay loam, sandy clay loam from the UK, and Italian sandy loam soils, respectively. Freundlich K_{oc} values were 76, 40, 22, 40, 305, 194, 20, 21, 253, 66, 13, and 46 for the NC sand, AR silt loam, Japanese loam, Japanese sandy clay loam, Japanese loam, Japanese loam, CA clay loam, ND loam, Italian silty clay loam, French silty clay loam, sandy clay loam from the UK, Italian sandy loam soils, respectively. Simple K_{oc} values were 130, 35, 14, 13, 73, and 19 for the silty clay sediment from AR silty clay sediment, Brazilian sandy loam, Brazilian clay loam, Brazilian sandy clay loam, Canadian clay loam, and Canadian clay loam soils, respectively.

At the end of the desorption phase, between 4.7 and 82.8% of the applied ^{14}C was desorbed. Freundlich K_{des} values were 1.56, 0.55, 4.16, 2.97, 20.77, 5.44, 2.88, 2.28, 5.09, 2.05, 0.87, and 0.86 for the NC sand, AR silt loam, Japanese loam, Japanese sandy clay loam, Japanese loam, Japanese loam, CA clay loam, ND loam, Italian silty clay loam, French silty clay loam, sandy clay loam from the UK, Italian sandy loam soils, respectively. Freundlich K_{oc} values were 296, 197, 279, 193, 2156, 713, 156, 150, 720, 264, 192, and 169 for the same 12 soils, NC sand, AR silt loam, Japanese loam, Japanese sandy clay loam, Japanese loam, Japanese loam, CA clay loam, ND loam, Italian silty clay loam, French silty clay loam, sandy clay loam from the UK, Italian sandy loam soils, respectively. No correlation was found for the relationship between Kd and percent organic carbon, pH or percent clay.

This study is classified as *acceptable*, and can be used to fulfill the data requirements for a mobility study for penoxsulam using unaged soil.

163-1 *Adsorption/Desorption* MRID #458308-02

The adsorption/desorption characteristics of three major penoxsulam metabolites, BSTCA, BST, and 5-OH-penoxsulam (see Table B6 for full Chemical Abstract Service names of transformation products), were studied in a batch equilibrium experiment in a NC sand soil (pH 5.6), an AR silt loam soil (pH 5.8), a CA clay loam soil (pH 6.5), a ND loam soil (pH 6.9), an Italian silty clay loam (pH 6.2), an Italian sandy loam soil (pH 6.3), a French silty clay loam soil (pH 6.2), and a UK sandy clay loam soil (pH 8.0).

The adsorption phase of the study was carried out by equilibrating soil with [^{14}C]BSTCA/BST and [^{14}C]5-OH-penoxsulam at a nominal concentration of 0.4 mg a.i/kg soil at 20°C in a 0.01M $CaCl_2$ solution with soil/solution ratios of 1:2 (w:v) for all soils. BSTCA was unstable in solution and continued to degrade to BST throughout the study. Desorption was not studied. The supernatants were analyzed for total radioactivity using LSC. The soil extracts were analyzed for total radioactivity using LSC. Portions of the extracts were further analyzed using HPLC. [^{14}C]Residues remaining in the extracted soil were quantified by LSC following combustion.

After 2 hours of equilibration, between 1.4 and 24.6% of the applied [^{14}C]BSTCA was adsorbed to the NC sand, AR silt loam, CA clay loam, Italian silty clay loam, French silty clay loam, and UK sandy clay loam soils, respectively. Calculated simple adsorption K_d values were 0.185, 1.515, 0.605, 4.395, 0.720, and 0.085 for the NC sand, AR silt loam, CA clay loam, Italian silty clay loam, French silty clay loam, and UK sandy clay loam soils, respectively. Corresponding K_{oc} values were 46, 156, 25, 444, 74, and 5.

After 2 hours of equilibration, between 3.2 and 33.5% of the applied [^{14}C]BST was adsorbed to the NC sand, AR silt loam, CA clay loam, ND loam, Italian silty clay loam, French silty clay loam, UK sandy clay loam, and Italian sandy loam soils, respectively. Calculated adsorption K_d values were 0.135, 0.590, 0.420, 0.545, 0.840, 0.470, 0.075, and 0.610 for the NC sand, AR silt loam, CA clay loam, ND loam, Italian silty clay loam, French silty clay loam, UK sandy clay loam, and Italian sandy loam soils, respectively. Corresponding K_{oc} values were 34, 61, 18, 21, 85, 48, 5, and 71.

After 24 hours of equilibration, between 6.6 and 39.6% of the applied [^{14}C]5-OH-penoxsulam was adsorbed to the NC sand, AR silt loam, CA clay loam, ND loam, Italian silty clay loam, French silty clay loam, UK sandy clay loam, and Italian sandy loam soils, respectively. Calculated K_d values were 0.140, 0.325, 0.455, 1.030, 1.425, 0.400, 0.280, and 0.295 for the NC sand, AR silt loam, CA clay loam, ND loam, Italian silty clay loam, French silty clay loam, UK sandy clay loam, and Italian sandy loam soils, respectively. Corresponding K_{oc} values were 34, 34, 18, 38, 144, 42, 18, and 34. No correlation was found for the relationship between Kd and percent organic carbon, pH or percent clay.

This study is classified as *supplemental*. The study cannot be used toward the fulfilment of the mobility data requirement guideline requirement for penoxsulam, because (1) the study was conducted using transformation products of penoxsulam rather than the parent compound. Additionally, desorption was not studied.

163-1 *Leaching/Aged Column* MRID #458348-02

In the preliminary study, [^{14}C]penoxsulam was applied to three of the four definitive study soils (Japanese sandy silt loam, Nagaoka clay loam, and Arkansas silt loam). After two days at room temperature, the [^{14}C]penoxsulam-treated soils were extracted, the extracts were analyzed by

LSC.

Leaching - Unaged Column

The column leaching of [triazolopyrimidine-2-^{14}C]penoxsulam was studied in the dark for 48 hours in four unaged soils: Japanese sandy silt loam (pH 6.5), Japanese clay loam (pH 5.8), AR silt loam (pH 5.7) and Italian sandy loam (pH 6.4). Two types of unaged soil column leaching experiments were performed in the study: a free-draining experiment and a saturated (flooded) experiment. All four soils were used in the free-draining experiment. Only the Japanese clay loam and the Italian sandy loam soils were used in the saturated experiment.

In the free-draining experiment, the flow of 0.01M $CaCl_2$ solution was controlled at the top of the column and uncontrolled at the bottom. In the saturated experiment, the flow of aqueous solution was restricted to maintain a 5 cm layer of the solvent on the top of the column. The application rate of penoxsulam was equivalent to 71 g/ha (approximately twice the maximum field application rate). The soils of the free-draining experiment were extracted, purified, and further analyzed by LSC and reverse-phase HPLC. The extracted soils were then combusted, analyzing for total radioactivity using LSC. Leachates were analyzed for total radioactivity using LSC and reverse-phase HPLC.

Free-draining experiment:

In unaged Japanese sandy silt loam soil treated with [triazolopyrimidine-2-^{14}C]penoxsulam, the distribution of total radioactivity was 40%, 26%, 20%, 13%, 1.5%, and not detected (the 0-5 cm, 5-10 cm, 10-15 cm, 15-20 cm, 20-25 cm, and 25-30 cm soil column depths, respectively. A minor, uncharacterized transformation product was only measured in the 5-10 cm and 10-15 cm soil column depths at < 1% of the applied respectively.

In unaged Japanese clay loam soil treated with [triazolopyrimidine-2-^{14}C]penoxsulam, the distribution of total radioactivity was 103% for the 0-5 cm and below the level of detection in all other soil column depths. The minor transformation product observed in the other test systems was not detected in any soil column depths.

In unaged Arkansas silt loam soil treated with [triazolopyrimidine-2-^{14}C]penoxsulam, the distribution of total radioactivity was 86% for the 0-5 cm soil layer, 12% for the 5-10 cm soil layer, and below the limit of detection in all other soil layers. A minor transformation product was reported at a maximum of 2% of the applied in the 0-5 cm soil column depth, accounted for 1% in the 5-10 cm, and was not detected in any other soil column depths.

In unaged Japanese sandy silt loam soil treated with [triazolopyrimidine-2-^{14}C]penoxsulam, the distribution of total radioactivity was 10%, 20%, 23%, 19%, 12%, and 13% for the 0-5 cm, 5-10 cm, 10-15 cm, 15-20 cm, 20-25 cm, and 25-30 cm soil column depths, respectively. A minor transformation product was reported at a maximum of 0.9% of the applied in the 10-15 cm soil

layer.

Volatile [^{14}C]organic compounds, $^{14}CO_2$, and bound residues were not measured individually in the free-draining experiment.

Saturated experiment:

In unaged Japanese clay loam soil treated with [triazolopyrimidine-2-^{14}C]penoxsulam, the distribution of total radioactivity was 36%, 16%, 15%, 10%, 15%, and 6% for the 0-5 cm, 5-10 cm, 10-15 cm, 15-20 cm, 20-25 cm, and 25-30 cm soil column depths, respectively.

In unaged Japanese sandy loam soil treated with [triazolopyrimidine-2-^{14}C]penoxsulam, the distribution of total radioactivity was 21%, 28%, 25%, 15%, 7%, and 1.5% for the 0-5 cm, 5-10 cm, 10-15 cm, 15-20 cm, 20-25 cm, and 25-30 cm soil column depths, respectively.

Total extractable [^{14}C]residues, nonextractable [^{14}C]residues, volatile [^{14}C]organic compounds, $^{14}CO_2$, and bound residues were not measured individually in either soil column of the saturated soil leaching experiment.

This study is classified supplemental. Both portions of this study, conducted using [triazolopyrimidine-2-^{14}C]penoxsulam in a free-draining and saturated leaching conditions, are scientifically valid, but do not satisfy data requirements for a mobility study using aged soil because: (1) only one ring in penoxsulam was radiolabeled, (2) the required minimum of four test soils were not studied in all portions of the primary study, (3) three test soils were foreign in origin and not completely characterized or compared to U.S. soils, (4) no test soil contained an organic matter content less than 1%, and (5) the test soils were leached with 20 cm of $CaCl_2$ solution, rather than the required 50.8 cm.

164-2 *Aquatic Field Dissipation* MRID #458308-04.

Penoxsulam, formulated as a liquid, was applied once at an application rate of 100 g a.i./ha (2 times the current proposed label rate) onto a bareground and a dry-seeded rice plot of Amagon silt loam soil in Arkansas, and onto a bareground and a wet-seeded rice plot of Oswald clay soil in California. The plots at the CA filed were flooded at application, while the AR field site were flooded 11 days after application, with both sites remaining flooded through the growing season.

Water samples were collected for analysis of penoxsulam and seven transformation products: 5-OH-penoxsulam, 2-amino-TP, BSTCA, BSA, TPSA, sulfonamide, and 5-OH-2-amino-TP (see Table B6 for full Chemical Abstract Service names of transformation products). Soil samples were collected for the analysis of penoxsulam and five transformation products: 5-OH-penoxsulam, 2-amino-TP, BSTCA, BSA, and sulfonamide for up to one year after application. The LOQ in water and soil were 0.003 µg/mL and 0.003 µg/g, respectively, for all analytes.

Arkansas field site

Dissipation of penoxsulam in the AR test plots was dominated by soil kinetics following

application to bareground and dry-seeded rice plots. Calculated half-life values for penoxsulam in soil were 13 days for the bareground plot and 14 days for the cropped plot. Penoxsulam dissipated in the ***paddy water with a calculated half-life value of 3.5 days in the bareground plot and 3.8 days in the cropped plot.*** Penoxsulam dissipated from the total system with a calculated half-life value of 16 days in both the bareground plot and in the cropped plot.

Penoxsulam dissipated in the 0 to 3 inch soil depth from a maximum concentration of 80-88 ppm at 1day, to 26-47 ppm by 7-13 days, and to less than the LOQ by 55 days posttreatment (bareground and cropped plots). Residues of penoxsulam and its transformation products were generally confined to the upper 9 inches of soil layers, but were detected above the LOQ in the cropped plot as deep as the 12 to 15 inch soil depth. The only transformation products detected in the soil were BSTCA, and 5-OH-penoxsulam, and BSA. The transformation products 2-amino-TP and sulfonamide were not detected in either test plot.

Penoxsulam was detected in the paddy water 2 days following flooding at maximum concentrations of 5 ppm in the bareground plot and 15 ppm in the cropped plot, then quickly dissipated. With the exception of BSTCA 7 days after flooding, penoxsulam transformation products were not detected in the paddy water at any sampling interval.

California field site

Dissipation of penoxsulam in the CA test plots was dominated by water kinetics following application to flooded bareground and wet-seeded rice plots. Calculated ***half-life values for penoxsulam in paddy water of 5 days in the bareground plot and 7 days in the cropped plot.*** Calculated half-life values for penoxsulam in soil were 14 days for the bareground plot and 26 days for the cropped plot. Penoxsulam dissipated from the total system with a calculated half-life value of 5 days in the bareground plot and 10 days in the cropped plot.

The only transformation products detected in the paddy water at a mean concentration above the LOQ were BSTCA and TPSA. The transformation product BSA was detected in the bareground plots, but was not detected above the LOQ. The transformation products 5-OH DE-638, sulfonamide, 2-amino-TP, and 5-OH-2-amino-TP were not detected in either test plots.

Penoxsulam dissipated in the 0 to 3 inch soil depth from a maximum concentration of 13-14 ppm at day 0 to less than the LOQ by 14 days in the bareground plot and by 60 days in the cropped plot. Residues of penoxsulam and its transformation products were generally confined to the upper 3 inch soil layer, but were detected above the LOQ in the cropped plot as deep as the 3 to 6 inch soil depth. The only transformation products detected in the soil were BSTCA and 5-OH-penoxsulam. The transformation product BSA was detected once in the cropped plot, below the LOQ, and the transformation products 2-amino-TP and sulfonamide were not detected in either test plot.

This study is classified *supplemental* and does not satisfy the data requirements for aquatic field dissipation because it was not possible to determine if the penoxsulam degradation products, which may be of toxicological concern, that formed in the paddy water through aqueous photolysis

partitioned into the sediment. However, no additional data is required at this time.

164-2 ***Aquatic Field Dissipation*** **MRID #458308-05.**

Penoxsulam, formulated as a granule mixture, was applied once at an application rate of 56 g a.i./ha onto a flooded plot of Oswald clay soil in Sutter County, California which had been planted with rice. Following application, water samples were collected for analysis of penoxsulam and seven transformation products: 5-OH-penoxsulam, 2-amino-TP, BSTCA, BSA, TPSA, sulfonamide, and 5-OH-2-amino-TP (see Table B6 for full Chemical Abstract Service names of transformation products) through 92 days after application (when the permanent floods were drained). Soil samples were collected for analysis of penoxsulam and the transformation products 5-OH-penoxsulam, 2-amino-TP, BSTCA, BSA, and sulfonamide through 306 days posttreatment.

Penoxsulam dissipated in the ***paddy water with a first-order calculated half-life value of 4 days***. Penoxsulam was detected in the paddy water at 33 ppm at day 0, decreased to 10 ppm by 7 days, and was below the LOQ by 14 days posttreatment. Transformation products of penoxsulam were not detected in the paddy water at any sampling interval except for a single detection of BSTCA at the LOD at 21 days posttreatment.

Penoxsulam was detected in the 0 to 3 inch depth of the soil at a maximum of 4.6 ppm at 2 days, and was below the LOQ by 21 days posttreatment. The only two transformation products detected in the soil at a mean concentration above the LOD were 5-OH-penoxsulam and BSTCA. 5-OH-penoxsulam was detected in the 0 to 3 inch soil depth at a maximum of 1.2 ppm at 14 days, and was not detected in soil following 30 days posttreatment. BSTCA was detected in the 0 to 3 inch soil depth at a maximum of 3 ppm at 14 days, and decreased to 2 ppm by 306 days. No analytes were detected below the 3 inch soil depth except for BSTCA, which was detected once in the 3 to 6 inch depth, at 1 pm at 306 days posttreatment. The data did not allow for the calculation of a half-life value for penoxsulam in soil.

This study is classified *acceptable* and partially satisfies the guideline data requirements for aquatic field dissipation.

165-5 ***Bioconcentration in Aquatic, Non-target Organisms*** **MRID #458300-01.**

The bioaccumulation of penoxsulam was studied in crayfish (*Procambarus clarkii*) at a concentration of 0.5 ppm under flow-through aquarium conditions. The test system consisted of two glass aquaria fitted with overflows to maintain a volume of 135 L (average flow rate of 94 mL/minute) at a loading rate of 70 crayfish per vessel. The exposure period was 14 days, and the subsequent depuration period was 7 days. The maximum concentration of total [^{14}C]residues in crayfish tail muscle was 14.4 µg/kg at 11 days.

The average steady-state calculated bioconcentration factor (BCF) was 0.02 mL/g. [^{14}C]Residues in the tissues were not characterized. After 5 days of depuration, total [^{14}C]residues were not detected in the crayfish tissue. [^{14}C]Residues in the crayfish during depuration were not characterized.

This study is classified as *acceptable*. The study is scientifically valid, and can be used towards fulfillment of the bioconcentration in aquatic, non-target organisms data requirements for penoxsulam.

Storage Stability **MRID #458307-18.**

The stability of penoxsulam was studied in soil that was treated at 0.03 mg a.i./kg and stored frozen (*ca.* -20°C) for up to 327 days. The penoxsulam transformation products: 5-OH-penoxsuolam, BSA, sulfonamide, BSTCA and 2-amino-TP (see Table B6 for full Chemical Abstract Service names of transformation products) were also studied in soil that was treated at 0.03 mg a.i./kg and stored frozen (*ca.* -20°C) for up to 327 days.

No significant degradation was observed during the frozen storage of penoxsulam, 5-OH, sulfonamide, BSA and 2-amino-TP. BSTCA degrade from an average of 89% of the applied at day 0 to 77% at 327 days.

Storage Stability **MRID #458308-03.**

The stability of penoxsulam was studied in water that was treated at 0.03 mg a.i./L and stored refrigerated (*ca.* 4°C) for up to 284 days, or frozen (-20°C) for up to 221 days. The penoxsulam transformation products: 5-OH-penoxsulam, BSA, sulfonamide, BSTCA, 2-amino-TP, TPSA and 5-OH-2-amino-TP (see Table B6 for full Chemical Abstract Service names of transformation products) were also studied in water that was treated at 0.03 mg a.i./L and stored refrigerated (*ca.* 4°C) for up to 284 days.

No significant degradation was observed during storage of the refrigerated transformation products. Penoxsulam showed no significant degradation for 130 days when stored refrigerated, and no significant degradation was observed in frozen storage for up to 221 days.

Ground and Surface Water Contamination Modeling **MRID #458308-11[5].**

Dow AgroSciences has submitted modeling that addresses both ground and surface water contamination from Penoxsulam applied to rice. For ground water, the registrant used SCI-GROW and generated EECs of 0.0014 and 0.0042 ug/L. Dow assumed effective "holding times"[6] when estimating surface water concentrations. For ecological effects from surface water (Table 1 in Dow document), the highest estimated concentrations for ecological effects occurred in wet-seeded rice in Louisiana on the Gulf Coast. Without imposing mandatory holding times, the highest peak concentration was 42.7 ug/L, which declined to 1.56 ug/L by 21 days after application, and 0.0031 ug/L by 60 days after application. For drinking water, the highest reported peak concentration in the

---

[5]Jim Breithaupt, Agronomist, ERB II, Environmental Fate and Effects Division (7507C)
Lucy Shanaman, Chemist, ERB II, Environmental Fate and Effects Division (7507C)

[6]See Penoxsulam Science Chapter, Appendix B for a more detailed discussion of this submission.

Index Reservoir from all scenarios was 0.26 ug/L after a 78 day effective "holding time", and the maximum chronic (365-day average) concentration was 0.005 ug/L. This concentration also occurred in the water-seeded rice grown on the Gulf Coast in Louisiana. The submitted estimates are of questionable value due to the use of inappropriate values for both degradation and partitioning, because the residues identified by HED as being of toxicological concern were not considered in the calculated half-life estimates, and because of the assumption of effective "holding times" not indicated on the label. This study can not be classified because it has not been submitted to be used towards fulfillment OPP data requirements for penoxsulam.

Structural Analysis (EPI Suite) Output Files

PENOXSULAM (proposed active ingredient)

SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM :
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37
---------- EPI SUMMARY (v3.10) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------

KOWWIN Program (v1.66) Results:
==========

Log Kow(version 1.66 estimate): 2.95

SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM :
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	1	C [aliphatic carbon - No H, not tert]	0.9723	0.9723
Frag	5	-F [fluorine, aliphatic attach]	-0.0031	-0.0155
Frag	11	Aromatic Carbon	0.2940	3.2340
Frag	1	Aromatic Nitrogen	-0.7324	-0.7324
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	3	-O- [oxygen, one aromatic attach]	-0.4664	-1.3992
Frag	1	-SO2-N [aromatic attach]	-0.2079	-0.2079
Frag	2	Aromatic Nitrogen [5-member ring]	-0.5262	-1.0524
Frag	1	Aromatic nitrogen [fused ring location]	-0.0001	-0.0001
Factor	1	o-Alkyloxy to 2 aromat nitrogens/pyrazine	0.8955	0.8955
Const		Equation Constant		0.2290

-------+-----+---------------------------------------+---------+--------

Log Kow = 2.9534

MPBPWIN (v1.40) Program Results:

Experimental Database Structure Match: no data

SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM :
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37
---------- SUMMARY MPBPWIN v1.40 ----------

Boiling Point: 526.67 deg C (Adapted Stein and Brown Method)

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 193.86 deg C (Gold and Ogle Method)
Mean Melt Pt : 271.85 deg C (Joback; Gold,Ogle Methods)
Selected MP: 225.05 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 526.67 deg C (estimated))
(Using MP: 225.05 deg C (estimated))
VP: 2.25E-013 mm Hg (Antoine Method)
VP: 4.14E-011 mm Hg (Modified Grain Method)
VP: 1.29E-010 mm Hg (Mackay Method)
Selected VP: 4.14E-011 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	2	-CH3	21.98	43.96
Group	1	-CH2-	24.22	24.22
Group	1	>CH-	11.86	11.86
Group	1	>C<	4.50	4.50
Group	5	-F	0.13	0.65
Group	3	-O- (nonring)	25.16	75.48
Group	1	>NH (nonring)	45.28	45.28
Group	4	CH (aromatic)	28.53	114.12
Group	6	-C (aromatic)	30.76	184.56
Group	1	C (3a aromatic)	45.46	45.46
Group	4	N (aromatic)	39.88	159.52
Group	1	>S(=O)(=O)	171.58	171.58

```
  *  |    | Equation Constant |        | 198.18
=============+=======================+==========+=========
RESULT-uncorr| BOILING POINT in deg Kelvin | 1079.37
RESULT- corr | BOILING POINT in deg Kelvin | 799.83
         | BOILING POINT in deg C      | 526.67
-------------------------------------------------

-------+-----+-------------------+----------+---------
 TYPE  |NUM | MELT DESCRIPTION | COEFF   | VALUE
-------+-----+-------------------+----------+---------
 Group | 2  | -CH3              |  -5.10 | -10.20
 Group | 1  | -CH2-             |  11.27 |  11.27
 Group | 1  | >CH-              |  12.64 |  12.64
 Group | 1  | >C<               |  46.43 |  46.43
 Group | 5  | -F                | -15.78 | -78.90
 Group | 3  | -O- (nonring)     |  22.23 |  66.69
 Group | 1  | >NH (nonring)     |  52.66 |  52.66
 Group | 4  | CH (aromatic)     |   8.13 |  32.52
 Group | 6  | -C (aromatic)     |  37.02 | 222.12
 Group | 1  | C (3a aromatic)   |  37.02 |  37.02
 Group | 4  | N (aromatic)      |  68.40 | 273.60
 Group | 1  | >S(=O)(=O)        | 150.00 | 150.00
  *  |    | Equation Constant |        | 122.50
=============+=======================+==========+=========
  RESULT    | MELTING POINT in deg Kelvin | 938.35
 RESULT-limit| MELTING POINT in deg Kelvin | 623.00
         | MELTING POINT in deg C      | 349.84
-------------------------------------------------

Water Sol from Kow (WSKOW v1.40) Results:
=========================================

        Water Sol: 2.749 mg/L

SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM   :
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37
---------- WSKOW v1.40 Results ----------
Log Kow  (estimated)  :  2.95
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  2.95
```

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -5.245
Water Solubility at 25 deg C (mg/L): 2.749

ECOSAR Program (v0.99g) Results:

SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37
Log Kow: 2.95 (KowWin estimate)
Melt Pt:
Wat Sol: 230.8 mg/L (calculated)

ECOSAR v0.99g Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**96.568**
Neutral Organics	**: Fish**	**96-hr**	**LC50**	**45.844**
Neutral Organics	**: Fish**	**14-day**	**LC50**	**96.568**
Neutral Organics	**: Daphnid**	**48-hr**	**LC50**	**52.454**
Neutral Organics	**: Green Algae**	**96-hr**	**EC50**	**34.636**
Neutral Organics	**: Fish**	**30-day**	**ChV**	**6.883**
Neutral Organics	**: Daphnid**	**16-day**	**EC50**	**4.076**
Neutral Organics	**: Green Algae**	**96-hr**	**ChV**	**5.998**

Neutral Organics : Fish (SW) 96-hr LC50 16.626
Neutral Organics : Mysid Shrimp 96-hr LC50 6.711

		mg/kg (ppm) dry wt soil		
Neutral Organics	**: Earthworm**	**14-day**	**LC50**	**1515.938 ***

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est : 1.42E-014 atm-m3/mole
Group Est: Incomplete

SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM :
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37

HENRYWIN v3.10 Results

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	9 Hydrogen to Carbon (aliphatic) Bonds		-1.0771
HYDROGEN	4 Hydrogen to Carbon (aromatic) Bonds		-0.6172
HYDROGEN	1 Hydrogen to Nitrogen Bonds		1.2835
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-Car		0.1619
FRAGMENT	3 C-O		3.2564
FRAGMENT	5 C-F		-2.0922
FRAGMENT	8 Car-Car		2.1105
FRAGMENT	7 Car-Nar		11.3975
FRAGMENT	1 Nar-Nar	ESTIMATE	3.0000
FRAGMENT	1 Car-S		0.6345
FRAGMENT	1 N-S	ESTIMATE	0.0000
FRAGMENT	1 Car-N		0.7304
FRAGMENT	3 Car-O		1.0418
FRAGMENT	2 O=S (sulfone-type)	ESTIMATE	2.1000

```
FACTOR  |  3  Additional aromatic nitrogen(s)      |       | -7.5000
FACTOR  |  1  -O-carbon ortho-position to Nar      |       | -0.9600
FACTOR  |  1  -SO2-N-  group                       |       | -1.3500
---------+-----------------------------------------+---------+----------
RESULT  |   BOND ESTIMATION METHOD for LWAPC VALUE  | TOTAL  | 12.236
---------+-----------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 1.42E-014 atm-m3/mole
                = 5.80E-013 unitless

--------+-----------------------------------------+-----------+--------
     |     GROUP CONTRIBUTION DESCRIPTION       | COMMENT | VALUE
--------+-----------------------------------------+-----------+--------
     |       2  CH3 (X)                  |        | -1.24
     |       1  CH2 (C)(O)               |        | -0.13
     |       1  CH (C)(F)(F)             |        |  0.70
     |       3  Car-H (Car)(Car)         |        |  0.33
     |       1  Car-H (Car)(Nar)         |        |  0.11
     |       1  Car (C)(Car)(Car)        |        |  0.70
     |       2  Car (Car)(Car)(O)        |        | -0.86
     |       1  Car (Car)(Car)(S)        |        | -0.25
     |       3  O (C)(Car)               |        |  3.75
     |       2  Nar (Car)(Car)           |        |  6.12
     |         MISSING Value for:  Nar (Nar)(Car)
     |         MISSING Value for:  Car (Nar)(N)(Nar)
     |         MISSING Value for:  Car (Car)(Nar)(Nar)
     |         MISSING Value for:  Nar (Nar)(Car)(Car)
     |         MISSING Value for:  Car (Nar)(O)(Nar)
     |         MISSING Value for:  NH (S)(Car)
     |         MISSING Value for:  S (=O)(=O)(Car)(N)
     |         MISSING Value for:  C (F)(F)(F)(Car)
--------+-----------------------------------------+-----------+--------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |
9.23
--------+-----------------------------------------+-----------+--------
```

Henrys LC [VP/WSol estimate using EPI values]:
HLC: 9.578E-012 atm-m3/mole
VP: 4.14E-011 mm Hg
WS: 2.75 mg/L

BIOWIN (v4.00) Program Results:
==========

SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM :
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37

---------- BIOWIN v4.00 Results ----------

Linear Model Prediction : Does Not Biodegrade Fast
Non-Linear Model Prediction: Does Not Biodegrade Fast
Ultimate Biodegradation Timeframe: Recalcitrant
Primary Biodegradation Timeframe: Weeks
MITI Linear Model Prediction : Does Not Biodegrade Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic ether [-O-aromatic carbon]	0.1319	0.3957
Frag	1	Trifluoromethyl group [-CF3]	-0.5204	-0.5204
MolWt	*	Molecular Weight Parameter		-0.2301
Const	*	Equation Constant		0.7475

RESULT	LINEAR BIODEGRADATION PROBABILITY		0.3927

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic ether [-O-aromatic carbon]	2.2483	6.7449
Frag	1	Trifluoromethyl group [-CF3]	-5.6696	-5.6696
MolWt	*	Molecular Weight Parameter		-6.8639

RESULT	NON-LINEAR BIODEGRADATION PROBABILITY		0.0584

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.1744
Frag	1	Trifluoromethyl group [-CF3]	-0.5130	-0.5130
MolWt	*	Molecular Weight Parameter		-1.0682
Const	*	Equation Constant		3.1992

RESULT	SURVEY MODEL - ULTIMATE BIODEGRADATION		1.4437

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic ether [-O-aromatic carbon]	0.0771	0.2314
Frag	1	Trifluoromethyl group [-CF3]	-0.2744	-0.2744
MolWt	*	Molecular Weight Parameter		-0.6974
Const	*	Equation Constant		3.8477

RESULT	SURVEY MODEL - PRIMARY BIODEGRADATION		3.1073

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic ether [-O-aromatic carbon]	0.1952	0.5857
Frag	5	Fluorine [-F]	0.0174	0.0869
Frag	4	Aromatic-H	0.0082	0.0329
Frag	2	Methyl [-CH3]	0.0004	0.0008
Frag	1	-CH2- [linear]	0.0494	0.0494
Frag	1	-CH- [linear]	-0.0507	-0.0507
MolWt	*	Molecular Weight Parameter		-1.4380
Const	*	Equation Constant		0.7121

RESULT	MITI LINEAR BIODEGRADATION PROBABILITY		-0.0209

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aromatic ether [-O-aromatic carbon]	1.3227	3.9681
Frag	5	Fluorine [-F]	-3.9878	-19.9392
Frag	4	Aromatic-H	0.1201	0.4806
Frag	2	Methyl [-CH3]	0.0194	0.0389
Frag	1	-CH2- [linear]	0.4295	0.4295

Frag | 1 | -CH- [linear] | -0.0998 | -0.0998
MolWt| * | Molecular Weight Parameter | |-13.9543
==========+==========+==========+==========+===

RESULT | MITI NON-LINEAR BIODEGRADATION PROBABILITY | | 0.0000
==========+==========+==========+==========+===

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.90) Results:
==========

SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM :
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 2.4599 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 0.6957 E-12 cm3/molecule-sec
**Addition to Fused Rings = 57.1137 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 60.2692 E-12 cm3/molecule-sec
HALF-LIFE = 0.177 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 2.130 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.90): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========

Koc (estimated): 2.72e+005
Koc may be sensitive to pH!
SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM :
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 14.974

Non-Corrected Log Koc ..... : 8.5851
Fragment Correction(s):
2 Ether, aromatic (-C-O-C-) ..... : -1.2862
1 Aromatic ring with 2 nitrogens ..... : -0.9650
1 Miscellaneous S(=O) group ..... : -0.9000
Corrected Log Koc ..... : 5.4339
Estimated Koc: 2.716e+005
NOTE:
The Koc of this structure may be sensitive to pH! The estimated Koc represents a best-fit to the majority of experimental values; however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========

SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM :
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!! For more information, (Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.14) Results:
==========

SMILES : n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F
CHEM :
MOL FOR: C16 H14 F5 N5 O5 S1
MOL WT : 483.37
---------- Bcfwin v2.14 ----------
Log Kow (estimated) : 2.95
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 2.95
Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction
Correction(s): Value
No Applicable Correction Factors
Estimated Log BCF = 1.574 (BCF = 37.51)

Volatization From Water

Chemical Name:
Molecular Weight : 483.37 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 1.42E-014 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	9.065E+010	9.889E+011
HALF-LIFE (days) :	3.777E+009	4.12E+010
HALF-LIFE (years) :	1.034E+007	1.128E+008

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

Molecular weight (g/mol)	483.37
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	1.42E-014
Air-water partition coefficient	5.80738E-013
Octanol-water partition coefficient (Kow)	891.251
Log Kow	2.95
Biomass to water partition coefficient	179.05
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	2636.77	10000.00
-Aeration tank	0.00	2636.77	10000.00
-Settling tank	0.00	2636.77	10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	2.1E-002	100.00
Primary sludge	2.31E-001	4.8E-004	2.31
Waste sludge	2.86E-001	5.9E-004	2.86

Primary volatilization	7.47E-012	1.5E-014	0.00
Settling volatilization	2.03E-011	4.2E-014	0.00
Aeration off gas	5.00E-011	1.0E-013	0.00
Primary biodegradation	2.30E-003	4.8E-006	0.02
Settling biodegradation	6.87E-004	1.4E-006	0.01
Aeration biodegradation	9.05E-003	1.9E-005	0.09
Final water effluent	9.47E+000	2.0E-002	94.71
Total removal	5.29E-001	1.1E-003	5.29
Total biodegradation	1.20E-002	2.5E-005	0.12

Level III Fugacity Model (Full-Output):

Chem Name :
Molecular Wt: 483.37
Henry's LC : 1.42e-014 atm-m3/mole (Henrywin program)
Vapor Press : 4.14e-011 mm Hg (Mpbpwin program)
Liquid VP : 3.94e-009 mm Hg (super-cooled)
Melting Pt : 225 deg C (Mpbpwin program)
Log Kow : 2.95 (Kowwin program)
Soil Koc : 365 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.36e-005	4.26	1000
Water	11.5	3.6e+003	1000
Soil	88.3	3.6e+003	1000
Sediment	0.259	1.44e+004	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.94e-018	0.217	0.0133	0.00723	0.000444
Water	1.65e-019	216	1.12e+003	7.19	37.4
Soil	1.55e-018	1.66e+003	0	55.4	0
Sediment	1.91e-019	1.22	0.507	0.0407	0.0169

Persistence Time: 3.26e+003 hr
Reaction Time: 5.2e+003 hr
Advection Time: 8.72e+003 hr
Percent Reacted: 62.6
Percent Advected: 37.4
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 4.26
Water: 3600
Soil: 3600

Sediment: 1.44e+004
Biowin estimate: 1.444 (recalcitrant)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

SFA (major degradate, 15% at study termination)

SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C10 H12 F5 N2 O3 S1
MOL WT : 335.27
---------- EPI SUMMARY (v3.10) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.66) Results:
==========

Log Kow(version 1.66 estimate): 1.64
SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C10 H12 F5 N2 O3 S1
MOL WT : 335.27

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH2- [aliphatic carbon]	0.4911	1.4733
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	1	-NH- [aliphatic attach]	-1.4962	-1.4962
Frag	5	-F [fluorine, aliphatic attach]	-0.0031	-0.0155
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	1	-SO2-N [aromatic attach]	-0.2079	-0.2079
Frag	1	-N=C [aliphatic attach]	-0.0010	-0.0010
Const		Equation Constant		0.2290

Log Kow = 1.6407

MPBPWIN (v1.40) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C10 H12 F5 N2 O3 S1

MOL WT : 335.27
---------- SUMMARY MPBPWIN v1.40 ----------

Boiling Point: 389.34 deg C (Adapted Stein and Brown Method)
Melting Point: 242.23 deg C (Adapted Joback Method)
Melting Point: 113.67 deg C (Gold and Ogle Method)
Mean Melt Pt : 177.95 deg C (Joback; Gold,Ogle Methods)
Selected MP: 145.81 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 389.34 deg C (estimated))
(Using MP: 145.81 deg C (estimated))
VP: 2.31E-007 mm Hg (Antoine Method)
VP: 8.98E-007 mm Hg (Modified Grain Method)
VP: 1.96E-006 mm Hg (Mackay Method)
Selected VP: 8.98E-007 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	3	-CH2-	24.22	72.66
Group	1	=CH-	27.95	27.95
Group	5	-F	0.13	0.65
Group	1	-O- (nonring)	25.16	25.16
Group	1	>NH (nonring)	45.28	45.28
Group	1	=NH	73.40	73.40
Group	3	CH (aromatic)	28.53	85.59
Group	3	-C (aromatic)	30.76	92.28
Group	1	>S(=O)(=O)	171.58	171.58
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 792.73
RESULT- corr | BOILING POINT in deg Kelvin | 662.50
| BOILING POINT in deg C | 389.34

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	3	-CH2-	11.27	33.81
Group	1	=CH-	8.73	8.73
Group	5	-F	-15.78	-78.90
Group	1	-O- (nonring)	22.23	22.23
Group	1	>NH (nonring)	52.66	52.66
Group	1	=NH	68.91	68.91

```
Group | 3 | CH (aromatic)    |  8.13 | 24.39
Group | 3 | -C (aromatic)    | 37.02 | 111.06
Group | 1 | >S(=O)(=O)       | 150.00 | 150.00
  *   |   | Equation Constant |       | 122.50
=============+=======================+==========+=========
  RESULT   | MELTING POINT in deg Kelvin | 515.39
           | MELTING POINT in deg C      | 242.23
-----------------------------------------------------

Water Sol from Kow (WSKOW v1.40) Results:
=========================================

        Water Sol: 301.6 mg/L
SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM   :
MOL FOR: C10 H12 F5 N2 O3 S1
MOL WT : 335.27
---------------------------------- WSKOW v1.40 Results ----------------------
Log Kow  (estimated)  :  1.64
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  1.64
Equation Used to Make Water Sol estimate:
  Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
    (used when Melting Point NOT available)
    Correction(s):       Value
    -------------------  -----
     No Applicable Correction Factors
  Log Water Solubility  (in moles/L) :  -3.046
  Water Solubility at 25 deg C (mg/L):  301.6

ECOSAR Program (v0.99g) Results:
================================
SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM   :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C10 H12 F5 N2 O3 S1
MOL WT : 335.27
Log Kow: 1.64  (KowWin estimate)
Melt Pt:
Wat Sol: 3472 mg/L  (calculated)
ECOSAR v0.99g Class(es) Found
```

Neutral Organics

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**926.735**
Neutral Organics	**: Fish**	**96-hr**	**LC50**	**541.746**
Neutral Organics	**: Fish**	**14-day**	**LC50**	**926.735**
Neutral Organics	**: Daphnid**	**48-hr**	**LC50**	**566.233**
Neutral Organics	**: Green Algae**	**96-hr**	**EC50**	**346.733**
Neutral Organics	**: Fish**	**30-day**	**ChV**	**65.856**
Neutral Organics	**: Daphnid**	**16-day**	**EC50**	**24.808**
Neutral Organics	**: Green Algae**	**96-hr**	**ChV**	**28.160**
Neutral Organics	**: Fish (SW)**	**96-hr**	**LC50**	**104.279**
Neutral Organics	**: Mysid Shrimp**	**96-hr**	**LC50**	**202.021**
		mg/kg (ppm) dry wt soil		
Neutral Organics	**: Earthworm**	**14-day**	**LC50**	**2662.413**

Note: * = asterick designates: Chemical may not be soluble
enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est: Incomplete
Group Est: Incomplete
SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C10 H12 F5 N2 O3 S1
MOL WT : 335.27

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	7 Hydrogen to Carbon (aliphatic) Bonds		-0.8377
HYDROGEN	3 Hydrogen to Carbon (aromatic) Bonds		-0.4629

```
HYDROGEN |  2  Hydrogen to Nitrogen Bonds          |       | 2.5670
FRAGMENT |  1  C-C                                 |       | 0.1163
FRAGMENT |  1  C-Car                               |       | 0.1619
FRAGMENT |  1  C-N                                 |       | 1.3010
FRAGMENT |  1  C-O                                 |       | 1.0855
FRAGMENT |  2  C-F                                 |       |-0.8369
FRAGMENT |  6  Car-Car                             |       | 1.5828
FRAGMENT |  1  Car-S                               |       | 0.6345
FRAGMENT |  1  N-S                                 |ESTIMATE| 0.0000
FRAGMENT |  1  Car-O                               |       | 0.3473
FRAGMENT |  1  C=N                                 |ESTIMATE| 0.0000
FRAGMENT |  2  O=S (sulfone-type)                  |ESTIMATE| 2.1000
FRAGMENT |     MISSING Value for:
FRAGMENT |     MISSING Value for:
FRAGMENT |     MISSING Value for:
---------+-----------------------------------------+--------+---------
RESULT   | BOND ESTIMATION METHOD for LWAPC VALUE *** INCOMPLETE| 7.759
---------+-----------------------------------------+--------+---------

--------+-----------------------------------------+-----------+--------
        |     GROUP CONTRIBUTION DESCRIPTION      | COMMENT | VALUE
--------+-----------------------------------------+-----------+--------
        |       1  CH2 (C)(O)                     |         |-0.13
        |       3  Car-H (Car)(Car)               |         | 0.33
        |       1  Car (C)(Car)(Car)              |         | 0.70
        |       1  Car (Car)(Car)(O)              |         |-0.43
        |       1  Car (Car)(Car)(S)              |         |-0.25
        |       1  O (C)(Car)                     |         | 1.25
        |          MISSING Value for: CH2 (C)(F)
        |          MISSING Value for: S (=O)(=O)(N)(Car)
        |          MISSING Value for: NH (C)(S)
        |          MISSING Value for: CH (=)(N)(N)
        |          MISSING Value for: NH (=)(C)
        |          MISSING Value for: CH2 (F)(Car)
--------+-----------------------------------------+-----------+--------
RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | INCOMPLETE |
1.47
--------+-----------------------------------------+-----------+--------
```

Henrys LC [VP/WSol estimate using EPI values]:
HLC: 1.313E-009 atm-m3/mole
VP: 8.98E-007 mm Hg
WS: 302 mg/L

BIOWIN (v4.00) Program Results:

SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C10 H12 F5 N2 O3 S1
MOL WT : 335.27

---------- BIOWIN v4.00 Results ----------

Linear Model Prediction : Biodegrades Fast
Non-Linear Model Prediction: Biodegrades Fast
Ultimate Biodegradation Timeframe: Weeks-Months
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model Prediction : Does Not Biodegrade Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1319	0.1319
MolWt	*	Molecular Weight Parameter		-0.1596
Const	*	Equation Constant		0.7475
RESULT		LINEAR BIODEGRADATION PROBABILITY		0.7198

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	2.2483	2.2483
MolWt	*	Molecular Weight Parameter		-4.7608
RESULT		NON-LINEAR BIODEGRADATION PROBABILITY		0.6216

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.0581
MolWt	*	Molecular Weight Parameter		-0.7409
Const	*	Equation Constant		3.1992

RESULT	SURVEY MODEL - ULTIMATE BIODEGRADATION		2.4001

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	0.0771	0.0771
MolWt	*	Molecular Weight Parameter		-0.4837
Const	*	Equation Constant		3.8477

RESULT	SURVEY MODEL - PRIMARY BIODEGRADATION		3.4411

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1952	0.1952
Frag	5	Fluorine [-F]	0.0174	0.0869
Frag	1	Aromatic-CH2	-0.0557	-0.0557
Frag	3	Aromatic-H	0.0082	0.0247
Frag	2	-CH2- [linear]	0.0494	0.0988
Frag	1	-CH- [linear]	-0.0507	-0.0507
MolWt	*	Molecular Weight Parameter		-0.9974
Const	*	Equation Constant		0.7121

RESULT	MITI LINEAR BIODEGRADATION PROBABILITY		0.0139

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	1.3227	1.3227
Frag	5	Fluorine [-F]	-3.9878	-19.9392
Frag	1	Aromatic-CH2	-0.1246	-0.1246
Frag	3	Aromatic-H	0.1201	0.3604
Frag	2	-CH2- [linear]	0.4295	0.8590
Frag	1	-CH- [linear]	-0.0998	-0.0998
MolWt	*	Molecular Weight Parameter		-9.6788

```
==========+==========================================================+========+===
======
  RESULT  | MITI NON-LINEAR BIODEGRADATION PROBABILITY |        | 0.0000
==========+==========================================================+========+===
======
```

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.90) Results:

SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C10 H12 F5 N2 O3 S1
MOL WT : 335.27
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
**Hydrogen Abstraction = 21.9125 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 5.3644 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 27.2769 E-12 cm3/molecule-sec
HALF-LIFE = 0.392 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 4.706 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.90): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:

Koc (estimated): 1.7e+004

SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C10 H12 F5 N2 O3 S1
MOL WT : 335.27
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 9.919
Non-Corrected Log Koc ..... : 5.8976
Fragment Correction(s):

1 Ether, aromatic (-C-O-C-) ..... : -0.6431
1 Nitrogen to Carbon (aliphatic) (-N-C).. : -0.1242
1 Miscellaneous S(=O) group ..... : -0.9000
Corrected Log Koc ..... : 4.2303
Estimated Koc: 1.699e+004

HYDROWIN Program (v1.67) Results:
==========

SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C10 H12 F5 N2 O3 S1
MOL WT : 335.27
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)
and Specific Alkyl Halides can be estimated!! For more information,
(Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.14) Results:
==========

SMILES : c1(OCCF(F))c(S(=O)(=O)NC=N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C10 H12 F5 N2 O3 S1
MOL WT : 335.27
---------- Bcfwin v2.14 ----------
Log Kow (estimated) : 1.64
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 1.64
Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction
Correction(s): Value
No Applicable Correction Factors
Estimated Log BCF = 0.563 (BCF = 3.659)

Volatization From Water
==========

Chemical Name:
Molecular Weight : 335.27 g/mole
Water Solubility : 301.6 ppm
Vapor Pressure : 8.98E-007 mm Hg
Henry's Law Constant: 1.31E-009 atm-m3/mole (calculated from VP/WS)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	8.162E+005	8.904E+006
HALF-LIFE (days) :	3.401E+004	3.71E+005
HALF-LIFE (years) :	93.11	1016

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

Molecular weight (g/mol)	335.27
Aqueous solubility (mg/l)	301.6
Vapour pressure (Pa)	0.000119723
(atm)	1.18158E-009
(mm Hg)	8.98E-007
Henry 's law constant (Atm-m3/mol)	1.31348E-009
Air-water partition coefficient	5.37176E-008
Octanol-water partition coefficient (Kow)	43.6516
Log Kow	1.64
Biomass to water partition coefficient	9.53032
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	187.04	10000.00
-Aeration tank	0.00	187.04	10000.00
-Settling tank	0.00	187.04	10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	3.0E-002	100.00
Primary sludge	3.54E-002	1.1E-004	0.35
Waste sludge	1.57E-001	4.7E-004	1.57
Primary volatilization	7.15E-007	2.1E-009	0.00
Settling volatilization	1.95E-006	5.8E-009	0.00
Aeration off gas	4.80E-006	1.4E-008	0.00
Primary biodegradation	1.79E-003	5.3E-006	0.02
Settling biodegradation	5.35E-004	1.6E-006	0.01
Aeration biodegradation	7.04E-003	2.1E-005	0.07

Final water effluent	9.80E+000	2.9E-002	97.98
Total removal	2.02E-001	6.0E-004	2.02
Total biodegradation	9.36E-003	2.8E-005	0.09

Level III Fugacity Model (Full-Output):

==========

Chem Name :
Molecular Wt: 335.27
Henry's LC : 1.31e-009 atm-m3/mole (calc VP/Wsol)
Vapor Press : 8.98e-007 mm Hg (Mpbpwin program)
Liquid VP : 1.41e-005 mm Hg (super-cooled)
Melting Pt : 146 deg C (Mpbpwin program)
Log Kow : 1.64 (Kowwin program)
Soil Koc : 17.9 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0209	9.41	1000
Water	36	900	1000
Soil	63.9	900	1000
Sediment	0.094	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	3.74e-013	40.2	5.46	1.34	0.182
Water	1.85e-014	725	942	24.2	31.4
Soil	4.98e-013	1.29e+003	0	42.9	0
Sediment	1.68e-014	0.473	0.0492	0.0158	0.00164

Persistence Time: 872 hr
Reaction Time: 1.27e+003 hr
Advection Time: 2.76e+003 hr
Percent Reacted: 68.4
Percent Advected: 31.6
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 9.41
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.400 (weeks-months)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

BSA (major degradate, 36% maximum)

SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23
---------- EPI SUMMARY (v3.10) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.66) Results:
==========

Log Kow(version 1.66 estimate): -0.17
SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH2- [aliphatic carbon]	0.4911	1.4733
Frag	5	-F [fluorine, aliphatic attach]	-0.0031	-0.0155
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	1	-SO2-OH [sulfonic], [coef*(1+0.3*(NUM-1))]	-3.1580	-3.1580
Const		Equation Constant		0.2290

Log Kow = -0.1736

MPBPWIN (v1.40) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23
---------- SUMMARY MPBPWIN v1.40 ----------

Boiling Point: 370.00 deg C (Adapted Stein and Brown Method)
Melting Point: 156.38 deg C (Adapted Joback Method)
Melting Point: 102.38 deg C (Gold and Ogle Method)
Mean Melt Pt : 129.38 deg C (Joback; Gold,Ogle Methods)
Selected MP: 120.38 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 370.00 deg C (estimated))
(Using MP: 120.38 deg C (estimated))
VP: 4.46E-008 mm Hg (Antoine Method)
VP: 1.57E-007 mm Hg (Modified Grain Method)
VP: 1.01E-005 mm Hg (Mackay Method)
Selected VP: 1.57E-007 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	3	-CH2-	24.22	72.66
Group	5	-F	0.13	0.65
Group	1	-OH (alcohol)	106.27	106.27
Group	1	-O- (nonring)	25.16	25.16
Group	3	CH (aromatic)	28.53	85.59
Group	3	-C (aromatic)	30.76	92.28
Group	1	>S(=O)(=O)	171.58	171.58
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 752.37
RESULT- corr | BOILING POINT in deg Kelvin | 643.16
| BOILING POINT in deg C | 370.00

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	3	-CH2-	11.27	33.81
Group	5	-F	-15.78	-78.90
Group	1	-OH (alcohol)	44.45	44.45
Group	1	-O- (nonring)	22.23	22.23
Group	3	CH (aromatic)	8.13	24.39
Group	3	-C (aromatic)	37.02	111.06
Group	1	>S(=O)(=O)	150.00	150.00
*		Equation Constant		122.50

RESULT | MELTING POINT in deg Kelvin | 429.54
| MELTING POINT in deg C | 156.38

Water Sol from Kow (WSKOW v1.40) Results:
==========

Water Sol: 1.525e+004 mg/L
SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23
---------- WSKOW v1.40 Results ----------
Log Kow (estimated) : -0.17
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -0.17
Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)
Correction(s): Value
---------- -----
No Applicable Correction Factors
Log Water Solubility (in moles/L) : -1.307
Water Solubility at 25 deg C (mg/L): 1.525e+004

ECOSAR Program (v0.99g) Results:
==========

SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23
Log Kow: -0.17 (KowWin estimate)
Melt Pt:
Wat Sol: 2.247E+005 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Neutral Organics-acid

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
==========	==========	==========	==========	==========

Neutral Organic SAR : Fish 14-day LC50 32236.725
(Baseline Toxicity)
--> Acid moeity found: Predicted values multiplied by 10
Neutral Organics-acid : Fish 96-hr LC50 2.51e+005 *
Neutral Organics-acid : Fish 14-day LC50 3.22e+005 *
Neutral Organics-acid : Daphnid 48-hr LC50 2.32e+005 *
Neutral Organics-acid : Green Algae 96-hr EC50 1.28e+005
Neutral Organics-acid : Fish 30-day ChV 22812.922
Neutral Organics-acid : Daphnid 16-day EC50 4599.186
Neutral Organics-acid : Green Algae 96-hr ChV 3648.051
Neutral Organics-acid : Fish (SW) 96-hr LC50 20154.912
Neutral Organics-acid : Mysid Shrimp 96-hr LC50 3.41e+005 *

mg/kg (ppm)
dry wt soil
==========

Neutral Organics-acid : Earthworm 14-day LC50 88642.273

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

HENRY (v3.10) Program Results:
==========

Bond Est: Incomplete
Group Est: Incomplete
SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	6 Hydrogen to Carbon (aliphatic) Bonds		-0.7181
HYDROGEN	3 Hydrogen to Carbon (aromatic) Bonds		-0.4629
HYDROGEN	1 Hydrogen to Oxygen Bonds		3.2318
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-Car		0.1619
FRAGMENT	1 C-O		1.0855
FRAGMENT	2 C-F		-0.8369

```
FRAGMENT |  6  Car-Car                          |          | 1.5828
FRAGMENT |  1  Car-S                            |          | 0.6345
FRAGMENT |  1  Car-O                            |          | 0.3473
FRAGMENT |  1  O-S                              | ESTIMATE | 0.2100
FRAGMENT |  2  O=S (sulfone-type)               | ESTIMATE | 2.1000
FRAGMENT |     MISSING Value for:
FRAGMENT |     MISSING Value for:
FRAGMENT |     MISSING Value for:
---------+-----------------------------------------+----------+----------
RESULT   | BOND ESTIMATION METHOD for LWAPC VALUE *** INCOMPLETE | 7.452
---------+-----------------------------------------+----------+----------

--------+-----------------------------------------+-----------+--------
        |     GROUP CONTRIBUTION DESCRIPTION      | COMMENT   | VALUE
--------+-----------------------------------------+-----------+--------
        |  1  CH2 (C)(O)                          |           | -0.13
        |  3  Car-H (Car)(Car)                    |           |  0.33
        |  1  Car (C)(Car)(Car)                   |           |  0.70
        |  1  Car (Car)(Car)(O)                   |           | -0.43
        |  1  Car (Car)(Car)(S)                   |           | -0.25
        |  1  O (C)(Car)                          |           |  1.25
        |     MISSING Value for:  CH2 (C)(F)
        |     MISSING Value for:  S (=O)(=O)(O)(Car)
        |     MISSING Value for:  O-H (S)
        |     MISSING Value for:  CH2 (F)(Car)
--------+-----------------------------------------+-----------+--------
RESULT  | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | INCOMPLETE |
1.47
--------+-----------------------------------------+-----------+--------

Henrys LC [VP/WSol estimate using EPI values]:
  HLC:  4.189E-012 atm-m3/mole
  VP:   1.57E-007 mm Hg
  WS:   1.53E+004 mg/L

BIOWIN (v4.00) Program Results:
==============================
SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM   :
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23
------------------------- BIOWIN v4.00 Results -------------------------
  Linear Model Prediction    : Biodegrades Fast
  Non-Linear Model Prediction: Does Not Biodegrade Fast
```

Ultimate Biodegradation Timeframe: Weeks-Months
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model Prediction : Does Not Biodegrade Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Sulfonic acid / salt -> aromatic attach	-0.2238	-0.2238
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1319	0.1319
MolWt	*	Molecular Weight Parameter		-0.1472
Const	*	Equation Constant		0.7475
RESULT		LINEAR BIODEGRADATION PROBABILITY		0.5085

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Sulfonic acid / salt -> aromatic attach	-1.0283	-1.0283
Frag	1	Aromatic ether [-O-aromatic carbon]	2.2483	2.2483
MolWt	*	Molecular Weight Parameter		-4.3911
RESULT		NON-LINEAR BIODEGRADATION PROBABILITY		0.4595

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Sulfonic acid / salt -> aromatic attach	0.1422	0.1422
Frag	1	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.0581
MolWt	*	Molecular Weight Parameter		-0.6834
Const	*	Equation Constant		3.1992
RESULT		SURVEY MODEL - ULTIMATE BIODEGRADATION		2.5999

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE

```
------+-----+-----------------------------------------+---------+---------
Frag | 1 | Sulfonic acid / salt -> aromatic attach  | 0.0216 | 0.0216
Frag | 1 | Aromatic ether  [-O-aromatic carbon]     | 0.0771 | 0.0771
MolWt| * | Molecular Weight Parameter               |        | -0.4461
Const| * | Equation Constant                        |        | 3.8477
=============+=========================================+=========+=====
======
  RESULT   | SURVEY MODEL - PRIMARY BIODEGRADATION    |        | 3.5003
=============+=========================================+=========+=====
======
Result Classification:  5.00 -> hours    4.00 -> days   3.00 -> weeks
 (Primary & Ultimate)   2.00 -> months   1.00 -> longer
------+-----+-----------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION         | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag | 1 | Sulfonic acid / salt -> aromatic attach  | 0.0221 | 0.0221
Frag | 1 | Aromatic ether  [-O-aromatic carbon]     | 0.1952 | 0.1952
Frag | 5 | Fluorine  [-F]                           | 0.0174 | 0.0869
Frag | 1 | Aromatic-CH2                             |-0.0557 |-0.0557
Frag | 3 | Aromatic-H                               | 0.0082 | 0.0247
Frag | 2 | -CH2-  [linear]                          | 0.0494 | 0.0988
MolWt| * | Molecular Weight Parameter               |        | -0.9200
Const| * | Equation Constant                        |        | 0.7121
=============+=========================================+=========+=====
======
  RESULT   | MITI LINEAR BIODEGRADATION PROBABILITY   |        | 0.1642
=============+=========================================+=========+=====
======
------+-----+-----------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION         | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag | 1 | Sulfonic acid / salt -> aromatic attach  | 0.6780 | 0.6780
Frag | 1 | Aromatic ether  [-O-aromatic carbon]     | 1.3227 | 1.3227
Frag | 5 | Fluorine  [-F]                           |-3.9878 |-19.9392
Frag | 1 | Aromatic-CH2                             |-0.1246 |-0.1246
Frag | 3 | Aromatic-H                               | 0.1201 | 0.3604
Frag | 2 | -CH2-  [linear]                          | 0.4295 | 0.8590
MolWt| * | Molecular Weight Parameter               |        | -8.9271
=============+=========================================+=========+=====
======
  RESULT   | MITI NON-LINEAR BIODEGRADATION PROBABILITY |        | 0.0000
=============+=========================================+=========+=====
======
```

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.90) Results:
==========
SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 3.8705 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 5.3644 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 9.3749 E-12 cm3/molecule-sec
HALF-LIFE = 1.141 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 13.691 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.90): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========
Koc (estimated): 490
Koc may be sensitive to pH!
SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 8.858
Non-Corrected Log Koc ..... : 5.3336
Fragment Correction(s):
1 Ether, aromatic (-C-O-C-) ..... : -0.6431
* Sulfonic acid (-S(=O)-OH) ..... : -2.0000
Corrected Log Koc ..... : 2.6905
Estimated Koc: 490.4
NOTE:

The Koc of this structure may be sensitive to pH! The estimated Koc represents a best-fit to the majority of experimental values; however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========

SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!! For more information, (Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.14) Results:
==========

SMILES : c1(OCCF(F))c(S(=O)(=O)O)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H10 F5 O4 S1
MOL WT : 309.23
---------- Bcfwin v2.14 ----------
Log Kow (estimated) : -0.17
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: -0.17
Equation Used to Make BCF estimate:
Log BCF = 0.50 (Ionic; Log Kow dependent)

Estimated Log BCF = 0.500 (BCF = 3.162)

Volatization From Water
==========

Chemical Name:
Molecular Weight : 309.23 g/mole
Water Solubility : 1.525E+004 ppm
Vapor Pressure : 1.57E-007 mm Hg
Henry's Law Constant: 4.19E-012 atm-m3/mole (calculated from VP/WS)

RIVER	LAKE

Water Depth (meters): 1 1
Wind Velocity (m/sec): 5 0.5
Current Velocity (m/sec): 1 0.05
HALF-LIFE (hours) : 2.458E+008 2.681E+009
HALF-LIFE (days) : 1.024E+007 1.117E+008
HALF-LIFE (years) : 2.804E+004 3.059E+005

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

Molecular weight (g/mol) 309.23
Aqueous solubility (mg/l) 15250
Vapour pressure (Pa) 2.09316E-005
(atm) 2.06579E-010
(mm Hg) 1.57E-007
Henry 's law constant (Atm-m3/mol) 4.18887E-012
Air-water partition coefficient 1.71312E-010
Octanol-water partition coefficient (Kow) 0.676083
Log Kow -0.17
Biomass to water partition coefficient 0.935217
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 0.04 18.67 10000.00
-Aeration tank 0.04 18.67 10000.00
-Settling tank 0.04 18.67 10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	3.2E-002	100.00
Primary sludge	2.51E-002	8.1E-005	0.25
Waste sludge	1.51E-001	4.9E-004	1.51
Primary volatilization	2.28E-009	7.4E-012	0.00
Settling volatilization	6.22E-009	2.0E-011	0.00
Aeration off gas	1.53E-008	5.0E-011	0.00
Primary biodegradation	1.76E-003	5.7E-006	0.02
Settling biodegradation	5.27E-004	1.7E-006	0.01
Aeration biodegradation	6.94E-003	2.2E-005	0.07
Final water effluent	9.82E+000	3.2E-002	98.15

Total removal	1.85E-001	6.0E-004	1.85
Total biodegradation	9.22E-003	3.0E-005	0.09

Level III Fugacity Model (Full-Output):

Chem Name :
Molecular Wt: 309.23
Henry's LC : 4.19e-012 atm-m3/mole (calc VP/Wsol)
Vapor Press : 1.57e-007 mm Hg (Mpbpwin program)
Liquid VP : 1.38e-006 mm Hg (super-cooled)
Melting Pt : 120 deg C (Mpbpwin program)
Log Kow : -0.17 (Kowwin program)
Soil Koc : 0.277 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.000119	27.4	1000
Water	49.4	900	1000
Soil	50.5	900	1000
Sediment	0.0917	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.35e-015	0.0717	0.0283	0.00239	0.000945
Water	7.95e-017	903	1.17e+003	30.1	39.1
Soil	2.94e-015	923	0	30.8	0
Sediment	7.32e-017	0.419	0.0435	0.014	0.00145

Persistence Time: 791 hr
Reaction Time: 1.3e+003 hr
Advection Time: 2.02e+003 hr
Percent Reacted: 60.9
Percent Advected: 39.1
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 27.38
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.600 (weeks-months)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

SULFONAMIDE (major degradate, 33% at study termination)

SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24
---------- EPI SUMMARY (v3.10) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.66) Results:
==========

Log Kow(version 1.66 estimate): 1.36
SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH2- [aliphatic carbon]	0.4911	1.4733
Frag	1	-NH2 [aliphatic attach]	-1.4148	-1.4148
Frag	5	-F [fluorine, aliphatic attach]	-0.0031	-0.0155
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	1	-SO2-N [aromatic attach]	-0.2079	-0.2079
Const		Equation Constant		0.2290

Log Kow = 1.3617

MPBPWIN (v1.40) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24
---------- SUMMARY MPBPWIN v1.40 ----------

Boiling Point: 348.78 deg C (Adapted Stein and Brown Method)
Melting Point: 178.82 deg C (Adapted Joback Method)
Melting Point: 89.99 deg C (Gold and Ogle Method)
Mean Melt Pt : 134.41 deg C (Joback; Gold,Ogle Methods)
Selected MP: 112.20 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 348.78 deg C (estimated))
(Using MP: 112.20 deg C (estimated))
VP: 9.25E-006 mm Hg (Antoine Method)
VP: 1.95E-005 mm Hg (Modified Grain Method)
VP: 3.83E-005 mm Hg (Mackay Method)
Selected VP: 1.95E-005 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	3	-CH2-	24.22	72.66
Group	5	-F	0.13	0.65
Group	1	-O- (nonring)	25.16	25.16
Group	1	-NH2	61.98	61.98
Group	3	CH (aromatic)	28.53	85.59
Group	3	-C (aromatic)	30.76	92.28
Group	1	>S(=O)(=O)	171.58	171.58
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 708.08
RESULT- corr | BOILING POINT in deg Kelvin | 621.94
| BOILING POINT in deg C | 348.78

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	3	-CH2-	11.27	33.81
Group	5	-F	-15.78	-78.90
Group	1	-O- (nonring)	22.23	22.23
Group	1	-NH2	66.89	66.89
Group	3	CH (aromatic)	8.13	24.39
Group	3	-C (aromatic)	37.02	111.06
Group	1	>S(=O)(=O)	150.00	150.00
*		Equation Constant		122.50

RESULT | MELTING POINT in deg Kelvin | 451.98
| MELTING POINT in deg C | 178.82

Water Sol from Kow (WSKOW v1.40) Results:
==========

Water Sol: 755.1 mg/L
SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24
---------- WSKOW v1.40 Results ----------
Log Kow (estimated) : 1.36
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 1.36
Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)
Correction(s): Value
---------- -----
No Applicable Correction Factors
Log Water Solubility (in moles/L) : -2.611
Water Solubility at 25 deg C (mg/L): 755.1

ECOSAR Program (v0.99g) Results:
==========
SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24
Log Kow: 1.36 (KowWin estimate)
Melt Pt:
Wat Sol: 6162 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)

Neutral Organic SAR : Fish 14-day LC50 1493.949
(Baseline Toxicity)
Neutral Organics : Fish 96-hr LC50 913.053
Neutral Organics : Fish 14-day LC50 1493.949
Neutral Organics : Daphnid 48-hr LC50 936.043
Neutral Organics : Green Algae 96-hr EC50 564.022
Neutral Organics : Fish 30-day ChV 106.095
Neutral Organics : Daphnid 16-day EC50 36.282
Neutral Organics : Green Algae 96-hr ChV 38.963
Neutral Organics : Fish (SW) 96-hr LC50 153.496
Neutral Organics : Mysid Shrimp 96-hr LC50 415.811
mg/kg (ppm)
dry wt soil
==========
Neutral Organics : Earthworm 14-day LC50 2985.491

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

HENRY (v3.10) Program Results:
==========

Bond Est: Incomplete
Group Est: Incomplete
SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	6 Hydrogen to Carbon (aliphatic) Bonds		-0.7181
HYDROGEN	3 Hydrogen to Carbon (aromatic) Bonds		-0.4629
HYDROGEN	2 Hydrogen to Nitrogen Bonds		2.5670
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-Car		0.1619
FRAGMENT	1 C-O		1.0855
FRAGMENT	2 C-F		-0.8369
FRAGMENT	6 Car-Car		1.5828
FRAGMENT	1 Car-S		0.6345

```
FRAGMENT |  1 N-S                          | ESTIMATE|  0.0000
FRAGMENT |  1 Car-O                        |         |  0.3473
FRAGMENT |  2 O=S (sulfone-type)           | ESTIMATE|  2.1000
FRAGMENT |    MISSING Value for:
FRAGMENT |    MISSING Value for:
FRAGMENT |    MISSING Value for:
----------+-----------------------------------------+---------+----------
RESULT   | BOND ESTIMATION METHOD for LWAPC VALUE *** INCOMPLETE|  6.578
----------+-----------------------------------------+---------+----------

--------+-----------------------------------------+-----------+--------
        |     GROUP CONTRIBUTION DESCRIPTION      |  COMMENT  | VALUE
--------+-----------------------------------------+-----------+--------
        |       1 CH2 (C)(O)                      |           | -0.13
        |       3 Car-H (Car)(Car)                |           |  0.33
        |       1 Car (C)(Car)(Car)               |           |  0.70
        |       1 Car (Car)(Car)(O)               |           | -0.43
        |       1 Car (Car)(Car)(S)               |           | -0.25
        |       1 O (C)(Car)                      |           |  1.25
        |         MISSING Value for: CH2 (C)(F)
        |         MISSING Value for: S (=O)(=O)(N)(Car)
        |         MISSING Value for: NH2 (S)
        |         MISSING Value for: CH2 (F)(Car)
--------+-----------------------------------------+-----------+--------
RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |
1.47
--------+-----------------------------------------+-----------+--------
```

Henrys LC [VP/WSol estimate using EPI values]:
HLC: 1.047E-008 atm-m3/mole
VP: 1.95E-005 mm Hg
WS: 755 mg/L

BIOWIN (v4.00) Program Results:
==========

SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24
---------- BIOWIN v4.00 Results ----------
Linear Model Prediction : Biodegrades Fast
Non-Linear Model Prediction: Biodegrades Fast
Ultimate Biodegradation Timeframe: Weeks-Months
Primary Biodegradation Timeframe: Days-Weeks

MITI Linear Model Prediction : Does Not Biodegrade Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1319	0.1319
MolWt	*	Molecular Weight Parameter		-0.1467
Const	*	Equation Constant		0.7475
RESULT		LINEAR BIODEGRADATION PROBABILITY		0.7327

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	2.2483	2.2483
MolWt	*	Molecular Weight Parameter		-4.3771
RESULT		NON-LINEAR BIODEGRADATION PROBABILITY		0.7068

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.0581
MolWt	*	Molecular Weight Parameter		-0.6812
Const	*	Equation Constant		3.1992
RESULT		SURVEY MODEL - ULTIMATE BIODEGRADATION		2.4599

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	0.0771	0.0771
MolWt	*	Molecular Weight Parameter		-0.4447
Const	*	Equation Constant		3.8477

```
=======
  RESULT   |  SURVEY MODEL - PRIMARY BIODEGRADATION   |        | 3.4801
===========+=========================================+========+====
======
Result Classification:  5.00 -> hours    4.00 -> days   3.00 -> weeks
 (Primary & Ultimate)   2.00 -> months   1.00 -> longer
------+-----+-----------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag |  1  | Aromatic ether  [-O-aromatic carbon]     | 0.1952 | 0.1952
Frag |  5  | Fluorine  [-F]                           | 0.0174 | 0.0869
Frag |  1  | Aromatic-CH2                             | -0.0557 | -0.0557
Frag |  3  | Aromatic-H                               | 0.0082 | 0.0247
Frag |  2  | -CH2-  [linear]                          | 0.0494 | 0.0988
MolWt|  *  | Molecular Weight Parameter               |        | -0.9170
Const|  *  | Equation Constant                        |        | 0.7121
===========+=========================================+========+====
======
  RESULT   |  MITI LINEAR BIODEGRADATION PROBABILITY   |        | 0.1450
===========+=========================================+========+====
======
------+-----+-----------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag |  1  | Aromatic ether  [-O-aromatic carbon]     | 1.3227 | 1.3227
Frag |  5  | Fluorine  [-F]                           | -3.9878 | -19.9392
Frag |  1  | Aromatic-CH2                             | -0.1246 | -0.1246
Frag |  3  | Aromatic-H                               | 0.1201 | 0.3604
Frag |  2  | -CH2-  [linear]                          | 0.4295 | 0.8590
MolWt|  *  | Molecular Weight Parameter               |        | -8.8986
===========+=========================================+========+====
======
  RESULT   | MITI NON-LINEAR BIODEGRADATION PROBABILITY |        | 0.0000
===========+=========================================+========+====
======
 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable


AOP Program (v1.90) Results:
============================
SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM   :
```

MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 3.8705 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 5.3644 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 9.2349 E-12 cm3/molecule-sec
HALF-LIFE = 1.158 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 13.899 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.90): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========
Koc (estimated): 6.17e+003

SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 8.858
Non-Corrected Log Koc ..... : 5.3336
Fragment Correction(s):
1 Ether, aromatic (-C-O-C-) ..... : -0.6431
1 Miscellaneous S(=O) group ..... : -0.9000
Corrected Log Koc ..... : 3.7905
Estimated Koc: 6173

HYDROWIN Program (v1.67) Results:
==========
SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for

the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)
and Specific Alkyl Halides can be estimated!! For more information,
(Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.14) Results:
==========
SMILES : c1(OCCF(F))c(S(=O)(=O)N)c(CF(F)(F))ccc1
CHEM :
MOL FOR: C9 H11 F5 N1 O3 S1
MOL WT : 308.24
---------- Bcfwin v2.14 ----------
Log Kow (estimated) : 1.36
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 1.36
Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction
Correction(s): Value
No Applicable Correction Factors
Estimated Log BCF = 0.349 (BCF = 2.231)

Volatization From Water
==========
Chemical Name:
Molecular Weight : 308.24 g/mole
Water Solubility : 755.1 ppm
Vapor Pressure : 1.95E-005 mm Hg
Henry's Law Constant: 1.05E-008 atm-m3/mole (calculated from VP/WS)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	9.814E+004	1.071E+006
HALF-LIFE (days) :	4089	4.462E+004
HALF-LIFE (years) :	11.2	122.2

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========
PROPERTIES OF:

Molecular weight (g/mol) 308.24

Aqueous solubility (mg/l) 755.1
Vapour pressure (Pa) 0.00259979
(atm) 2.56579E-008
(mm Hg) 1.95E-005
Henry 's law constant (Atm-m3/mol) 1.04738E-008
Air-water partition coefficient 4.28347E-007
Octanol-water partition coefficient (Kow) 22.9087
Log Kow 1.36
Biomass to water partition coefficient 5.38174
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 0.01 106.49 10000.00
-Aeration tank 0.01 106.49 10000.00
-Settling tank 0.01 106.49 10000.00
STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	3.2E-002	100.00
Primary sludge	3.04E-002	9.9E-005	0.30
Waste sludge	1.54E-001	5.0E-004	1.54
Primary volatilization	5.70E-006	1.9E-008	0.00
Settling volatilization	1.55E-005	5.0E-008	0.00
Aeration off gas	3.83E-005	1.2E-007	0.00
Primary biodegradation	1.77E-003	5.7E-006	0.02
Settling biodegradation	5.31E-004	1.7E-006	0.01
Aeration biodegradation	6.99E-003	2.3E-005	0.07
Final water effluent	9.81E+000	3.2E-002	98.06
Total removal	1.94E-001	6.3E-004	1.94
Total biodegradation	9.29E-003	3.0E-005	0.09

Level III Fugacity Model (Full-Output):

Chem Name :
Molecular Wt: 308.24
Henry's LC : 1.05e-008 atm-m3/mole (calc VP/Wsol)
Vapor Press : 1.95e-005 mm Hg (Mpbpwin program)
Liquid VP : 0.000142 mm Hg (super-cooled)
Melting Pt : 112 deg C (Mpbpwin program)
Log Kow : 1.36 (Kowwin program)

Soil Koc : 9.39 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.155	27.8	1000
Water	41.1	900	1000
Soil	58.7	900	1000
Sediment	0.0923	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.98e-012	94.2	37.8	3.14	1.26
Water	1.7e-013	769	999	25.6	33.3
Soil	5.13e-012	1.1e+003	0	36.6	0
Sediment	1.56e-013	0.432	0.0449	0.0144	0.0015

Persistence Time: 811 hr
Reaction Time: 1.24e+003 hr
Advection Time: 2.35e+003 hr
Percent Reacted: 65.4
Percent Advected: 34.6
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 27.79
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.460 (weeks-months)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

BSTCA (major degradate, 39% at study termination)

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28

---------- EPI SUMMARY (v3.11) ----------

Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------

KOWWIN Program (v1.67) Results:

==========

Log Kow(version 1.67 estimate): 1.10

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	1	C [aliphatic carbon - No H, not tert]	0.9723	0.9723
Frag	5	-F [fluorine, aliphatic attach]	-0.0031	-0.0155
Frag	8	Aromatic Carbon	0.2940	2.3520
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	1	-COOH [acid, aromatic attach]	-0.1186	-0.1186
Frag	1	-SO2-N [aromatic attach]	-0.2079	-0.2079
Frag	3	Aromatic Nitrogen [5-member ring]	-0.5262	-1.5786
Const		Equation Constant		0.2290

Log Kow = 1.1018

MPBPWIN (v1.41) Program Results:

==========

Experimental Database Structure Match: no data

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2

CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 536.69 deg C (Adapted Stein and Brown Method)
Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 199.71 deg C (Gold and Ogle Method)
Mean Melt Pt : 274.78 deg C (Joback; Gold,Ogle Methods)
Selected MP: 229.74 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 536.69 deg C (estimated))
(Using MP: 229.74 deg C (estimated))
VP: 7.19E-014 mm Hg (Antoine Method)
VP: 2.02E-011 mm Hg (Modified Grain Method)
VP: 6.42E-011 mm Hg (Mackay Method)
Selected VP: 2.02E-011 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH2-	24.22	24.22
Group	1	>CH-	11.86	11.86
Group	1	>C<	4.50	4.50
Group	5	-F	0.13	0.65
Group	1	-O- (nonring)	25.16	25.16
Group	1	-COOH (acid)	169.83	169.83
Group	1	>NH (nonring)	45.28	45.28
Group	3	CH (aromatic)	28.53	85.59
Group	5	-C (aromatic)	30.76	153.80
Group	3	N (aromatic)	39.88	119.64
Group	1	>S(=O)(=O)	171.58	171.58
Corr	1	Triazole [NH]	90.00	90.00
*		Equation Constant		198.18

RESULT-uncorr	BOILING POINT in deg Kelvin	1100.29
RESULT- corr	BOILING POINT in deg Kelvin	809.85
	BOILING POINT in deg C	536.69

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH2-	11.27	11.27

Group	1	>CH-	12.64	12.64
Group	1	>C<	46.43	46.43
Group	5	-F	-15.78	-78.90
Group	1	-O- (nonring)	22.23	22.23
Group	1	-COOH (acid)	155.50	155.50
Group	1	>NH (nonring)	52.66	52.66
Group	3	CH (aromatic)	8.13	24.39
Group	5	-C (aromatic)	37.02	185.10
Group	3	N (aromatic)	68.40	205.20
Group	1	>S(=O)(=O)	150.00	150.00
*		Equation Constant		122.50

RESULT	MELTING POINT in deg Kelvin	909.02
RESULT-limit	MELTING POINT in deg Kelvin	623.00
	MELTING POINT in deg C	349.84

Water Sol from Kow (WSKOW v1.41) Results:

==========

Water Sol: 277.9 mg/L
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : 1.10
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 1.10
Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
Acid, aromatic	0.000

Log Water Solubility (in moles/L) : -3.175
Water Solubility at 25 deg C (mg/L): 277.9

WATERNT Program (v1.01) Results:

==========

Water Sol (v1.01 est): 14.55 mg/L
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1

MOL WT : 416.28

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	-0.5370	-0.5370
Frag	1	-CH [aliphatic carbon]	-0.5285	-0.5285
Frag	1	C [aliphatic carbon - No H, not tert]	-1.0516	-1.0516
Frag	5	-F [fluorine, aliphatic attach]	-0.1580	-0.7900
Frag	3	Aromatic Carbon (C-H type)	-0.3359	-1.0076
Frag	1	-N [aliphatic N, one aromatic attach]	1.2749	1.2749
Frag	1	-O- [oxygen, one aromatic attach]	0.1980	0.1980
Frag	1	-COOH [acid, aromatic attach]	0.0568	0.0568
Frag	5	Aromatic Carbon (C-substituent type)	-0.5400	-2.6998
Frag	1	-SO2-N [aromatic attach]	-1.2003	-1.2003
Frag	3	Aromatic Nitrogen [5-member ring]	0.5265	1.5795
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -4.4565
Water Solubility (mg/L) at 25 dec C = 14.55

ECOSAR Program (v0.99g) Results:

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28
Log Kow: 1.10 (KowWin estimate)
Melt Pt:
Wat Sol: 1.532E+004 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Neutral Organics-acid

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**3398.495**

--> Acid moeity found: Predicted values multiplied by 10

Neutral Organics-acid : Fish 96-hr LC50 21646.445 *
Neutral Organics-acid : Fish 14-day LC50 33984.945 *
Neutral Organics-acid : Daphnid 48-hr LC50 21796.492 *
Neutral Organics-acid : Green Algae 96-hr EC50 12938.578
Neutral Organics-acid : Fish 30-day ChV 2412.052
Neutral Organics-acid : Daphnid 16-day EC50 754.026
Neutral Organics-acid : Green Algae 96-hr ChV 769.107
Neutral Organics-acid : Fish (SW) 96-hr LC50 3209.125
Neutral Organics-acid : Mysid Shrimp 96-hr LC50 11868.248
mg/kg (ppm)
dry wt soil
==========
Neutral Organics-acid : Earthworm 14-day LC50 48482.676 *

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

HENRY (v3.10) Program Results:
==========

Bond Est : 3.59E-015 atm-m3/mole
Group Est: Incomplete
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	3 Hydrogen to Carbon (aliphatic) Bonds		-0.3590
HYDROGEN	3 Hydrogen to Carbon (aromatic) Bonds		-0.4629
HYDROGEN	1 Hydrogen to Oxygen Bonds		3.2318
HYDROGEN	1 Hydrogen to Nitrogen Bonds		1.2835
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-Car		0.1619
FRAGMENT	1 C-O		1.0855
FRAGMENT	5 C-F		-2.0922
FRAGMENT	6 Car-Car		1.5828
FRAGMENT	1 Car-CO		1.2387

```
FRAGMENT |  4  Car-Nar                          |          | 6.5129
FRAGMENT |  1  Nar-Nar                          | ESTIMATE | 3.0000
FRAGMENT |  1  Car-S                            |          | 0.6345
FRAGMENT |  1  CO-O                             |          | 0.0714
FRAGMENT |  1  N-S                              | ESTIMATE | 0.0000
FRAGMENT |  1  Car-N                            |          | 0.7304
FRAGMENT |  1  Car-O                            |          | 0.3473
FRAGMENT |  2  O=S (sulfone-type)               | ESTIMATE | 2.1000
FACTOR   |  2  Additional aromatic nitrogen(s)  |          | -5.0000
FACTOR   |  1  -SO2-N-  group                   |          | -1.3500
---------+--------------------------------------+----------+----------
RESULT   |  BOND ESTIMATION METHOD for LWAPC VALUE  | TOTAL | 12.833
---------+--------------------------------------+----------+----------
HENRYs LAW CONSTANT at 25 deg C = 3.59E-015 atm-m3/mole
                = 1.47E-013 unitless
--------+-------------------------------------+-----------+--------
        |     GROUP CONTRIBUTION DESCRIPTION  |  COMMENT  | VALUE
--------+-------------------------------------+-----------+--------
        |  1  CH2 (C)(O)                      |           | -0.13
        |  1  CH (C)(F)(F)                    |           | 0.70
        |  3  Car-H (Car)(Car)                |           | 0.33
        |  1  Car (C)(Car)(Car)               |           | 0.70
        |  1  Car (Car)(Car)(O)               |           | -0.43
        |  1  Car (Car)(Car)(S)               |           | -0.25
        |  1  CO (O)(Car)                     |           | 4.57
        |  1  O-H (CO)                        |           | 1.45
        |  1  O (C)(Car)                      |           | 1.25
        |  1  Nar (Car)(Car)                  |           | 3.06
        |     MISSING Value for:  C (F)(F)(F)(Car)
        |     MISSING Value for:  S (=O)(=O)(N)(Car)
        |     MISSING Value for:  NH (Car)(S)
        |     MISSING Value for:  Car (Nar)(Nar)(N)
        |     MISSING Value for:  Car (CO)(Nar)(Nar)
        |     MISSING Value for:  Nar (Nar)(Car)
        |     MISSING Value for:  Nar (Car)(Nar)
--------+-------------------------------------+-----------+--------
RESULT  |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |
11.25
--------+-------------------------------------+-----------+--------
```

Henrys LC [VP/WSol estimate using EPI values]:
HLC: 3.981E-014 atm-m3/mole
VP: 2.02E-011 mm Hg

WS: 278 mg/L

BIOWIN (v4.01) Program Results:

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28

---------- BIOWIN v4.01 Results ----------

Linear Model Prediction : Does Not Biodegrade Fast
Non-Linear Model Prediction: Does Not Biodegrade Fast
Ultimate Biodegradation Timeframe: Months
Primary Biodegradation Timeframe: Weeks
MITI Linear Model Prediction : Does Not Biodegrade Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	0.1769	0.1769
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1319	0.1319
Frag	1	Trifluoromethyl group [-CF3]	-0.5204	-0.5204
MolWt	*	Molecular Weight Parameter		-0.1982
Const	*	Equation Constant		0.7475
RESULT		LINEAR BIODEGRADATION PROBABILITY		0.3377

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	2.4224	2.4224
Frag	1	Aromatic ether [-O-aromatic carbon]	2.2483	2.2483
Frag	1	Trifluoromethyl group [-CF3]	-5.6696	-5.6696
MolWt	*	Molecular Weight Parameter		-5.9112
RESULT		NON-LINEAR BIODEGRADATION PROBABILITY		0.0198

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	0.0879	0.0879
Frag	1	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.0581
Frag	1	Trifluoromethyl group [-CF3]	-0.5130	-0.5130
MolWt	*	Molecular Weight Parameter		-0.9199
Const	*	Equation Constant		3.1992

RESULT	SURVEY MODEL - ULTIMATE BIODEGRADATION		1.7960

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	0.0077	0.0077
Frag	1	Aromatic ether [-O-aromatic carbon]	0.0771	0.0771
Frag	1	Trifluoromethyl group [-CF3]	-0.2744	-0.2744
MolWt	*	Molecular Weight Parameter		-0.6006
Const	*	Equation Constant		3.8477

RESULT	SURVEY MODEL - PRIMARY BIODEGRADATION		3.0576

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	0.3770	0.3770
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1952	0.1952
Frag	5	Fluorine [-F]	0.0174	0.0869
Frag	3	Aromatic-H	0.0082	0.0247
Frag	1	-CH2- [linear]	0.0494	0.0494
Frag	1	-CH- [linear]	-0.0507	-0.0507
MolWt	*	Molecular Weight Parameter		-1.2384
Const	*	Equation Constant		0.7121

RESULT	MITI LINEAR BIODEGRADATION PROBABILITY		0.1562

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	2.4449	2.4449
Frag	1	Aromatic ether [-O-aromatic carbon]	1.3227	1.3227
Frag	5	Fluorine [-F]	-3.9878	-19.9392
Frag	3	Aromatic-H	0.1201	0.3604
Frag	1	-CH2- [linear]	0.4295	0.4295
Frag	1	-CH- [linear]	-0.0998	-0.0998
MolWt	*	Molecular Weight Parameter		-12.0175

RESULT	MITI NON-LINEAR BIODEGRADATION PROBABILITY		0.0000

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:
==========

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28
---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.8007 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.5200 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 0.7957 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 2.1164 E-12 cm3/molecule-sec
HALF-LIFE = 5.054 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 60.647 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========

Koc (estimated): 1.42e+003
Koc may be sensitive to pH!
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28
---------- PCKOCWIN v1.66 Results ----------

First Order Molecular Connectivity Index ..... : 12.415
Non-Corrected Log Koc ..... : 7.2244
Fragment Correction(s):
* Nitrogen to non-fused aromatic ring ... : -0.7770
1 Ether, aromatic (-C-O-C-) ..... : -0.6431
* Organic Acid (-CO-OH) ..... : -1.7512
1 Miscellaneous S(=O) group ..... : -0.9000
Corrected Log Koc ..... : 3.1531
Estimated Koc: 1423
NOTE:
The Koc of this structure may be sensitive to pH! The estimated Koc represents a best-fit to the majority of experimental values; however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28
---------- HYDROWIN v1.67 Results ----------

Currently, this program can NOT estimate a hydrolysis rate constant for the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!! For more information, (Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:
==========

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)O)nn2
CHEM :
MOL FOR: C12 H9 F5 N4 O5 S1
MOL WT : 416.28
---------- Bcfwin v2.15 ----------

Log Kow (estimated) : 1.10
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 1.10
Equation Used to Make BCF estimate:
Log BCF = 0.50 (Ionic; Log Kow dependent)

Estimated Log BCF = 0.500 (BCF = 3.162)

Volatization From Water

Chemical Name:
Molecular Weight : 416.28 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 3.59E-015 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	3.327E+011	3.63E+012
HALF-LIFE (days) :	1.386E+010	1.512E+011
HALF-LIFE (years) :	3.796E+007	4.141E+008

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

Molecular weight (g/mol)	416.28
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	3.59E-015
Air-water partition coefficient	1.4682E-013
Octanol-water partition coefficient (Kow)	12.5893
Log Kow	1.1
Biomass to water partition coefficient	3.31785
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.01	65.92	10000.00
-Aeration tank	0.01	65.92	10000.00

-Settling tank 0.01 65.92 10000.00

STP Overall Chemical Mass Balance:

---

	g/h	mol/h	percent
Influent	1.00E+001	2.4E-002	100.00
Primary sludge	2.80E-002	6.7E-005	0.28
Waste sludge	1.52E-001	3.7E-004	1.52
Primary volatilization	1.96E-012	4.7E-015	0.00
Settling volatilization	5.33E-012	1.3E-014	0.00
Aeration off gas	1.31E-011	3.2E-014	0.00
Primary biodegradation	1.77E-003	4.2E-006	0.02
Settling biodegradation	5.29E-004	1.3E-006	0.01
Aeration biodegradation	6.96E-003	1.7E-005	0.07
Final water effluent	9.81E+000	2.4E-002	98.10
Total removal	1.90E-001	4.6E-004	1.90
Total biodegradation	9.26E-003	2.2E-005	0.09

Level III Fugacity Model (Full-Output):

==========

Chem Name :
Molecular Wt: 416.28
Henry's LC : 3.59e-015 atm-m3/mole (Henrywin program)
Vapor Press : 2.02e-011 mm Hg (Mpbpwin program)
Liquid VP : 2.14e-009 mm Hg (super-cooled)
Melting Pt : 230 deg C (Mpbpwin program)
Log Kow : 1.1 (Kowwin program)
Soil Koc : 5.16 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.92e-005	121	1000
Water	44.9	1.44e+003	1000
Soil	55	1.44e+003	1000
Sediment	0.0956	5.76e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	8.62e-019	0.00354	0.0062	0.000118	0.000207
Water	6.25e-020	697	1.45e+003	23.2	48.3
Soil	2.01e-018	854	0	28.5	0
Sediment	5.92e-020	0.371	0.0617	0.0124	0.00206

Persistence Time: 1.08e+003 hr
Reaction Time: 2.08e+003 hr
Advection Time: 2.23e+003 hr
Percent Reacted: 51.7
Percent Advected: 48.3
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 121.3
Water: 1440
Soil: 1440
Sediment: 5760
Biowin estimate: 1.796 (months)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

BSTCA methyl (major degradate, 13% maximum)

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM :
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31

---------- EPI SUMMARY (v3.11) ----------

Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------

KOWWIN Program (v1.67) Results:

==========

Log Kow(version 1.67 estimate): 1.06

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM :
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	1	C [aliphatic carbon - No H, not tert]	0.9723	0.9723
Frag	5	-F [fluorine, aliphatic attach]	-0.0031	-0.0155
Frag	8	Aromatic Carbon	0.2940	2.3520
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	1	-C(=O)O [ester, aromatic attach]	-0.7121	-0.7121
Frag	1	-SO2-N [aromatic attach]	-0.2079	-0.2079
Frag	3	Aromatic Nitrogen [5-member ring]	-0.5262	-1.5786
Const		Equation Constant		0.2290

Log Kow = 1.0556

MPBPWIN (v1.41) Program Results:

==========

Experimental Database Structure Match: no data

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM :
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 503.63 deg C (Adapted Stein and Brown Method)
Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 180.41 deg C (Gold and Ogle Method)
Mean Melt Pt : 265.12 deg C (Joback; Gold,Ogle Methods)
Selected MP: 214.29 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 503.63 deg C (estimated))
(Using MP: 214.29 deg C (estimated))
VP: 2.82E-012 mm Hg (Antoine Method)
VP: 2.15E-010 mm Hg (Modified Grain Method)
VP: 6.33E-010 mm Hg (Mackay Method)
Selected VP: 2.15E-010 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	1	-CH2-	24.22	24.22
Group	1	>CH-	11.86	11.86
Group	1	>C<	4.50	4.50
Group	5	-F	0.13	0.65
Group	1	-O- (nonring)	25.16	25.16
Group	1	-COO- (ester)	78.85	78.85
Group	1	>NH (nonring)	45.28	45.28
Group	3	CH (aromatic)	28.53	85.59
Group	5	-C (aromatic)	30.76	153.80
Group	3	N (aromatic)	39.88	119.64
Group	1	>S(=O)(=O)	171.58	171.58
Corr	1	Triazole [NH]	90.00	90.00
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 1031.29
RESULT- corr | BOILING POINT in deg Kelvin | 776.79
| BOILING POINT in deg C | 503.63

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE

```
-------+-----+--------------------+----------+---------
Group | 1 | -CH3              |  -5.10 |  -5.10
Group | 1 | -CH2-             |  11.27 |  11.27
Group | 1 | >CH-              |  12.64 |  12.64
Group | 1 | >C<               |  46.43 |  46.43
Group | 5 | -F                | -15.78 | -78.90
Group | 1 | -O- (nonring)     |  22.23 |  22.23
Group | 1 | -COO- (ester)     |  53.60 |  53.60
Group | 1 | >NH (nonring)     |  52.66 |  52.66
Group | 3 | CH (aromatic)     |   8.13 |  24.39
Group | 5 | -C (aromatic)     |  37.02 | 185.10
Group | 3 | N (aromatic)      |  68.40 | 205.20
Group | 1 | >S(=O)(=O)        | 150.00 | 150.00
  *   |   | Equation Constant |        | 122.50
==========+====================+==========+=========
  RESULT    | MELTING POINT in deg Kelvin | 802.02
 RESULT-limit| MELTING POINT in deg Kelvin | 623.00
           | MELTING POINT in deg C      | 349.84
-----------------------------------------------------

Water Sol from Kow (WSKOW v1.41) Results:
=========================================

        Water Sol: 248.7 mg/L
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM   :
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31
---------------------------------- WSKOW v1.41 Results ----------------------
Log Kow  (estimated)  :  1.06
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  1.06
Equation Used to Make Water Sol estimate:
  Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
    (used when Melting Point NOT available)
    Correction(s):       Value
    -------------------  -----
     No Applicable Correction Factors
  Log Water Solubility  (in moles/L) :  -3.238
  Water Solubility at 25 deg C (mg/L):  248.7

WATERNT Program (v1.01) Results:
================================

            Water Sol (v1.01 est): 31.606 mg/L
```

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM :
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	-0.3213	-0.3213
Frag	1	-CH2- [aliphatic carbon]	-0.5370	-0.5370
Frag	1	-CH [aliphatic carbon]	-0.5285	-0.5285
Frag	1	C [aliphatic carbon - No H, not tert]	-1.0516	-1.0516
Frag	5	-F [fluorine, aliphatic attach]	-0.1580	-0.7900
Frag	3	Aromatic Carbon (C-H type)	-0.3359	-1.0076
Frag	1	-N [aliphatic N, one aromatic attach]	1.2749	1.2749
Frag	1	-O- [oxygen, one aromatic attach]	0.1980	0.1980
Frag	1	-C(=O)O [ester, aromatic attach]	0.7006	0.7006
Frag	5	Aromatic Carbon (C-substituent type)	-0.5400	-2.6998
Frag	1	-SO2-N [aromatic attach]	-1.2003	-1.2003
Frag	3	Aromatic Nitrogen [5-member ring]	0.5265	1.5795
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -4.1340
Water Solubility (mg/L) at 25 dec C = 31.606

ECOSAR Program (v0.99g) Results:
==========
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31
Log Kow: 1.06 (KowWin estimate)
Melt Pt:
Wat Sol: 1.74E+004 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Esters

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)

Neutral Organic SAR : Fish 14-day LC50 3806.445
(Baseline Toxicity)
Esters : Fish 96-hr LC50 207.338
Esters : Daphnid 48-hr LC50 2450.076
Esters : Green Algae 96-hr EC50 15.946
Esters : Green Algae ChV 12.111
Esters : Fish ChV 150.349
Note: * = asterick designates: Chemical may not be soluble
enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est : 1.15E-012 atm-m3/mole
Group Est: Incomplete
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM :
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	6 Hydrogen to Carbon (aliphatic) Bonds		-0.7181
HYDROGEN	3 Hydrogen to Carbon (aromatic) Bonds		-0.4629
HYDROGEN	1 Hydrogen to Nitrogen Bonds		1.2835
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-Car		0.1619
FRAGMENT	2 C-O		2.1709
FRAGMENT	5 C-F		-2.0922
FRAGMENT	6 Car-Car		1.5828
FRAGMENT	1 Car-CO		1.2387
FRAGMENT	4 Car-Nar		6.5129
FRAGMENT	1 Nar-Nar	ESTIMATE	3.0000
FRAGMENT	1 Car-S		0.6345
FRAGMENT	1 CO-O		0.0714
FRAGMENT	1 N-S	ESTIMATE	0.0000
FRAGMENT	1 Car-N		0.7304

```
FRAGMENT |  1  Car-O                          |          | 0.3473
FRAGMENT |  2  O=S (sulfone-type)             | ESTIMATE| 2.1000
FACTOR   |  2  Additional aromatic nitrogen(s)|          |-5.0000
FACTOR   |  1  -SO2-N-  group                 |          |-1.3500
---------+-------------------------------------+---------+---------
RESULT   |   BOND ESTIMATION METHOD for LWAPC VALUE  | TOTAL | 10.328
---------+-------------------------------------+---------+---------
HENRYs LAW CONSTANT at 25 deg C = 1.15E-012 atm-m3/mole
                = 4.70E-011 unitless
--------+-------------------------------------+-----------+--------
        |     GROUP CONTRIBUTION DESCRIPTION  |  COMMENT  | VALUE
--------+-------------------------------------+-----------+--------
        |       1  CH3 (X)                    |           |-0.62
        |       1  CH2 (C)(O)                 |           |-0.13
        |       1  CH (C)(F)(F)               |           | 0.70
        |       3  Car-H (Car)(Car)           |           | 0.33
        |       1  Car (C)(Car)(Car)          |           | 0.70
        |       1  Car (Car)(Car)(O)          |           |-0.43
        |       1  Car (Car)(Car)(S)          |           |-0.25
        |       1  CO (O)(Car)                |           | 4.57
        |       1  O (C)(Car)                 |           | 1.25
        |       1  O (C)(CO)                  |           |-0.53
        |       1  Nar (Car)(Car)             |           | 3.06
        |         MISSING Value for:  C (F)(F)(F)(Car)
        |         MISSING Value for:  S (=O)(=O)(N)(Car)
        |         MISSING Value for:  NH (Car)(S)
        |         MISSING Value for:  Car (Nar)(Nar)(N)
        |         MISSING Value for:  Car (CO)(Nar)(Nar)
        |         MISSING Value for:  Nar (Nar)(Car)
        |         MISSING Value for:  Nar (Car)(Nar)
--------+-------------------------------------+-----------+--------
RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | INCOMPLETE |
8.65
--------+-------------------------------------+-----------+--------

Henrys LC [VP/WSol estimate using EPI values]:
  HLC:  4.895E-013 atm-m3/mole
  VP:   2.15E-010 mm Hg
  WS:   249 mg/L

BIOWIN (v4.01) Program Results:
==============================

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
```

CHEM :
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31

---------- BIOWIN v4.01 Results ----------

Linear Model Prediction : Does Not Biodegrade Fast
Non-Linear Model Prediction: Does Not Biodegrade Fast
Ultimate Biodegradation Timeframe: Months
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model Prediction : Does Not Biodegrade Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Ester [-C(=O)-O-C]	0.1742	0.1742
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1319	0.1319
Frag	1	Trifluoromethyl group [-CF3]	-0.5204	-0.5204
MolWt	*	Molecular Weight Parameter		-0.2049
Const	*	Equation Constant		0.7475
RESULT		LINEAR BIODEGRADATION PROBABILITY		0.3284

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Ester [-C(=O)-O-C]	4.0795	4.0795
Frag	1	Aromatic ether [-O-aromatic carbon]	2.2483	2.2483
Frag	1	Trifluoromethyl group [-CF3]	-5.6696	-5.6696
MolWt	*	Molecular Weight Parameter		-6.1104
RESULT		NON-LINEAR BIODEGRADATION PROBABILITY		0.0799

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Ester [-C(=O)-O-C]	0.1402	0.1402
Frag	1	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.0581
Frag	1	Trifluoromethyl group [-CF3]	-0.5130	-0.5130

MolWt| * | Molecular Weight Parameter | | -0.9509
Const| * | Equation Constant | | 3.1992

RESULT | SURVEY MODEL - ULTIMATE BIODEGRADATION | | 1.8174

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Ester [-C(=O)-O-C]	0.2290	0.2290
Frag	1	Aromatic ether [-O-aromatic carbon]	0.0771	0.0771
Frag	1	Trifluoromethyl group [-CF3]	-0.2744	-0.2744
MolWt	*	Molecular Weight Parameter		-0.6208
Const	*	Equation Constant		3.8477

RESULT | SURVEY MODEL - PRIMARY BIODEGRADATION | | 3.2586

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Ester [-C(=O)-O-C]	0.3437	0.3437
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1952	0.1952
Frag	5	Fluorine [-F]	0.0174	0.0869
Frag	3	Aromatic-H	0.0082	0.0247
Frag	1	Methyl [-CH3]	0.0004	0.0004
Frag	1	-CH2- [linear]	0.0494	0.0494
Frag	1	-CH- [linear]	-0.0507	-0.0507
MolWt	*	Molecular Weight Parameter		-1.2802
Const	*	Equation Constant		0.7121

RESULT | MITI LINEAR BIODEGRADATION PROBABILITY | | 0.0816

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Ester [-C(=O)-O-C]	2.4462	2.4462

```
Frag |  1  | Aromatic ether  [-O-aromatic carbon]     | 1.3227 |  1.3227
Frag |  5  | Fluorine  [-F]                          |-3.9878 |-19.9392
Frag |  3  | Aromatic-H                              | 0.1201 |  0.3604
Frag |  1  | Methyl  [-CH3]                          | 0.0194 |  0.0194
Frag |  1  | -CH2-  [linear]                         | 0.4295 |  0.4295
Frag |  1  | -CH-  [linear]                          |-0.0998 | -0.0998
MolWt|  *  | Molecular Weight Parameter              |        |-12.4225
============+=========================================+========+=====
======
  RESULT   | MITI NON-LINEAR BIODEGRADATION PROBABILITY |        | 0.0000
============+=========================================+========+=====
======
 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:
============================
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM  :
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31
---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction     =  1.0183 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds  =  0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings =  0.7957 E-12 cm3/molecule-sec
Addition to Fused Rings   =  0.0000 E-12 cm3/molecule-sec
  OVERALL OH Rate Constant =  1.8140 E-12 cm3/molecule-sec
  HALF-LIFE =    5.896 Days (12-hr day; 1.5E6 OH/cm3)
  HALF-LIFE =   70.757 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
          ******  NO OZONE REACTION ESTIMATION ******
          (ONLY Olefins and Acetylenes are Estimated)
Experimental Database:  NO Structure Matches

PCKOC Program (v1.66) Results:
==============================
            Koc (estimated): 7.61e+003
           Koc may be sensitive to pH!
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM  :
```

MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31
---------- PCKOCWIN v1.66 Results ----------

First Order Molecular Connectivity Index ..... : 12.953
Non-Corrected Log Koc ..... : 7.5105
Fragment Correction(s):
* Nitrogen to non-fused aromatic ring ... : -0.7770
1 Ether, aromatic (-C-O-C-) ..... : -0.6431
1 Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -1.3089
1 Miscellaneous S(=O) group ..... : -0.9000
Corrected Log Koc ..... : 3.8815
Estimated Koc: 7611
NOTE:
The Koc of this structure may be sensitive to pH! The estimated Koc represents a best-fit to the majority of experimental values; however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM :
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31
---------- HYDROWIN v1.67 Results ----------

NOTE: Fragment(s) on this compound are NOT available from the fragment library. Substitute(s) have been used!!! Substitute R1, R2, R3, or R4 fragments are marked with double astericks "**".
ESTER: R1-C(=O)-O-R2 ** R1: -Phenyl
R2: -CH3
Kb hydrolysis at atom # 23: 3.998E-002 L/mol-sec
Total Kb for pH > 8 at 25 deg C : 3.998E-002 L/mol-sec
Kb Half-Life at pH 8: 200.670 days
Kb Half-Life at pH 7: 5.494 years

BCF Program (v2.15) Results:
==========

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc(C(=O)OC)nn2
CHEM :
MOL FOR: C13 H11 F5 N4 O5 S1
MOL WT : 430.31
---------- Bcfwin v2.15 ----------

Log Kow (estimated) : 1.06
Log Kow (experimental): not available from database

Log Kow used by BCF estimates: 1.06
Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction
Correction(s): Value
No Applicable Correction Factors
Estimated Log BCF = 0.113 (BCF = 1.297)

Volatization From Water

Chemical Name:
Molecular Weight : 430.31 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 1.15E-012 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	1.056E+009	1.152E+010
HALF-LIFE (days) :	4.4E+007	4.8E+008
HALF-LIFE (years) :	1.205E+005	1.314E+006

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

Molecular weight (g/mol)	430.31
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	1.15E-012
Air-water partition coefficient	4.70316E-011
Octanol-water partition coefficient (Kow)	11.4815
Log Kow	1.06
Biomass to water partition coefficient	3.09631
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.01	61.55	10000.00
-Aeration tank	0.01	61.55	10000.00
-Settling tank	0.01	61.55	10000.00

STP Overall Chemical Mass Balance:

---

	g/h	mol/h	percent
Influent	1.00E+001	2.3E-002	100.00
Primary sludge	2.77E-002	6.4E-005	0.28
Waste sludge	1.52E-001	3.5E-004	1.52
Primary volatilization	6.27E-010	1.5E-012	0.00
Settling volatilization	1.71E-009	4.0E-012	0.00
Aeration off gas	4.21E-009	9.8E-012	0.00
Primary biodegradation	1.77E-003	4.1E-006	0.02
Settling biodegradation	5.29E-004	1.2E-006	0.01
Aeration biodegradation	6.96E-003	1.6E-005	0.07
Final water effluent	9.81E+000	2.3E-002	98.11
Total removal	1.89E-001	4.4E-004	1.89
Total biodegradation	9.26E-003	2.2E-005	0.09

Level III Fugacity Model (Full-Output):

==========

Chem Name :
Molecular Wt: 430.31
Henry's LC : 1.15e-012 atm-m3/mole (Henrywin program)
Vapor Press : 2.15e-010 mm Hg (Mpbpwin program)
Liquid VP : 1.6e-008 mm Hg (super-cooled)
Melting Pt : 214 deg C (Mpbpwin program)
Log Kow : 1.06 (Kowwin program)
Soil Koc : 4.71 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.000838	142	1000
Water	45.4	1.44e+003	1000
Soil	54.5	1.44e+003	1000
Sediment	0.0957	5.76e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.67e-016	0.132	0.269	0.00439	0.00896
Water	1.95e-017	701	1.46e+003	23.4	48.6
Soil	6.28e-016	841	0	28	0
Sediment	1.84e-017	0.369	0.0614	0.0123	0.00205

Persistence Time: 1.07e+003 hr
Reaction Time: 2.08e+003 hr

Advection Time: 2.2e+003 hr
Percent Reacted: 51.4
Percent Advected: 48.6
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 141.5
Water: 1440
Soil: 1440
Sediment: 5760
Biowin estimate: 1.817 (months)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

5-OH penoxsulam (major degradate, 63% maximun)

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM :
MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35
---------- EPI SUMMARY (v3.11) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 2.25
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM :
MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	1	C [aliphatic carbon - No H, not tert]	0.9723	0.9723
Frag	5	-F [fluorine, aliphatic attach]	-0.0031	-0.0155
Frag	11	Aromatic Carbon	0.2940	3.2340
Frag	1	Aromatic Nitrogen	-0.7324	-0.7324
Frag	1	-OH [hydroxy, aromatic attach]	-0.4802	-0.4802
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	2	-O- [oxygen, one aromatic attach]	-0.4664	-0.9328
Frag	1	-SO2-N [aromatic attach]	-0.2079	-0.2079
Frag	2	Aromatic Nitrogen [5-member ring]	-0.5262	-1.0524
Frag	1	Aromatic nitrogen [fused ring location]	-0.0001	-0.0001
Factor	1	Ring rx -> -OH ortho to aromatic nitrogen	0.7500	0.7500
Const		Equation Constant		0.2290

Log Kow = 2.2468

MPBPWIN (v1.41) Program Results:

==========

Experimental Database Structure Match: no data

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM :
MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 537.85 deg C (Adapted Stein and Brown Method)
Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 200.39 deg C (Gold and Ogle Method)
Mean Melt Pt : 275.11 deg C (Joback; Gold,Ogle Methods)
Selected MP: 230.28 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 537.85 deg C (estimated))
(Using MP: 230.28 deg C (estimated))
VP: 4.18E-015 mm Hg (Antoine Method)
VP: 2E-012 mm Hg (Modified Grain Method)
VP: 5.93E-011 mm Hg (Mackay Method)
Selected VP: 2E-012 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	1	-CH2-	24.22	24.22
Group	1	>CH-	11.86	11.86
Group	1	>C<	4.50	4.50
Group	5	-F	0.13	0.65
Group	1	-OH (phenol)	70.48	70.48
Group	2	-O- (nonring)	25.16	50.32
Group	1	>NH (nonring)	45.28	45.28
Group	4	CH (aromatic)	28.53	114.12
Group	6	-C (aromatic)	30.76	184.56
Group	1	C (3a aromatic)	45.46	45.46
Group	4	N (aromatic)	39.88	159.52
Group	1	>S(=O)(=O)	171.58	171.58
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 1102.71
RESULT- corr | BOILING POINT in deg Kelvin | 811.01
| BOILING POINT in deg C | 537.85

```
-------------------------------------------------
-------+-----+-------------------+----------+---------
 TYPE  |NUM| MELT DESCRIPTION  | COEFF    | VALUE
-------+-----+-------------------+----------+---------
 Group | 1  | -CH3              |  -5.10 |  -5.10
 Group | 1  | -CH2-             |  11.27 |  11.27
 Group | 1  | >CH-              |  12.64 |  12.64
 Group | 1  | >C<               |  46.43 |  46.43
 Group | 5  | -F                | -15.78 | -78.90
 Group | 1  | -OH (phenol)      |  82.83 |  82.83
 Group | 2  | -O- (nonring)     |  22.23 |  44.46
 Group | 1  | >NH (nonring)     |  52.66 |  52.66
 Group | 4  | CH (aromatic)     |   8.13 |  32.52
 Group | 6  | -C (aromatic)     |  37.02 | 222.12
 Group | 1  | C (3a aromatic)   |  37.02 |  37.02
 Group | 4  | N (aromatic)      |  68.40 | 273.60
 Group | 1  | >S(=O)(=O)        | 150.00 | 150.00
   *   |    | Equation Constant |        | 122.50
=============+=====================+==========+=========
  RESULT    | MELTING POINT in deg Kelvin | 1004.05
 RESULT-limit| MELTING POINT in deg Kelvin | 623.00
           | MELTING POINT in deg C      | 349.84
-------------------------------------------------

Water Sol from Kow (WSKOW v1.41) Results:
=========================================

        Water Sol: 13.55 mg/L
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM   :
MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35
---------------------------------- WSKOW v1.41 Results ----------------------
Log Kow  (estimated)  :  2.25
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  2.25
Equation Used to Make Water Sol estimate:
  Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
     (used when Melting Point NOT available)
    Correction(s):        Value
    -------------------   -----
     No Applicable Correction Factors
  Log Water Solubility  (in moles/L) :  -4.540
  Water Solubility at 25 deg C (mg/L):  13.55
```

WATERNT Program (v1.01) Results:

Water Sol (v1.01 est): 1.4002 mg/L
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM :
MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	-0.3213	-0.3213
Frag	1	-CH2- [aliphatic carbon]	-0.5370	-0.5370
Frag	1	-CH [aliphatic carbon]	-0.5285	-0.5285
Frag	1	C [aliphatic carbon - No H, not tert]	-1.0516	-1.0516
Frag	5	-F [fluorine, aliphatic attach]	-0.1580	-0.7900
Frag	4	Aromatic Carbon (C-H type)	-0.3359	-1.3435
Frag	1	Aromatic Nitrogen [max count of 1 allowed]	1.9255	1.9255
Frag	1	-OH [hydroxy, aromatic attach]	1.6578	1.6578
Frag	1	-N [aliphatic N, one aromatic attach]	1.2749	1.2749
Frag	2	-O- [oxygen, one aromatic attach]	0.1980	0.3959
Frag	7	Aromatic Carbon (C-substituent type)	-0.5400	-3.7797
Frag	1	-SO2-N [aromatic attach]	-1.2003	-1.2003
Frag	2	Aromatic Nitrogen [5-member ring]	0.5265	1.0530
Frag	1	Aromatic nitrogen [fused ring location]	0.0000	0.0000
Factor	1	Reaction -> -OH / nitrogen (arom 6-ring)	-2.5298	-2.5298
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -5.5253
Water Solubility (mg/L) at 25 dec C = 1.4002

ECOSAR Program (v0.99g) Results:

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35
Log Kow: 2.25 (KowWin estimate)
Melt Pt:
Wat Sol: 1160 mg/L (calculated)

ECOSAR v0.99g Class(es) Found

Phenols

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**381.718**
Phenols	**: Fish**	**96-hr**	**LC50**	**48.361**
Phenols	**: Daphnid**	**48-hr**	**LC50**	**19.964**
Phenols	**: Green Algae**	**96-hr**	**EC50**	**140.037**
Phenols	**: Fish**	**30-day**	**ChV**	**7.315**
Phenols	**: Fish**	**90-day**	**ChV**	**0.433**
Phenols	**: Daphnid**	**21-day**	**ChV**	**5.212**
Phenols	**: Green Algae**	**96-hr**	**ChV**	**16.181**

Note: * = asterick designates: Chemical may not be soluble
enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 7.0
Green algal EC50 toxicity log Kow cutoff: 7.0
Chronic toxicity log Kow cutoff: 9.0
MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est : 2.74E-018 atm-m3/mole
Group Est: Incomplete
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM :
MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	6 Hydrogen to Carbon (aliphatic) Bonds		-0.7181
HYDROGEN	4 Hydrogen to Carbon (aromatic) Bonds		-0.6172
HYDROGEN	1 Hydrogen to Oxygen Bonds		3.2318
HYDROGEN	1 Hydrogen to Nitrogen Bonds		1.2835
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-Car		0.1619
FRAGMENT	2 C-O		2.1709

```
FRAGMENT |  5  C-F                              |        | -2.0922
FRAGMENT |  8  Car-Car                          |        |  2.1105
FRAGMENT |  1  Car-OH                           |        |  0.5967
FRAGMENT |  7  Car-Nar                          |        | 11.3975
FRAGMENT |  1  Nar-Nar                          | ESTIMATE|  3.0000
FRAGMENT |  1  Car-S                            |        |  0.6345
FRAGMENT |  1  N-S                              | ESTIMATE|  0.0000
FRAGMENT |  1  Car-N                            |        |  0.7304
FRAGMENT |  2  Car-O                            |        |  0.6945
FRAGMENT |  2  O=S (sulfone-type)               | ESTIMATE|  2.1000
FACTOR   |  3  Additional aromatic nitrogen(s)  |        | -7.5000
FACTOR   |  1  -SO2-N-  group                   |        | -1.3500
---------+--------------------------------------+--------+---------
RESULT   |  BOND ESTIMATION METHOD for LWAPC VALUE  | TOTAL | 15.951
---------+--------------------------------------+--------+---------
HENRYs LAW CONSTANT at 25 deg C = 2.74E-018 atm-m3/mole
                = 1.12E-016 unitless
--------+-------------------------------------+-----------+--------
        |    GROUP CONTRIBUTION DESCRIPTION   | COMMENT   | VALUE
--------+-------------------------------------+-----------+--------
        |  1  CH3 (X)                         |           | -0.62
        |  1  CH2 (C)(O)                      |           | -0.13
        |  1  CH (C)(F)(F)                    |           |  0.70
        |  3  Car-H (Car)(Car)                |           |  0.33
        |  1  Car-H (Car)(Nar)                |           |  0.11
        |  1  Car (C)(Car)(Car)               |           |  0.70
        |  2  Car (Car)(Car)(O)               |           | -0.86
        |  1  Car (Car)(Car)(S)               |           | -0.25
        |  1  O-H (Car)                       |           |  4.45
        |  2  O (C)(Car)                      |           |  2.50
        |  2  Nar (Car)(Car)                  |           |  6.12
        |     MISSING Value for:  C (F)(F)(F)(Car)
        |     MISSING Value for:  S (=O)(=O)(N)(Car)
        |     MISSING Value for:  NH (Car)(S)
        |     MISSING Value for:  Car (Nar)(Nar)(N)
        |     MISSING Value for:  Car (Nar)(Car)(Nar)
        |     MISSING Value for:  Car (O)(Nar)(Nar)
        |     MISSING Value for:  Nar (Car)(Nar)(Car)
        |     MISSING Value for:  Nar (Car)(Nar)
--------+-------------------------------------+-----------+--------
RESULT  |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |
13.05
--------+-------------------------------------+-----------+--------
```

Henrys LC [VP/WSol estimate using EPI values]:
HLC: 9.115E-014 atm-m3/mole
VP: 2E-012 mm Hg
WS: 13.6 mg/L

BIOWIN (v4.01) Program Results:

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM :
MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35

---------- BIOWIN v4.01 Results ----------

Linear Model Prediction : Does Not Biodegrade Fast
Non-Linear Model Prediction: Does Not Biodegrade Fast
Ultimate Biodegradation Timeframe: Recalcitrant
Primary Biodegradation Timeframe: Weeks
MITI Linear Model Prediction : Does Not Biodegrade Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.1158	0.1158
Frag	2	Aromatic ether [-O-aromatic carbon]	0.1319	0.2638
Frag	1	Trifluoromethyl group [-CF3]	-0.5204	-0.5204
MolWt	*	Molecular Weight Parameter		-0.2234
Const	*	Equation Constant		0.7475
RESULT		LINEAR BIODEGRADATION PROBABILITY		0.3833

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.9086	0.9086
Frag	2	Aromatic ether [-O-aromatic carbon]	2.2483	4.4966
Frag	1	Trifluoromethyl group [-CF3]	-5.6696	-5.6696
MolWt	*	Molecular Weight Parameter		-6.6647
RESULT		NON-LINEAR BIODEGRADATION PROBABILITY		0.0194

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0564	0.0564
Frag	2	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.1162
Frag	1	Trifluoromethyl group [-CF3]	-0.5130	-0.5130
MolWt	*	Molecular Weight Parameter		-1.0372
Const	*	Equation Constant		3.1992

RESULT	SURVEY MODEL - ULTIMATE BIODEGRADATION		1.5892

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0397	0.0397
Frag	2	Aromatic ether [-O-aromatic carbon]	0.0771	0.1542
Frag	1	Trifluoromethyl group [-CF3]	-0.2744	-0.2744
MolWt	*	Molecular Weight Parameter		-0.6772
Const	*	Equation Constant		3.8477

RESULT	SURVEY MODEL - PRIMARY BIODEGRADATION		3.0901

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0642	0.0642
Frag	2	Aromatic ether [-O-aromatic carbon]	0.1952	0.3905
Frag	5	Fluorine [-F]	0.0174	0.0869
Frag	4	Aromatic-H	0.0082	0.0329
Frag	1	Methyl [-CH3]	0.0004	0.0004
Frag	1	-CH2- [linear]	0.0494	0.0494
Frag	1	-CH- [linear]	-0.0507	-0.0507
MolWt	*	Molecular Weight Parameter		-1.3963
Const	*	Equation Constant		0.7121

```
=======
  RESULT   | MITI LINEAR BIODEGRADATION PROBABILITY   |        | -0.1106
============+=========================================+=========+===
=======

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION       | COEFF   | VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  | Aromatic alcohol  [-OH]                 |  0.4884 |  0.4884
 Frag |  2  | Aromatic ether  [-O-aromatic carbon]    |  1.3227 |  2.6454
 Frag |  5  | Fluorine  [-F]                          | -3.9878 | -19.9392
 Frag |  4  | Aromatic-H                              |  0.1201 |  0.4806
 Frag |  1  | Methyl  [-CH3]                          |  0.0194 |  0.0194
 Frag |  1  | -CH2-  [linear]                         |  0.4295 |  0.4295
 Frag |  1  | -CH-  [linear]                          | -0.0998 | -0.0998
 MolWt|  *  | Molecular Weight Parameter              |         | -13.5494
============+=========================================+=========+===
======
  RESULT   | MITI NON-LINEAR BIODEGRADATION PROBABILITY |        | 0.0000
============+=========================================+=========+===
======
 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

 AOP Program (v1.91) Results:
 ============================
 SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
 CHEM   :
 MOL FOR: C15 H12 F5 N5 O5 S1
 MOL WT : 469.35
 ---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
 Hydrogen Abstraction      =  1.6303 E-12 cm3/molecule-sec
 Reaction with N, S and -OH =  0.1400 E-12 cm3/molecule-sec
 Addition to Triple Bonds  =  0.0000 E-12 cm3/molecule-sec
 Addition to Olefinic Bonds =  0.0000 E-12 cm3/molecule-sec
 **Addition to Aromatic Rings =  0.6957 E-12 cm3/molecule-sec
 **Addition to Fused Rings   =  63.4308 E-12 cm3/molecule-sec
   OVERALL OH Rate Constant =  65.8968 E-12 cm3/molecule-sec
   HALF-LIFE =    0.162 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =    1.948 Hrs
 ..... ** Designates Estimation(s) Using ASSUMED Value(s)
 ---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
            ******  NO OZONE REACTION ESTIMATION ******
            (ONLY Olefins and Acetylenes are Estimated)
```

NOTE: Reaction with Nitrate Radicals May Be Important!
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========

Koc (estimated): 1.41e+005
Koc may be sensitive to pH!
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM :
MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35
---------- PCKOCWIN v1.66 Results ----------

First Order Molecular Connectivity Index ..... : 14.436
Non-Corrected Log Koc ..... : 8.2991
Fragment Correction(s):
2 Ether, aromatic (-C-O-C-) ..... : -1.2862
1 Aromatic ring with 2 nitrogens ..... : -0.9650
1 Miscellaneous S(=O) group ..... : -0.9000
Corrected Log Koc ..... : 5.1479
Estimated Koc: 1.406e+005
NOTE:
The Koc of this structure may be sensitive to pH! The estimated Koc represents a best-fit to the majority of experimental values; however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM :
MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35
---------- HYDROWIN v1.67 Results ----------

Currently, this program can NOT estimate a hydrolysis rate constant for the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!! For more information, (Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:
==========

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(OC)cnc(O)n3n2
CHEM :

MOL FOR: C15 H12 F5 N5 O5 S1
MOL WT : 469.35
---------- Bcfwin v2.15 ----------
Log Kow (estimated) : 2.25
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 2.25
Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction
Correction(s): Value
No Applicable Correction Factors
Estimated Log BCF = 1.030 (BCF = 10.72)

Volatization From Water

Chemical Name:
Molecular Weight : 469.35 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 2.74E-018 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	4.629E+014	5.05E+015
HALF-LIFE (days) :	1.929E+013	2.104E+014
HALF-LIFE (years) :	5.281E+010	5.761E+011

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

Molecular weight (g/mol)	469.35
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	2.74E-018
Air-water partition coefficient	1.12058E-016
Octanol-water partition coefficient (Kow)	177.828
Log Kow	2.25
Biomass to water partition coefficient	36.3656
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	678.00	10000.00
-Aeration tank	0.00	678.00	10000.00
-Settling tank	0.00	678.00	10000.00

STP Overall Chemical Mass Balance:

---

	g/h	mol/h	percent
Influent	1.00E+001	2.1E-002	100.00
Primary sludge	6.71E-002	1.4E-004	0.67
Waste sludge	1.78E-001	3.8E-004	1.78
Primary volatilization	1.48E-015	3.2E-018	0.00
Settling volatilization	4.04E-015	8.6E-018	0.00
Aeration off gas	9.95E-015	2.1E-017	0.00
Primary biodegradation	1.87E-003	4.0E-006	0.02
Settling biodegradation	5.60E-004	1.2E-006	0.01
Aeration biodegradation	7.37E-003	1.6E-005	0.07
Final water effluent	9.74E+000	2.1E-002	97.45
Total removal	2.55E-001	5.4E-004	2.55
Total biodegradation	9.80E-003	2.1E-005	0.10

Level III Fugacity Model (Full-Output):

==========

Chem Name :
Molecular Wt: 469.35
Henry's LC : 2.74e-018 atm-m3/mole (Henrywin program)
Vapor Press : 2e-012 mm Hg (Mpbpwin program)
Liquid VP : 2.14e-010 mm Hg (super-cooled)
Melting Pt : 230 deg C (Mpbpwin program)
Log Kow : 2.25 (Kowwin program)
Soil Koc : 72.9 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	6.2e-008	3.9	1000
Water	20.3	3.6e+003	1000
Soil	79.6	3.6e+003	1000
Sediment	0.114	1.44e+004	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	5.84e-022	0.000838	4.71e-005	2.79e-005	1.57e-006

Water 4.5e-023 296 1.54e+003 9.88 51.3
Soil 9.56e-022 1.16e+003 0 38.8 0
Sediment 4.58e-023 0.415 0.173 0.0138 0.00575
Persistence Time: 2.53e+003 hr
Reaction Time: 5.2e+003 hr
Advection Time: 4.93e+003 hr
Percent Reacted: 48.7
Percent Advected: 51.3
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 3.895
Water: 3600
Soil: 3600
Sediment: 1.44e+004
Biowin estimate: 1.589 (recalcitrant)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

2-amino TP (major degradate, 18% maximum)

SMILES : Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O2
MOL WT : 195.18
---------- EPI SUMMARY (v3.11) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 1.26
SMILES : Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O2
MOL WT : 195.18

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	5	Aromatic Carbon	0.2940	1.4700
Frag	1	Aromatic Nitrogen	-0.7324	-0.7324
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	2	-O- [oxygen, one aromatic attach]	-0.4664	-0.9328
Frag	2	Aromatic Nitrogen [5-member ring]	-0.5262	-1.0524
Frag	1	Aromatic nitrogen [fused ring location]	-0.0001	-0.0001
Factor	1	o-Alkyloxy to 2 aromat nitrogens/pyrazine	0.8955	0.8955
Factor	1	Imidazole type -> 2-amino type correction	0.5596	0.5596
Factor	1	Additional amino-type triazole correction	0.6500	0.6500
Const		Equation Constant		0.2290

Log Kow = 1.2640

MPBPWIN (v1.41) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : Nc1nc2c(OC)cnc(OC)n2n1

CHEM :
MOL FOR: C7 H9 N5 O2
MOL WT : 195.18
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 347.25 deg C (Adapted Stein and Brown Method)
Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 89.10 deg C (Gold and Ogle Method)
Mean Melt Pt : 219.47 deg C (Joback; Gold,Ogle Methods)
Selected MP: 141.24 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 347.25 deg C (estimated))
(Using MP: 141.24 deg C (estimated))
VP: 4.96E-006 mm Hg (Antoine Method)
VP: 1.03E-005 mm Hg (Modified Grain Method)
VP: 2.14E-005 mm Hg (Mackay Method)
Selected VP: 1.03E-005 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	2	-CH3	21.98	43.96
Group	2	-O- (nonring)	25.16	50.32
Group	1	CH (aromatic)	28.53	28.53
Group	3	-C (aromatic)	30.76	92.28
Group	1	C (3a aromatic)	45.46	45.46
Group	1	-NH2 (to arom)	86.63	86.63
Group	4	N (aromatic)	39.88	159.52
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 704.88
RESULT- corr | BOILING POINT in deg Kelvin | 620.41
| BOILING POINT in deg C | 347.25

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	2	-CH3	-5.10	-10.20
Group	2	-O- (nonring)	22.23	44.46
Group	1	CH (aromatic)	8.13	8.13
Group	3	-C (aromatic)	37.02	111.06
Group	1	C (3a aromatic)	37.02	37.02
Group	1	-NH2 (to arom)	66.89	66.89

```
Group | 4 | N (aromatic)     | 68.40 | 273.60
  *   |   | Equation Constant |       | 122.50
=============+=======================+==========+=========
  RESULT     | MELTING POINT in deg Kelvin | 653.46
RESULT-limit | MELTING POINT in deg Kelvin | 623.00
             | MELTING POINT in deg C      | 349.84
-----------------------------------------------------
```

Water Sol from Kow (WSKOW v1.41) Results:

==========

Water Sol: 3855 mg/L

SMILES : Nc1nc2c(OC)cnc(OC)n2n1

CHEM :

MOL FOR: C7 H9 N5 O2

MOL WT : 195.18

---------- WSKOW v1.41 Results ----------

Log Kow (estimated) : 1.26

Log Kow (experimental): not available from database

Log Kow used by Water solubility estimates: 1.26

Equation Used to Make Water Sol estimate:

Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction

(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -1.704

Water Solubility at 25 deg C (mg/L): 3855

WATERNT Program (v1.01) Results:

==========

Water Sol (v1.01 est): 1e+006 mg/L

SMILES : Nc1nc2c(OC)cnc(OC)n2n1

CHEM :

MOL FOR: C7 H9 N5 O2

MOL WT : 195.18

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	-0.3213	-0.6425
Frag	1	Aromatic Carbon (C-H type)	-0.3359	-0.3359
Frag	1	Aromatic Nitrogen [max count of 1 allowed]	1.9255	1.9255
Frag	1	-N [aliphatic N, one aromatic attach]	1.2749	1.2749
Frag	2	-O- [oxygen, one aromatic attach]	0.1980	0.3959

Frag	4	Aromatic Carbon (C-substituent type)	-0.5400	-2.1598
Frag	2	Aromatic Nitrogen [5-member ring]	0.5265	1.0530
Frag	1	Aromatic nitrogen [fused ring location]	0.0000	0.0000
Const		Equation Constant		0.2492

NOTE		Maximum Solubility (1,000,000 mg/L) Applied!	

Log Water Sol (moles/L) at 25 dec C = 0.7096
Water Solubility (mg/L) at 25 dec C = 1e+006

ECOSAR Program (v0.99g) Results:

SMILES : Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C7 H9 N5 O2
MOL WT : 195.18
Log Kow: 1.26 (KowWin estimate)
Melt Pt:
Wat Sol: 4934 mg/L (calculated)

ECOSAR v0.99g Class(es) Found

Aromatic Amines

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**1156.058**
Aromatic Amines	**: Fish**	**96-hr**	**LC50**	**206.681**
Aromatic Amines	**: Fish**	**14-day**	**LC50**	**116.295**
Aromatic Amines	**: Daphnid**	**48-hr**	**LC50**	**2.118**
Aromatic Amines	**: Fish**		**ChV**	**0.970**
Aromatic Amines	**: Daphnid**		**ChV**	**0.052**
Aromatic Amines	**: Green Algae**		**ChV**	**13.758**

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 7.0
Green algal EC50 toxicity log Kow cutoff: 7.0

Chronic toxicity log Kow cutoff: 9.0
MW cutoff: 1000

HENRY (v3.10) Program Results:
==========

Bond Est : 4.29E-014 atm-m3/mole
Group Est: Incomplete
SMILES : Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O2
MOL WT : 195.18

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	6 Hydrogen to Carbon (aliphatic) Bonds		-0.7181
HYDROGEN	1 Hydrogen to Carbon (aromatic) Bonds		-0.1543
HYDROGEN	2 Hydrogen to Nitrogen Bonds		2.5670
FRAGMENT	2 C-O		2.1709
FRAGMENT	2 Car-Car		0.5276
FRAGMENT	7 Car-Nar		11.3975
FRAGMENT	1 Nar-Nar	ESTIMATE	3.0000
FRAGMENT	1 Car-N		0.7304
FRAGMENT	2 Car-O		0.6945
FACTOR	3 Additional aromatic nitrogen(s)		-7.5000
FACTOR	1 -O-carbon ortho-position to Nar		-0.9600
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	11.756

HENRYs LAW CONSTANT at 25 deg C = 4.29E-014 atm-m3/mole
= 1.76E-012 unitless

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	1 NH2 (Car)	ESTIMATE	4.00
	2 CH3 (X)		-1.24
	1 Car-H (Car)(Nar)		0.11
	1 Car (Car)(Car)(O)		-0.43
	2 O (C)(Car)		2.50
	2 Nar (Car)(Car)		6.12
	MISSING Value for: Car (Nar)(Nar)(N)		
	MISSING Value for: Car (Nar)(Car)(Nar)		
	MISSING Value for: Car (O)(Nar)(Nar)		

```
|          MISSING Value for:  Nar (Car)(Nar)(Car)
|          MISSING Value for:  Nar (Car)(Nar)
--------+-----------------------------------------+-----------+--------
 RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | INCOMPLETE |
11.06
--------+-----------------------------------------+-----------+--------

Henrys LC [VP/WSol estimate using EPI values]:
  HLC:  6.862E-010 atm-m3/mole
  VP:   1.03E-005 mm Hg
  WS:   3.86E+003 mg/L

BIOWIN (v4.01) Program Results:
==============================
SMILES : Nc1nc2c(OC)cnc(OC)n2n1
CHEM   :
MOL FOR: C7 H9 N5 O2
MOL WT : 195.18
-------------------------- BIOWIN v4.01 Results --------------------------
  Linear Model Prediction    :  Biodegrades Fast
  Non-Linear Model Prediction:  Biodegrades Fast
  Ultimate Biodegradation Timeframe:  Weeks-Months
  Primary  Biodegradation Timeframe:  Days-Weeks
  MITI Linear Model Prediction    :  Does Not Biodegrade Fast
  MITI Non-Linear Model Prediction:  Does Not Biodegrade Fast
------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF  | VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  | Aromatic amine  [-NH2  or  -NH-]        | -0.2338 | -0.2338
 Frag |  2  | Aromatic ether  [-O-aromatic carbon]    |  0.1319 |  0.2638
 MolWt|  *  | Molecular Weight Parameter              |         | -0.0929
 Const|  *  | Equation Constant                       |         |  0.7475
============+=========================================+=========+=====
======
  RESULT   |    LINEAR BIODEGRADATION PROBABILITY    |         | 0.6847
============+=========================================+=========+=====
======
------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF  | VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  | Aromatic amine  [-NH2  or  -NH-]        | -1.9070 | -1.9070
 Frag |  2  | Aromatic ether  [-O-aromatic carbon]    |  2.2483 |  4.4966
 MolWt|  *  | Molecular Weight Parameter              |         | -2.7716
```

RESULT	NON-LINEAR BIODEGRADATION PROBABILITY		0.9441

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.1349	-0.1349
Frag	2	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.1162
MolWt	*	Molecular Weight Parameter		-0.4313
Const	*	Equation Constant		3.1992

RESULT	SURVEY MODEL - ULTIMATE BIODEGRADATION		2.5167

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.1084	-0.1084
Frag	2	Aromatic ether [-O-aromatic carbon]	0.0771	0.1542
MolWt	*	Molecular Weight Parameter		-0.2816
Const	*	Equation Constant		3.8477

RESULT	SURVEY MODEL - PRIMARY BIODEGRADATION		3.6120

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.1577	-0.1577
Frag	2	Aromatic ether [-O-aromatic carbon]	0.1952	0.3905
Frag	1	Aromatic-H	0.0082	0.0082
Frag	2	Methyl [-CH3]	0.0004	0.0008
MolWt	*	Molecular Weight Parameter		-0.5807
Const	*	Equation Constant		0.7121

```
=======
  RESULT   | MITI LINEAR BIODEGRADATION PROBABILITY   |       | 0.3733
============+=========================================+=========+=====
======

------+-----+-----------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag |  1  | Aromatic amine  [-NH2  or  -NH-]        |-1.2264 |-1.2264
Frag |  2  | Aromatic ether  [-O-aromatic carbon]    | 1.3227 | 2.6454
Frag |  1  | Aromatic-H                              | 0.1201 | 0.1201
Frag |  2  | Methyl  [-CH3]                          | 0.0194 | 0.0389
MolWt|  *  | Molecular Weight Parameter              |        |-5.6347
============+=========================================+=========+=====
======
  RESULT   | MITI NON-LINEAR BIODEGRADATION PROBABILITY |       | 0.1778
============+=========================================+=========+=====
======
 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:
============================
SMILES : Nc1nc2c(OC)cnc(OC)n2n1
CHEM   :
MOL FOR: C7 H9 N5 O2
MOL WT : 195.18
---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction     =  1.6592 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds  =  0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =  0.0000 E-12 cm3/molecule-sec
**Addition to Fused Rings   =  90.7277 E-12 cm3/molecule-sec
  OVERALL OH Rate Constant =  92.3869 E-12 cm3/molecule-sec
  HALF-LIFE =    0.116 Days (12-hr day; 1.5E6 OH/cm3)
  HALF-LIFE =    1.389 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
          ******  NO OZONE REACTION ESTIMATION ******
          (ONLY Olefins and Acetylenes are Estimated)
Experimental Database:  NO Structure Matches

PCKOC Program (v1.66) Results:
```

Koc (estimated): 92.3
Koc may be sensitive to pH!
SMILES : Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O2
MOL WT : 195.18
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 6.758
Non-Corrected Log Koc ..... : 4.2166
Fragment Correction(s):
2 Ether, aromatic (-C-O-C-) ..... : -1.2862
1 Aromatic ring with 2 nitrogens ..... : -0.9650
Corrected Log Koc ..... : 1.9654
Estimated Koc: 92.34
NOTE:
The Koc of this structure may be sensitive to pH! The estimated Koc represents a best-fit to the majority of experimental values; however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:

SMILES : Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O2
MOL WT : 195.18
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!! For more information, (Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:

SMILES : Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O2
MOL WT : 195.18
---------- Bcfwin v2.15 ----------
Log Kow (estimated) : 1.26
Log Kow (experimental): not available from database

Log Kow used by BCF estimates: 1.26
Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction
Correction(s): Value
No Applicable Correction Factors
Estimated Log BCF = 0.273 (BCF = 1.876)

Volatization From Water

Chemical Name:
Molecular Weight : 195.18 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 4.29E-014 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	1.907E+010	2.08E+011
HALF-LIFE (days) :	7.944E+008	8.667E+009
HALF-LIFE (years) :	2.175E+006	2.373E+007

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

Molecular weight (g/mol)	195.18
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	4.29E-014
Air-water partition coefficient	1.75448E-012
Octanol-water partition coefficient (Kow)	18.197
Log Kow	1.26
Biomass to water partition coefficient	4.4394
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.01	88.01	10000.00
-Aeration tank	0.01	88.01	10000.00
-Settling tank	0.01	88.01	10000.00

STP Overall Chemical Mass Balance:

---

	g/h	mol/h	percent
Influent	1.00E+001	5.1E-002	100.00
Primary sludge	2.93E-002	1.5E-004	0.29
Waste sludge	1.53E-001	7.9E-004	1.53
Primary volatilization	2.34E-011	1.2E-013	0.00
Settling volatilization	6.37E-011	3.3E-013	0.00
Aeration off gas	1.57E-010	8.0E-013	0.00
Primary biodegradation	1.77E-003	9.1E-006	0.02
Settling biodegradation	5.30E-004	2.7E-006	0.01
Aeration biodegradation	6.98E-003	3.6E-005	0.07
Final water effluent	9.81E+000	5.0E-002	98.08
Total removal	1.92E-001	9.8E-004	1.92
Total biodegradation	9.28E-003	4.8E-005	0.09

Level III Fugacity Model (Full-Output):

==========

Chem Name :
Molecular Wt: 195.18
Henry's LC : 4.29e-014 atm-m3/mole (Henrywin program)
Vapor Press : 1.03e-005 mm Hg (Mpbpwin program)
Liquid VP : 0.000145 mm Hg (super-cooled)
Melting Pt : 141 deg C (Mpbpwin program)
Log Kow : 1.26 (Kowwin program)
Soil Koc : 7.46 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	6.99e-007	2.78	1000
Water	41.7	900	1000
Soil	58.2	900	1000
Sediment	0.0903	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.2e-017	0.00441	0.000177	0.000147	5.89e-006
Water	1.16e-018	812	1.05e+003	27.1	35.2
Soil	3.75e-017	1.13e+003	0	37.7	0
Sediment	1.06e-018	0.44	0.0457	0.0147	0.00152

Persistence Time: 843 hr
Reaction Time: 1.3e+003 hr

Advection Time: 2.4e+003 hr
Percent Reacted: 64.8
Percent Advected: 35.2
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 2.779
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.517 (weeks-months)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

TPSA (major degradate, 56% maximum)

SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24
---------- EPI SUMMARY (v3.11) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): -3.10
SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	5	Aromatic Carbon	0.2940	1.4700
Frag	1	Aromatic Nitrogen	-0.7324	-0.7324
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	2	-O- [oxygen, one aromatic attach]	-0.4664	-0.9328
Frag	1	-SO2-OH [sulfonic], [coef*(1+0.3*(NUM-1))]	-3.1580	-3.1580
Frag	2	Aromatic Nitrogen [5-member ring]	-0.5262	-1.0524
Frag	1	Aromatic nitrogen [fused ring location]	-0.0001	-0.0001
Factor	1	o-Alkyloxy to 2 aromat nitrogens/pyrazine	0.8955	0.8955
Const		Equation Constant		0.2290

Log Kow = -3.1036

MPBPWIN (v1.41) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM :

MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 460.56 deg C (Adapted Stein and Brown Method)
Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 155.26 deg C (Gold and Ogle Method)
Mean Melt Pt : 252.55 deg C (Joback; Gold,Ogle Methods)
Selected MP: 194.17 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 460.56 deg C (estimated))
(Using MP: 194.17 deg C (estimated))
VP: 1.37E-012 mm Hg (Antoine Method)
VP: 4.89E-011 mm Hg (Modified Grain Method)
VP: 1.2E-008 mm Hg (Mackay Method)
Selected VP: 4.89E-011 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	2	-CH3	21.98	43.96
Group	1	-OH (alcohol)	106.27	106.27
Group	2	-O- (nonring)	25.16	50.32
Group	1	>NH (nonring)	45.28	45.28
Group	1	CH (aromatic)	28.53	28.53
Group	3	-C (aromatic)	30.76	92.28
Group	1	C (3a aromatic)	45.46	45.46
Group	4	N (aromatic)	39.88	159.52
Group	1	>S(=O)(=O)	171.58	171.58
*		Equation Constant		198.18

RESULT-uncorr	BOILING POINT in deg Kelvin	941.38	
RESULT- corr	BOILING POINT in deg Kelvin	733.72	
	BOILING POINT in deg C	460.56	

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	2	-CH3	-5.10	-10.20
Group	1	-OH (alcohol)	44.45	44.45
Group	2	-O- (nonring)	22.23	44.46
Group	1	>NH (nonring)	52.66	52.66
Group	1	CH (aromatic)	8.13	8.13

```
Group | 3 | -C (aromatic)     |  37.02 | 111.06
Group | 1 | C (3a aromatic)   |  37.02 |  37.02
Group | 4 | N (aromatic)      |  68.40 | 273.60
Group | 1 | >S(=O)(=O)        | 150.00 | 150.00
  *   |   | Equation Constant |        | 122.50
======================+=========================+==========+=========
  RESULT    | MELTING POINT in deg Kelvin | 833.68
RESULT-limit| MELTING POINT in deg Kelvin | 623.00
            | MELTING POINT in deg C      | 349.84
-------------------------------------------------------

Water Sol from Kow (WSKOW v1.41) Results:
=========================================

        Water Sol: 7.628e+004 mg/L
SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM   :
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24
---------------------------------- WSKOW v1.41 Results -----------------------
Log Kow  (estimated)  : -3.10
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -3.10
Equation Used to Make Water Sol estimate:
  Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
    (used when Melting Point NOT available)
    Correction(s):        Value
    --------------------  -----
     Amino/sulfonic acid  -2.000
  Log Water Solubility  (in moles/L) :  -0.557
  Water Solubility at 25 deg C (mg/L):  7.628e+004

WATERNT Program (v1.01) Results:
================================

             Water Sol (v1.01 est): 1e+006 mg/L
SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM   :
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24
-------+-----+-------------------------------------------+----------+---------
 TYPE  |NUM |   WATER SOLUBILITY FRAGMENT DESCRIPTION     | COEFF    | VALUE
-------+-----+-------------------------------------------+----------+---------
 Frag  | 2  | -CH3   [aliphatic carbon]                  |-0.3213   | -0.6425
 Frag  | 1  | Aromatic Carbon  (C-H type)                |-0.3359   | -0.3359
```

```
Frag  |  1  | Aromatic Nitrogen [max count of 1 allowed]| 1.9255  | 1.9255
Frag  |  1  | -N   [aliphatic N, one aromatic attach]  | 1.2749  | 1.2749
Frag  |  2  | -O-  [oxygen, one aromatic attach]       | 0.1980  | 0.3959
Frag  |  4  | Aromatic Carbon  (C-substituent type)    |-0.5400  | -2.1598
Frag  |  2  | Aromatic Nitrogen [5-member ring]        | 0.5265  | 1.0530
Frag  |  1  | Aromatic nitrogen  [fused ring location] | 0.0000  | 0.0000
Frag  |  1  | -SO2-OH [sulfonic], [coef*(1+0.3*(NUM-1))]| 3.8495  | 3.8495
Const |     | Equation Constant                        |         | 0.2492
-------+-----+------------------------------------------+---------+---------
NOTE  |     | Maximum Solubility (1,000,000 mg/L) Applied!       |
-------+-----+------------------------------------------+---------+---------
                    Log Water Sol (moles/L) at 25 dec C =   0.5603
                    Water Solubility (mg/L) at 25 dec C =   1e+006
```

ECOSAR Program (v0.99g) Results:

SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24
Log Kow: -3.10 (KowWin estimate)
Melt Pt:
Wat Sol: 1.949E+008 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**1.02e+007**
Neutral Organics	**: Fish**	**96-hr**	**LC50**	**1.27e+007**
Neutral Organics	**: Fish**	**14-day**	**LC50**	**1.02e+007**
Neutral Organics	**: Daphnid**	**48-hr**	**LC50**	**9.57e+006**
Neutral Organics	**: Green Algae**	**96-hr**	**EC50**	**4.46e+006**
Neutral Organics	**: Fish**	**30-day**	**ChV**	**7.19e+005**
Neutral Organics	**: Daphnid**	**16-day**	**EC50**	**52688.023**

Neutral Organics : Green Algae 96-hr ChV 23394.395
Neutral Organics : Fish (SW) 96-hr LC50 2.47e+005
Neutral Organics : Mysid Shrimp 96-hr LC50 1.4e+008

mg/kg (ppm)
dry wt soil

Neutral Organics : Earthworm 14-day LC50 63024.848

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est : 5.30E-017 atm-m3/mole
Group Est: Incomplete
SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	6 Hydrogen to Carbon (aliphatic) Bonds		-0.7181
HYDROGEN	1 Hydrogen to Carbon (aromatic) Bonds		-0.1543
HYDROGEN	1 Hydrogen to Oxygen Bonds		3.2318
HYDROGEN	1 Hydrogen to Nitrogen Bonds		1.2835
FRAGMENT	2 C-O		2.1709
FRAGMENT	2 Car-Car		0.5276
FRAGMENT	7 Car-Nar		11.3975
FRAGMENT	1 Nar-Nar	ESTIMATE	3.0000
FRAGMENT	1 N-S	ESTIMATE	0.0000
FRAGMENT	1 Car-N		0.7304
FRAGMENT	2 Car-O		0.6945
FRAGMENT	1 O-S	ESTIMATE	0.2100
FRAGMENT	2 O=S (sulfone-type)	ESTIMATE	2.1000
FACTOR	3 Additional aromatic nitrogen(s)		-7.5000
FACTOR	1 -O-carbon ortho-position to Nar		-0.9600
FACTOR	1 -SO2-N- group		-1.3500

```
 RESULT  |   BOND ESTIMATION METHOD for LWAPC VALUE   | TOTAL | 14.664
---------+-------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 5.30E-017 atm-m3/mole
                  = 2.17E-015 unitless
--------+-------------------------------------------+-----------+--------
      |     GROUP CONTRIBUTION DESCRIPTION        | COMMENT | VALUE
--------+-------------------------------------------+-----------+--------
      |       2  CH3 (X)                  |         | -1.24
      |       1  Car-H (Car)(Nar)           |         |  0.11
      |       1  Car (Car)(Car)(O)          |         | -0.43
      |       2  O (C)(Car)               |         |  2.50
      |       2  Nar (Car)(Car)             |         |  6.12
      |         MISSING Value for:  O-H (S)
      |         MISSING Value for:  S (=O)(=O)(N)(O)
      |         MISSING Value for:  NH (Car)(S)
      |         MISSING Value for:  Car (Nar)(Nar)(N)
      |         MISSING Value for:  Car (Nar)(Car)(Nar)
      |         MISSING Value for:  Car (O)(Nar)(Nar)
      |         MISSING Value for:  Nar (Car)(Nar)(Car)
      |         MISSING Value for:  Nar (Car)(Nar)
--------+-------------------------------------------+-----------+--------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |
7.06
--------+-------------------------------------------+-----------+--------

Henrys LC [VP/WSol estimate using EPI values]:
  HLC:  2.322E-016 atm-m3/mole
  VP:   4.89E-011 mm Hg
  WS:   7.63E+004 mg/L

BIOWIN (v4.01) Program Results:
==============================
SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM   :
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24
-------------------------- BIOWIN v4.01 Results --------------------------
  Linear Model Prediction    : Biodegrades Fast
  Non-Linear Model Prediction: Biodegrades Fast
  Ultimate Biodegradation Timeframe: Weeks-Months
  Primary  Biodegradation Timeframe: Days-Weeks
  MITI Linear Model Prediction    : Does Not Biodegrade Fast
  MITI Non-Linear Model Prediction: Does Not Biodegrade Fast
```

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic ether [-O-aromatic carbon]	0.1319	0.2638
MolWt	*	Molecular Weight Parameter		-0.1310
Const	*	Equation Constant		0.7475

RESULT	LINEAR BIODEGRADATION PROBABILITY		0.8803

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic ether [-O-aromatic carbon]	2.2483	4.4966
MolWt	*	Molecular Weight Parameter		-3.9084

RESULT	NON-LINEAR BIODEGRADATION PROBABILITY		0.9733

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.1162
MolWt	*	Molecular Weight Parameter		-0.6082
Const	*	Equation Constant		3.1992

RESULT	SURVEY MODEL - ULTIMATE BIODEGRADATION		2.4747

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic ether [-O-aromatic carbon]	0.0771	0.1542
MolWt	*	Molecular Weight Parameter		-0.3971
Const	*	Equation Constant		3.8477

RESULT	SURVEY MODEL - PRIMARY BIODEGRADATION		3.6049

```
=============+=========================================+=========+=====
======
 Result Classification:  5.00 -> hours    4.00 -> days   3.00 -> weeks
  (Primary & Ultimate)   2.00 -> months   1.00 -> longer
------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  | Aromatic ether  [-O-aromatic carbon]     | 0.1952 | 0.3905
 Frag |  1  | Aromatic-H                               | 0.0082 | 0.0082
 Frag |  2  | Methyl  [-CH3]                           | 0.0004 | 0.0008
 MolWt|  *  | Molecular Weight Parameter               |        | -0.8188
 Const|  *  | Equation Constant                        |        | 0.7121
=============+=========================================+=========+=====
======
   RESULT    | MITI LINEAR BIODEGRADATION PROBABILITY   |         | 0.2928
=============+=========================================+=========+=====
======
------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  | Aromatic ether  [-O-aromatic carbon]     | 1.3227 | 2.6454
 Frag |  1  | Aromatic-H                               | 0.1201 | 0.1201
 Frag |  2  | Methyl  [-CH3]                           | 0.0194 | 0.0389
 MolWt|  *  | Molecular Weight Parameter               |        | -7.9458
=============+=========================================+=========+=====
======
   RESULT    | MITI NON-LINEAR BIODEGRADATION PROBABILITY |       | 0.0681
=============+=========================================+=========+=====
======
 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:
============================
SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM   :
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24
---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction      =  1.6592 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds  =  0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  0.0000 E-12 cm3/molecule-sec
```

Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
**Addition to Fused Rings = 57.1137 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 58.9129 E-12 cm3/molecule-sec
HALF-LIFE = 0.182 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 2.179 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========

Koc (estimated): 91.4
Koc may be sensitive to pH!
SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 8.442
Non-Corrected Log Koc ..... : 5.1122
Fragment Correction(s):
2 Ether, aromatic (-C-O-C-) ..... : -1.2862
1 Aromatic ring with 2 nitrogens ..... : -0.9650
1 Miscellaneous S(=O) group ..... : -0.9000
Corrected Log Koc ..... : 1.9610
Estimated Koc: 91.41
NOTE:
The Koc of this structure may be sensitive to pH! The estimated
Koc represents a best-fit to the majority of experimental values;
however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========
SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)

and Specific Alkyl Halides can be estimated!! For more information,
(Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:
==========

SMILES : OS(=O)(=O)Nc1nc2c(OC)cnc(OC)n2n1
CHEM :
MOL FOR: C7 H9 N5 O5 S1
MOL WT : 275.24
---------- Bcfwin v2.15 ----------
Log Kow (estimated) : -3.10
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: -3.10
Equation Used to Make BCF estimate:
Log BCF = 0.50 (Ionic; Log Kow dependent)

Estimated Log BCF = 0.500 (BCF = 3.162)

Volatization From Water
==========

Chemical Name:
Molecular Weight : 275.24 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 5.3E-017 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	1.833E+013	1.999E+014
HALF-LIFE (days) :	7.636E+011	8.33E+012
HALF-LIFE (years) :	2.091E+009	2.281E+010

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========

PROPERTIES OF:

Molecular weight (g/mol)	275.24
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0

(mm Hg) 0
Henry 's law constant (Atm-m3/mol) 5.3E-017
Air-water partition coefficient 2.16754E-015
Octanol-water partition coefficient (Kow) 0.000794328
Log Kow -3.1
Biomass to water partition coefficient 0.800159
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 0.04 15.98 10000.00
-Aeration tank 0.04 15.98 10000.00
-Settling tank 0.04 15.98 10000.00
STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	3.6E-002	100.00
Primary sludge	2.50E-002	9.1E-005	0.25
Waste sludge	1.50E-001	5.5E-004	1.50
Primary volatilization	2.89E-014	1.0E-016	0.00
Settling volatilization	7.87E-014	2.9E-016	0.00
Aeration off gas	1.94E-013	7.0E-016	0.00
Primary biodegradation	1.76E-003	6.4E-006	0.02
Settling biodegradation	5.27E-004	1.9E-006	0.01
Aeration biodegradation	6.93E-003	2.5E-005	0.07
Final water effluent	9.82E+000	3.6E-002	98.15
Total removal	1.85E-001	6.7E-004	1.85
Total biodegradation	9.22E-003	3.3E-005	0.09

Level III Fugacity Model (Full-Output):

Chem Name :
Molecular Wt: 275.24
Henry's LC : 5.3e-017 atm-m3/mole (Henrywin program)
Vapor Press : 4.89e-011 mm Hg (Mpbpwin program)
Liquid VP : 2.3e-009 mm Hg (super-cooled)
Melting Pt : 194 deg C (Mpbpwin program)
Log Kow : -3.1 (Kowwin program)
Soil Koc : 0.000326 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)

Air 3.59e-007 4.36 1000
Water 49.8 900 1000
Soil 50.1 900 1000
Sediment 0.0919 3.6e+003 0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.93e-020	0.00135	8.5e-005	4.5e-005	2.83e-006
Water	1.14e-021	908	1.18e+003	30.3	39.3
Soil	4.23e-020	912	0	30.4	0
Sediment	1.05e-021	0.418	0.0435	0.0139	0.00145

Persistence Time: 789 hr
Reaction Time: 1.3e+003 hr
Advection Time: 2.01e+003 hr
Percent Reacted: 60.7
Percent Advected: 39.3
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 4.358
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.475 (weeks-months)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

5-OH 2-amino TP (major degradate, 32% maximum)
SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15
---------- EPI SUMMARY (v3.11) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 0.56
SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	5	Aromatic Carbon	0.2940	1.4700
Frag	1	Aromatic Nitrogen	-0.7324	-0.7324
Frag	1	-OH [hydroxy, aromatic attach]	-0.4802	-0.4802
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	2	Aromatic Nitrogen [5-member ring]	-0.5262	-1.0524
Frag	1	Aromatic nitrogen [fused ring location]	-0.0001	-0.0001
Factor	1	Imidazole type -> 2-amino type correction	0.5596	0.5596
Factor	1	Ring rx -> -OH ortho to aromatic nitrogen	0.7500	0.7500
Factor	1	Additional amino-type triazole correction	0.6500	0.6500
Const		Equation Constant		0.2290

Log Kow = 0.5574

MPBPWIN (v1.41) Program Results:
==========

Experimental Database Structure Match: no data

SMILES : Nc1nc2c(OC)cnc(O)n2n1

CHEM :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 358.43 deg C (Adapted Stein and Brown Method)
Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 95.63 deg C (Gold and Ogle Method)
Mean Melt Pt : 222.73 deg C (Joback; Gold,Ogle Methods)
Selected MP: 146.47 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 358.43 deg C (estimated))
(Using MP: 146.47 deg C (estimated))
VP: 4.84E-007 mm Hg (Antoine Method)
VP: 1.25E-006 mm Hg (Modified Grain Method)
VP: 1.04E-005 mm Hg (Mackay Method)
Selected VP: 1.25E-006 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	1	-OH (phenol)	70.48	70.48
Group	1	-O- (nonring)	25.16	25.16
Group	1	CH (aromatic)	28.53	28.53
Group	3	-C (aromatic)	30.76	92.28
Group	1	C (3a aromatic)	45.46	45.46
Group	1	-NH2 (to arom)	86.63	86.63
Group	4	N (aromatic)	39.88	159.52
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 728.22
RESULT- corr | BOILING POINT in deg Kelvin | 631.59
| BOILING POINT in deg C | 358.43

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH3	-5.10	-5.10
Group	1	-OH (phenol)	82.83	82.83
Group	1	-O- (nonring)	22.23	22.23
Group	1	CH (aromatic)	8.13	8.13
Group	3	-C (aromatic)	37.02	111.06

```
Group | 1 | C (3a aromatic)  |  37.02 |  37.02
Group | 1 | -NH2 (to arom)   |  66.89 |  66.89
Group | 4 | N (aromatic)     |  68.40 | 273.60
  *   |   | Equation Constant |       | 122.50
=============+=======================+==========+=========
  RESULT   | MELTING POINT in deg Kelvin | 719.16
RESULT-limit| MELTING POINT in deg Kelvin | 623.00
          | MELTING POINT in deg C      | 349.84
-----------------------------------------------------
```

Water Sol from Kow (WSKOW v1.41) Results:

```
==========================================
        Water Sol: 1.816e+004 mg/L
SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM   :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15
---------------------------------- WSKOW v1.41 Results ----------------------
Log Kow  (estimated)  :  0.56
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  0.56
Equation Used to Make Water Sol estimate:
  Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
     (used when Melting Point NOT available)
    Correction(s):       Value
    -------------------  -----
     No Applicable Correction Factors
  Log Water Solubility  (in moles/L) :  -0.999
  Water Solubility at 25 deg C (mg/L):  1.816e+004
```

WATERNT Program (v1.01) Results:

```
==================================
            Water Sol (v1.01 est): 1e+006 mg/L
SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM   :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15
-------+-----+-------------------------------------------+---------+---------
 TYPE  |NUM |   WATER SOLUBILITY FRAGMENT DESCRIPTION     | COEFF   | VALUE
-------+-----+-------------------------------------------+---------+---------
 Frag  |  1  | -CH3   [aliphatic carbon]                 |-0.3213  | -0.3213
 Frag  |  1  | Aromatic Carbon  (C-H type)               |-0.3359  | -0.3359
 Frag  |  1  | Aromatic Nitrogen [max count of 1 allowed]| 1.9255  |  1.9255
```

```
Frag | 1 | -OH    [hydroxy, aromatic attach]       | 1.6578  | 1.6578
Frag | 1 | -N   [aliphatic N, one aromatic attach] | 1.2749  | 1.2749
Frag | 1 | -O-  [oxygen, one aromatic attach]      | 0.1980  | 0.1980
Frag | 4 | Aromatic Carbon  (C-substituent type)   |-0.5400  | -2.1598
Frag | 2 | Aromatic Nitrogen [5-member ring]       | 0.5265  | 1.0530
Frag | 1 | Aromatic nitrogen  [fused ring location] | 0.0000  | 0.0000
Factor| 1 | Reaction ->  -OH / nitrogen (arom 6-ring) |-2.5298  | -2.5298
Const |   | Equation Constant                       |         | 0.2492
-------+-----+-----------------------------------------+---------+---------
NOTE |   | Maximum Solubility (1,000,000 mg/L) Applied!      |
-------+-----+-----------------------------------------+---------+---------
                    Log Water Sol (moles/L) at 25 dec C =   0.7419
                    Water Solubility (mg/L) at 25 dec C =   1e+006
```

ECOSAR Program (v0.99g) Results:

SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15
Log Kow: 0.56 (KowWin estimate)
Melt Pt:
Wat Sol: 2.371E+004 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Aromatic Amines
Phenols

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**4368.075**
Aromatic Amines	**: Fish**	**96-hr**	**LC50**	**631.263**
Aromatic Amines	**: Fish**	**14-day**	**LC50**	**530.603**
Aromatic Amines	**: Daphnid**	**48-hr**	**LC50**	**3.043**
Aromatic Amines	**: Fish**		**ChV**	**2.466**
Aromatic Amines	**: Daphnid**		**ChV**	**0.086**
Aromatic Amines	**: Green Algae**		**ChV**	**32.944**

Phenols : Fish 96-hr LC50 205.159
Phenols : Daphnid 48-hr LC50 37.845
Phenols : Green Algae 96-hr EC50 1692.194
Phenols : Fish 30-day ChV 32.140
Phenols : Fish 90-day ChV 0.952
Phenols : Daphnid 21-day ChV 21.939
Phenols : Green Algae 96-hr ChV 73.622

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.

Aromatic Amines:
Fish and daphnid acute toxicity log Kow cutoff: 7.0
Green algal EC50 toxicity log Kow cutoff: 7.0
Chronic toxicity log Kow cutoff: 9.0
MW cutoff: 1000

Phenols:
Fish and daphnid acute toxicity log Kow cutoff: 7.0
Green algal EC50 toxicity log Kow cutoff: 7.0
Chronic toxicity log Kow cutoff: 9.0
MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est : 8.28E-018 atm-m3/mole
Group Est: Incomplete
SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	3 Hydrogen to Carbon (aliphatic) Bonds		-0.3590
HYDROGEN	1 Hydrogen to Carbon (aromatic) Bonds		-0.1543
HYDROGEN	1 Hydrogen to Oxygen Bonds		3.2318
HYDROGEN	2 Hydrogen to Nitrogen Bonds		2.5670
FRAGMENT	1 C-O		1.0855
FRAGMENT	2 Car-Car		0.5276
FRAGMENT	1 Car-OH		0.5967
FRAGMENT	7 Car-Nar		11.3975
FRAGMENT	1 Nar-Nar	ESTIMATE	3.0000
FRAGMENT	1 Car-N		0.7304
FRAGMENT	1 Car-O		0.3473

```
FACTOR  |  3  Additional aromatic nitrogen(s)      |       | -7.5000
---------+-------------------------------------------+---------+---------
RESULT  |   BOND ESTIMATION METHOD for LWAPC VALUE  | TOTAL | 15.470
---------+-------------------------------------------+---------+---------
HENRYs LAW CONSTANT at 25 deg C = 8.28E-018 atm-m3/mole
                    = 3.38E-016 unitless
--------+-------------------------------------------+-----------+--------
     |     GROUP CONTRIBUTION DESCRIPTION       | COMMENT | VALUE
--------+-------------------------------------------+-----------+--------
     |        1  NH2 (Car)                 | ESTIMATE | 4.00
     |        1  CH3 (X)                   |          | -0.62
     |        1  Car-H (Car)(Nar)          |          |  0.11
     |        1  Car (Car)(Car)(O)         |          | -0.43
     |        1  O-H (Car)                 |          |  4.45
     |        1  O (C)(Car)                |          |  1.25
     |        2  Nar (Car)(Car)            |          |  6.12
     |          MISSING Value for:  Car (Nar)(Nar)(N)
     |          MISSING Value for:  Car (Nar)(Car)(Nar)
     |          MISSING Value for:  Car (O)(Nar)(Nar)
     |          MISSING Value for:  Nar (Car)(Nar)(Car)
     |          MISSING Value for:  Nar (Car)(Nar)
--------+-------------------------------------------+-----------+--------
RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | INCOMPLETE |
14.88
--------+-------------------------------------------+-----------+--------

Henrys LC [VP/WSol estimate using EPI values]:
  HLC:  1.641E-011 atm-m3/mole
  VP:   1.25E-006 mm Hg
  WS:   1.82E+004 mg/L

BIOWIN (v4.01) Program Results:
==============================
SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM   :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15
------------------------- BIOWIN v4.01 Results -------------------------
  Linear Model Prediction    : Biodegrades Fast
  Non-Linear Model Prediction: Biodegrades Fast
  Ultimate Biodegradation Timeframe:  Weeks-Months
  Primary  Biodegradation Timeframe:  Days-Weeks
  MITI Linear Model Prediction    : Does Not Biodegrade Fast
```

MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.1158	0.1158
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.2338	-0.2338
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1319	0.1319
MolWt	*	Molecular Weight Parameter		-0.0862
Const	*	Equation Constant		0.7475
RESULT		LINEAR BIODEGRADATION PROBABILITY		0.6753

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.9086	0.9086
Frag	1	Aromatic amine [-NH2 or -NH-]	-1.9070	-1.9070
Frag	1	Aromatic ether [-O-aromatic carbon]	2.2483	2.2483
MolWt	*	Molecular Weight Parameter		-2.5724
RESULT		NON-LINEAR BIODEGRADATION PROBABILITY		0.8437

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0564	0.0564
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.1349	-0.1349
Frag	1	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.0581
MolWt	*	Molecular Weight Parameter		-0.4003
Const	*	Equation Constant		3.1992
RESULT		SURVEY MODEL - ULTIMATE BIODEGRADATION		2.6622

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE

Frag	1	Aromatic alcohol [-OH]	0.0397	0.0397
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.1084	-0.1084
Frag	1	Aromatic ether [-O-aromatic carbon]	0.0771	0.0771
MolWt	*	Molecular Weight Parameter		-0.2614
Const	*	Equation Constant		3.8477

RESULT	SURVEY MODEL - PRIMARY BIODEGRADATION	3.5948

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0642	0.0642
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.1577	-0.1577
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1952	0.1952
Frag	1	Aromatic-H	0.0082	0.0082
Frag	1	Methyl [-CH3]	0.0004	0.0004
MolWt	*	Molecular Weight Parameter		-0.5389
Const	*	Equation Constant		0.7121

RESULT	MITI LINEAR BIODEGRADATION PROBABILITY	0.2836

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.4884	0.4884
Frag	1	Aromatic amine [-NH2 or -NH-]	-1.2264	-1.2264
Frag	1	Aromatic ether [-O-aromatic carbon]	1.3227	1.3227
Frag	1	Aromatic-H	0.1201	0.1201
Frag	1	Methyl [-CH3]	0.0194	0.0194
MolWt	*	Molecular Weight Parameter		-5.2297

RESULT	MITI NON-LINEAR BIODEGRADATION PROBABILITY	0.1213

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable

A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:

SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15
---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.8296 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
**Addition to Fused Rings = 100.7627 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 101.7323 E-12 cm3/molecule-sec
HALF-LIFE = 0.105 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 1.262 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
NOTE: Reaction with Nitrate Radicals May Be Important!
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:

Koc (estimated): 210
Koc may be sensitive to pH!
SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 6.220
Non-Corrected Log Koc ..... : 3.9305
Fragment Correction(s):
1 Ether, aromatic (-C-O-C-) ..... : -0.6431
1 Aromatic ring with 2 nitrogens ..... : -0.9650
Corrected Log Koc ..... : 2.3224
Estimated Koc: 210.1
NOTE:
The Koc of this structure may be sensitive to pH! The estimated

Koc represents a best-fit to the majority of experimental values;
however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========

SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)
and Specific Alkyl Halides can be estimated!! For more information,
(Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:
==========

SMILES : Nc1nc2c(OC)cnc(O)n2n1
CHEM :
MOL FOR: C6 H7 N5 O2
MOL WT : 181.15
---------- Bcfwin v2.15 ----------
Log Kow (estimated) : 0.56
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 0.56
Equation Used to Make BCF estimate:
Log BCF = 0.50
Correction(s): Value
Correction Factors Not Used for Log Kow < 1
Estimated Log BCF = 0.500 (BCF = 3.162)

Volatization From Water
==========

Chemical Name:
Molecular Weight : 181.15 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 8.28E-018 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1

Wind Velocity (m/sec): 5 0.5
Current Velocity (m/sec): 1 0.05
HALF-LIFE (hours) : 9.517E+013 1.038E+015
HALF-LIFE (days) : 3.965E+012 4.326E+013
HALF-LIFE (years) : 1.086E+010 1.184E+011

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

Molecular weight (g/mol) 181.15
Aqueous solubility (mg/l) 0
Vapour pressure (Pa) 0
(atm) 0
(mm Hg) 0
Henry 's law constant (Atm-m3/mol) 8.28E-018
Air-water partition coefficient 3.38627E-016
Octanol-water partition coefficient (Kow) 3.63078
Log Kow 0.56
Biomass to water partition coefficient 1.52616
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 0.02 30.43 10000.00
-Aeration tank 0.02 30.43 10000.00
-Settling tank 0.02 30.43 10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	5.5E-002	100.00
Primary sludge	2.58E-002	1.4E-004	0.26
Waste sludge	1.51E-001	8.3E-004	1.51
Primary volatilization	4.51E-015	2.5E-017	0.00
Settling volatilization	1.23E-014	6.8E-017	0.00
Aeration off gas	3.03E-014	1.7E-016	0.00
Primary biodegradation	1.76E-003	9.7E-006	0.02
Settling biodegradation	5.27E-004	2.9E-006	0.01
Aeration biodegradation	6.94E-003	3.8E-005	0.07
Final water effluent	9.81E+000	5.4E-002	98.14
Total removal	1.86E-001	1.0E-003	1.86

Total biodegradation 9.23E-003 5.1E-005 0.09

Level III Fugacity Model (Full-Output):

==========

Chem Name :
Molecular Wt: 181.15
Henry's LC : 8.28e-018 atm-m3/mole (Henrywin program)
Vapor Press : 1.25e-006 mm Hg (Mpbpwin program)
Liquid VP : 1.99e-005 mm Hg (super-cooled)
Melting Pt : 146 deg C (Mpbpwin program)
Log Kow : 0.56 (Kowwin program)
Soil Koc : 1.49 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.47e-010	2.52	1000
Water	47.8	900	1000
Soil	52.1	900	1000
Sediment	0.0911	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	4.57e-021	9.73e-007	3.54e-008	3.24e-008	1.18e-009
Water	2.63e-022	885	1.15e+003	29.5	38.3
Soil	9.49e-021	966	0	32.2	0
Sediment	2.42e-022	0.422	0.0438	0.0141	0.00146

Persistence Time: 802 hr
Reaction Time: 1.3e+003 hr
Advection Time: 2.09e+003 hr
Percent Reacted: 61.7
Percent Advected: 38.3
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 2.522
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.662 (weeks-months)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

5,8-di-OH (major degradate, 11% at study termination)

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM :
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32
---------- EPI SUMMARY (v3.11) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 1.69
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM :
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	1	C [aliphatic carbon - No H, not tert]	0.9723	0.9723
Frag	5	-F [fluorine, aliphatic attach]	-0.0031	-0.0155
Frag	11	Aromatic Carbon	0.2940	3.2340
Frag	1	Aromatic Nitrogen	-0.7324	-0.7324
Frag	2	-OH [hydroxy, aromatic attach]	-0.4802	-0.9604
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	1	-SO2-N [aromatic attach]	-0.2079	-0.2079
Frag	2	Aromatic Nitrogen [5-member ring]	-0.5262	-1.0524
Frag	1	Aromatic nitrogen [fused ring location]	-0.0001	-0.0001
Factor	1	Ring rx -> -OH ortho to aromatic nitrogen	0.7500	0.7500
Const		Equation Constant		0.2290

Log Kow = 1.6857

MPBPWIN (v1.41) Program Results:
==========

Experimental Database Structure Match: no data

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM :
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 549.03 deg C (Adapted Stein and Brown Method)
Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 206.92 deg C (Gold and Ogle Method)
Mean Melt Pt : 278.38 deg C (Joback; Gold,Ogle Methods)
Selected MP: 235.50 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 549.03 deg C (estimated))
(Using MP: 235.50 deg C (estimated))
VP: 8.44E-017 mm Hg (Antoine Method)
VP: 1.1E-013 mm Hg (Modified Grain Method)
VP: 2.72E-011 mm Hg (Mackay Method)
Selected VP: 1.1E-013 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH2-	24.22	24.22
Group	1	>CH-	11.86	11.86
Group	1	>C<	4.50	4.50
Group	5	-F	0.13	0.65
Group	2	-OH (phenol)	70.48	140.96
Group	1	-O- (nonring)	25.16	25.16
Group	1	>NH (nonring)	45.28	45.28
Group	4	CH (aromatic)	28.53	114.12
Group	6	-C (aromatic)	30.76	184.56
Group	1	C (3a aromatic)	45.46	45.46
Group	4	N (aromatic)	39.88	159.52
Group	1	>S(=O)(=O)	171.58	171.58
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 1126.05
RESULT- corr | BOILING POINT in deg Kelvin | 822.19
| BOILING POINT in deg C | 549.03

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH2-	11.27	11.27
Group	1	>CH-	12.64	12.64
Group	1	>C<	46.43	46.43
Group	5	-F	-15.78	-78.90
Group	2	-OH (phenol)	82.83	165.66
Group	1	-O- (nonring)	22.23	22.23
Group	1	>NH (nonring)	52.66	52.66
Group	4	CH (aromatic)	8.13	32.52
Group	6	-C (aromatic)	37.02	222.12
Group	1	C (3a aromatic)	37.02	37.02
Group	4	N (aromatic)	68.40	273.60
Group	1	>S(=O)(=O)	150.00	150.00
*		Equation Constant		122.50

RESULT	MELTING POINT in deg Kelvin	1069.75
RESULT-limit	MELTING POINT in deg Kelvin	623.00
	MELTING POINT in deg C	349.84

Water Sol from Kow (WSKOW v1.41) Results:

==========

Water Sol: 50.12 mg/L
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM :
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32

---------- WSKOW v1.41 Results ----------

Log Kow (estimated) : 1.69
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 1.69
Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -3.958
Water Solubility at 25 deg C (mg/L): 50.12

WATERNT Program (v1.01) Results:

==========

Water Sol (v1.01 est): 16.681 mg/L
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM :
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	-0.5370	-0.5370
Frag	1	-CH [aliphatic carbon]	-0.5285	-0.5285
Frag	1	C [aliphatic carbon - No H, not tert]	-1.0516	-1.0516
Frag	5	-F [fluorine, aliphatic attach]	-0.1580	-0.7900
Frag	4	Aromatic Carbon (C-H type)	-0.3359	-1.3435
Frag	1	Aromatic Nitrogen [max count of 1 allowed]	1.9255	1.9255
Frag	1	-N [aliphatic N, one aromatic attach]	1.2749	1.2749
Frag	1	-O- [oxygen, one aromatic attach]	0.1980	0.1980
Frag	7	Aromatic Carbon (C-substituent type)	-0.5400	-3.7797
Frag	1	-SO2-N [aromatic attach]	-1.2003	-1.2003
Frag	2	Aromatic Nitrogen [5-member ring]	0.5265	1.0530
Frag	1	-OH [combined multiple aromatic attach]	2.6237	2.6237
Frag	1	Aromatic nitrogen [fused ring location]	0.0000	0.0000
Factor	1	Reaction -> -OH / nitrogen (arom 6-ring)	-2.5298	-2.5298
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -4.4361
Water Solubility (mg/L) at 25 dec C = 16.681

ECOSAR Program (v0.99g) Results:
==========
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32
Log Kow: 1.69 (KowWin estimate)
Melt Pt:
Wat Sol: 4193 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Phenols

Quinone/Hydroquinone

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**1138.478**
Phenols	**: Fish**	**96-hr**	**LC50**	**103.818**
Phenols	**: Daphnid**	**48-hr**	**LC50**	**32.817**
Phenols	**: Green Algae**	**96-hr**	**EC50**	**425.270**
Phenols	**: Fish**	**30-day**	**ChV**	**15.888**
Phenols	**: Fish**	**90-day**	**ChV**	**0.748**
Phenols	**: Daphnid**	**21-day**	**ChV**	**11.160**
Phenols	**: Green Algae**	**96-hr**	**ChV**	**35.551**
Quinone/Hydroquinone	**: Fish [CLOGP]**	**96-hr**	**LC50**	**0.311**
Quinone/Hydroquinone	**: Daphnid [CLOGP]**	**48-hr**	**LC50**	**0.334**
Quinone/Hydroquinone	**: Green Algae [CLOGP]**	**96-hr**	**EC50**	**0.702**
Quinone/Hydroquinone	**: Fish [CLOGP]**	**96-hr**	**LC50**	**0.311**
Quinone/Hydroquinone	**: Fish (SW) [CLOGP]**	**96-hr**	**LC50**	**0.264**
Quinone/Hydroquinone	**: Mysid [CLOGP]**	**96-hr**	**LC50**	**1.491**
Quinone/Hydroquinone	**: G Algae (SW)[CLOGP]**	**96-hr**	**EC50**	**0.029**
Quinone/Hydroquinone	**: G Algae (SW)[CLOGP]**		**ChV**	**0.004**

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.

Phenols:
Fish and daphnid acute toxicity log Kow cutoff: 7.0
Green algal EC50 toxicity log Kow cutoff: 7.0
Chronic toxicity log Kow cutoff: 9.0
MW cutoff: 1000

Quinone/Hydroquinone:
Fish and daphnid acute toxicity log Kow cutoff: 7.0
Green algal EC50 toxicity log Kow cutoff: 7.0
Chronic toxicity log Kow cutoff: 7.0
MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est : 4.81E-021 atm-m3/mole
Group Est: Incomplete
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM :
MOL FOR: C14 H10 F5 N5 O5 S1

MOL WT : 455.32

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	3 Hydrogen to Carbon (aliphatic) Bonds		-0.3590
HYDROGEN	4 Hydrogen to Carbon (aromatic) Bonds		-0.6172
HYDROGEN	2 Hydrogen to Oxygen Bonds		6.4635
HYDROGEN	1 Hydrogen to Nitrogen Bonds		1.2835
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-Car		0.1619
FRAGMENT	1 C-O		1.0855
FRAGMENT	5 C-F		-2.0922
FRAGMENT	8 Car-Car		2.1105
FRAGMENT	2 Car-OH		1.1934
FRAGMENT	7 Car-Nar		11.3975
FRAGMENT	1 Nar-Nar	ESTIMATE	3.0000
FRAGMENT	1 Car-S		0.6345
FRAGMENT	1 N-S	ESTIMATE	0.0000
FRAGMENT	1 Car-N		0.7304
FRAGMENT	1 Car-O		0.3473
FRAGMENT	2 O=S (sulfone-type)	ESTIMATE	2.1000
FACTOR	3 Additional aromatic nitrogen(s)		-7.5000
FACTOR	1 -SO2-N- group		-1.3500
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	18.706

HENRYs LAW CONSTANT at 25 deg C = 4.81E-021 atm-m3/mole
= 1.97E-019 unitless

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	1 CH2 (C)(O)		-0.13
	1 CH (C)(F)(F)		0.70
	3 Car-H (Car)(Car)		0.33
	1 Car-H (Car)(Nar)		0.11
	1 Car (C)(Car)(Car)		0.70
	2 Car (Car)(Car)(O)		-0.86
	1 Car (Car)(Car)(S)		-0.25
	2 O-H (Car)		8.90
	1 O (C)(Car)		1.25
	2 Nar (Car)(Car)		6.12
	MISSING Value for: C (F)(F)(F)(Car)		

```
        |          MISSING Value for:  S (=O)(=O)(N)(Car)
        |          MISSING Value for:  NH (Car)(S)
        |          MISSING Value for:  Car (Nar)(Nar)(N)
        |          MISSING Value for:  Car (Nar)(Car)(Nar)
        |          MISSING Value for:  Car (O)(Nar)(Nar)
        |          MISSING Value for:  Nar (Car)(Nar)(Car)
        |          MISSING Value for:  Nar (Car)(Nar)
--------+-----------------------------------------------+------------+--------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |
16.87
--------+-----------------------------------------------+------------+--------

Henrys LC [VP/WSol estimate using EPI values]:
   HLC:  1.315E-015 atm-m3/mole
   VP:   1.1E-013 mm Hg
   WS:   50.1 mg/L

BIOWIN (v4.01) Program Results:
================================
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM   :
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32
-------------------------- BIOWIN v4.01 Results ---------------------------
   Linear Model Prediction    :  Does Not Biodegrade Fast
   Non-Linear Model Prediction:  Does Not Biodegrade Fast
   Ultimate Biodegradation Timeframe:  Recalcitrant
   Primary  Biodegradation Timeframe:  Weeks
   MITI Linear Model Prediction    :  Does Not Biodegrade Fast
   MITI Non-Linear Model Prediction:  Does Not Biodegrade Fast
------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION       | COEFF   | VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Aromatic alcohol  [-OH]                | 0.1158  |  0.2316
 Frag |  1  |  Aromatic ether  [-O-aromatic carbon]   | 0.1319  |  0.1319
 Frag |  1  |  Trifluoromethyl group  [-CF3]          |-0.5204  | -0.5204
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.2168
 Const|  *  |  Equation Constant                      |         |  0.7475
==============+=========================================+=========+=========
  RESULT   |    LINEAR BIODEGRADATION PROBABILITY    |         |  0.3739
==============+=========================================+=========+=========
```

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.9086	1.8172
Frag	1	Aromatic ether [-O-aromatic carbon]	2.2483	2.2483
Frag	1	Trifluoromethyl group [-CF3]	-5.6696	-5.6696
MolWt	*	Molecular Weight Parameter		-6.4655

RESULT	NON-LINEAR BIODEGRADATION PROBABILITY		0.0063

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0564	0.1128
Frag	1	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.0581
Frag	1	Trifluoromethyl group [-CF3]	-0.5130	-0.5130
MolWt	*	Molecular Weight Parameter		-1.0062
Const	*	Equation Constant		3.1992

RESULT	SURVEY MODEL - ULTIMATE BIODEGRADATION		1.7347

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic alcohol [-OH]	0.0397	0.0794
Frag	1	Aromatic ether [-O-aromatic carbon]	0.0771	0.0771
Frag	1	Trifluoromethyl group [-CF3]	-0.2744	-0.2744
MolWt	*	Molecular Weight Parameter		-0.6569
Const	*	Equation Constant		3.8477

RESULT	SURVEY MODEL - PRIMARY BIODEGRADATION		3.0729

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

```
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION       | COEFF | VALUE
------+-----+----------------------------------------+--------+--------
Frag | 2 | Aromatic alcohol [-OH]                | 0.0642 | 0.1285
Frag | 1 | Aromatic ether [-O-aromatic carbon]    | 0.1952 | 0.1952
Frag | 5 | Fluorine [-F]                         | 0.0174 | 0.0869
Frag | 4 | Aromatic-H                            | 0.0082 | 0.0329
Frag | 1 | -CH2- [linear]                        | 0.0494 | 0.0494
Frag | 1 | -CH- [linear]                         |-0.0507 |-0.0507
MolWt| * | Molecular Weight Parameter            |        |-1.3546
Const| * | Equation Constant                     |        | 0.7121
============+=======================================================+=========+===
======
  RESULT   | MITI LINEAR BIODEGRADATION PROBABILITY   |        |-0.2002
============+=======================================================+=========+===
======

------+-----+----------------------------------------+--------+--------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION       | COEFF | VALUE
------+-----+----------------------------------------+--------+--------
Frag | 2 | Aromatic alcohol [-OH]                | 0.4884 | 0.9768
Frag | 1 | Aromatic ether [-O-aromatic carbon]    | 1.3227 | 1.3227
Frag | 5 | Fluorine [-F]                         |-3.9878 |-19.9392
Frag | 4 | Aromatic-H                            | 0.1201 | 0.4806
Frag | 1 | -CH2- [linear]                        | 0.4295 | 0.4295
Frag | 1 | -CH- [linear]                         |-0.0998 |-0.0998
MolWt| * | Molecular Weight Parameter            |        |-13.1445
============+=======================================================+=========+===
======
  RESULT   | MITI NON-LINEAR BIODEGRADATION PROBABILITY |        | 0.0000
============+=======================================================+=========+===
======
 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:
============================
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM  :
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32
---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction     =  0.8007 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  0.2800 E-12 cm3/molecule-sec
Addition to Triple Bonds  =  0.0000 E-12 cm3/molecule-sec
```

Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 0.6957 E-12 cm3/molecule-sec
**Addition to Fused Rings = 70.4466 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 72.2230 E-12 cm3/molecule-sec
HALF-LIFE = 0.148 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 1.777 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
NOTE: Reaction with Nitrate Radicals May Be Important!
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========

Koc (estimated): 3.2e+005
Koc may be sensitive to pH!
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM :
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 13.898
Non-Corrected Log Koc ..... : 8.0130
Fragment Correction(s):
1 Ether, aromatic (-C-O-C-) ..... : -0.6431
1 Aromatic ring with 2 nitrogens ..... : -0.9650
1 Miscellaneous S(=O) group ..... : -0.9000
Corrected Log Koc ..... : 5.5049
Estimated Koc: 3.198e+005
NOTE:
The Koc of this structure may be sensitive to pH! The estimated
Koc represents a best-fit to the majority of experimental values;
however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM :
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for

the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)
and Specific Alkyl Halides can be estimated!! For more information,
(Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:
==========
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2nc3c(O)cnc(O)n3n2
CHEM :
MOL FOR: C14 H10 F5 N5 O5 S1
MOL WT : 455.32
---------- Bcfwin v2.15 ----------
Log Kow (estimated) : 1.69
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 1.69
Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction
Correction(s): Value
No Applicable Correction Factors
Estimated Log BCF = 0.598 (BCF = 3.963)

Volatization From Water
==========
Chemical Name:
Molecular Weight : 455.32 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 4.81E-021 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	2.597E+017	2.833E+018
HALF-LIFE (days) :	1.082E+016	1.181E+017
HALF-LIFE (years) :	2.963E+013	3.232E+014

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========
PROPERTIES OF:

Molecular weight (g/mol) 455.32

Aqueous solubility (mg/l) 0
Vapour pressure (Pa) 0
(atm) 0
(mm Hg) 0
Henry 's law constant (Atm-m3/mol) 4.81E-021
Air-water partition coefficient 1.96715E-019
Octanol-water partition coefficient (Kow) 48.9779
Log Kow 1.69
Biomass to water partition coefficient 10.5956
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 0.00 207.51 10000.00
-Aeration tank 0.00 207.51 10000.00
-Settling tank 0.00 207.51 10000.00
STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	2.2E-002	100.00
Primary sludge	3.66E-002	8.0E-005	0.37
Waste sludge	1.58E-001	3.5E-004	1.58
Primary volatilization	2.62E-018	5.7E-021	0.00
Settling volatilization	7.13E-018	1.6E-020	0.00
Aeration off gas	1.76E-017	3.9E-020	0.00
Primary biodegradation	1.79E-003	3.9E-006	0.02
Settling biodegradation	5.36E-004	1.2E-006	0.01
Aeration biodegradation	7.05E-003	1.5E-005	0.07
Final water effluent	9.80E+000	2.2E-002	97.96
Total removal	2.04E-001	4.5E-004	2.04
Total biodegradation	9.38E-003	2.1E-005	0.09

Level III Fugacity Model (Full-Output):

Chem Name :
Molecular Wt: 455.32
Henry's LC : 4.81e-021 atm-m3/mole (Henrywin program)
Vapor Press : 1.1e-013 mm Hg (Mpbpwin program)
Liquid VP : 1.33e-011 mm Hg (super-cooled)
Melting Pt : 236 deg C (Mpbpwin program)
Log Kow : 1.69 (Kowwin program)

Soil Koc : 20.1 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.37e-009	3.55	1000
Water	34	3.6e+003	1000
Soil	65.9	3.6e+003	1000
Sediment	0.0995	1.44e+004	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.06e-024	2.6e-005	1.33e-006	8.67e-007	4.45e-008
Water	1.01e-025	369	1.92e+003	12.3	63.9
Soil	2.78e-024	714	0	23.8	0
Sediment	9.99e-026	0.27	0.112	0.00899	0.00374

Persistence Time: 1.88e+003 hr
Reaction Time: 5.2e+003 hr
Advection Time: 2.94e+003 hr
Percent Reacted: 36.1
Percent Advected: 63.9
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 3.554
Water: 3600
Soil: 3600
Sediment: 1.44e+004
Biowin estimate: 1.735 (recalcitrant)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

2-amino TCA (major degradate, 85% at study termination)

SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- EPI SUMMARY (v3.11) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): -0.59

SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic Carbon	0.2940	0.5880
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	1	-COOH [acid, aromatic attach]	-0.1186	-0.1186
Frag	3	Aromatic Nitrogen [5-member ring]	-0.5262	-1.5786
Factor	1	Imidazole type -> 2-amino type correction	0.5596	0.5596
Factor	1	Additional amino-type triazole correction	0.6500	0.6500
Const		Equation Constant		0.2290

Log Kow = -0.5876

MPBPWIN (v1.41) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 357.27 deg C (Adapted Stein and Brown Method)
Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 94.95 deg C (Gold and Ogle Method)
Mean Melt Pt : 222.39 deg C (Joback; Gold,Ogle Methods)
Selected MP: 145.93 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 357.27 deg C (estimated))
(Using MP: 145.93 deg C (estimated))
VP: 2.23E-006 mm Hg (Antoine Method)
VP: 5.26E-006 mm Hg (Modified Grain Method)
VP: 1.12E-005 mm Hg (Mackay Method)
Selected VP: 5.26E-006 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-COOH (acid)	169.83	169.83
Group	2	-C (aromatic)	30.76	61.52
Group	1	-NH2 (to arom)	86.63	86.63
Group	3	N (aromatic)	39.88	119.64
Corr	1	Triazole [NH]	90.00	90.00
*		Equation Constant		198.18

RESULT-uncorr	BOILING POINT in deg Kelvin	725.80	
RESULT- corr	BOILING POINT in deg Kelvin	630.43	
	BOILING POINT in deg C	357.27	

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-COOH (acid)	155.50	155.50
Group	2	-C (aromatic)	37.02	74.04
Group	1	-NH2 (to arom)	66.89	66.89
Group	3	N (aromatic)	68.40	205.20
*		Equation Constant		122.50

RESULT	MELTING POINT in deg Kelvin	624.13	
RESULT-limit	MELTING POINT in deg Kelvin	623.00	
	MELTING POINT in deg C	349.84	

Water Sol from Kow (WSKOW v1.41) Results:

Water Sol: 2.97e+005 mg/L
SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : -0.59
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -0.59
Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)
Correction(s): Value
---------- -----
No Applicable Correction Factors
Log Water Solubility (in moles/L) : 0.365
Water Solubility at 25 deg C (mg/L): 2.97e+005

WATERNT Program (v1.01) Results:
==========

Water Sol (v1.01 est): 1e+006 mg/L
SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-N [aliphatic N, one aromatic attach]	1.2749	1.2749
Frag	1	-COOH [acid, aromatic attach]	0.0568	0.0568
Frag	2	Aromatic Carbon (C-substituent type)	-0.5400	-1.0799
Frag	3	Aromatic Nitrogen [5-member ring]	0.5265	1.5795
Const		Equation Constant		0.2492
NOTE		Maximum Solubility (1,000,000 mg/L) Applied!		

Log Water Sol (moles/L) at 25 dec C = 0.8925
Water Solubility (mg/L) at 25 dec C = 1e+006

ECOSAR Program (v0.99g) Results:
==========

SMILES : Nc1nc(C(=O)O)nn1
CHEM :

CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
Log Kow: -0.59 (KowWin estimate)
Melt Pt:
Wat Sol: 2.496E+005 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Aromatic Amines-acid

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	31003.322
--> Acid moeity found: Predicted values multiplied by 10				
Aromatic Amines-acid	: Fish	96-hr	LC50	31588.445
Aromatic Amines-acid	: Fish	14-day	LC50	51337.914
Aromatic Amines-acid	: Daphnid	48-hr	LC50	44.097
Aromatic Amines-acid	: Fish		ChV	91.257
Aromatic Amines-acid	: Daphnid		ChV	1.585
Aromatic Amines-acid	: Green Algae		ChV	1105.193

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 7.0
Green algal EC50 toxicity log Kow cutoff: 7.0
Chronic toxicity log Kow cutoff: 9.0
MW cutoff: 1000

HENRY (v3.10) Program Results:
Bond Est : 1.09E-014 atm-m3/mole
Group Est: Incomplete
SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- HENRYWIN v3.10 Results ----------
---------+----------+---------+----------

```
  CLASS |    BOND CONTRIBUTION DESCRIPTION          | COMMENT |  VALUE
---------+-------------------------------------------+---------+----------
HYDROGEN |  1  Hydrogen to Oxygen Bonds              |         |  3.2318
HYDROGEN |  2  Hydrogen to Nitrogen Bonds            |         |  2.5670
FRAGMENT |  1  Car-CO                                |         |  1.2387
FRAGMENT |  4  Car-Nar                               |         |  6.5129
FRAGMENT |  1  Nar-Nar                               | ESTIMATE|  3.0000
FRAGMENT |  1  CO-O                                  |         |  0.0714
FRAGMENT |  1  Car-N                                 |         |  0.7304
FACTOR   |  2  Additional aromatic nitrogen(s)       |         | -5.0000
---------+-------------------------------------------+---------+----------
RESULT   |   BOND ESTIMATION METHOD for LWAPC VALUE  |  TOTAL  | 12.352
---------+-------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 1.09E-014 atm-m3/mole
                = 4.44E-013 unitless
--------+-------------------------------------------+-----------+--------
        |     GROUP CONTRIBUTION DESCRIPTION        |  COMMENT  |  VALUE
--------+-------------------------------------------+-----------+--------
        |       1  NH2 (Car)                        | ESTIMATE  |  4.00
        |       1  CO (O)(Car)                      |           |  4.57
        |       1  O-H (CO)                         |           |  1.45
        |       1  Nar (Car)(Car)                   |           |  3.06
        |          MISSING Value for:  Car (Nar)(Nar)(N)
        |          MISSING Value for:  Car (CO)(Nar)(Nar)
        |          MISSING Value for:  Nar (Nar)(Car)
        |          MISSING Value for:  Nar (Car)(Nar)
--------+-------------------------------------------+-----------+--------
RESULT  |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |
13.08
--------+-------------------------------------------+-----------+--------

Henrys LC [VP/WSol estimate using EPI values]:
  HLC:  2.985E-012 atm-m3/mole
  VP:   5.26E-006 mm Hg
  WS:   2.97E+005 mg/L

BIOWIN (v4.01) Program Results:
==============================
SMILES : Nc1nc(C(=O)O)nn1
CHEM   :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
-------------------------- BIOWIN v4.01 Results ---------------------------
```

Linear Model Prediction : Biodegrades Fast
Non-Linear Model Prediction: Biodegrades Fast
Ultimate Biodegradation Timeframe: Weeks
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model Prediction : Biodegrades Fast
MITI Non-Linear Model Prediction: Biodegrades Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	0.1769	0.1769
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.2338	-0.2338
MolWt	*	Molecular Weight Parameter		-0.0610
Const	*	Equation Constant		0.7475
RESULT		LINEAR BIODEGRADATION PROBABILITY		0.6297

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	2.4224	2.4224
Frag	1	Aromatic amine [-NH2 or -NH-]	-1.9070	-1.9070
MolWt	*	Molecular Weight Parameter		-1.8189
RESULT		NON-LINEAR BIODEGRADATION PROBABILITY		0.8462

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	0.0879	0.0879
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.1349	-0.1349
MolWt	*	Molecular Weight Parameter		-0.2831
Const	*	Equation Constant		3.1992
RESULT		SURVEY MODEL - ULTIMATE BIODEGRADATION		2.8690

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	0.0077	0.0077
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.1084	-0.1084
MolWt	*	Molecular Weight Parameter		-0.1848
Const	*	Equation Constant		3.8477
RESULT		SURVEY MODEL - PRIMARY BIODEGRADATION		3.5623

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	0.3770	0.3770
Frag	1	Aromatic amine [-NH2 or -NH-]	-0.1577	-0.1577
MolWt	*	Molecular Weight Parameter		-0.3811
Const	*	Equation Constant		0.7121
RESULT		MITI LINEAR BIODEGRADATION PROBABILITY		0.5503

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic acid [-C(=O)-OH]	2.4449	2.4449
Frag	1	Aromatic amine [-NH2 or -NH-]	-1.2264	-1.2264
MolWt	*	Molecular Weight Parameter		-3.6978
RESULT		MITI NON-LINEAR BIODEGRADATION PROBABILITY		0.5116

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:
==========

SMILES : Nc1nc(C(=O)O)nn1

CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.5200 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.1000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 0.6200 E-12 cm3/molecule-sec
HALF-LIFE = 17.252 Days (12-hr day; 1.5E6 OH/cm3)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========

Koc (estimated): 2.13
Koc may be sensitive to pH!
SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 4.198
Non-Corrected Log Koc ..... : 2.8559
Fragment Correction(s):
* Nitrogen to non-fused aromatic ring ... : -0.7770
* Organic Acid (-CO-OH) ..... : -1.7512
Corrected Log Koc ..... : 0.3277
Estimated Koc: 2.127
NOTE:
The Koc of this structure may be sensitive to pH! The estimated
Koc represents a best-fit to the majority of experimental values;
however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========

SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2

MOL WT : 128.09
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)
and Specific Alkyl Halides can be estimated!! For more information,
(Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:
==========

SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- Bcfwin v2.15 ----------
Log Kow (estimated) : -0.59
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: -0.59
Equation Used to Make BCF estimate:
Log BCF = 0.50 (Ionic; Log Kow dependent)

Estimated Log BCF = 0.500 (BCF = 3.162)

Volatization From Water
==========

Chemical Name:
Molecular Weight : 128.09 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 1.09E-014 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	6.079E+010	6.632E+011
HALF-LIFE (days) :	2.533E+009	2.763E+010
HALF-LIFE (years) :	6.935E+006	7.565E+007

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========

PROPERTIES OF:

Molecular weight (g/mol) 128.09
Aqueous solubility (mg/l) 0
Vapour pressure (Pa) 0
(atm) 0
(mm Hg) 0
Henry 's law constant (Atm-m3/mol) 1.09E-014
Air-water partition coefficient 4.45778E-013
Octanol-water partition coefficient (Kow) 0.25704
Log Kow -0.59
Biomass to water partition coefficient 0.851408
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.04	17.00	10000.00
-Aeration tank	0.04	17.00	10000.00
-Settling tank	0.04	17.00	10000.00

STP Overall Chemical Mass Balance:

---

	g/h	mol/h	percent
Influent	1.00E+001	7.8E-002	100.00
Primary sludge	2.50E-002	2.0E-004	0.25
Waste sludge	1.51E-001	1.2E-003	1.51
Primary volatilization	5.94E-012	4.6E-014	0.00
Settling volatilization	1.62E-011	1.3E-013	0.00
Aeration off gas	3.99E-011	3.1E-013	0.00
Primary biodegradation	1.76E-003	1.4E-005	0.02
Settling biodegradation	5.27E-004	4.1E-006	0.01
Aeration biodegradation	6.93E-003	5.4E-005	0.07
Final water effluent	9.82E+000	7.7E-002	98.15
Total removal	1.85E-001	1.4E-003	1.85
Total biodegradation	9.22E-003	7.2E-005	0.09

Level III Fugacity Model (Full-Output):

==========

Chem Name :
Molecular Wt: 128.09
Henry's LC : 1.09e-014 atm-m3/mole (Henrywin program)
Vapor Press : 5.26e-006 mm Hg (Mpbpwin program)
Liquid VP : 8.26e-005 mm Hg (super-cooled)

Melting Pt : 146 deg C (Mpbpwin program)
Log Kow : -0.59 (Kowwin program)
Soil Koc : 0.105 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	3.57e-007	414	1000
Water	45.2	360	1000
Soil	54.7	360	1000
Sediment	0.0755	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	8.51e-018	7.55e-006	4.51e-005	2.52e-007	1.5e-006
Water	2.43e-019	1.1e+003	571	36.6	19
Soil	1.08e-017	1.33e+003	0	44.3	0
Sediment	2.02e-019	0.459	0.0191	0.0153	0.000636

Persistence Time: 421 hr
Reaction Time: 520 hr
Advection Time: 2.21e+003 hr
Percent Reacted: 81
Percent Advected: 19
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 414
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.869 (weeks)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- EPI SUMMARY (v3.11) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------

Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): -0.59
SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic Carbon	0.2940	0.5880
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	1	-COOH [acid, aromatic attach]	-0.1186	-0.1186
Frag	3	Aromatic Nitrogen [5-member ring]	-0.5262	-1.5786
Factor	1	Imidazole type -> 2-amino type correction	0.5596	0.5596
Factor	1	Additional amino-type triazole correction	0.6500	0.6500
Const		Equation Constant		0.2290

Log Kow = -0.5876

MPBPWIN (v1.41) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 357.27 deg C (Adapted Stein and Brown Method)
Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 94.95 deg C (Gold and Ogle Method)
Mean Melt Pt : 222.39 deg C (Joback; Gold,Ogle Methods)
Selected MP: 145.93 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 357.27 deg C (estimated))
(Using MP: 145.93 deg C (estimated))
VP: 2.23E-006 mm Hg (Antoine Method)
VP: 5.26E-006 mm Hg (Modified Grain Method)
VP: 1.12E-005 mm Hg (Mackay Method)

Selected VP: 5.26E-006 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-COOH (acid)	169.83	169.83
Group	2	-C (aromatic)	30.76	61.52
Group	1	-NH2 (to arom)	86.63	86.63
Group	3	N (aromatic)	39.88	119.64
Corr	1	Triazole [NH]	90.00	90.00
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 725.80
RESULT- corr | BOILING POINT in deg Kelvin | 630.43
| BOILING POINT in deg C | 357.27

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-COOH (acid)	155.50	155.50
Group	2	-C (aromatic)	37.02	74.04
Group	1	-NH2 (to arom)	66.89	66.89
Group	3	N (aromatic)	68.40	205.20
*		Equation Constant		122.50

RESULT | MELTING POINT in deg Kelvin | 624.13
RESULT-limit| MELTING POINT in deg Kelvin | 623.00
| MELTING POINT in deg C | 349.84

Water Sol from Kow (WSKOW v1.41) Results:

Water Sol: 2.97e+005 mg/L
SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : -0.59
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -0.59
Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction

(used when Melting Point NOT available)
Correction(s): Value

No Applicable Correction Factors
Log Water Solubility (in moles/L) : 0.365
Water Solubility at 25 deg C (mg/L): 2.97e+005

WATERNT Program (v1.01) Results:
==========

Water Sol (v1.01 est): 1e+006 mg/L
SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-N [aliphatic N, one aromatic attach]	1.2749	1.2749
Frag	1	-COOH [acid, aromatic attach]	0.0568	0.0568
Frag	2	Aromatic Carbon (C-substituent type)	-0.5400	-1.0799
Frag	3	Aromatic Nitrogen [5-member ring]	0.5265	1.5795
Const		Equation Constant		0.2492
NOTE		Maximum Solubility (1,000,000 mg/L) Applied!		

Log Water Sol (moles/L) at 25 dec C = 0.8925
Water Solubility (mg/L) at 25 dec C = 1e+006

ECOSAR Program (v0.99g) Results:
==========

SMILES : Nc1nc(C(=O)O)nn1
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
Log Kow: -0.59 (KowWin estimate)
Melt Pt:
Wat Sol: 2.496E+005 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Aromatic Amines-acid

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**31003.322**
--> Acid moeity found: Predicted values multiplied by 10				
Aromatic Amines-acid	**: Fish**	**96-hr**	**LC50**	**31588.445**
Aromatic Amines-acid	**: Fish**	**14-day**	**LC50**	**51337.914**
Aromatic Amines-acid	**: Daphnid**	**48-hr**	**LC50**	**44.097**
Aromatic Amines-acid	**: Fish**		**ChV**	**91.257**
Aromatic Amines-acid	**: Daphnid**		**ChV**	**1.585**
Aromatic Amines-acid	**: Green Algae**		**ChV**	**1105.193**

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 7.0
Green algal EC50 toxicity log Kow cutoff: 7.0
Chronic toxicity log Kow cutoff: 9.0
MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est : 1.09E-014 atm-m3/mole
Group Est: Incomplete
SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	1 Hydrogen to Oxygen Bonds		3.2318
HYDROGEN	2 Hydrogen to Nitrogen Bonds		2.5670
FRAGMENT	1 Car-CO		1.2387
FRAGMENT	4 Car-Nar		6.5129
FRAGMENT	1 Nar-Nar	ESTIMATE	3.0000
FRAGMENT	1 CO-O		0.0714
FRAGMENT	1 Car-N		0.7304
FACTOR	2 Additional aromatic nitrogen(s)		-5.0000

```
RESULT  |   BOND ESTIMATION METHOD for LWAPC VALUE   | TOTAL | 12.352
---------+-------------------------------------------+---------+---------
HENRYs LAW CONSTANT at 25 deg C = 1.09E-014 atm-m3/mole
                  = 4.44E-013 unitless
--------+-------------------------------------------+-----------+--------
      |     GROUP CONTRIBUTION DESCRIPTION        |  COMMENT  | VALUE
--------+-------------------------------------------+-----------+--------
      |        1  NH2 (Car)                 | ESTIMATE | 4.00
      |        1  CO (O)(Car)               |          | 4.57
      |        1  O-H (CO)                  |          | 1.45
      |        1  Nar (Car)(Car)            |          | 3.06
      |          MISSING Value for:  Car (Nar)(Nar)(N)
      |          MISSING Value for:  Car (CO)(Nar)(Nar)
      |          MISSING Value for:  Nar (Nar)(Car)
      |          MISSING Value for:  Nar (Car)(Nar)
--------+-------------------------------------------+-----------+--------
RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |
13.08
--------+-------------------------------------------+-----------+--------

Henrys LC [VP/WSol estimate using EPI values]:
  HLC:  2.985E-012 atm-m3/mole
  VP:   5.26E-006 mm Hg
  WS:   2.97E+005 mg/L

BIOWIN (v4.01) Program Results:
==============================
SMILES : Nc1nc(C(=O)O)nn1
CHEM   :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
-------------------------- BIOWIN v4.01 Results ---------------------------
  Linear Model Prediction    : Biodegrades Fast
  Non-Linear Model Prediction: Biodegrades Fast
  Ultimate Biodegradation Timeframe:  Weeks
  Primary  Biodegradation Timeframe:  Days-Weeks
  MITI Linear Model Prediction    : Biodegrades Fast
  MITI Non-Linear Model Prediction: Biodegrades Fast
------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION          | COEFF   | VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aromatic acid   [-C(=O)-OH]              | 0.1769  | 0.1769
 Frag |  1  |  Aromatic amine  [-NH2  or  -NH-]         | -0.2338 | -0.2338
```

```
MolWt| * | Molecular Weight Parameter           |       | -0.0610
Const| * | Equation Constant                   |       | 0.7475
============+=============================================+=========+=====
=======
  RESULT  |   LINEAR BIODEGRADATION PROBABILITY     |       | 0.6297
============+=============================================+=========+=====
=======
------+-----+-------------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION          | COEFF | VALUE
------+-----+-------------------------------------------+---------+---------
Frag | 1  | Aromatic acid  [-C(=O)-OH]              | 2.4224 | 2.4224
Frag | 1  | Aromatic amine  [-NH2 or -NH-]          | -1.9070 | -1.9070
MolWt| * | Molecular Weight Parameter              |       | -1.8189
============+=============================================+=========+=====
=======
  RESULT  |  NON-LINEAR BIODEGRADATION PROBABILITY  |       | 0.8462
============+=============================================+=========+=====
=======
A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast
------+-----+-------------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION          | COEFF | VALUE
------+-----+-------------------------------------------+---------+---------
Frag | 1  | Aromatic acid  [-C(=O)-OH]              | 0.0879 | 0.0879
Frag | 1  | Aromatic amine  [-NH2 or -NH-]          | -0.1349 | -0.1349
MolWt| * | Molecular Weight Parameter              |       | -0.2831
Const| * | Equation Constant                   |       | 3.1992
============+=============================================+=========+=====
======
  RESULT  |  SURVEY MODEL - ULTIMATE BIODEGRADATION  |       | 2.8690
============+=============================================+=========+=====
======
------+-----+-------------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION          | COEFF | VALUE
------+-----+-------------------------------------------+---------+---------
Frag | 1  | Aromatic acid  [-C(=O)-OH]              | 0.0077 | 0.0077
Frag | 1  | Aromatic amine  [-NH2 or -NH-]          | -0.1084 | -0.1084
MolWt| * | Molecular Weight Parameter              |       | -0.1848
Const| * | Equation Constant                   |       | 3.8477
============+=============================================+=========+=====
=======
  RESULT  |  SURVEY MODEL - PRIMARY BIODEGRADATION  |       | 3.5623
============+=============================================+=========+=====
```

```
=======
Result Classification:  5.00 -> hours    4.00 -> days    3.00 -> weeks
 (Primary & Ultimate)   2.00 -> months   1.00 -> longer
------+-----+-----------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag |  1  | Aromatic acid   [-C(=O)-OH]             | 0.3770 |  0.3770
Frag |  1  | Aromatic amine  [-NH2 or -NH-]          |-0.1577 | -0.1577
MolWt|  *  | Molecular Weight Parameter              |        | -0.3811
Const|  *  | Equation Constant                       |        |  0.7121
============+=========================================+========+=========+===
=======
  RESULT   | MITI LINEAR BIODEGRADATION PROBABILITY   |        |  0.5503
============+=========================================+========+=========+===
=======
------+-----+-----------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag |  1  | Aromatic acid   [-C(=O)-OH]             | 2.4449 |  2.4449
Frag |  1  | Aromatic amine  [-NH2 or -NH-]          |-1.2264 | -1.2264
MolWt|  *  | Molecular Weight Parameter              |        | -3.6978
============+=========================================+========+=========+===
=======
  RESULT   |MITI NON-LINEAR BIODEGRADATION PROBABILITY |        |  0.5116
============+=========================================+========+=========+===
=======
 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:
============================
SMILES : Nc1nc(C(=O)O)nn1
CHEM   :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction      =  0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  0.5200 E-12 cm3/molecule-sec
Addition to Triple Bonds  =  0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =  0.1000 E-12 cm3/molecule-sec
Addition to Fused Rings   =  0.0000 E-12 cm3/molecule-sec
  OVERALL OH Rate Constant =  0.6200 E-12 cm3/molecule-sec
```

HALF-LIFE = 17.252 Days (12-hr day; 1.5E6 OH/cm3)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========

Koc (estimated): 2.13
Koc may be sensitive to pH!
SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 4.198
Non-Corrected Log Koc ..... : 2.8559
Fragment Correction(s):
* Nitrogen to non-fused aromatic ring ... : -0.7770
* Organic Acid (-CO-OH) ..... : -1.7512
Corrected Log Koc ..... : 0.3277
Estimated Koc: 2.127
NOTE:
The Koc of this structure may be sensitive to pH! The estimated
Koc represents a best-fit to the majority of experimental values;
however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========
SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)
and Specific Alkyl Halides can be estimated!! For more information,
(Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:
==========

SMILES : Nc1nc(C(=O)O)nn1
CHEM :
MOL FOR: C3 H4 N4 O2
MOL WT : 128.09
---------- Bcfwin v2.15 ----------
Log Kow (estimated) : -0.59
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: -0.59
Equation Used to Make BCF estimate:
Log BCF = 0.50 (Ionic; Log Kow dependent)

Estimated Log BCF = 0.500 (BCF = 3.162)

Volatization From Water
==========

Chemical Name:
Molecular Weight : 128.09 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 1.09E-014 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	6.079E+010	6.632E+011
HALF-LIFE (days) :	2.533E+009	2.763E+010
HALF-LIFE (years) :	6.935E+006	7.565E+007

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========

PROPERTIES OF:

Molecular weight (g/mol)	128.09
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	1.09E-014
Air-water partition coefficient	4.45778E-013
Octanol-water partition coefficient (Kow)	0.25704
Log Kow	-0.59
Biomass to water partition coefficient	0.851408

Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 0.04 17.00 10000.00
-Aeration tank 0.04 17.00 10000.00
-Settling tank 0.04 17.00 10000.00
STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	7.8E-002	100.00
Primary sludge	2.50E-002	2.0E-004	0.25
Waste sludge	1.51E-001	1.2E-003	1.51
Primary volatilization	5.94E-012	4.6E-014	0.00
Settling volatilization	1.62E-011	1.3E-013	0.00
Aeration off gas	3.99E-011	3.1E-013	0.00
Primary biodegradation	1.76E-003	1.4E-005	0.02
Settling biodegradation	5.27E-004	4.1E-006	0.01
Aeration biodegradation	6.93E-003	5.4E-005	0.07
Final water effluent	9.82E+000	7.7E-002	98.15
Total removal	1.85E-001	1.4E-003	1.85
Total biodegradation	9.22E-003	7.2E-005	0.09

Level III Fugacity Model (Full-Output):

Chem Name :
Molecular Wt: 128.09
Henry's LC : 1.09e-014 atm-m3/mole (Henrywin program)
Vapor Press : 5.26e-006 mm Hg (Mpbpwin program)
Liquid VP : 8.26e-005 mm Hg (super-cooled)
Melting Pt : 146 deg C (Mpbpwin program)
Log Kow : -0.59 (Kowwin program)
Soil Koc : 0.105 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	3.57e-007	414	1000
Water	45.2	360	1000
Soil	54.7	360	1000
Sediment	0.0755	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)

Air 8.51e-018 7.55e-006 4.51e-005 2.52e-007 1.5e-006
Water 2.43e-019 1.1e+003 571 36.6 19
Soil 1.08e-017 1.33e+003 0 44.3 0
Sediment 2.02e-019 0.459 0.0191 0.0153 0.000636
Persistence Time: 421 hr
Reaction Time: 520 hr
Advection Time: 2.21e+003 hr
Percent Reacted: 81
Percent Advected: 19
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 414
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.869 (weeks)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

---

di-FESA (minor degradate, 8% maximum)

SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
CHEM :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16
---------- EPI SUMMARY (v3.11) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 2.37
SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
CHEM :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	2	-F [fluorine, aliphatic attach]	-0.0031	-0.0062
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	1	-OH [hydroxy, aromatic attach]	-0.4802	-0.4802
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	1	-COOH [acid, aromatic attach]	-0.1186	-0.1186
Factor	1	Ortho reaction -> hydroxy/acid correc	1.1930	1.1930
Factor	1	Ring reaction -> ortho to aromatic acid	-0.3425	-0.3425
Factor	1	Ring reaction -> alkyloxy ortho to -OH	-0.2560	-0.2560
Const		Equation Constant		0.2290

Log Kow = 2.3686

MPBPWIN (v1.41) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1

CHEM :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 333.86 deg C (Adapted Stein and Brown Method)
Melting Point: 237.70 deg C (Adapted Joback Method)
Melting Point: 81.28 deg C (Gold and Ogle Method)
Mean Melt Pt : 159.49 deg C (Joback; Gold,Ogle Methods)
Selected MP: 120.39 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 333.86 deg C (estimated))
(Using MP: 120.39 deg C (estimated))
VP: 5.56E-006 mm Hg (Antoine Method)
VP: 1.03E-005 mm Hg (Modified Grain Method)
VP: 7.06E-005 mm Hg (Mackay Method)
Selected VP: 1.03E-005 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH2-	24.22	24.22
Group	1	>CH-	11.86	11.86
Group	2	-F	0.13	0.26
Group	1	-OH (phenol)	70.48	70.48
Group	1	-O- (nonring)	25.16	25.16
Group	1	-COOH (acid)	169.83	169.83
Group	3	CH (aromatic)	28.53	85.59
Group	3	-C (aromatic)	30.76	92.28
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 677.86
RESULT- corr | BOILING POINT in deg Kelvin | 607.02
| BOILING POINT in deg C | 333.86

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH2-	11.27	11.27
Group	1	>CH-	12.64	12.64
Group	2	-F	-15.78	-31.56
Group	1	-OH (phenol)	82.83	82.83
Group	1	-O- (nonring)	22.23	22.23

```
Group | 1 | -COOH (acid)      | 155.50 | 155.50
Group | 3 | CH (aromatic)     |  8.13 |  24.39
Group | 3 | -C (aromatic)     | 37.02 | 111.06
  *   |   | Equation Constant |       | 122.50
======================================================================
  RESULT   | MELTING POINT in deg Kelvin | 510.86
           | MELTING POINT in deg C      | 237.70
----------------------------------------------------
```

Water Sol from Kow (WSKOW v1.41) Results:

```
==========================================
        Water Sol: 334 mg/L
SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
CHEM   :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16
---------------------------------- WSKOW v1.41 Results -----------------------
Log Kow  (estimated)  :  2.37
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  2.37
Equation Used to Make Water Sol estimate:
  Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
    (used when Melting Point NOT available)
    Correction(s):       Value
    -------------------  -----
    Acid, aromatic       0.000
  Log Water Solubility  (in moles/L) :  -2.815
  Water Solubility at 25 deg C (mg/L):  334
```

WATERNT Program (v1.01) Results:

```
==================================
            Water Sol (v1.01 est): 235.09 mg/L
SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
CHEM   :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16
-------+-----+-------------------------------------------+----------+---------
 TYPE  |NUM|   WATER SOLUBILITY FRAGMENT DESCRIPTION      | COEFF    | VALUE
-------+-----+-------------------------------------------+----------+---------
 Frag  | 1   | -CH2-  [aliphatic carbon]                  |-0.5370   | -0.5370
 Frag  | 1   | -CH    [aliphatic carbon]                  |-0.5285   | -0.5285
 Frag  | 2   | -F     [fluorine, aliphatic attach]        |-0.1580   | -0.3160
 Frag  | 3   | Aromatic Carbon  (C-H type)                |-0.3359   | -1.0076
```

Frag	1	-OH [hydroxy, aromatic attach]	1.6578	1.6578
Frag	1	-O- [oxygen, one aromatic attach]	0.1980	0.1980
Frag	1	-COOH [acid, aromatic attach]	0.0568	0.0568
Frag	3	Aromatic Carbon (C-substituent type)	-0.5400	-1.6199
Factor	1	Ring reaction -> ortho to aromatic acid	0.6563	0.6563
Factor	1	Ring ortho reaction -> -OH / -COOH	-1.7766	-1.7766
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -2.9675
Water Solubility (mg/L) at 25 dec C = 235.09

ECOSAR Program (v0.99g) Results:

SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16
Log Kow: 2.37 (KowWin estimate)
Melt Pt:
Wat Sol: 406.8 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Phenols-acid
Salicylic Acid-acid

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**139.477**
--> Acid moeity found: Predicted values multiplied by 10				
Phenols-acid	**: Fish**	**96-hr**	**LC50**	**189.606**
Phenols-acid	**: Daphnid**	**48-hr**	**LC50**	**82.878**
Phenols-acid	**: Green Algae**	**96-hr**	**EC50**	**509.708 ***
Phenols-acid	**: Fish**	**30-day**	**ChV**	**28.610**
Phenols-acid	**: Fish**	**90-day**	**ChV**	**1.780**
Phenols-acid	**: Daphnid**	**21-day**	**ChV**	**20.445**
Phenols-acid	**: Green Algae**	**96-hr**	**ChV**	**63.124**

Note: * = asterick designates: Chemical may not be soluble
enough to measure this predicted effect.
Phenols:
Fish and daphnid acute toxicity log Kow cutoff: 7.0
Green algal EC50 toxicity log Kow cutoff: 7.0
Chronic toxicity log Kow cutoff: 9.0
MW cutoff: 1000
Salicylic Acid:
Fish and daphnid acute toxicity log Kow cutoff: none
Green algal EC50 toxicity log Kow cutoff: none
Chronic toxicity log Kow cutoff: none
MW cutoff: none

HENRY (v3.10) Program Results:
==========

Bond Est : 4.42E-009 atm-m3/mole
Group Est: 2.94E-013 atm-m3/mole
SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
CHEM :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	3 Hydrogen to Carbon (aliphatic) Bonds		-0.3590
HYDROGEN	3 Hydrogen to Carbon (aromatic) Bonds		-0.4629
HYDROGEN	2 Hydrogen to Oxygen Bonds		6.4635
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-O		1.0855
FRAGMENT	2 C-F		-0.8369
FRAGMENT	6 Car-Car		1.5828
FRAGMENT	1 Car-OH		0.5967
FRAGMENT	1 Car-CO		1.2387
FRAGMENT	1 CO-O		0.0714
FRAGMENT	1 Car-O		0.3473
FACTOR	1 ortho-C(=O) to -OH		-3.1000
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	6.743

HENRYs LAW CONSTANT at 25 deg C = 4.42E-009 atm-m3/mole
= 1.81E-007 unitless

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	1 CH2 (C)(O)		-0.13
	1 CH (C)(F)(F)		0.70
	3 Car-H (Car)(Car)		0.33
	2 Car (Car)(Car)(O)		-0.86
	1 Car (Car)(Car)(CO)		-0.84
	1 CO (O)(Car)		4.57
	1 O-H (Car)		4.45
	1 O-H (CO)		1.45
	1 O (C)(Car)		1.25
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	10.92

HENRYs LAW CONSTANT at 25 deg C = 2.94E-013 atm-m3/mole
= 1.20E-011 unitless

Henrys LC [VP/WSol estimate using EPI values]:
HLC: 8.852E-009 atm-m3/mole
VP: 1.03E-005 mm Hg
WS: 334 mg/L

BIOWIN (v4.01) Program Results:

SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
CHEM :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16

---------- BIOWIN v4.01 Results ----------

Linear Model Prediction : Biodegrades Fast
Non-Linear Model Prediction: Biodegrades Fast
Ultimate Biodegradation Timeframe: Weeks
Primary Biodegradation Timeframe: Days-Weeks
MITI Linear Model Prediction : Biodegrades Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.1158	0.1158
Frag	1	Aromatic acid [-C(=O)-OH]	0.1769	0.1769
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1319	0.1319
MolWt	*	Molecular Weight Parameter		-0.1039
Const	*	Equation Constant		0.7475

```
=============+=============================================+==========+===
======
  RESULT   |    LINEAR BIODEGRADATION PROBABILITY     |       | 1.0683
=============+=============================================+==========+===
======
------+-----+---------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION       | COEFF | VALUE
------+-----+---------------------------------------+---------+---------
Frag |  1  | Aromatic alcohol  [-OH]                | 0.9086 | 0.9086
Frag |  1  | Aromatic acid   [-C(=O)-OH]            | 2.4224 | 2.4224
Frag |  1  | Aromatic ether  [-O-aromatic carbon]   | 2.2483 | 2.2483
MolWt|  *  | Molecular Weight Parameter             |        | -3.0978
=============+=============================================+==========+===
======
  RESULT   |  NON-LINEAR BIODEGRADATION PROBABILITY   |       | 0.9959
=============+=============================================+==========+===
======
A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast
------+-----+---------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION       | COEFF | VALUE
------+-----+---------------------------------------+---------+---------
Frag |  1  | Aromatic alcohol  [-OH]                | 0.0564 | 0.0564
Frag |  1  | Aromatic acid   [-C(=O)-OH]            | 0.0879 | 0.0879
Frag |  1  | Aromatic ether  [-O-aromatic carbon]   |-0.0581 |-0.0581
MolWt|  *  | Molecular Weight Parameter             |        | -0.4821
Const|  *  | Equation Constant                      |        | 3.1992
=============+=============================================+==========+===
======
  RESULT   |  SURVEY MODEL - ULTIMATE BIODEGRADATION  |       | 2.8032
=============+=============================================+==========+===
======
------+-----+---------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION       | COEFF | VALUE
------+-----+---------------------------------------+---------+---------
Frag |  1  | Aromatic alcohol  [-OH]                | 0.0397 | 0.0397
Frag |  1  | Aromatic acid   [-C(=O)-OH]            | 0.0077 | 0.0077
Frag |  1  | Aromatic ether  [-O-aromatic carbon]   | 0.0771 | 0.0771
MolWt|  *  | Molecular Weight Parameter             |        | -0.3147
Const|  *  | Equation Constant                      |        | 3.8477
=============+=============================================+==========+===
======
  RESULT   |  SURVEY MODEL - PRIMARY BIODEGRADATION   |       | 3.6575
```

```
=============+=========================================+=========+===
======
Result Classification:  5.00 -> hours    4.00 -> days   3.00 -> weeks
 (Primary & Ultimate)   2.00 -> months   1.00 -> longer
------+-----+-----------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag |  1  | Aromatic alcohol  [-OH]                 | 0.0642 | 0.0642
Frag |  1  | Aromatic acid  [-C(=O)-OH]              | 0.3770 | 0.3770
Frag |  1  | Aromatic ether  [-O-aromatic carbon]    | 0.1952 | 0.1952
Frag |  2  | Fluorine  [-F]                          | 0.0174 | 0.0348
Frag |  3  | Aromatic-H                              | 0.0082 | 0.0247
Frag |  1  | -CH2-  [linear]                         | 0.0494 | 0.0494
Frag |  1  | -CH-  [linear]                          |-0.0507 |-0.0507
MolWt|  *  | Molecular Weight Parameter              |        |-0.6490
Const|  *  | Equation Constant                       |        | 0.7121
=============+=========================================+=========+===
======
  RESULT   | MITI LINEAR BIODEGRADATION PROBABILITY   |        | 0.7577
=============+=========================================+=========+===
======
------+-----+-----------------------------------------+---------+---------
TYPE | NUM |      BIOWIN FRAGMENT DESCRIPTION        | COEFF | VALUE
------+-----+-----------------------------------------+---------+---------
Frag |  1  | Aromatic alcohol  [-OH]                 | 0.4884 | 0.4884
Frag |  1  | Aromatic acid  [-C(=O)-OH]              | 2.4449 | 2.4449
Frag |  1  | Aromatic ether  [-O-aromatic carbon]    | 1.3227 | 1.3227
Frag |  2  | Fluorine  [-F]                          |-3.9878 |-7.9757
Frag |  3  | Aromatic-H                              | 0.1201 | 0.3604
Frag |  1  | -CH2-  [linear]                         | 0.4295 | 0.4295
Frag |  1  | -CH-  [linear]                          |-0.0998 |-0.0998
MolWt|  *  | Molecular Weight Parameter              |        |-6.2980
=============+=========================================+=========+===
======
  RESULT   | MITI NON-LINEAR BIODEGRADATION PROBABILITY |        | 0.0011
=============+=========================================+=========+===
======
A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:
============================
SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
```

CHEM :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16
---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.8007 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.6600 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 10.6743 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 12.1350 E-12 cm3/molecule-sec
HALF-LIFE = 0.881 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 10.577 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
NOTE: Reaction with Nitrate Radicals May Be Important!
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========

Koc (estimated): 91.6
Koc may be sensitive to pH!
SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
CHEM :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 7.020
Non-Corrected Log Koc ..... : 4.3560
Fragment Correction(s):
1 Ether, aromatic (-C-O-C-) ..... : -0.6431
* Organic Acid (-CO-OH) ..... : -1.7512
Corrected Log Koc ..... : 1.9617
Estimated Koc: 91.56
NOTE:
The Koc of this structure may be sensitive to pH! The estimated
Koc represents a best-fit to the majority of experimental values;
however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:
==========

SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
CHEM :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16
---------- HYDROWIN v1.67 Results ----------
Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens)
and Specific Alkyl Halides can be estimated!! For more information,
(Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:
==========

SMILES : FC(F)COc1c(O)c(C(=O)O)ccc1
CHEM :
MOL FOR: C9 H8 F2 O4
MOL WT : 218.16
---------- Bcfwin v2.15 ----------
Log Kow (estimated) : 2.37
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 2.37
Equation Used to Make BCF estimate:
Log BCF = 0.50 (Ionic; Log Kow dependent)

Estimated Log BCF = 0.500 (BCF = 3.162)

Volatization From Water
==========

Chemical Name:
Molecular Weight : 218.16 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 4.42E-009 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	1.957E+005	2.135E+006
HALF-LIFE (days) :	8152	8.894E+004
HALF-LIFE (years) :	22.32	243.5

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

Molecular weight (g/mol)	218.16
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	4.42E-009
Air-water partition coefficient	1.80765E-007
Octanol-water partition coefficient (Kow)	234.423
Log Kow	2.37
Biomass to water partition coefficient	47.6846
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	870.66	10000.00
-Aeration tank	0.00	870.66	10000.00
-Settling tank	0.00	870.66	10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	4.6E-002	100.00
Primary sludge	8.04E-002	3.7E-004	0.80
Waste sludge	1.87E-001	8.6E-004	1.87
Primary volatilization	2.39E-006	1.1E-008	0.00
Settling volatilization	6.50E-006	3.0E-008	0.00
Aeration off gas	1.60E-005	7.3E-008	0.00
Primary biodegradation	1.90E-003	8.7E-006	0.02
Settling biodegradation	5.70E-004	2.6E-006	0.01
Aeration biodegradation	7.51E-003	3.4E-005	0.08
Final water effluent	9.72E+000	4.5E-002	97.22
Total removal	2.78E-001	1.3E-003	2.78
Total biodegradation	9.98E-003	4.6E-005	0.10

Level III Fugacity Model (Full-Output):

Chem Name :
Molecular Wt: 218.16

Henry's LC : 4.42e-009 atm-m3/mole (Henrywin program)
Vapor Press : 1.03e-005 mm Hg (Mpbpwin program)
Liquid VP : 9.04e-005 mm Hg (super-cooled)
Melting Pt : 120 deg C (Mpbpwin program)
Log Kow : 2.37 (Kowwin program)
Soil Koc : 96.1 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.128	21.2	1000
Water	30.7	360	1000
Soil	69.1	360	1000
Sediment	0.138	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.87e-012	55.1	16.8	1.84	0.561
Water	4.08e-014	776	403	25.9	13.4
Soil	3.92e-013	1.75e+003	0	58.3	0
Sediment	2.78e-014	0.873	0.0363	0.0291	0.00121

Persistence Time: 438 hr
Reaction Time: 510 hr
Advection Time: 3.13e+003 hr
Percent Reacted: 86
Percent Advected: 14
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 21.15
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.803 (weeks)
Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

BST (minor degradate, 6% maximum)

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM :
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27
---------- EPI SUMMARY (v3.11) ----------
Physical Property Inputs:
Water Solubility (mg/L): ------
Vapor Pressure (mm Hg) : ------
Henry LC (atm-m3/mole) : ------
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 1.22
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM :
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	1	C [aliphatic carbon - No H, not tert]	0.9723	0.9723
Frag	5	-F [fluorine, aliphatic attach]	-0.0031	-0.0155
Frag	8	Aromatic Carbon	0.2940	2.3520
Frag	1	-N [aliphatic N, one aromatic attach]	-0.9170	-0.9170
Frag	1	-O- [oxygen, one aromatic attach]	-0.4664	-0.4664
Frag	1	-SO2-N [aromatic attach]	-0.2079	-0.2079
Frag	3	Aromatic Nitrogen [5-member ring]	-0.5262	-1.5786
Const		Equation Constant		0.2290

Log Kow = 1.2204

MPBPWIN (v1.41) Program Results:
==========

Experimental Database Structure Match: no data

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM :

MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27
---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 454.26 deg C (Adapted Stein and Brown Method)
Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 151.58 deg C (Gold and Ogle Method)
Mean Melt Pt : 250.71 deg C (Joback; Gold,Ogle Methods)
Selected MP: 191.23 deg C (Weighted Value)
Vapor Pressure Estimations (25 deg C):
(Using BP: 454.26 deg C (estimated))
(Using MP: 191.23 deg C (estimated))
VP: 4.29E-010 mm Hg (Antoine Method)
VP: 6.96E-009 mm Hg (Modified Grain Method)
VP: 1.84E-008 mm Hg (Mackay Method)
Selected VP: 6.96E-009 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH2-	24.22	24.22
Group	1	>CH-	11.86	11.86
Group	1	>C<	4.50	4.50
Group	5	-F	0.13	0.65
Group	1	-O- (nonring)	25.16	25.16
Group	1	>NH (nonring)	45.28	45.28
Group	4	CH (aromatic)	28.53	114.12
Group	4	-C (aromatic)	30.76	123.04
Group	3	N (aromatic)	39.88	119.64
Group	1	>S(=O)(=O)	171.58	171.58
Corr	1	Triazole [NH]	90.00	90.00
*		Equation Constant		198.18

RESULT-uncorr| BOILING POINT in deg Kelvin | 928.23
RESULT- corr | BOILING POINT in deg Kelvin | 727.42
| BOILING POINT in deg C | 454.26

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH2-	11.27	11.27
Group	1	>CH-	12.64	12.64
Group	1	>C<	46.43	46.43

```
Group | 5 | -F              | -15.78 | -78.90
Group | 1 | -O- (nonring)   |  22.23 |  22.23
Group | 1 | >NH (nonring)   |  52.66 |  52.66
Group | 4 | CH (aromatic)   |   8.13 |  32.52
Group | 4 | -C (aromatic)   |  37.02 | 148.08
Group | 3 | N (aromatic)    |  68.40 | 205.20
Group | 1 | >S(=O)(=O)      | 150.00 | 150.00
  *   |   | Equation Constant |      | 122.50
------------+--------------------+--------+--------
  RESULT    | MELTING POINT in deg Kelvin | 724.63
RESULT-limit| MELTING POINT in deg Kelvin | 623.00
            | MELTING POINT in deg C      | 349.84
---------------------------------------------------

Water Sol from Kow (WSKOW v1.41) Results:
=========================================

        Water Sol: 411.6 mg/L
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM   :
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27
---------------------------------- WSKOW v1.41 Results ----------------------
Log Kow  (estimated)  :  1.22
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  1.22
Equation Used to Make Water Sol estimate:
  Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
    (used when Melting Point NOT available)
    Correction(s):        Value
    --------------------  -----
     No Applicable Correction Factors
  Log Water Solubility  (in moles/L) :  -2.956
  Water Solubility at 25 deg C (mg/L):  411.6

WATERNT Program (v1.01) Results:
================================

            Water Sol (v1.01 est): 18.266 mg/L
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM   :
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27
-------+-----+-----------------------------------------+----------+---------
 TYPE  | NUM |   WATER SOLUBILITY FRAGMENT DESCRIPTION  | COEFF    | VALUE
```

Frag	1	-CH2- [aliphatic carbon]	-0.5370	-0.5370
Frag	1	-CH [aliphatic carbon]	-0.5285	-0.5285
Frag	1	C [aliphatic carbon - No H, not tert]	-1.0516	-1.0516
Frag	5	-F [fluorine, aliphatic attach]	-0.1580	-0.7900
Frag	4	Aromatic Carbon (C-H type)	-0.3359	-1.3435
Frag	1	-N [aliphatic N, one aromatic attach]	1.2749	1.2749
Frag	1	-O- [oxygen, one aromatic attach]	0.1980	0.1980
Frag	4	Aromatic Carbon (C-substituent type)	-0.5400	-2.1598
Frag	1	-SO2-N [aromatic attach]	-1.2003	-1.2003
Frag	3	Aromatic Nitrogen [5-member ring]	0.5265	1.5795
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -4.3092
Water Solubility (mg/L) at 25 dec C = 18.266

ECOSAR Program (v0.99g) Results:

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27
Log Kow: 1.22 (KowWin estimate)
Melt Pt:
Wat Sol: 1.034E+004 mg/L (calculated)
ECOSAR v0.99g Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	**: Fish**	**14-day**	**LC50**	**2389.127**
Neutral Organics	**: Fish**	**96-hr**	**LC50**	**1492.998**
Neutral Organics	**: Fish**	**14-day**	**LC50**	**2389.127**
Neutral Organics	**: Daphnid**	**48-hr**	**LC50**	**1515.861**
Neutral Organics	**: Green Algae**	**96-hr**	**EC50**	**906.065**

Neutral Organics : Fish 30-day ChV 169.613
Neutral Organics : Daphnid 16-day EC50 55.266
Neutral Organics : Green Algae 96-hr ChV 57.727
Neutral Organics : Fish (SW) 96-hr LC50 234.563
Neutral Organics : Mysid Shrimp 96-hr LC50 751.379

mg/kg (ppm)
dry wt soil
==========

Neutral Organics : Earthworm 14-day LC50 3981.982

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

HENRY (v3.10) Program Results:
==========

Bond Est : 1.79E-010 atm-m3/mole
Group Est: Incomplete
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM :
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27

---------- HENRYWIN v3.10 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	3 Hydrogen to Carbon (aliphatic) Bonds		-0.3590
HYDROGEN	4 Hydrogen to Carbon (aromatic) Bonds		-0.6172
HYDROGEN	1 Hydrogen to Nitrogen Bonds		1.2835
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-Car		0.1619
FRAGMENT	1 C-O		1.0855
FRAGMENT	5 C-F		-2.0922
FRAGMENT	6 Car-Car		1.5828
FRAGMENT	4 Car-Nar		6.5129
FRAGMENT	1 Nar-Nar	ESTIMATE	3.0000
FRAGMENT	1 Car-S		0.6345
FRAGMENT	1 N-S	ESTIMATE	0.0000
FRAGMENT	1 Car-N		0.7304
FRAGMENT	1 Car-O		0.3473
FRAGMENT	2 O=S (sulfone-type)	ESTIMATE	2.1000

```
FACTOR  |  2  Additional aromatic nitrogen(s)      |      | -5.0000
FACTOR  |  1  -SO2-N-  group                       |      | -1.3500
---------+-----------------------------------------+--------+---------
RESULT  |   BOND ESTIMATION METHOD for LWAPC VALUE  | TOTAL  | 8.137
---------+-----------------------------------------+--------+---------
HENRYs LAW CONSTANT at 25 deg C = 1.79E-010 atm-m3/mole
                  = 7.30E-009 unitless
--------+-----------------------------------------+-----------+--------
     |     GROUP CONTRIBUTION DESCRIPTION       | COMMENT | VALUE
--------+-----------------------------------------+-----------+--------
     |       1  CH2 (C)(O)                      |         | -0.13
     |       1  CH (C)(F)(F)                    |         |  0.70
     |       3  Car-H (Car)(Car)                |         |  0.33
     |       1  Car (C)(Car)(Car)               |         |  0.70
     |       1  Car (Car)(Car)(O)               |         | -0.43
     |       1  Car (Car)(Car)(S)               |         | -0.25
     |       1  O (C)(Car)                      |         |  1.25
     |       1  Nar (Car)(Car)                  |         |  3.06
     |          MISSING Value for:  C (F)(F)(F)(Car)
     |          MISSING Value for:  S (=O)(=O)(N)(Car)
     |          MISSING Value for:  NH (Car)(S)
     |          MISSING Value for:  Car (Nar)(Nar)(N)
     |          MISSING Value for:  CarH (Nar)(Nar)
     |          MISSING Value for:  Nar (Nar)(Car)
     |          MISSING Value for:  Nar (Car)(Nar)
--------+-----------------------------------------+-----------+--------
RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | INCOMPLETE |
5.23
--------+-----------------------------------------+-----------+--------

Henrys LC [VP/WSol estimate using EPI values]:
  HLC:  8.283E-012 atm-m3/mole
  VP:   6.96E-009 mm Hg
  WS:   412 mg/L

BIOWIN (v4.01) Program Results:
==============================

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM   :
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27
------------------------- BIOWIN v4.01 Results --------------------------
  Linear Model Prediction    :  Does Not Biodegrade Fast
```

Non-Linear Model Prediction: Does Not Biodegrade Fast
Ultimate Biodegradation Timeframe: Months
Primary Biodegradation Timeframe: Weeks
MITI Linear Model Prediction : Does Not Biodegrade Fast
MITI Non-Linear Model Prediction: Does Not Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1319	0.1319
Frag	1	Trifluoromethyl group [-CF3]	-0.5204	-0.5204
MolWt	*	Molecular Weight Parameter		-0.1772
Const	*	Equation Constant		0.7475
RESULT		LINEAR BIODEGRADATION PROBABILITY		0.1818

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	2.2483	2.2483
Frag	1	Trifluoromethyl group [-CF3]	-5.6696	-5.6696
MolWt	*	Molecular Weight Parameter		-5.2862
RESULT		NON-LINEAR BIODEGRADATION PROBABILITY		0.0033

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.0581
Frag	1	Trifluoromethyl group [-CF3]	-0.5130	-0.5130
MolWt	*	Molecular Weight Parameter		-0.8227
Const	*	Equation Constant		3.1992
RESULT		SURVEY MODEL - ULTIMATE BIODEGRADATION		1.8054

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	0.0771	0.0771
Frag	1	Trifluoromethyl group [-CF3]	-0.2744	-0.2744
MolWt	*	Molecular Weight Parameter		-0.5371
Const	*	Equation Constant		3.8477

RESULT	SURVEY MODEL - PRIMARY BIODEGRADATION		3.1134

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1952	0.1952
Frag	5	Fluorine [-F]	0.0174	0.0869
Frag	4	Aromatic-H	0.0082	0.0329
Frag	1	-CH2- [linear]	0.0494	0.0494
Frag	1	-CH- [linear]	-0.0507	-0.0507
MolWt	*	Molecular Weight Parameter		-1.1075
Const	*	Equation Constant		0.7121

RESULT	MITI LINEAR BIODEGRADATION PROBABILITY		-0.0816

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic ether [-O-aromatic carbon]	1.3227	1.3227
Frag	5	Fluorine [-F]	-3.9878	-19.9392
Frag	4	Aromatic-H	0.1201	0.4806
Frag	1	-CH2- [linear]	0.4295	0.4295
Frag	1	-CH- [linear]	-0.0998	-0.0998
MolWt	*	Molecular Weight Parameter		-10.7470

RESULT	MITI NON-LINEAR BIODEGRADATION PROBABILITY		0.0000

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable

A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:
==========
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM :
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27
---------- SUMMARY (AOP v1.91): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.8007 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 2.8835 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec
OVERALL OH Rate Constant = 3.6841 E-12 cm3/molecule-sec
HALF-LIFE = 2.903 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 34.839 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION ----------
****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches

PCKOC Program (v1.66) Results:
==========
Koc (estimated): 1.62e+004
Koc may be sensitive to pH!
SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM :
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27
---------- PCKOCWIN v1.66 Results ----------
First Order Molecular Connectivity Index ..... : 11.110
Non-Corrected Log Koc ..... : 6.5308
Fragment Correction(s):
* Nitrogen to non-fused aromatic ring ... : -0.7770
1 Ether, aromatic (-C-O-C-) ..... : -0.6431
1 Miscellaneous S(=O) group ..... : -0.9000
Corrected Log Koc ..... : 4.2107
Estimated Koc: 1.624e+004
NOTE:

The Koc of this structure may be sensitive to pH! The estimated Koc represents a best-fit to the majority of experimental values; however, the Koc may vary significantly with pH.

HYDROWIN Program (v1.67) Results:

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM :
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27

---------- HYDROWIN v1.67 Results ----------

Currently, this program can NOT estimate a hydrolysis rate constant for the type of chemical structure entered!!
ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!! For more information, (Click OVERVIEW in Help or see the User's Guide)
***** CALCULATION NOT PERFORMED *****

BCF Program (v2.15) Results:

SMILES : FC(F)COc1cccc(C(F)(F)F)c1S(=O)(=O)Nc2ncnn2
CHEM :
MOL FOR: C11 H9 F5 N4 O3 S1
MOL WT : 372.27

---------- Bcfwin v2.15 ----------

Log Kow (estimated) : 1.22
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 1.22
Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction
Correction(s): Value
No Applicable Correction Factors
Estimated Log BCF = 0.240 (BCF = 1.737)

Volatization From Water

Chemical Name:
Molecular Weight : 372.27 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 1.79E-010 atm-m3/mole (estimated by Bond SAR Method)

RIVER	LAKE

Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	6.311E+006	6.885E+007
HALF-LIFE (days) :	2.63E+005	2.869E+006
HALF-LIFE (years) :	719.9	7854

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

Molecular weight (g/mol)	372.27
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	1.79E-010
Air-water partition coefficient	7.32057E-009
Octanol-water partition coefficient (Kow)	16.5959
Log Kow	1.22
Biomass to water partition coefficient	4.11917
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.01	81.71	10000.00
-Aeration tank	0.01	81.71	10000.00
-Settling tank	0.01	81.71	10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	2.7E-002	100.00
Primary sludge	2.89E-002	7.8E-005	0.29
Waste sludge	1.53E-001	4.1E-004	1.53
Primary volatilization	9.75E-008	2.6E-010	0.00
Settling volatilization	2.66E-007	7.1E-010	0.00
Aeration off gas	6.55E-007	1.8E-009	0.00
Primary biodegradation	1.77E-003	4.8E-006	0.02
Settling biodegradation	5.30E-004	1.4E-006	0.01
Aeration biodegradation	6.97E-003	1.9E-005	0.07
Final water effluent	9.81E+000	2.6E-002	98.09

Appendix B - Aquatic Environmental Effects Concentrations (EECs)

Applying the method outlined in the current EFED interim policy for calculating estimated environmental concentrations (EECs) and estimated drinking water concentrations (EDWC) resulting from the use of pesticides on rice crops produced an ***upper bound screening estimation***, using the lowest K_d value (0.13) for a non-sand soil, of ***45 ppb*** (ug/L) ***in paddy waters***. This estimated EEC should be used for both acute and chronic EECs, as well as for both aquatic ecological risk assessments and for drinking water exposure (EDWCs) in human health risk assessments. A value of 43 ppb (ug/L) was calculated from the average K_d value for non-sand, non-volcanic soils/sediments, excluding Canadian soils which are not typical of rice growing regions.

Modeling aquatic concentrations using the standard Tier 1 model, SCI-GROW, estimated parent-only ***ground water concentrations of 0.67 ppb*** (ug/L). Even so, EFED does not regard ground water contamination from a pesticide applied to rice to be a significant route of dissipation.

Method for Estimating Aquatic Concentrations

EFED does not currently have an approved model for estimating aqueous concentrations resulting from pesticides use on rice crops. An interim policy has been issued by EFED Division Director, Steven Bradbury on October 29, 2002, outlining a method to estimate screening level concentrations in water in order to support regulatory decisions for pesticides used in rice agriculture that require ecological and human health risk assessments. The guidance document can be located on the f-drive of the LAN at F:\USER\SHARE\Policies, Guidance, and Formats\EFED Policies\Final Policies\Rice Policy Memo.

The policy establishes a method for calculating estimated environmental concentrations (EECs) and estimated drinking water concentrations (EDWC) for the use of pesticides in rice paddies until a more complete rice modeling method becomes available. EECs/EDWCs are estimated by applying the total annual application to the paddy[1] and partitioning the pesticide between the water and the paddy sediment according to a linear or K_d partitioning model. The EEC/EDWC ($\mu g.\ L^{-1}$) represents the dissolved concentration occurring in the water column and the concentration in water released from the paddy. Movement of pesticide on suspended sediment is not considered. The equation (**EQ B1**) to use for this calculation is:

$$EEC = \frac{10^9 M_T}{V_T + m_{sed} K_d} \qquad \textbf{(EQ B1)}$$

[1]Since penoxsulam is a single application pesticide, the maximum single application is the annual application rate.

where M_T is the total mass of pesticide in kg applied per ha of paddy, V_T is 1.067 x10^6 L ha^{-1} which is the volume of water in a paddy 4 inches (10.16 cm) deep, and includes the pore space in a 1 cm sediment interaction zone. The mass of sediment, m_{sed}, is the amount found in the top 1 cm interaction zone and is 130,000 kg ha^{-1} when the sediment bulk density was assumed to be 1.3 kg L^{-1}, a standard assumption for the bulk density of surface horizons of mineral soils (Brady, 1984; Hillel, 1982). The 10^9 constant converts the units of mass from kg to µg. For chemicals that have a valid K_{oc}, the K_d can be calculated using a sediment carbon content of 2% (K_{oc}*0.02). An organic carbon content of 2% represents a typical value for a high clay soil that might be used to grow rice in the Mississippi Valley or gulf coast regions. Both K_d and K_{oc} should be estimated according to the methods recommended for other surface water models in EFED's Input Parameter Guidance (USEPA, 2002).

The estimated EEC/EDWC value should be used for both acute and chronic EECs as well as for aquatic ecological risk assessments and for drinking water exposure (EDWCs) in human health risk assessments. EECs/EDWCs calculated by this method are screening estimates, and as such are expected to exceed the true values found in the environment the great majority of the time. Based on preliminary assessment of rice monitoring data, predicted pesticide concentrations as derived above (assuming a 1 cm sediment interaction zone) exceed the observed peak pesticide concentrations. These EECs/EDWCs are expected to exceed the concentrations measured in the paddy, because degradation processes and dilution with uncontaminated water outside the paddy is not considered.

While this approach is extremely conservative for estimating chronic environmental concentrations for quickly degrading compounds with short half lives, it also helps prevent underestimation in cases where little is known about major degradates and when labels do not contain explicit holding times for treated paddy water. It also provides some margin of safety in acute exposure assessments to reflect the paucity of information relating to the amount of paddy water that could reasonably be expected to impact any given acre of adjoining semi-aquatic areas[2]. It is less conservative than the approach taken to modeling aquatic pesticides where there is direct application to waterways.

It is worth emphasizing that the result of this calculation does not represent a concentration that we would expect to find in drinking water, as it represents paddy discharge water. Rather, it represents an upper bound on the drinking water concentrations, and is therefore suitable for use in screening assessments. The concentrations found at drinking water facilities impacted by rice culture would be expected to be less than this value (in some cases much less) because of the aforementioned degradation processes, dilution by water from areas in the basin not in rice culture, and the fact that in most cases less than 100% of the rice paddies in a specific area will be treated with the pesticide.

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[2]This lack of information is in marked contrast to the conventional PRZM/EXAMS scenarios where one or ten acres of runoff are projected to impinge upon a one acre pond.

When the level of concern in a risk assessment is not exceeded using an EEC/EDWC calculated by this screening method, there is high confidence that there will be little or no risk above the level of concern from exposure through water resources. The size of the area and the length of time for which the estimate is reasonable depends upon how fast the pesticide degrades, the rate of removal onto uncontaminated bed sediments, the nature of the local stream network, and all other relevant environmental fate factors. However, because of the uncertainties associated with this method, when a level of concern is exceeded it cannot be determined whether the exceedance will in fact occur or whether this method has overestimated the exposure. While this method is conservative it does represent the exposure experience by aquatic organisms whose habitat lies close to the discharge from the paddies during and shortly after discharge.

The size of the area and length of time for which the estimate is reasonable depends upon how fast the pesticide degrades, the rate of removal onto uncontaminated bed sediments, and the nature of the local stream network.

Estimated Aquatic Concentrations of Penoxsulam in Rice Paddy Water

Applying the method outlined in the current EFED interim policy for calculating both estimated environmental concentrations (EEC's) and estimated drinking water concentrations (EDWCs), using the lowest K_d value for a non-sand soil, that would result from the use of pesticides on rice crops which have been outlined above, produced an upper bound screening estimation of ***45 ppb*** (ug/L) ***in paddy waters***. This estimated EEC/EDWC should be used for the estimated acute and chronic exposure concentrations, for both aquatic ecological risk assessments and for drinking water exposure in human health risk assessments. An EEC/EDWC value of 43 ppb (ug/L) was calculated from the average K_d value for non-sand, non-volcanic soils/sediments, and excluding Canadian soils which are not typical of rice growing regions.

Individual EEC/EDWC values calculated from adsorption/desorption data submitted for the individual soil/sediment systems for non-sand, non-volcanic soils/sediments appears in **Table B1** below. K_d values for submitted non-sand, non-volcanic soils/sediments are also tabulated below. EEC/EDWC values were not calculated for those excluded test systems. Mobility data submitted for three penoxsulam transformation products (including BSTCA and 5-OH-penoxsulam) indicates that the three degradates examined are of generally equivalent mobility when compared to the parent compound, penoxsulam.. Therefore, EDWCs were estimated using submitted adsorption/desorption data for the parent compound.

Table B 1. Estimated Interim Model Surface Water EECs for Penoxsulam Used on Rice Crops

Soil/Sediment Type	Soil/Sediment Source	K_d	K_{oc}	EEC in ppb
Silt loam	Arkansas	0.37	40	43.9
Silty clay sediment	Arkansas	1.4	1100	39.2
Clay loam	California	0.49	20	43.3
Loam	North Dakota	0.45	20	43.5
Sandy clay loam	Japan	0.56	40	43.0
Silty clay loam	Italy	2.0	250	37.1
Sandy loam	Italy	0.32	46	44.2
Sandy clay loam	United Kingdom	0.16	13	45.0
Silty clay loam	France	0.48	66	43.4
Sandy loam	Brazil	0.51	35	43.2
Clay loam	Brazil	0.64	14	42.6
Sandy clay loam	**Brazil**	**0.13**	**13**	**45.2**
All soils	***average Kd***	***0.92***	***average EEC***	***41.3***
All soils	***median Kd***	***0.54***	***median EEC***	***43.1***
Sand	North Carolina	0.27	76	Not calculated
Loam (volcanic)	Japan	0.59	22	Not calculated
Loam (volcanic)	Japan	4.7	310	Not calculated
Loam (volcanic)	Japan	1.6	200	Not calculated
Clay loam	Canada	1.4	73	Not calculated
Clay loam	Canada	0.67	19	Not calculated

Estimated Aquatic Ecological Effects Concentrations of Penoxsulam in Ground Water

Modeling ground water concentrations using SCI-GROW (input parameters **Table B2**) estimated ***ground water concentrations of 0.67 ug/L.*** However, rice paddies are designed and constructed to hold water. EFED does not expect subsurface transport of paddy water into ground water to be a significant route of dissipation.

Table B2. Parent-Only and Combined Residue Environmental Fate Input Parameters for SCIGROW :

Parameters	Values & Units	Sources
Application Rate (1 application)	0.044 lbs. a.i./acre/season	Product Label
Organic Carbon Partition Coefficient	13	Lowest Non-Sand K_{oc} MRID 458308-01
Parent-Only Aerobic Soil Metabolism Half-life	116 days	MRID 458307-24
Combined Residue Aerobic Soil Metabolism Half-life	410 days	Calculated from Combined Residues MRID 458307-24

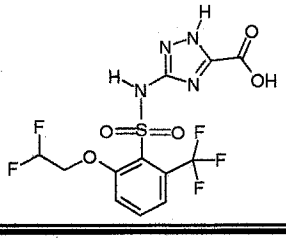
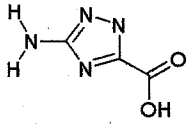
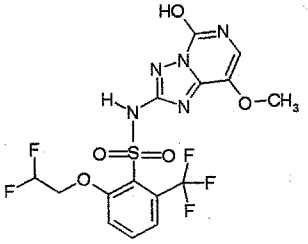
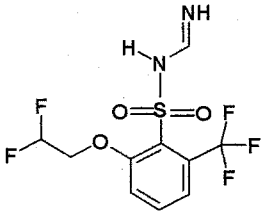
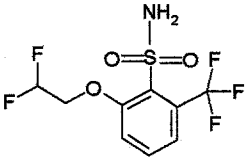
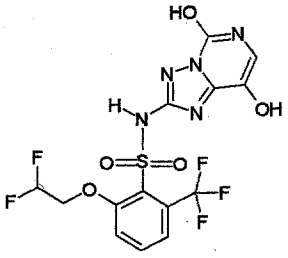
Penoxsulam Residues of Toxicological Concern in Drinking Water

On March 19, 2004, the Health Effects Division MARC determined that six penoxsulam transformation products (see **Table B6** below) should be included with the parent compound in the risk assessment for water. Data are not available to fully characterize these degradates and their respective potential degradation pathways. However, the EFED interim policy for estimating water concentrations does not consider degradation of the pesticide. ***The result of not considering degradation in the risk assessment is the same as considering all degradation products to be of toxicological concern.*** Therefore, applying current EFED policy produces an even more conservative estimate than the inclusion of these six individual degradation products.

Estimated Drinking Water Concentrations of Penoxsulam in Ground Water

Modeling screening level ***drinking water concentrations*** using SCI-GROW (input parameters **TableB 2**) produced estimated ground water concentrations of 5.9 ppb (ug/L). for the ***combined residues*** of penoxsulam and the six degradates identified by HED to be of toxicological concern. Mobility data submitted for three penoxsulam degradates indicated a mobility approximately equivalent to the parent compound, so the K_{oc} value for penoxsulam was used as the combined residue input values. However, EFED does not regard ground water contamination from a pesticide applied to rice to be a significant route of dissipation.

Table B3. Penoxsulam Residues of Human Toxicological Concern

Degradate Name	Structure	Maximum %	Study Type
BSTCA 3-[[[2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)phenyl]-sulfonyl]amino]-1H-1,2,4-triazole-5-carboxylic acid		39.4%*	aerobic aquatic metabolism
2-amino TCA 2-amino-1,2,4-triazole carboxylic acid		85%*	aqueous photolysis
5-OH-penoxsulam 2-(2,2-Difluoroethoxy) -N-(5,6-dihydro-8-methoxy-5-oxo[1,2,4] triazolo[1,5-c] pyrimidin-2-yl)-6-(trifluoromethyl) benzenesulfonamide		62.6%	aerobic soil metabolism
SFA 2-2,2-Difluoroethoxy)-N-(iminomethyl-6-(trifluoromethyl)-benzenesulfonamide		14.7%*	aerobic soil metabolism
Sulfonamide 2-(2,2-Difluoroethoxy) -6-(trifluoromethyl)-benzenesulfonamide		33.0%*	aerobic soil metabolism
5,8-diOH 2-(2,2-Difluoroethoxy) -6-trifluoromethyl-N-(5,8-dihydroxy-[1,2,4] triazolo[1,5-c] pyrimidin-2-yl) benzenesulfonamide		11.0%*	anaerobic aquatic metabolism

*Maximum % of applied reported at study termination indicating that amounts may have continued to increased with time

Estimated Holding Times Necessary to Reduce Aquatic Concentrations of Penoxsulam in Rice Paddy Water to Levels Below Ecological Effects LOCs

As a further refinement to calculating the maximum surface water ecological effects concentrations with the interim model, the modeling approach used for the refined assessment associated with the propanil RED was utilized (see Product Code 028201, Bar Code D290202[3]). With the EFED interim model, peak concentrations for paddy water before degradation are calculated by considering only dilution and sorption as factors. The refinement introduced in the propanil RED, which has not been officially approved for general use by EFED, partitions the pesticide between the paddy water and the soil, degrades the pesticide using the rate constant from the dominant mechanism for the environmental compartment, and calculates concentrations which can be useful for suggesting potential holding times of paddy water. A K_d value of 0.49, reported for soils typical of those found in rice growing regions, was used for this holding time estimation. This value was used instead of the lowest non-sand K_d value of 0.13, as recommended by EFED policy for selecting modeling input parameters. The choice of K_d values had little effect upon EECs (see **Table B1**).

The simplifying assumption of a single degradation mechanism can result in estimating concentrations which may or may not be as conservative as those from officially approved modeling methods which consider interaction between competing degradation mechanisms in connected environmental compartments. It is uncertain to what degree the simplifying assumptions made in this model may underestimate the predicted aquatic concentrations.

The dominant route of dissipation for penoxsulam in paddy water is expected to be through aqueous photolysis. Using the initial acute concentration and the 90th percent tile mean photolysis rate constant from the three submitted water only test systems produced the aqueous concentrations used for estimating the suggested potential holding times for rice crops. Including the photolysis half-life for the flooded silt loam test system in when calculating the half-life value would increase the estimated holding times.

However, the photolytic degradation rate can be reduced by environmental conditions which limit the amount of solar energy impinging upon the aquatic system. ***A more realistic approach*** would be to accept the suggestion by the Dow AgroScience in their submitted aquatic modeling assessment (MRID 458308-11) to use aquatic field dissipation rates in paddy water to estimate suggested holding times. Estimated values derived from both aqueous photolysis (**Figure B1**) and paddy water aquatic field dissipation (**Figure B2**) and total system aquatic field dissipation (**Figure B3**) rate constants are plotted below.

Estimated concentrations in soil were calculated by degradation of the initial concentrations partitioned into the paddy soil through aerobic soil metabolism. While anaerobic degradation half-lives are significantly shorter than the aerobic half-lives, anaerobic conditions are

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[3]EFED Response to Registrant Request for a Seven (7) Day Holding Period for Propanil Use in Rice Paddies; DP Barcode: D290202; PC Code: 028201; 9/11/03.

not expected to exist to any great extent in rice paddies. Persistent anaerobic conditions would damage the roots of the rice plants, jeopardizing a successful harvest.

Within the limits of the simplifying assumptions used in previous EFED assessments for rice crops, the results from the modeling approach using the aqueous photolysis rate constant, combined with the calculated RQ values for ecological risk, estimates that a holding time of approximately 13 days would be sufficient to bring the aquatic concentrations in paddy water below any level of concern identified in this science chapter.

A more ***realistic approach*** would be to modify If the simplifying assumptions adopted in this model had been modified to account for competing degradation pathways, use a conservative rather than typical estimate of partitioning, and the interactions and effects of other environmental compartments and/or factors, the suggested holding times would be greater. For example, assuming that the degradation rate in paddy water from the aquatic field dissipation would accurately account for competing degradation pathways and environmental processes, an ***estimated holding time of approximately 23 days*** would be indicated.

Further, if the total system aquatic field dissipation rate constant is used for estimating water concentrations, and combined with the calculated RQ values for ecological risk, an estimated holding time of approximately 58 days would be required to bring the aquatic concentrations in paddy water below any level of concern identified in this science chapter. Using aerobic degradation half-lives would produce even longer estimated holding times.

Figure B1: Estimated Concentrations for Paddy Water and Soil for Dry-Seeded Rice Using Photolysis Degradation Rate

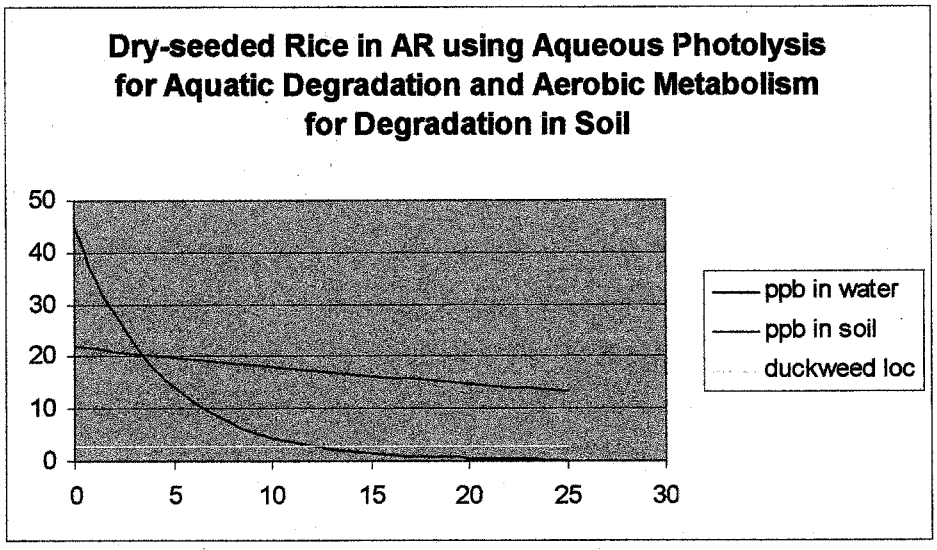

Figure B2: Estimated Concentrations for Paddy Water and Soil for Dry-Seeded Rice Using Aquatic Field Dissipation Paddy Water Degradation Rates

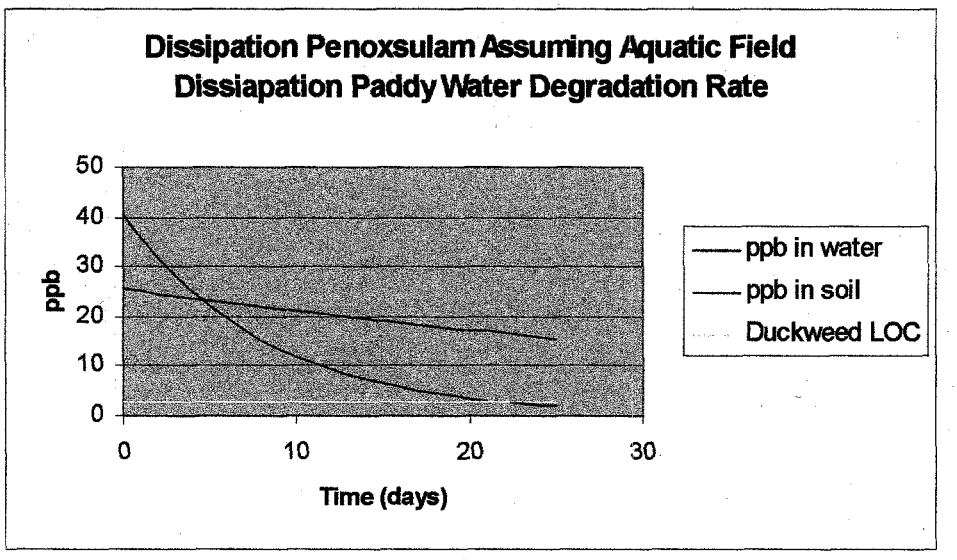

Figure B3: Estimated Concentrations for Paddy Water and Soil for Dry-Seeded Rice Using Aquatic Field Dissipation Total System Degradation Rates

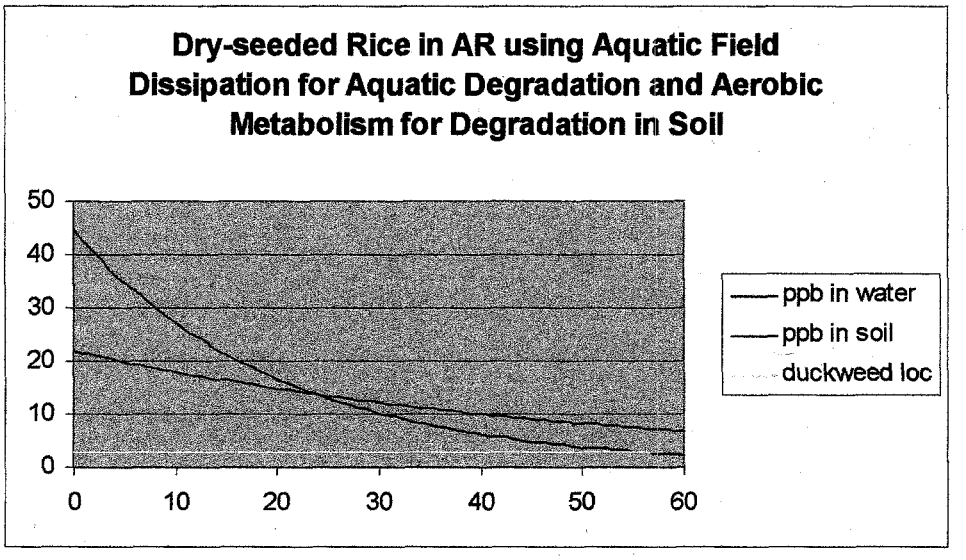

Table B 4. Environmental Fate Input Parameters for Propanil RED[4] Refinement Model:

Input Parameter	Dry Seeded Rice
Planting Date	May 30
Emergence	June 9
Application Date	June 29
Date of Flooding	July 10
Days of Aerobic Soil Metabolism Degradation Before Flooding	11
Aerobic Soil Metabolism Half-life (days)	66.9
Application Rate (lb a.i./acre)	0.05
Soil Bulk Density	1.31
Kd	0.49
Aqueous Photolysis Half-life (days)	4
Paddy Water Aquatic Field Dissipation Half-life (days)	5.4
Total System Aquatic Field Dissipation Half-life (days)	14
Aerobic Aquatic Half-life (days)	35.1

Suggested Alternate Method of Estimating Aquatic Concentrations

Dow Agrosciences has submitted a document (MRID 458308-11) that addresses modeling of penoxsulam concentrations in drinking water, and modeling ecological effects concentrations for both ground water and surface water from the proposed use on rice. Dow assumes effective "holding times" when estimating aqueous concentrations by calculating concentrations by reporting estimated acute concentrations 28 to 78 days after application. For this EFED Science Chapter, the results from the more conservative, Interim Rice Model were used, as indicated by current policy. Dow provided modeling of ground water using the SCI-GROW model, which they state is not relevant to applied compounds in rice fields because of relatively impermeable layers that hold a flood. While this conclusion is consistent with the molinate and thiobencarb REDs, the registrant did calculate a ground water concentration using the SCI-GROW model as an "extremely conservative Tier I EEC." EFED notes that (1) the registrant used field dissipation half-lives instead of laboratory aerobic soil metabolism half-lives, (2) the lowest partitioning coefficient from a non-sand, non-volcanic soil was not used, and (3) the degradates identified to be of toxicological concern were not considered for human drinking water concentrations.

For surface water, Dow AgroScience assumed effective "holding times" by reporting

[4]EFED Response to Registrant Request for a Seven (7) Day Holding Period for Propanil Use in Rice Paddies; DP Barcode: D290202; PC Code: 028201; 9/11/03.

estimated acute concentrations 28 to 78 days after application with the modeling approach from the modified propanil RED and cyhalofop butyl Section 3 documents Dow noted that EFED has no official model for surface water exposure from pesticides applied to rice. While most of these modifications were reasonable and scientifically sound, the registrant used the parent-only, "average" aerobic soil metabolism half-lives prior to flooding instead of upper 90th confidence bound values for the combined residues. The registrant also used the parent-only "average" aquatic field dissipation half-lives. Dow justified the use of field dissipation half-lives because penoxsulam degrades by both abiotic and biotic processes. Additionally, the registrant used a much higher soil to water partitioning coefficient than the recommended lowest reported value for a non-sand, non-volcanic soil. The half-life values used for drinking water estimates do not address the degradates of toxicological concern, as identified by HED. Additionally, assuming effective "holding times" between 28 and 78 days[5] may not be appropriate for this assessment. For example, the application date on the proposed label for penoxsualm differs depending upon the target weed, and would not necessarily coincide with the application date(s) of other pesticides. Furthermore, even if the Dow "holding time" assumptions[6] were valid for human drinking water, ecological effects are possible at the point where the flood water leaves the paddy, not at the drinking water intake.

For drinking water derived from surface water, Dow drained all the fields at once into the Index Reservoir and calculated peak and annual mean values for acute and chronic exposure. The peak concentration leaving the fields was divided by two (2) because the volume of water from the rice paddies and the volume of the Index Reservoir were very similar. The chronic exposure were determined by degrading the peak concentrations from California (continuous flood rice), the Mississippi Delta (dry-seeded rice), and South Louisiana (pinpoint flood or delayed flood rice) for one year to get an annual mean concentration for each location.

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[5]Precedent cited from EFED Estimated Environmental Concentrations in Unfinished Drinking Water for use of Cyhalofop-Butyl on Rice; D P Barcode D275810; PC Code: 082583; 8/10/01.

[6]The "effective holding time" assumptions discussed in this text were adopted by EFED for refining estimates of human drinking water concentrations. These "holding times" assume that either (1) water is circulated through a series of connected paddies during the permanent flood period, (2) that California Water Reclamation Districts hold agricultural water throughout an entire growing season, or that (3) drinking water intakes would not be located adjacent to rice fields, and released tail water would not immediately contact an intake site.

SCIGROW
VERSION 2.3
ENVIRONMENTAL FATE AND EFFECTS DIVISION
OFFICE OF PESTICIDE PROGRAMS
U.S. ENVIRONMENTAL PROTECTION AGENCY
SCREENING MODEL
FOR AQUATIC PESTICIDE EXPOSURE

SciGrow version 2.3
chemical:penoxsulam parent only
time is 7/ 7/2004 16:11:27

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.044	1.0	0.044	1.30E+01	116.0

groundwater screening cond (ppb) = 6.71E-01
****

SCIGROW
VERSION 2.3

ENVIRONMENTAL FATE AND EFFECTS DIVISION
OFFICE OF PESTICIDE PROGRAMS
U.S. ENVIRONMENTAL PROTECTION AGENCY
SCREENING MODEL
FOR AQUATIC PESTICIDE EXPOSURE

SciGrow version 2.3
chemical:penoxsulam combined residues
time is 7/ 7/2004 16:12:32

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
0.044	1.0	0.044	1.30E+01	410.0

groundwater screening cond (ppb) = 5.86E+00
****

Ground and Surface Water Contamination Modeling of Penoxsulam Applied to Rice (MRID 458308-11)

"Expected Environmental Concentrations of XDE-638 in Ground Water and Surface Water Using US EPA Tier I Screening Models"; Krieger M.S.; Regulatory Laboratories-Indianapolis Lab, Dow AgroSciences LLC, 9330 Zionsville Road, Indianapolis, Indiana 46268; October 28, 2002.

Reviewed by: Jim Breithaupt[7]
Agronomist, ERB II
Environmental Fate and Effects Division (7507C)

Approved by: Lucy Shanaman[7]
Chemist, ERB III
Environmental Fate and Effects Division (7507C)

Conclusions:

Dow Agrosciences has submitted a non-standard study which provides supplemental data for penoxsulam. The study is a modeling effort that addresses both ground and surface water contamination from Penoxsulam applied to rice. For ground water, the registrant used SCI-GROW and generated EECs of 0.0014 and 0.0042 ug/L. For ecological effects from surface water (Table 1 in Dow document), the highest estimated concentrations for ecological effects occurred in wet-seeded rice in Louisiana on the Gulf Coast. Based on the modeling results (Table 1 in Dow document), the highest estimated concentrations for ecological effects occurred in water-seeded rice in Louisiana on the Gulf Coast. The highest peak concentration was 42.7 ug/L, which declined to 1.56 ug/L by 21 days after application, and 0.0031 ug/L by 60 days after application. For drinking water, assuming effective "holding times" between 28 and 78 days, the highest peak concentration in the Index Reservoir from all scenarios was 0.26 ug/L, and the maximum chronic (365-day average) concentration was 0.005 ug/L. This concentration occurred in the water-seeded rice grown on the Gulf Coast in Louisiana. The Dow estimates are of questionable value due to (1) the use of inappropriate values for both degradation and partitioning, (2) because the residues identified by HED as being of toxicological concern were not considered in the calculated half-life estimates, and (3) because penoxsulam application dates differ, and therefore their assumed effective "holding times" should differ, from those of the rice herbicides used as the example for Dow's exposure modeling.

Ground Water Contamination from Penoxsulam Use on Rice

Dow provided modeling of ground water using the SCI-GROW model, which they state is not relevant to applied compounds in rice fields because of relatively impermeable layers that hold a flood. This conclusion is consistent with the molinate and thiobencarb REDs, However, the

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[7]September 7, 2004

registrant did calculate ground water concentrations of 0.0014 and 0.0042 ug/L assuming wet-seeded and dry-seeded rice, respectively, using the SCI-GROW model as an "extremely conservative Tier I EEC." EFED notes that the registrant used field dissipation half-lives instead of laboratory aerobic soil metabolism half-lives as an input into the model, which may be inappropriate. Even so, EFED does not regard ground water contamination from a pesticide applied to rice to be a significant route of dissipation.

Surface Water Contamination from Penoxsulam Use on Rice

For surface water, Dow used the modeling approach from the propanil RED and cyhalofop butyl Section 3 documents with some modifications. Dow noted that EFED has no official Tier II model for surface water exposure from pesticides applied to rice. While most of these modifications were reasonable and scientifically sound, the registrant used "average" aerobic soil metabolism half-lives prior to flooding instead of upper 90th CB values. The registrant also used "average" aquatic field dissipation half-lives instead of aerobic aquatic metabolism half-lives. The use of field dissipation half-lives is questionable because field studies are not generally conducted under the same rigorous conditions, with good material balances verified, as required for acceptable laboratory studies. The registrant justified the use of field dissipation half-lives because penoxsulam degrades by both abiotic and biotic processes, and aquatic field dissipation rates they incorporate the results of many dissipation processes.

Ecological Effects Concentrations

Based on the modeling results (Table 1 in Dow document), the highest estimated concentrations for ecological effects occurred in water-seeded rice in Louisiana on the Gulf Coast. Without imposing mandatory holding times, the highest peak concentration was 42.7 ug/L, which declined to 1.56 ug/L by 21 days after application, and 0.0031 ug/L by 60 days after application.

Estimated Drinking Water Concentrations from Surface Water

For drinking water, assuming effective "holding times" between 28 and 78 days, the highest peak concentration in the Index Reservoir from all scenarios was 0.26 ug/L, and the maximum chronic (365-day average) concentration was 0.005 ug/L. This concentration occurred in the water-seeded rice grown on the Gulf Coast in Louisiana. Assumed effective "holding time" values were adopted directly from the exposure modeling EFED had conducted for the rice herbicides propanil and cyhalofop-butyl. The Dow estimates are of questionable value due to (1) the use of inappropriate values for both degradation and partitioning, (2) because the residues identified by HED as being of toxicological concern were not considered in the calculated half-life estimates, and (3) because penoxsulam application dates differ, and therefore their assumed effective "holding times" should differ, from those of the rice herbicides used as an example for Dow's exposure modeling.

For drinking water derived from surface water, Dow drained all the fields at once into the Index Reservoir and calculated peak and annual mean values for acute and chronic exposure. The

peak concentration leaving the fields was divided by two (2) because the volume of water from the rice paddies and the volume of the Index Reservoir were very similar. The chronic exposure was determined by degrading the peak concentrations from California (continuous flood rice), the Mississippi Delta (dry-seeded rice), and South Louisiana (pinpoint flood or delayed flood rice) for one year to get an annual mean concentration for each location.

Ground and Surface Water Modeling Inputs

- Application Rate–0.045 lb ai/acre
- No. Apps–1
- Koc (l/kg)–90
- $T_{1/2}$ (for water-seeded rice)–6.5 days (average total system half-life from water-seeded aquatic field dissipation studies)
- $T^{1/2}$ (for dry-seeded rice)–14.6 days (average total system half-life from dry-seeded aquatic field dissipation studies)

Appendix I EFED Modeling Approaches

Interim Rice Model

EFED has used different modeling approaches for rice tailwater runoff to date. The first appproach, known as the Interim Rice Model, includes only sorption as a dissipation process. It provides a conservative Tier I estimate of the concentration of an applied pesticide in surface water with the following assumptions:

- Sorption is the only dissipation process the model considers
- 100 % of perfectly-normal application is applied to flooded field, reaches the flood water, and instantaneously partitions between water and soil
- No degradation, drift, volatility, foliar interception, runoff, or leaching occurs in the field
- The field is drained the day of application

Refined Modeling used for Propanil RED

Dry-seeded Rice

EFED modeled the dissipation of propanil in the field by incorporating both degradation (aerobic soil and aerobic aquatic metabolism) and partitioning between water and soil. For dry-seeded rice, the refined modeling used for propanil estimates the concentration in paddy water 10 days after the day of application to a non-flooded field. Most of the rice grown in the U.S. is produced using this cultural practice, and is primarily located in the lower Mississippi River Delta and in southeastern Texas. This modeling approach provides a maximum concentration in paddy water, after an effective "holding time" incorporated into the calculations in order to estimate the time required for paddy tail water to reach drinking water intakes. It also predicts concentrations for ecological effects to organisms living at the edge of the rice paddy. Required water-holding times to reduce aquatic exposure below a given level of concern can be estimated. The assumptions for dry-seeded rice and application to non-flooded soil include:

- 100 % of application reaches the soil and instantaneously sorbs
- Degradation occurs by aerobic soil metabolism (average $T_{1/2}$=46 days for propanil) for non-flooded fields
- Degradation occurs by aquatic field dissipation (average $T_{1/2}$=4.4 days for propanil) for flooded fields.
- No drift, volatility, foliar interception, runoff, or leaching occurs
- Flooding over the entire field is instantaneous
- The field is flooded 10 days after the day of application, followed by immediate partitioning between soil and water.
- No outflow or overflow from the fields occurs after flooding.
- For ecological effects, the concentration of paddy water was used as exposure to aquatic organisms
- For drinking water, the paddy water was drained to the Index Reservoir, diluted, and then degraded using the aerobic aquatic metabolism rate

Water-Seeded Rice

Water-seeded rice is grown in southwestern Louisiana and in California. The primary method of water-seeded rice production in Louisiana that uses propanil is called "delayed flood rice." The pregerminated seeds are dropped into standing water, which is drained 1-2 days later. A permanent flood is established about 3-4 weeks after planting and is held for about 10 weeks in the first crop. The modeling assumes that the compound is applied before the permanent flood, and that the water is held until 28 days after herbicide application when drainage is necessary due to a rainfall event causing overflow. California uses the "permanent flood" method of producing rice. Pregerminated seeds are dropped into standing water where a flow of aerobic water is established, but is NOT normally drained totally until a postemergence herbicide is applied about 30 days later. After treatment with a herbicide, a 4-inch flood is reestablished and later increased to 8 inches of depth in Mid-July to ensure proper seed formation. It is drained about 2-3 weeks prior to harvest. The maximum surface water concentration is that achieved on the day of application, and the later concentrations are predicted for drinking water assuming California agricultural waters are held within a water management district for up to 78 days after propanil application. The aerobic aquatic metabolism rate is used to degrade the pesticide. The modeling assumptions used in the propanil modeling follow:

- 100 % of perfectly-normal application reaches flooded soil and instantaneously partitions between the soil and floodwater
- Degradation occurs by aquatic field dissipation half-life of 4.4 days for propanil
- No drift, volatility, foliar interception, runoff, or leaching occurs
- Flooding over the entire field is instantaneous
- The flood water is released 28 days later for southern Louisiana and 78 days in California.
- No outflow or overflow from the fields occurs after flooding prior to release.
- For ecological effects, the concentration of paddy water was used as exposure to aquatic organisms
- For drinking water, the paddy water was drained to the Index Reservoir, diluted, and then

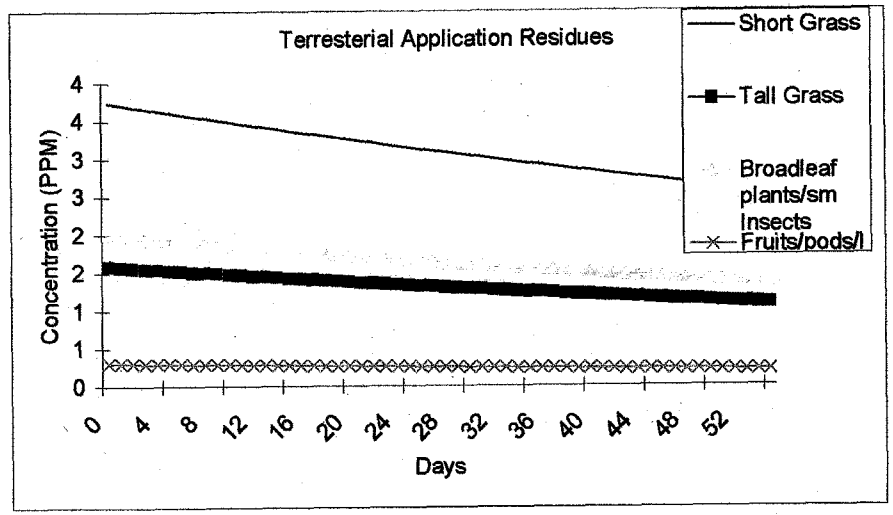
degraded using aerobic aquatic metabolism

Appendix C – ELL Fate Model and Results
Mean Residues

Chemical Name:	Penoxsulam
Use	Rice
Formulation	Soluble Concentrate

Inputs

Application Rate	0.04	lbs a.i./acre
Half-life	100	days
Frequency of Application	1	days
Maximum # Apps./Year	1	



Outputs

	Maximum Concentration (PPM)	56 day Average Concentration (PPM)	
Short Grass	**3.74**	**3.11**	
Tall Grass	**1.58**	**1.32**	# days
Broadleaf plants/sm			
insects	**1.98**	**1.65**	Exceeded
Fruits/pods/lg insects	**0.31**	**0.26**	on short grass (in first 56)

Avian	Acute LC50 (ppm)	2025	0
	Chronic NOAEC (p	4411	0

	Acute RQ	Chronic RQ	
		(Max. res. mult. apps.)	
Short Grass	**0.00**	**0.00**	
Tall Grass	**0.00**	**0.00**	# days
Broadleaf plants/sm			
Insects	**0.00**	**0.00**	Exceeded
Fruits/pods/lg insects	**0.00**	**0.00**	on short grass (in first 56)

Max Single Application which does NOT exceed

Avian Acute	8.438	
Avian Chronic	18.379	(lb a.i.)
Mammalian Acute	138.89	
Mammalian Chronic	2.50	

Mammalian

Acute LD50 (mg/kg	5000	0	Rat Calculated LC50 (ppm	100000
Chronic NOAEL (m	600	0	Rat Calculated NOAEL (p	12000

	15 g mammal		35 g mammal		1000 g mammal	Rat Acute Dietary RQ	Rat Chronic Dietary RQ
	Acute RQ (mult. apps)		Acute RQ (mult. apps)		Acute RQ (mult. apps)		
Short Grass	**0.00**		**0.00**		**0.00**	**0.00**	0.01
Tall Grass	**0.00**		**0.00**		**0.00**	**0.00**	0.00
Broadleaf plants/sm insects	**0.00**		**0.00**		**0.00**	**0.00**	0.00
Fruits/pods/lg insects	**0.00**		**0.00**		**0.00**	**0.00**	0.00
Seeds (granivore)	**0.00**		**0.00**		**0.00**	**0.00**	

Length of Simulation 1 year

Level of Concern 193.00 (ppm)

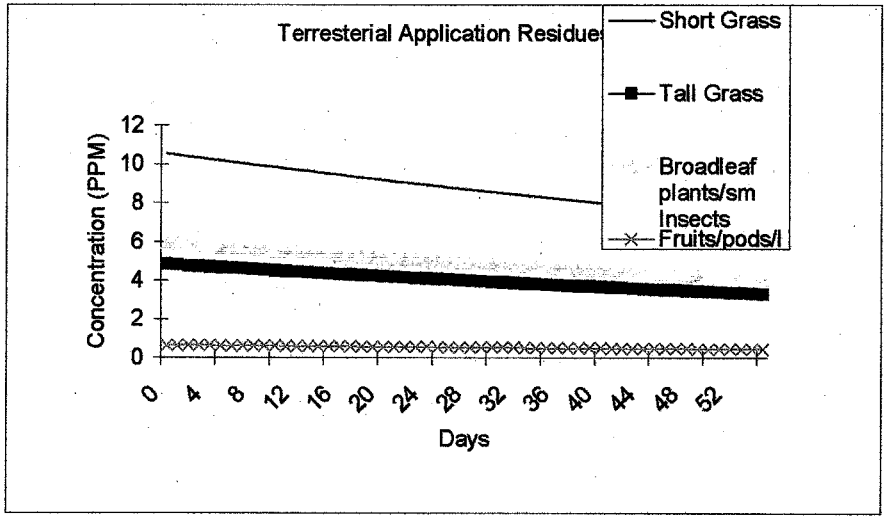
			Acute Mammalian RQs			
Mammalian Class	Body Wgt	% body wgt consumed	Short grass	Tall grass	Broadleaf pla	Fruit/pods/lg insects
	15	95	**0.00**	**0.00**	**0.00**	**0.00**
Herbivores/	35	66	**0.00**	**0.00**	**0.00**	**0.00**
insectivores	1000	15	**0.00**	**0.00**	**0.00**	**0.00**
	21	21				**0.00**
Grainivores	35	15				**0.00**
	1000	3				**0.00**
			Chronic Mammalian RQs			
			0.01	0.00	0.00	0.00

Maximum Residues

Chemical Name:	Penoxsulam
Use	Rice
Formulation	Soluble Concentrate

Inputs

Application Rate	0.044	lbs a.i./acre
Half-life	100	days
Frequency of Application	1	days
Maximum # Apps./Year	1	



Outputs

	Maximum Concentration (PPM)	56 day Average Concentration (PPM)	
Short Grass	**10.56**	**8.78**	
Tall Grass	**4.84**	**4.03**	# days
Broadleaf plants/sm			
Insects	**5.94**	**4.94**	Exceeded
Fruits/pods/lg insects	**0.66**	**0.55**	on short grass (in first 56)

Avian	Acute LC50 (ppm)	2025	0
	Chronic NOAEC (p	4411	0

	Acute RQ	Chronic RQ (Max. res. mult. apps.)	
Short Grass	**0.01**	**0.00**	
Tall Grass	**0.00**	**0.00**	# days
Broadleaf plants/sm			
Insects	**0.00**	**0.00**	Exceeded
Fruits/pods/lg insects	**0.00**	**0.00**	on short grass (in first 56)

Max Single Application which does NOT exceed

Avian Acute	8.438	
Avian Chronic	18.379	(lb a.i.)
Mammalian Acute	138.89	
Mammalian Chronic	2.50	

Mammalian

Acute LD50 (mg/kg	5000	0	Rat Calculated LC50 (ppm	100000
Chronic NOAEL (m	600	0	Rat Calculated NOAEL (p	12000

	15 g mammal		35 g mammal		1000 g mammal	Rat Acute Dietary RQ	Rat Chronic Dietary RQ
	Acute RQ (mult. apps)		Acute RQ (mult. apps)		Acute RQ (mult. apps)		
Short Grass	**0.00**		**0.00**		**0.00**	**0.00**	0.02
Tall Grass	**0.00**		**0.00**		**0.00**	**0.00**	0.01
Broadleaf plants/sm insects	**0.00**		**0.00**		**0.00**	**0.00**	0.01
Fruits/pods/lg insects	**0.00**		**0.00**		**0.00**	**0.00**	0.00
Seeds (granivore)	**0.00**		**0.00**		**0.00**	**0.00**	

Length of Simulation 1 year

Level of Concern 193.00 (ppm)

			Acute Mammalian RQs			
Mammalian Class	Body Wgt	% body wgt consumed	Short grass	Tall grass	Broadleaf pla	Fruit/pods/lg insects
	15	95	**0.00**	**0.00**	**0.00**	**0.00**
Herbivores/	35	66	**0.00**	**0.00**	**0.00**	**0.00**
insectivores	1000	15	**0.00**	**0.00**	**0.00**	**0.00**
	21	21				**0.00**
Grainivores	35	15				**0.00**
	1000	3				**0.00**
			Chronic Mammalian RQs			
			0.02	0.01	0.01	0.00

APPENDIX D - Ecological Effects Data

§71-1a. MRID 45830928 Acute oral toxicity to northern bobwhite quail.
No mortalities or treatment-related sub-lethal effects were observed during the study. There were no significant differences in body weights or feed consumption, and no abnormalities were observed at terminal necropsy.

The 14-day acute oral LD_{50} is >2025 mg a.i./kg bw, which categorizes XDE-638 as practically nontoxic to Northern Bobwhite quail. This study is classified as CORE.

§71-1a. MRID 45830929 Acute oral toxicity mallard ducks.
No mortalities or treatment-related sub-lethal effects were observed during the study. There were no significant differences in body weights or feed consumption, and no abnormalities were observed at terminal necropsy. The 14-day acute oral LD_{50} is >1900 mg a.i./kg bw, which categorizes penoxsulam as practically nontoxic to Mallard ducks on an acute oral basis. This toxicity study is scientifically sound but does not fulfill the guideline requirements for an acute toxicity study using the Mallard duck (§71-1), because the experimental concentrations were not determined.

This study is classified as SUPPLEMENTAL. Since the nominal concentrations are very high, the study need not be repeated. The NOAEL, *etc.* will be recorded as > 1,900 mg a.i./kg bw.

§71-1b. MRID 45831001 Acute oral toxicity of GF-443 (21.7% penoxsulam) to bobwhite quail
The acute oral toxicity of GF-443(a 21.9% EUP) to 21-week-old Northern Bobwhite quail (*Colinus virginianus*) was assessed for 14 days. GF-443 was administered to the birds via gavage at nominal concentrations of the active ingredient of 170, 283,473, 778, 1314, 2190 mg ai/kg. No mortalities or treatment-related sub-lethal effects or significant differences in body weights were observed. A statistically-significant reduction in feed consumption was observed on Days 0-3 at the 2190 mg ai/kg bw dose group compared to the control (15 versus 19 g/bird/day). Feed consumption recovered for the remainder of the study. No treatment-related abnormalities were observed at terminal necropsy.

The 14-day acute oral LD_{50} is >2190 mg ai/kg bw, which categorizes GF-443 as practically nontoxic to Northern Bobwhite quail on an acute oral basis. This study is classified as CORE.

§71-2a. MRID 45831002 Acute dietary toxicity bobwhite quail
Mean-measured concentrations were <LOD (control), 877, 1456, 2091, 3110, and 4411 ppm a.i., respectively. No mortalities occurred during the 8-day study, there were no sub-lethal signs of toxicity, or treatment-related effects on body weights or feed consumption. No significant gross pathological findings were observed.

The 8-day acute dietary LC_{50} was >4411 ppm a.i., the highest concentration tested, which categorizes it as slightly toxic to the Bobwhite quail on an acute dietary basis. This toxicity study is scientifically sound. However, since the concentration of acetone used in the preparation of the treated feed was not reported, this study does not fulfill the guideline requirements for an avian dietary study using the Northern Bobwhite quail (§71-2a). This study is classified as SUPPLEMENTAL, but need not be repeated.

§71-2b. MRID 45831003 Acute dietary toxicity to the mallard duck

Mean-measured concentrations were <LOD (control), 733, 1210, 1870, 2620, and 4310 ppm a.i. No mortalities occurred, there were no sub-lethal signs of toxicity, or treatment-related effects on feed consumption. Statistically-significant reductions in body weight gains were observed at the 2620 ppm a.i. level after the exposure period, and at all test levels after the recovery period. No significant gross pathological findings were observed.

The 8-day acute dietary LC_{50} was >4310 ppm a.i., the highest concentration tested, which categorizes it as slightly toxic to the Mallard duck on an acute dietary basis. Based on reductions in body weight gains, the NOAEC was <733 ppm a.i., the lowest concentration tested. The study is scientifically sound. However, since the concentration of acetone used in the preparation of the treated feed was not reported, this study does not fulfill the guideline requirements for an avian dietary study using the Mallard duck (§71-2b). This study is classified as SUPPLEMENTAL, but it need not be repeated.

§71-4a. MRID 45831006 Reproductive toxicity bobwhite quail

XDE-638 was administered to the birds in the diet at mean-measured concentrations of <1.10 (<LOQ, control), 231, 501, and 958 ppm a.i. There were no significant treatment-related effects on any reproductive parameter; however, adult food consumption, and male and female body weights were adversely affected. There was a significant reduction in food consumption at the 501 ppm a.i. treatment level and significant reductions in male and female body weight gain at the highest treatment level.

The NOAEC and LOAEC levels were 231 and 501 ppm a.i. diet, respectively. This toxicity study is scientifically sound. However, because the amount of solvent (acetone) used in the test diet preparations was not specified, nor was it stated that the acetone was allowed to completely evaporate prior to offering, and because the only endpoints adversely affected (*e.g.*, food consumption and male and female body weight gain) may have been related to this deviation, this study is classified as SUPPLEMENTAL but need not be redone.

§71-4b. MRID 46276401 Reproductive toxicity to mallard ducks.

Penoxsulam was administered in the diet at mean-measured concentrations of <70.7 (<LOQ, control), 231, 501, and 958 ppm a.i. Adult male body weight gain was adversely affected at the highest treatment level. There were no other significant adverse effects on any adult parameter. In addition, no treatment-related effects were observed on egg production or quality, fertility,

embryonic development, hatchability, or survival of hatchlings. No treatment-related effects on hatchling body weights were observed; however, 14-day-old body weights of ducklings were statistically-reduced compared to the control at all test levels. The mean body weights of the 14-day old ducklings were 240, 218, 211, and 215 g in the control, 250, 500, and 1000 ppm test groups, respectively. A hatchling brooder density test was provided as a supplement to this study (MRID 46276402) and it provided strong evidence that brooder density may have been the primary factor contributing to the survivor body weight reductions.

As a result, the LOAEC for this study is defined by reductions in adult male body weight at the 958 ppm a.i. treatment level. The NOAEC was 501 ppm a.i. This study is scientifically sound, fulfills guideline requirements for the reproductive toxicity of penoxsulam to Mallard duck (§71-4b), and is classified as CORE.

§72-1. MRID 45831009 96-hour acute toxicity study with juvenile common carp

Carp were exposed to mean-measured concentrations of <10 (LOQ, controls) and 101 ppm a.i. After 96 hours of exposure, no mortality or sub-lethal effects were observed in any control or test group.

The 96-hour LC_{50} was >101 ppm a.i., which categorizes XDE-638 as practically nontoxic to juvenile common carp (*Cyprinus carpio*) on an acute toxicity basis. The NOAEC and LOAEC were 101 and >101 ppm a.i., respectively. This study is scientifically sound. However, since the common carp is not recognized as an acceptable species for use in an acute toxicity study with freshwater fish (§72-1), this study is classified as SUPPLEMENTAL.

§72-1a. MRID 45831010 Acute toxicity study with the bluegill sunfish.

Mean-measured concentrations were <12 (LOQ, controls) and 103 ppm a.i. After 96 hours of exposure, there was 7% mortality in the solvent control and 103 ppm a.i. treatment group. No mortality occurred in the control. No significant sub-lethal effects were observed. The LC_{50} was >103 mg a.i./L, which categorizes it as practically nontoxic to juvenile bluegill sunfish on an acute toxicity basis.

The NOAEC and LOAEC were 103 and >103 ppm a.i., respectively. Since the mean fish weight of 0.199 g was less than the required initial weight range of 0.5 to 5 g, this study does not fulfill guideline requirements for an acute toxicity study with the bluegill sunfish (§72-1a) and is classified SUPPLEMENTAL, but need not be repeated.

§72-1c. MRID 45834804 Acute toxicity study with rainbow trout

Trout were exposed under static conditions to mean-measured concentrations of <12 (LOQ, controls) and 102 ppm a.i. No mortality or sub-lethal effects were observed in any control or test group.

The 96-hour LC_{50} was >102 ppm a.i., which categorizes it as practically nontoxic to juvenile rainbow trout on an acute toxicity basis. The NOAEC and LOAEC were 102 and >102 ppm a.i., respectively. Since the mean fish weight of 0.287 g was less than the required initial

weight range of 0.5 to 5 g, this study does not fulfill guideline requirements for an acute toxicity study with the Rainbow trout (§72-1c) and is classified SUPPLEMENTAL, but it need not be repeated.

§72-1c. MRID 45831011 Acute toxicity of an EUP to the rainbow trout

Trout exposed under static conditions to GF-443 [an end-use product containing 22%] at mean-measured concentrations of <5.91 (LOQ, negative control), 13.3, 20.8, 37.1, 57.0, 91.4, and 147 ppm a.i. Ten percent mortality was observed in the 91.4 ppm a.i. treatment group. No other mortalities or sub-lethal effects were observed.

The LC_{50} was >147 ppm a.i., which categorizes GF-443 as practically nontoxic to juvenile Rainbow trout on an acute toxicity basis. The NOAEC (for mortality) was 91.4 ppm a.i. This study was classified as SUPPLEMENTAL because of turbidity and aeration, but it need not be repeated. It is scientifically sound and fulfills the guideline requirements for an acute toxicity test with freshwater fish (72-1c) using an end-use product.

§72-2. MRID 45831012 Acute toxicity to the water flea.

Daphnids were exposed to the test material under static conditions at mean-measured concentrations of <12 (LOQ, negative and solvent controls) and 98.3 ppm a.i. After 48 hours, no immobilization was observed in the controls or 98.3 ppm a.i. treatment group.

The 48-hour LC/EC_{50} was >98.3 ppm a.i., which categorizes it as slightly toxic to the water flea on an acute toxicity basis. The 48-hour NOAEC level, based on mortality and immobilization, was 98.3 ppm a.i., the only concentration tested. This study is scientifically sound and satisfies the guideline requirements. Because of the very high water hardness, this study is classified as SUPPLEMENTAL, but it need not be redone.

§72-2. MRID 45831021 Acute toxicity to the amphipod, *Gammarus pseudolimnaeus*.

Gammarids were exposed to the test material at mean-measured concentrations of <0.00902 (LOQ, negative control), 16.3, 26.9, 44.6, 75.5, and 126 ppm a.i. The study found a wide range of mortality; there were some deaths in every concentration level, including the control. After 96 hours, survival was 95% in the control and 16.3 ppm a.i. test group, 75% in the 26.9 ppm a.i. test group, 70% in the 44.6 and 75.5 ppm a.i. test groups, and 55% in the 126 ppm a.i. test group. The 96-hour LC_{50} was >126 ppm a.i., which categorizes it as practically nontoxic to the gammarid on an acute toxicity basis.

No sub-lethal effects were observed during the study. The LC_{50} could be determined visually because mortality did not exceed 50% in this study. The NOAEC could not be determined, but the LOAEC was 16.3.

This study is scientifically sound but does not satisfy the guideline requirements for an acute toxicity study with freshwater invertebrates (§72-2) because of the range of mortality. This study is classified as SUPPLEMENTAL, but it need not be repeated, because it is not a required study.

§72-2a. MRID 45831019 Acute toxicity of 2-AMINO-TP to freshwater invertebrates - *Daphnia magna*.

The 48-hour acute toxicity of 2-AMINO-TP (a metabolite of penoxsulam) to *Daphnia magna*, was studied under static conditions. Daphnids were exposed to the study material at a single nominal concentration 1.0 ppm with a negative control. The mean-measured concentration was not determined. No mortality or immobilization was observed in either the control or study group during the 48-hour study.

The 48-hour LC/EC_{50} was >1.0 ppm, which categorizes 2-AMINO-TP as moderately toxic to *Daphnia magna* on an acute toxicity basis. The 48-hour NOAEC level, based on mortality or immobilization, was 1.0 ppm, the only concentration studied. This study is scientifically sound. However, since only ten daphnids were used in a limit study and analytical measurements of metabolite in the dilution water was not performed, this study does not fulfill guideline requirements. The study is classified SUPPLEMENTAL.

§72-2a. MRID 45831014 Acute toxicity of XDE-638 metabolite (BSTCA) to freshwater invertebrates - *Daphnia magna*.

The 48-hour acute toxicity of XDE-638 Metabolite (BSTCA; a metabolite of penoxsulam) *Daphnia magna*, was studied under static conditions. Mean-measured concentrations were <0.70 (LOQ, controls), 6.4, 13, 25, 51, and 100 ppm a.i. No immobilization or sub-lethal effects were observed.

The 48-hour LC/EC_{50} was >100 ppm a.i.., which categorizes BSTCA as practically nontoxic to the *Daphnia magna* on an acute toxicity basis. The 48-hour NOAEC level was 100 ppm a.i. This study is scientifically sound and satisfies the guideline requirements. This study is classified as CORE.

§72-2. MRID 45831018 Acute toxicity of XDE-638 metabolite TPSA to freshwater invertebrates - *Daphnia magna*.

The 48-hour acute toxicity of XDE-638 Metabolite TPSA (a metabolite of penoxsulam) to *Daphnia magna*, was studied under static conditions. Ten Daphnids were exposed to the test material at a single nominal concentration 1.4 ppm with a negative control. The mean-measured concentration was not determined. No mortality or immobilization was observed in either the control or test group during the 48-hour study.

The 48-hour LC/EC_{50} was >1.4 ppm, which categorizes TPSA as moderately toxic to *Daphnia magna* on an acute toxicity basis. The 48-hour NOAEC, was 1.4 ppm, the only concentration tested. This study is scientifically sound. However, since analytical measurements of metabolite in the dilution water was not performed and only ten daphnids were used per level in a limit study, this study does not fulfill guideline requirements for an acute toxicity study with the daphnia (§72-2) using a metabolite of penoxsulam and is classified SUPPLEMENTAL.

§72-2a. MRID 45831015 Acute toxicity of XDE-638 metabolite (BST) to freshwater invertebrates -*Daphnia magna*.

The 48-hour acute toxicity of XDE-638 Metabolite BST to *Daphnia magna*, was studied under static conditions. Daphnids were exposed to the test material at mean-measured concentrations of <0.52 (LOQ, controls), 5.2, 13, 26, 51, and 96 ppm a.i. recommended. No immobilization or sub-lethal effects were observed at any control or test level during the 48-hour study.

The 48-hour LC/EC_{50} was >96 ppm a.i., which categorizes XDE-638 metabolite (BST; a metabolite of penoxsulam) as slightly toxic to *Daphnia magna* on an acute toxicity basis. The 48-hour NOAEC level was 96 ppm a.i. This study is scientifically sound and satisfies the guideline requirements for an acute toxicity study with freshwater invertebrates (§72-2) using a metabolite of penoxsulam. This study is classified as CORE.

§72-2a. MRID 45831017 Acute toxicity of XDE-638 metabolite BSA to freshwater invertebrates - *Daphnia magna* .

The 48-hour acute toxicity of XDE-638 Metabolite BSA to *Daphnia magna*, was studied under static conditions. Daphnids were exposed to the test material at a single nominal concentration 1.6 ppm with a negative control. The mean-measured concentration was not determined. No mortality or immobilization was observed in either the control or test group during the 48-hour study.

The 48-hour LC/EC_{50} was >1.6 ppm, which categorizes BSA as moderately toxic to *Daphnia magna* on an acute toxicity basis. The 48-hour NOAEC level, based on mortality or immobilization, was 1.6 ppm, the only concentration tested. This study is scientifically sound. However, since analytical measurements of metabolite in the dilution water was not performed, this study does not fulfill guideline requirements for an acute toxicity study with the daphnia (§72-2) using a metabolite of penoxsulam and is classified SUPPLEMENTAL.

§72-2a. MRID 45831016 Acute Toxicity of 5-OH,2-AMINO-TP to freshwater invertebrates - *Daphnia magna*.

The 48-hour acute toxicity of 5-OH,2-AMINO-TP to *Daphnia magna*, was studied under static conditions. Daphnids were exposed to the test material at a single nominal concentration 1.0 ppm with a negative control. After 48 hours, 3% mortality or immobilization was observed in the 1.0 ppm treatment group and no mortality or immobility was observed in the control.

The 48-hour LC/EC_{50} was >1.0 ppm, which categorizes 5-OH,2-AMINO-TP as moderately toxic to *Daphnia magna* on an acute toxicity basis. The 48-hour NOAEC level, based on mortality or immobilization, was 1.0 ppm, the only concentration tested. This study is scientifically sound. However, since only ten daphnids were used in this limit study and since analytical measurements of metabolite in the dilution water was not performed, this study does not fulfill guideline requirements for an acute toxicity study with the daphnia (§72-2) using a metabolite of penoxsulam and is classified SUPPLEMENTAL.

§72-2a. MRID 45831013 Acute toxicity of 5-Hydroxy-XDE-638 to freshwater invertebrates - *Daphnia magna*.

The 48-hour acute toxicity of 5-Hydroxy-XDE-638 (a metabolite of penoxsulam) to *Daphnia magna*, was studied under static conditions. Daphnids were exposed to mean-measured concentrations of <0.54 (LOQ, controls), 5.8, 13, 26, 50, and 100 ppm a.i. No sub-lethal effects were observed.

The 48-hour LC/EC_{50} was >100 ppm a.i., which categorizes 5-Hydroxy-XDE-638 as practically nontoxic to *Daphnia magna* on an acute toxicity basis. The 48-hour NOAEC level was 100 ppm a.i. This study is scientifically sound, but, since the water hardness was higher than recommended and there were only four treatment levels with only five daphnids each., it does not satisfy the guideline requirements for an acute toxicity study with freshwater invertebrates (§72-2) using a metabolite of penoxsulam. This study is classified as SUPPLEMENTAL, but it need not be repeated.

§72-2b. MRID 45831020 Acute toxicity of the TEP, GF-443, to freshwater invertebrates - *Daphnia magna*.

The 48-hour acute toxicity of GF-443 [an end-use product containing 22% penoxsulam] to *Daphnia magna*, was studied under static conditions. Daphnids were exposed to the test material at mean-measured concentrations were <0.6 (LOQ, negative control), 7.92, 13.3, 22.2, 36.5, 58.0, and 90.1 ppm a.i. The water hardness was higher than recommended. No mortality was observed during the study. Incidental immobilization was observed at 5, 10, 10, and 5% in the 13.3, 22.2, 36.5, and 58.0 ppm a.i. test levels. No immobilization was observed in the negative control group, the 7.92 ppm a.i. test group, or the highest level tested, 90.1 ppm a.i.

The 48-hour LC/EC_{50} was >90.1 ppm a.i., which categorizes GF-443 as slightly toxic to *Daphnia magna* on an acute toxicity basis. The 48-hour NOAEC level, based on mortality or immobilization, was 90.1 ppm a.i. This study is classified as SUPPLEMENTAL, but it need not be repeated. It is scientifically sound and fulfills the guideline requirements for an acute toxicity test with freshwater invertebrate (72-2) using an end-use product.

§72-3a. MRID 45831022 Acute toxicity of XDE-638 to silverside (*Menidia beryllina*).

In a 96-hour acute toxicity study, juvenile silverside (*Menidia beryllina*) were exposed under static conditions to XDE-638 (penoxsulam) at mean measured concentrations were <0.0553 (LOQ, negative control), 17.0, 28.5, 44.5, 76.0, and 129 ppm a.i. After 96 hours of exposure, mortality was 5% in the 44.5 ppm a.i. treatment group. No other mortalities were observed in the control or treatment groups, therefore, the mortality is not considered significant. The 96-hour LC_{50} was >129 ppm a.i., which categorizes penoxsulam as practically nontoxic to the silverside, *Menidia beryllina*, on an acute toxicity basis. No sub-lethal effects were observed during the study. Based on lack of effects, the NOAEC and LOAEC were 129 and >129 ppm a.i., respectively. This study is scientifically sound. However, since the average terminal control wet fish weight was less than the required initial weight of 0.5-5 g, this study does not fulfill

guideline requirements for an acute toxicity study with the silverside (§72-3a). This study provides useful information, and is classified SUPPLEMENTAL, but it need not be repeated.

§72-3b. MRID 45831023 Acute EC_{50} study with an estuarine/marine mollusk shell deposition.

In this 96-hour, flow-through acute EC_{50} test with an estuarine/marine mollusk, the eastern oyster (*Crassostrea virginica*) was exposed to XDE-638 (penoxsulam) at mean-measured concentrations of ≤0.00673 (LOQ, control), 15.8, 26.4, 45.4, 73.6, and 127 ppm a.i. (99-106% of nominal values). After 96 hours of exposure, there was one mortality in the control and no mortalities in the treatment groups. No significant reductions were shell deposition were observed at any test level. Mean shell growth was 2.4 mm for the negative control, and 2.4, 2.4, 2.6, 2.6, and 2.1 mm for the 15.8, 26.4, 45.4, 73.6, and 127 mg a.i./L groups, respectively.

The EC_{50} is >127 ppm a.i., which categorizes XDE-638 (penoxsulam) as practically nontoxic to the eastern oyster on an acute toxicity basis. The NOAEC was 127 ppm a.i. This study is scientifically valid and fulfills the requirements of an acute toxicity test with an estuarine/marine mollusk (§72-3b). This study is classified as CORE

§72-3c. MRID 45831024 XDE-638: Acute toxicity to the mysid, *Americamysis bahia*.

The 96-hour acute toxicity of XDE-638 (penoxsulam) to the saltwater mysid, *Americamysis bahia*, was studied under static conditions. Mysids were exposed to mean-measured concentrations of <0.0270 (LOQ; control), 14.4, 25.6, 42.8, 71.1, and 114 ppm a.i. (90-100% of nominal values). After 96 hours, mortality was 5% in the 114 ppm a.i. test level. No other mortality or sub-lethal effects were observed in any control or test level.

The 96-hour LC_{50} value was >114 ppm a.i., which categorizes XDE-638 as practically nontoxic to the saltwater mysid, *Americamysis bahia*, on an acute toxicity basis. Based on mortality and sub-lethal effects, the NOAEC value was 114 ppm a.i., the highest concentration tested. This study is scientifically valid and fulfills the requirements of an acute LC_{50} test with an estuarine/marine organism (§72-3c). This study is classified as CORE.

§72-4a. MRID 45831027 Toxicity of XDE-638 to the early life stage of fathead minnow (*Pimephales promelas*).

The chronic toxicity of XDE-638 (penoxsulam) to the early life-stage of fathead minnows (*Pimephales promelas)* was studied under flow-through conditions for 36 days. Fertilized eggs/embryos (100 embryos/treatment), approximately 18-22 hours old, were exposed to XDE-638 at mean-measured concentrations of <0.08 (<LOQ, control), 0.802, 1.28, 2.09, 3.65, 6.19, and 10.2 ppm a.i. Hatching commenced on Day 3 and was complete by Day 5, with no treatment-related differences observed in the day-to-mean hatch. No treatment-related effects on the percent hatch, or the survival of post-hatch larvae were observed. At test termination, all surviving larvae were normal, and no treatment-related effects on terminal growth (dry weight and length) were observed.

the NOAEC and LOAEC were 10.2 and >10.2 ppm a.i. Since no endpoint was affected by treatment up to 10.2 ppm a.i., this study does not fulfill guideline requirements for an early life-stage toxicity study with the Fathead minnow (§72-4a) and is classified SUPPLEMENTAL, but it need not be repeated.

§72-4b. MRID 45831026. Chronic toxicity of XDE-638 to freshwater invertebrates - *Daphnia* sp.

The 21-day chronic toxicity of XDE-638 (penoxsulam) to *Daphnia magna* was studied under static renewal conditions. Daphnids were exposed to mean-measured concentrations of <0.01(LOQ, control), 0.040, 0.111, 0.376, 0.942, 2.95, and 9.76 ppm a.i..Immobility was observed in 10% of daphnids in the 0.942 and 2.95 ppm a.i. treatment groups; no other sub-lethal effects were observed. No treatment-related effects were observed on the day of first eggs observed, the day to first brood release, the total number of offspring produced, the number of offspring per adult, or terminal lengths. However, a statistically-significant reduction in the number of live offspring produced was observed at the 9.76 ppm a.i. level compared to the control group (922 versus 1395).

The 21-day LC_{50} was >9.76 ppm a.i. The 21-day EC_{50} was >9.76 ppm a.i. Based on the number of live offspring (the only endpoint affected), the NOAEC and LOAEC values were 2.95 and 9.76, respectively. This study is scientifically sound, fulfills the guideline requirements for an aquatic invertebrate life cycle test with *Daphnia magna* (§ 72-4b), and is classified CORE.

§72-4c. MRID 45831028 XDE-638: Chronic toxicity test to the mysid, *Americamysis bahia*.

In a 28-day life-cycle test, *Americamysis bahia* neonates were exposed under flow-through conditions to XDE-638 (penoxsulam) to mean-measured concentrations <0.0881 (LOD, control), 8.08, 15.2, 29.4, 59.3, and 119 ppm a.i. First-generation mysids were observed for mortality and signs of abnormal behavior once daily throughout the study.. Data endpoints included percent survival of first-generation mysids at study termination (Day 28; combined sexes), number of young produced per female, and length, wet weight, and dry weight of surviving first-generation mysids (Day 28; sex-specific and combined sexes). Dry weights males averaged 0.64 mg for the negative control group, and ranged from 0.46 to 0.54 mg for the treatment groups. In addition, a treatment-related reduction in length was observed in combined sexes at the 119 ppm a.i. test level compared to the control group (8.4 versus 9.2 mm). No other treatment-related effects were observed during the study.

Based on significant reductions in dry weights of males, the NOAEC and LOAEC values were <8.08 and 8.08 ppm a.i., respectively. This study is scientifically sound. However, since the survival of male mysids following pairing was not monitored, since offspring were not maintained and observed for 4 days, and since a NOAEC was not established, this study does not fulfill the guideline requirements for an aquatic invertebrate life-cycle toxicity test using the *Americamysis bahia* (72-4c), and is classified SUPPLEMENTAL, but it need not be repeated

§81-1 870.1100 An Acute Oral Toxicity Study in Rats.

Five male and 5 female Fischer 344 rats were used in the study (Age: 10 weeks. Weight: males 170-211g, females 122-149g). On the day before study initiation animals were weighed and fasted overnight. On day "0" of the study a single dose of XDE-638 was administered by gavage to both sexes; for administration the test article was mixed with 0.5% w/v methylcellulose in distilled water. The dosage was at 10 mL/kg. Animals were observed for signs of clinical abnormalities twice on day "0" and daily thereafter. Health and mortality checks were made twice daily. Body weights were taken on day -1, prior to test substance ingestion and again on days 7 and 14.

No animals died during the study. Clinical abnormalities (transient, and only in a few animals) observed during the study included dark material around the mouth during the first 2 days of the study, mucoid stools, abnormal colored feces, and fecal/urine stain.

At necropsy, "3 incidences of foci on the lungs were observed on day 14. The relationship of these foci to the test material could not be determined." The Oral LD_{50} is greater than 5000 mg/kg for both male and female rats. Penoxsulam is classified as Tox category IV for acute oral toxicity based on the lack of mortality in male and female rats following dosage at 5000 mg/kg.

§84-3 OPPTS 870.3800 MRID 45830920. Penoxsulam:13-week dietary probe study in CD rats.

In a two-generation reproduction toxicity study, penoxsulam (97.7% a.i.) was administered to 30 male and 30 female rats at dietary concentrations that provided 0, 30, 100, or 300 mg/kg/day. One litter was produced in each generation. F_0 and F_1 parental animals were administered test or control diets for 10 weeks prior to mating, throughout mating, gestation, and lactation and until sacrifice.

At necropsy, mid- and high-dose males of both generations had increased and/or relative liver weights due to slight hapatocellar hypertrophy that was not considered to be adverse. High-dose females of both generations had significantly increased absolute and relative kidney weights. Microscopic lesions of the kidney of high-dose F_0 and F_1 females included epithelial hyperplasia, inflammation, and crystal formation in the pelvis and tubular degeneration. The incidences (severity) of kidney lesions in control and high-dose females were 1-2/30 (1.00) and 25-26 (1.58-2.04), respectively, for hyperplasia, 0/30 and 7-8/30 (1.25-2.14), respectively, for inflammation, and 3/30 (1.00) and 20-21/30(1.62-1.85),respectively, for degeneration. Crystals were observed in 0, 0, 2, and 16 F_0 females and in 2, 1, 7, and 11 F_1 females in the control, low-, mid-, and high-dose groups, respectively. The parental systemic toxicity LOAEL for female rats is 100 mg/kg/day based on kidney lesions (crystals) and for male rats is 300 mg/kg/day based on reduced absolute body weights of the F_1 males. The parental systemic toxicity NOAEL for female rats is 30 mg/kg/day and for male rats is 100 mg/kg/day.

Preputial separation, an indicator of sexual maturation, was significantly ($p \leq 0.05$) delayed in mid- and high-dose F_1 males. The mean age at which preputial separation was attained for the control, low-, mid-, and high-dose groups was 43.6, 44.0, 45.5, and 46.0 days, respectively. This delay was considered to be a treatment-related effect. The reproductive/offspring toxicity LOAEL is 100 mg/kg/day based on delay is preputial separation in F_1 males. The

reproduction/offspring toxicity NOAEL is 30 mg/kg/day. The study is Acceptable/Guideline and satisfies the guideline requirement for a two-generation reproduction study in rats.

§122-2. MRID 45831113 Acute toxicity of penoxsulam metabolite on the alga, *Selenastrum capricornutum*.

In a 96-hour acute toxicity study, cultures of *Selenastrum capricornutum* were exposed to penoxsulam metabolite, TPSA, under static conditions. A single nominal concentration was tested (1.4 mg a.i./L), which was compared to a dilution water control; analytical verification of the nominal test concentration was not conducted. The 96-hour cell density, growth rates, and biomass percent inhibitions were -12.4, -2.0, and -8.3%, respectively, in the 1.4 mg a.i./L treatment group (negative values indicate stimulations, no inhibitory effect).

The EC_{50} was >1.4 mg a.i./L, the EC_{05} could not be determined, and the NOAEC was 1.4 mg a.i./L for all endpoints. This toxicity study is scientifically sound, however, it does not satisfy the Guideline §122-2 because the nominal test concentration was not analytically verified and the concentrations were too low. As a result, this study is classified as SUPPLEMENTAL.

§122-2. MRID 45831114 Acute toxicity of penoxsulam metabolite to the alga, *Selenastrum capricornutum.*

In a 96-hour acute toxicity study, cultures of *Selenastrum capricornutum* were exposed to penoxsulam metabolite, 5-OH,2-AMINO-TP, under static conditions. A single nominal concentration was tested (1.0 mg a.i./L), which was compared to a dilution water control; analytical verification of the nominal test concentration was not conducted. The 96-hour cell density and growth rate percent inhibitions were -9.2 and -1.5%, respectively, in the 1.0 mg a.i./L treatment group (negative values indicate stimulations, no inhibitory effect). The mean area under the growth curve (biomass) had 2.0% inhibition.

The EC_{50} was >1.0 mg a.i./L, the EC_{05} could not be determined, and the NOAEC was 1.0 mg a.i./L for all endpoints. This toxicity study is scientifically sound, however, it does not satisfy §122-2 because the nominal test concentration was not analytically verified. As a result, this study is classified as SUPPLEMENTAL.

§122-2. MRID 45831112 Acute toxicity of penoxsulam metabolite to the alga, *Selenastrum capricornutum.*

In a 96-hour acute toxicity study, cultures of *Selenastrum capricornutum* were exposed to penoxsulam metabolite, BSA, under static conditions. A single nominal concentration was tested (1.6 mg a.i./L), which was compared to a dilution water control; analytical verification of the nominal test concentration was not conducted. The 96-hour cell density, growth rates, and biomass percent inhibitions were -9.7, -1.6, and -9.5%, respectively, in the 1.6 mg a.i./L treatment group (negative values indicate stimulations, no inhibitory effect).

The EC_{50} was >1.6 mg a.i./L, the EC_{05} could not be determined, and the NOAEC was 1.6 mg a.i./L for all endpoints. This toxicity study is scientifically sound, however, it does not satisfy

guideline §122-2 because the nominal test concentration was not analytically verified. As a result, this study is classified as SUPPLEMENTAL.

§122-2. MRID 45831115 Acute toxicity of penoxsulam metabolite to the alga, *Selenastrum capricornutum*.

In a 96-hour acute toxicity study, cultures of *Selenastrum capricornutum* were exposed to penoxsulam metabolite, 2-AMINO-TP, under static conditions. A single nominal concentration was tested (1.0 mg a.i./L), which was compared to a dilution water control; analytical verification of the nominal test concentration was not conducted. The 96-hour cell density, growth rates, and biomass percent inhibitions were -7.2, -1.3, and -3.0%, respectively, in the 1.0 mg a.i./L treatment group (negative values indicate stimulations, no inhibitory effect).

The EC_{50} was >1.0 mg a.i./L, the EC_{05} could not be determined, and the NOAEC was 1.0 mg a.i./L for all endpoints. This toxicity study is scientifically sound, however, it does not satisfy guideline §122-2 because the nominal test concentration was not analytically verified. As a result, this study is classified as SUPPLEMENTAL.

§122-2. MRID 45831109 Acute toxicity of penoxsulam metabolite to aquatic vascular plants- *Lemna gibba*.

In a 14-day acute toxicity study, freshwater aquatic vascular plants Duckweed, *Lemna gibba* G3, were exposed to penoxsulam metabolite TPSA at a single, nominal concentration of 1.4 mg a.i./L under static conditions. The mean frond numbers, dry weights, areas under the growth curve, and growth rates were not affected in the 1.4 mg a.i./L treatment group compared to the control.

The NOAEC was 1.4 mg a.i./L, but the EC_{05} could not be determined. The frond number EC_{50} was >1.4 mg a.i./L. This toxicity study is scientifically sound, but it does not satisfy guideline §122-2 because the single nominal test concentration was not analytically determined. As a result, this study is classified as SUPPLEMENTAL.

§122-2. MRID 45831108 Acute toxicity of penoxsulam metabolite to aquatic vascular plants *Lemna gibba*.

In a 14-day acute toxicity study, freshwater aquatic vascular plants Duckweed, *Lemna gibba* G3, were exposed to penoxsulam metabolite 5-OH,2-AMINO-TP at a single, nominal concentration of 1.25 mg a.i./L under static conditions. The mean frond numbers, areas under the growth curve, and growth rates were not affected in the 1.25 mg a.i./L treatment group compared to the control. The dry weight percent inhibition was 0.7% for the 1.25 mg a.i./L treatment group.

The NOAEC was 1.25 mg a.i./L. The frond number EC_{50} was >1.25 mg a.i./L. The EC_{05} could not be determined. This toxicity study is scientifically sound, but it does not satisfy guideline §122-2 because the single nominal test concentration was not analytically determined. As a result, this study is classified as SUPPLEMENTAL.

§122-2. MRID 45831111 Acute toxicity of penoxsulam metabolite to aquatic vascular plants *Lemna gibba*.

In a 14-day acute toxicity study, freshwater aquatic vascular plants Duckweed, *Lemna gibba* G3, were exposed to penoxsulam metabolite 2-AMINO-TP at a single, nominal concentration of 1.0 mg a.i./L under static conditions. The mean frond numbers, dry weights, areas under the growth curve, and growth rates were not affected in the 1.0 mg a.i./L treatment group compared to the control.

The NOAEC as 1.0 mg a.i./L and the EC_{50} was >1.0 mg a.i./L. The EC_{05} could not be determined. This toxicity study is scientifically sound, but it does not satisfy guideline §122-2 because the single nominal test concentration was not analytically determined. As a result, this study is classified as SUPPLEMENTAL.

§122-2. MRID 45831110 Acute Toxicity of penoxsulam metabolite to aquatic vascular plants *Lemna gibba*.

In a 14-day acute toxicity study, freshwater aquatic vascular plants Duckweed, *Lemna gibba* G3, were exposed to penoxsulam metabolite BSA at a single, nominal concentration of 1.6 mg a.i./L under static conditions. The mean frond numbers, dry weights, areas under the growth curve, and growth rates were not affected in the 1.6 mg a.i./L treatment group compared to the control.

The NOAEC/EC_{05} was 1.6 mg a.i./L and the EC_{50} was >1.6 mg a.i./L, but the EC_{05} could not be determined. This toxicity study is scientifically sound, but it does not satisfy guideline §122-2 because the single nominal test concentration was not analytically determined. As a result, this study is classified as SUPPLEMENTAL.

§123-2. MRID 45831120 Acute toxicity of penoxsulam to aquatic vascular plants *Lemna gibba*.

In a 14-day acute toxicity study, freshwater aquatic vascular plants Duckweed, *Lemna gibba* G3, were exposed to XDE-638 (penoxsulam) at mean measured concentrations of 0.491, 1.05, 1.93, 3.84, 7.21, and 14.5 µg a.i./L under static conditions. Nominal concentrations were 0 (negative and solvent controls), 0.5, 1, 2, 4, 8, and 16 µg a.i./L.

The NOAEC, EC_{05} , and EC_{50} values for frond number were 1.05, 0.74, and 3.0 µg a.i./L, respectively. This toxicity study is scientifically sound and satisfies guideline §123-2 for an aquatic vascular plant study with *Lemna gibba*. As a result, this study is classified as CORE.

§123-2. MRID 45831104 Acute toxicity of penoxsulam metabolite (5-Hydroxy-XDE-638) to aquatic vascular plants *Lemna gibba*.

In a 14-day acute toxicity study, freshwater aquatic vascular plants Duckweed, *Lemna gibba* G3, were exposed to penoxsulam metabolite 5-Hydroxy-XDE-638 at mean measured concentrations <0.013-0.016 (<LOQ, negative and solvent controls), 0.081, 0.22, 0.62, 1.6, 4.6, and 11 mg a.i./L under static conditions. The most sensitive variable was frond numbers

The NOAEC was 0.22 mg/L, LOAEC was 0.62 mg/L/L, EC_{05} was 0.095 mg/L, and the EC_{50} >11 mg/L. This toxicity study is scientifically sound and satisfies the guideline §123-2 for an aquatic vascular plant study with *Lemna gibba*. The study is classified as Core.

§123-2. MRID 45831105 Acute toxicity of penoxsulam metabolite (BST) to aquatic vascular plants *Lemna gibba*.

In a 14-day acute toxicity study, freshwater aquatic vascular plants Duckweed, *Lemna gibba* G3, were exposed to penoxsulam metabolite (BST) at mean measured concentrations <0.014 (<LOQ, negative and solvent controls), 0.10, 0.27, 0.68, 1.7, 4.2, and 6.2 mg a.i./L under static conditions. The percent reductions for frond number were significant in all treatment groups, however, significance did not exceed 10% in the highest treatment group. The percent reduction for growth rate was significantly reduced at the lowest treatment level and not significantly reduced for dry weight at any treatment level.

The NOAEC and EC_{50} were not determined, the LOAEC was 0.10 mg/L, and the EC_{50} was >6.2 mg/L. This toxicity study is scientifically sound, but it does not satisfy guideline §123-2 for an aquatic vascular plant study with *Lemna gibba* because a NOAEC could not be determined (for frond number and growth rate) and the US EPA-recommended Probit method (for determining EC_x values) could not be used to determine EC_{05} values, due to the non-monotonic nature of the responses. As a result, this study is classified as SUPPLEMENTAL.

§123-2. MRID 45831106 Acute toxicity of penoxsulam metabolite (BSTCA) to aquatic vascular plants *Lemna gibba*.

In a 14-day acute toxicity study, freshwater aquatic vascular plants Duckweed, *Lemna gibba* G3, were exposed to penoxsulam metabolite (BSTCA) at mean measured concentrations <0.027 (<LOQ, negative and solvent controls), 0.11, 0.27, 0.65, 1.6, 4.1, and 10 mg a.i./L under static conditions. The percent reductions for number of fronds, growth rate, and dry weight were not significant in any treatment group. The NOAEC was 10 mg a.i./L, the EC_{50} >10 mg a.i./L, but the EC_{05} could not be determined. This toxicity study is scientifically sound and satisfies guideline §123-2 for an aquatic vascular plant study with *Lemna gibba*. As a result, this study is classified as SUPPLEMENTAL.

§123-2. MRID 45831123 Acute toxicity of penoxsulam on the saltwater diatom, *Skeletonema costatum*.

In a 120-hour acute toxicity study, cultures of *Skeletonema costatum* were exposed to penoxsulam, as XDE-638, under static conditions. The 0-hour measured concentrations were <0.12 (LOQ, negative control), 1.14, 2.33, 4.62, 9.42, 21.0, and 46.7 mg a.i./L; 0-hour measured concentrations were used to determine toxicity values because measured concentrations after 120 hours declined below 70% of nominal. There were effects on cell density in the 4.62, 9.42, and 46.7 treatment groups. Neither cell density nor biomass was inhibited greater than 50%, so the EC_{50} value for these endpoints was >46.7 mg a.i./L.

The NOAEC based on cell density was 2.33 mg a.i./L and the EC_{05} is 0.43 mg a.i./L. The study is scientifically sound and satisfies guideline §123-2 for an aquatic nonvascular plant study with *Skeletonema costatum*. This study is classified as CORE.

§123-2. MRID 45831121 Acute toxicity of penoxsulam on the freshwater diatom, *Navicula pelliculosa.*

In a 120-hour acute toxicity study, cultures of *Navicula pelliculosa* were exposed to penoxsulam, as XDE-638, under static conditions. The mean measured concentrations were <0.12 (LOQ, negative control), 1.38, 2.65, 5.2, 10.7, 24, and 49.6 mg a.i./L. The 120-hour cell density percent inhibitions were 24.0, 28.5, 15.9, 28.0, 32.8, and 18.6% for the 1.38, 2.65, 5.20, 10.7, 24.0, and 49.6 mg a.i./L treatment groups, respectively. There were no significant effects on cell density.

The EC_{50} was >49.6 mg a.i./L, the EC_{05}: could not be determined, and the NOAEC was 49.6 mg a.i./L for cell density. The study is scientifically sound; however, because the replicate number was lower than recommended and there was high cell density variability within and among the treatment groups, this study does not satisfy guideline §123-2 for an aquatic nonvascular plant study with *Navicula pelliculosa*. As a result, this study is classified as SUPPLEMENTAL.

§123-2. MRID 45831122 Acute toxicity of penoxsulam on the freshwater alga, *Anabaena flos-aquae.*

In a 120-hour acute toxicity study, cultures of *Anabaena flos-aquae* were exposed to penoxsulam under static conditions. The mean measured concentrations were <0.01 (LOQ, negative control), 0.100, 0.194, 0.387, 0.788, 1.59, and 3.22 mg a.i./L. The 120-hour cell density percent inhibitions were -27.5, 15.9, 75.1, 88.8, 88.1, and 86.6% for the 0.100, 0.194, 0.387, 0.788, 1.59, and 3.22 mg a.i./L treatment groups, respectively. There were significant effects on cell density in the 0.387, 0.788, 1.59, and 3.22 mg a.i./L treatment groups.

Cell density was the more sensitive endpoint, with an EC_{50} of 0.27 mg a.i./L; the NOAEC was 0.194 mg a.i./L. The study is scientifically sound and satisfies guideline §123-2 for an aquatic nonvascular plant study with *Anabaena flos-aquae*. This study is classified as CORE.

§123-2. MRID 45831107 Acute toxicity of penoxsulam end-use product , GF-443, on the freshwater alga *Selenastrum capricornutum.*

In a 96-hour acute toxicity study, cultures of *Selenastrum capricornutum* were exposed to GF-443 under static conditions. The mean measured concentrations were <1.77 (control), 8.76, 15.8, 27.9, 41.2, 86.7, and 168 µg a.i./L.

Biomass was the most sensitive endpoint, with an EC_{50} of 94 µg a.i./L; the NOAEC for biomass was 8.76 µg a.i./L. The EC_{05} was 5.1 µg a.i./L and the EC_{50} 94 µg a.i./L. The study is scientifically sound and satisfies guideline §123-2 for an aquatic nonvascular plant study with *Selenastrum capricornutum*. This study is classified as CORE.

§123-2. MRID 45834805 Acute toxicity of penoxsulam to the algae, *Selenastrum capricornutum.*

In a 96-hour acute toxicity study, cultures of *Selenastrum capricornutum* were exposed to penoxsulam, as XDE-638, under static conditions. The mean measured concentrations were 4.62, 11.3, 14.6, 34.9, 74.3, 122, and 233 µg a.i./L. The 96-hour cell density percent inhibitions were 9.7, 10.1, 16.2, 20.6, 34.6, 44.2, 58.3, and 75.5% for the 4.62, 11.3, 14.6, 34.9, 74.3, 122, and 233 µg a.i./L treatment groups, respectively. The solvent control had 9.7% inhibition compared to the negative (dilution water) control. Cell density was significantly reduced at treatment levels equal to and greater than 11.3 µg a.i./L.

The cell density EC_{50} was 92.0 µg a.i./L, the EC_{05} was 6.5 µg a.i./L, and the NOAEC was 4.62 µg a.i./L. The study is scientifically sound and satisfies guideline §123-2 for an aquatic nonvascular plant study with *Selenastrum capricornutum*. This study is classified as CORE.

§123-2. MRID 45831119 Acute toxicity of penoxsulam to the freshwater alga, *Pseudokirchneriella subcapitata.*

In a 96-hour acute toxicity study, cultures of *Pseudokirchneriella subcapitata* were exposed to penoxsulam metabolite BSTCA under static conditions. The mean measured concentrations were <0.026 (LOQ, negative and solvent controls), 0.10, 0.27, 0.64, 1.7, 4.2, and 10 mg a.i./L.

No endpoint was significantly affected by treatment. The EC_{50} was >10 mg a.i./L the EC_{50} could not be determined for cell density or biomass, but was >10 mg a.i./L for growth rate, and the NOAEC was 10 mg a.i./L. The study is scientifically sound and satisfies guideline §123-2 for an aquatic nonvascular plant study with *Pseudokirchneriella subcapitata*. This study is classified as CORE.

§123-2. MRID 45831118 Acute toxicity of penoxsulam metabolite (5-Hydroxy-XDE-638) to the alga, *Pseudokirchneriella subcapitata.*

In a 96-hour acute toxicity study, cultures of *Pseudokirchneriella subcapitata* were exposed to penoxsulam metabolite 5-Hydroxy-XDE-638, under static conditions. The mean measured concentrations were <0.014-0.015 (<LOQ, negative and solvent controls), 0.10, 0.25, 0.62, 1.5, 4.0, and 10.0 mg a.i./L.

The EC_{50} was >10 mg a.i./L for all endpoints, the EC_{05} was 0.58 mg a.i./L, and the NOAEC was 10.0 mg a.i./L. The study is scientifically sound and satisfies the guideline, §123-2 for an aquatic nonvascular plant study with *Pseudokirchneriella subcapitata*. This study is classified as CORE.

§123-2. MRID 45831117 Acute toxicity of penoxsulam metabolite to the freshwater alga, *Pseudokirchneriella subcapitata.*

In a 96-hour acute toxicity study, cultures of *Pseudokirchneriella subcapitata* were exposed to penoxsulam, as its metabolite (BST), under static conditions. The mean measured concentrations were <0.011-0.012 (LOQ, negative and solvent controls), 0.093, 0.22, 0.58, 1.4, 3.9, and 9.6

mg a.i./L. There were significant effects on growth rate and biomass in the 9.6 mg a.i./L treatment group; however, no reductions exceeded 50% for any endpoint.

The EC_{50} was >9.6 mg a.i./L and the NOAEC was 3.9 mg a.i./L (based on biomass and growth rate). The EC_{05}: could not be determined. The study is scientifically sound and satisfies guideline §123-2 for an aquatic nonvascular plant study with *Pseudokirchneriella subcapitata.* This study is classified as CORE.

§123-1 850.4225 and 850.4250 MRID 45831116. Effects of penoxsulam on the Emergence and Vegetative Vigor of Non-Target Terrestrial Plants (Tier II).

The effect of XDE-638 on the seedling emergence and vegetative vigor of dicot (*Gossypium hirsutum,* cotton; *Cucumis sativus,* cucumber; *Beta vulgaris altissima,* sugarbeet; *Brassica oleracea acephala,* kale; *Glycine max,* soybean; and *Lycopersicon esculentum*, tomato) and monocot (*Zea mays,* corn; *Triticum aestivum,* wheat; *Lolium perenne,* ryegrass; and *Allium cepa*, onion) crops was studied at nominal concentrations of 0.14, 0.41, 1.2, 3.7, 11.1, 33.3, and 100 g a.i./ha. The growth medium used in the seedling emergence and vegetative vigor test was natural soil (sandy loam, pH 6.4, organic carbon 1.2%). On day 21, the surviving plants per pot were recorded and cut at soil level for measuring the plant height and dry weight in the seedling emergence and vegetative vigor test, respectively.

The **seedling emergence** test was performed at rates of 0.14, 0.41, 1.2, 3.7, 11.1, 33.3, and 100 g a.i./ha (for corn and wheat), 0.046, 0.14, 0.41, 1.2, 3.7, 11.1, and 33.3 g a.i./ha (for cotton, cucumber, kale, onion, ryegrass, soybean, and tomato), and 0.015, 0.046, 0.14, 0.41, 1.2, 3.7, and 11.1 g a.i./ha (soybean). Corn, cotton, cucumber, ryegrass, soybean, and wheat were not sensitive to treatment (as defined by inhibition of 25% or greater for at least one endpoint). Of the species that were sensitive to treatment with penoxsulam, onion (a monocot) was the most sensitive species (based on shoot weight) with an EC_{25} of 1.1 g a.i./ha; the NOAEC value for this species was 0.41 g a.i./ha. The most sensitive dicot was sugarbeet (based on shoot weight) with an EC_{25} of 3.2 g a.i./ha; the NOAEC value for this species was 1.2 g a.i./ha.

The **vegetative vigor** test was performed at rates of 0.14, 0.41, 1.2, 3.7, 11.1, 33.3, and 100 g a.i./ha (for corn, cotton, cucumber, onion, ryegrass, tomato, and wheat), and 0.015, 0.046, 0.14, 0.41, 1.2, 3.7, and 11.1 g a.i./ha (for kale, soybean, and sugarbeet). Corn and wheat were not sensitive to treatment. Of the species that were sensitive to treatment with penoxsulam, soybean (a dicot) was the most sensitive species (based on shoot weight) with an EC_{25} of 3.9 g a.i./ha; the NOAEC value for this species was 1.2 g a.i./ha. The most sensitive monocot was ryegrass (based on shoot weight) with an EC_{25} of 17.0 g a.i./ha; the NOAEC value for this species was 0.41 g a.i./ha.

This study fulfills the US EPA guideline requirements for seedling emergence and vegetative vigor studies (Subdivision J, §123-1 (a & b; TIER II)). This study is classified as CORE.

§141-1. MRID 45831124 XDE-638: Acute Contact Toxicity Test with the Honeybee, *Apis mellifera*

The honey bee, *Apis mellifera*, was exposed to XDE-638 for 48 hours, at a single nominal concentration of 100 µg a.i./bee. By 48 hours, mortality was 13% in the 100 µg a.i./bee treatment group. There was 3% negative control mortality and 0% solvent control mortality. No sublethal effects were observed during the study.

The LD_{50} value was >100 µg a.i./bee. As a result, XDE-638 is categorized as practically nontoxic to honeybees on an acute contact basis. This study is scientifically sound and it satisfies the EFED concerning the guideline requirements. It is CORE

§141-1. MRID 45831127 *[Penoxsulam end-use product]* GF-443: Acute Contact Toxicity Test with the Honeybee *(Apis mellifera)*

The honey bee, *Apis mellifera*, was exposed to GF-443 for 48 hours, at nominal concentrations of 0.1, 1.0, 10, and 100 µg a.i./bee. Since GF-443 is only 21.9% a.i., penoxsulam, the test concentrations were 0.02, 0.22, 2.19, and 21.9 µg a.i./bee.

The LD_{50} was >22 µg a.i./bee and the NOAEC was 22 µg a.i./bee. This study is scientifically sound but does not fully satisfy the EFED guideline requirements for a contact toxicity test with honey bees (§141-1 or 850.3020). It is classified as Supplemental. It can be used for a risk assessment and need not be repeated.

OPPTS DRAFT 850.1735. MRID 45831102 XDE-638 - The Full Life-Cycle Toxicity To Midge (*Chironomus riparius*) Under Static Conditions Using Spiked Sediment and Spiked Water.

Mean-measured concentrations were <0.33 (<LOQ; control), 7.1, 15, 31, 61, and 140 mg a.i./L. . No treatment-related effects on percent emergence were observed; mean percent emergence ranged from 90-96% for all test and control groups.

Based on reductions in the development rate, the NOAEC and LOAEC were 7.1 and 15 mg a.i./L, respectively. This study was designed to fulfill OECD DRAFT Guidelines 218 and 219, and does not fulfill any current U.S. EPA guideline. This study is scientifically sound, and provides useful information on the 28-day toxicity of XDE-638 Technical to the midge, *Chironomus riparius*, under static conditions. Dry weight by sex, which has been found to be the most sensitive pen-point (MRID 45831028) was not assessed. This study is classified as SUPPLEMENTAL.

Appendix E Screening Level Risk Quotients Presumptive Levels of Concern

Table E1. Risk Presumptions for Terrestrial Organisms

Risk Presumptions	RQ	LOC
Birds		
Acute High Risk	EEC [a]/LC_{50} or LD_{50}/sqft [b] or LD_{50}/day [c]	0.5
Acute Restricted Use	EEC/LC_{50} or LD_{50}/sqft or LD_{50}/day (or LD_{50} < 50 mg/kg)	0.2
Acute Species	EEC/LC_{50} or LD_{50}/sqft or LD_{50}/day	0.1
Chronic Risk	EEC/NOAEC	1
Wild Mammals		
Acute High Risk	EEC/LC_{50} or LD_{50}/sqft or LD_{50}/day	0.5
Acute Restricted Use	EEC/LC_{50} or LD_{50}/sqft or LD_{50}/day (or LD_{50} < 50 mg/kg)	0.2
Acute Species	EEC/LC_{50} or LD_{50}/sqft or LD_{50}/day	0.1
Chronic Risk	EEC/NOAEC	1

[a] abbreviation for Estimated Environmental Concentrations (ppm) on avian/mammalian food items

[b] $\frac{mg/ft^2}{LD_{50} * wt. of bird}$ [c] $\frac{mg\ of\ toxicant\ consumed/day}{LD_{50} * wt. of bird}$

Table E2. Risk presumptions for aquatic organisms

Risk Presumptions	RQ	LOC
Acute High Risk	EEC [a]/LC_{50} or EC_{50}	0.5
Acute Restricted Use	EEC/LC_{50} or EC_{50}	0.1
Acute Species	EEC/LC_{50} or EC_{50}	0.005
Chronic Risk	EEC/NOAEC	1

[a] EEC = (ppm or ppb) in water

Table E3. Risk presumptions for plants

Risk Presumptions	RQ	LOC
Plant Inhibiting Terrestrial and Semi-Aquatic Areas		
Acute High Risk	EEC [a] /EC_{25}	1
Acute Species	EEC/EC_{05} or NOAEC	1
Aquatic Plants		
Acute High Risk	EEC [b] /EC_{50}	1
Acute Species	EEC/EC_{05} or NOAEC	1

[a] EEC = lbs a.i./acre

[b] EEC = (ppm or ppb) in water

Appendix F
AgDRIFT Modeling Approach and Results

The AgDRIFT model (Version 2.01) was used to refine the spray drift exposure estimate for terrestrial plants. Downwind spray drift buffers were developed for possible use in mitigating risks for endangered terrestrial plants that grow in close proximity to rice fields that may be treated with liquid spray applications of penoxsulam. The model was used to estimate spray buffer distances for ground and aerial application to reach the NOAEC and EC_{25} doses for the most sensitive monocot and dicot species in the seedling emergence and the vegetative vigor studies. The standard toxicity level EFED uses for calculating risk quotients for non-endangered terrestrial plants is the EC_{25}. For endangered plants, the NOAEC (or EC_{05} if a NOAEC value is not available) is used. Seedling emergence endpoints are representative of exposure through soil to germinating plants, while vegetative vigor endpoints are representative of foliar exposure. The terrestrial plant measurement endpoints used in the model are specified in Table F- 1.

Table F-1. Agdrift Input Parameters for Terrestrial Plant Measurement Endpoints

Test Type/ Crop	Most Sensitive Study Species	NOAEC (g ai/ha) /Fraction Applied[1]	EC_{25} (g ai/ha) / Fraction Applied[1]	Most sensitive parameter
Seedling Emergence: Monocot	Onion	0.41 / 0.0082	1.1 / 0.022	Shoot Weight
Seedling Emergence: Dicot	Sugarbeet	1.2 / 0.024	3.2 / 0.064	Shoot Weight
Vegetative Vigor: Monocot	Ryegrass	0.41 / 0.0082	17 / 0.34	Shoot Weight
Vegetative Vigor: Dicot	Soybean	1.2 / 0.024	3.9 / 0.078	Shoot Weight

[1] The fraction of the application rate = NOAEC or the EC_{25}/maximum application rate of penoxsulam (50 g ai/ha of 0.0446 lb ai/A).

A summary of the results of the AgDRIFT modeling for ground and aerial application of penoxsulam is presented in Table F-2. Downwind spray drift buffers or distances required to dissipate spray drift to NOAEC levels are estimated for both monocot and dicot terrestrial plant species and for ground and aerial applications of penoxsulam. Dissipation to the no effect level was modeled in order to provide potential buffer distances that are protective of endangered terrestrial plant species. Dissipation distances to the EC_{25} level were also modeled in order to provide potential buffer distances required to protect non-endangered terrestrial plant species. The range of dissipation distances is dependant on a number of input variables including droplet size, release height, etc., which are discussed in further detail for ground and aerial applications below. As expected, modeled ground boom applications resulted in lower drift deposition distances than modeled aerial applications in all instances. Modeled high end dissipation

distances for aerial application of penoxsulam are approximately 5 and 3 times higher than ground boom applications for endangered monocots and dicots, respectively.

Table F-2. Summary of AgDRIFT Modeling Results for Endangered Plant Species		
Crop	**Dissipation Distance for Ground Application (feet)**	**Dissipation Distance for Aerial Application (feet)**
Monocots	46 - 282	466 - 1,385
Dicots	13 - 105	187 - 341

Ground Application

The most important factors affecting drift from ground boom applications are spray quality (droplet size), release height, and wind speed. The ground boom part of AgDRIFT is based on field trial data from bare ground applications. The results of the model reflect the quality and conditions of the data on which it was based. The data from the field trials were grouped into categories by spray quality (droplet size) and release height. Results from field trials conducted with different wind speeds were averaged. The average wind speed over all trials was approximately 10 mph, which is consistent with the label language for penoxsulam. AgDRIFT outputs for ground boom applications estimate the 50^{th} and 90^{th} percentile of data collected from field trials. For this analysis, the 90^{th} percentile was used to provide protective dissipation distances.

Because the label for penoxsulam does not specify release height or droplet size for ground applications, the AgDRIFT model was run for all four scenarios (high boom and fine spray, low boom and fine spray, high boom and medium/coarse spray, and low boom and medium/coarse spray) to provide a range of possible buffer distances. All drop size descriptions are based on ASAE S-572 standard definitions. High and low boom heights are representative of 4 and 2 foot release heights, respectively. The output of the AgDRIFT model provides distances (in feet) required to dissipate spray drift to the NOAEC and EC_{25} levels. Buffer distances are provided for both types of tests (i.e., seedling emergence (SE) and vegetative vigor (VV)) using the most sensitive monocot and dicot species (Table F-1). The results of the AgDRIFT model for ground application of penoxsulam are provided in Table F- 3.

Table F-3. Results of AgDRIFT Modeling for Ground Application of Penoxsulam					
Species	**Test Type**	**Distance Required to Dissipate Spray Drift to NOAEC/EC_{25} Levels (feet)**			
		High boom; fine spray (NOAEC/EC_{25})	**Low boom; fine spray (NOAEC/EC_{25})**	**High boom; med/coarse spray (NOAEC/EC_{25})**	**Low boom; med/coarse spray (NOAEC/ EC_{25})**
Onion (Monocot)	SE	282 / 115	118 / 43	82 / 26	46 / 13
Sugarbeet (Dicot)	SE	105 / 39	39 / 16	23 / 10	13 / 7
Ryegrass (Monocot)	VV	282 / 10	118 / 3	82 / 3	46 / 3
Soybean (Dicot)	VV	105 / 33	39 / 13	23 / 7	13 / 7

The results of the AgDRIFT modeling for ground application of penoxsulam show that a buffer distance of 282 feet is required to dissipate spray drift to NOAEC levels (under worst case conditions of high boom and fine spray) for seedling emergence and vegetative vigor, based on the most sensitive species, which are both monocots. Dissipation distances required for no effects to the most sensitive species are reduced to 118 feet (based on low boom and fine spray), 82 feet (based on high boom and medium/course spray), and 46 feet (based on low boom and medium/course spray). Dissipation distances for dicots are less than those predicted for monocots, with NOAEC-level values ranging from 13 to 105 feet. As expected, ground boom dissipation distances were affected by both droplet size and release height. Therefore, spray drift can be reduced by lowering the release height and/or increasing the spray droplet size. Resulting label language should identify ASAE S-572 as the droplet sizing standard.

Aerial Application

The most important factors affecting drift from aerial applications are spray droplet size, release height, and wind speed. The aerial part of the AgDRIFT model predicts mean values based on the inputs provided. The Tier I aerial results were generated using the specified droplet size spectra, 10 foot release height, and a 10 mph wind speed. When wind speed and/or release height is lower than the modeled values, the spray drift levels would expected to be lower. Conversely, in instances where applications may be made in higher wind speeds or at a higher release height, these inputs may not be adequately conservative and higher tier modeling may be necessary.

Label guidelines for aerial application of penoxsulam specify a medium to coarse droplet size category (per S-572 ASAE standard), and a spray volume of 10 gallons per acre. In addition, the

distance between the outer most nozzles on the boom must not exceed two-thirds (2/3) of the wingspan of fixed-wing aircraft (or 3/4 of the helicopter rotor width), and nozzles must always point backward parallel to the air stream and never downward more than 45 degrees. Although the label specifies a medium to coarse droplet size for aerial application of penoxsulam, fixed winged applications (applications made by airplanes) are limited in the coarsest droplet size that can be sprayed. Typical fixed wing aerial application speeds exceed 120 mph. At these speeds, coarse droplets shatter and produce medium or finer sprays. Thus, it is generally inappropriate to model coarse sprays for fixed wing applications without some restriction on flight speed. For the purpose of AgDRIFT modeling, fine to medium spray droplet size was modeled as a high end drift scenario. In addition, other ASAE droplet sizes including medium and medium/coarse sprays were also considered.

Tier I Aerial Modeling

The AgDRIFT Tier I model for aerial application limits the input parameters to droplet size only. As stated above, the Tier I model was run for both fine to medium sprays (as a high end scenario) and medium/coarse sprays. The output of the Tier I AgDRIFT model provides distances required to dissipate spray drift to the NOAEC and EC_{25} levels. Similar to the ground application modeling, buffer distances are provided for both types of tests using the most sensitive monocot and dicot species. The results of the AgDRIFT Tier I model for aerial application of penoxsulam are provided in Table F-4.

Table F-4. Results of AgDRIFT Tier I Modeling for Aerial Application of Penoxsulam

Species	Test Type	Distance Required to Dissipate Spray Drift to NOAEC/EC_{25} Levels (feet)	
		Fine to Medium Spray (NOAEC/EC_{25})	Medium to Coarse Spray (NOAEC/EC_{25})
Onion (Monocot)	SE	>1,000* / 430	555 / 223
Sugarbeet (Dicot)	SE	390 / 151	207 / 89
Ryegrass (Monocot)	VV	>1,000* / 10	555 / 10
Soybean (Dicot)	VV	390 / 125	207 / 79

* The maximum dissipation distance from the edge of the field in the Tier I aerial model is 1000 feet.

The results of the Tier I aerial AgDRIFT modeling show that a buffer distance of greater than 1,000 feet is required to dissipate spray drift to no effect levels for monocots under high end conditions of fine to medium spray drift. The dissipation distance for monocot plant species decreases to 555 feet, based on the use of a medium to coarse droplet size. Dissipation distances for no effect levels to dicots are 390 feet for fine to medium sprays and 207 feet for medium to

coarse sprays.

Tier II Aerial Modeling

Tier II aerial spray drift estimates were also derived for penoxsulam because this level of modeling allows for greater control over input and output options. A list of the non-default input parameters used in the Tier II aerial modeling is provided in Table F-5. For Tier II modeling, a wind speed of 10 mph (maximum recommended wind speed on the label) and a release height of 10 feet are assumed. The results of the AgDRIFT Tier II model for aerial application of penoxsulam are provided in Table F-6.

Table F-5. Tier II Aerial AgDRIFT Model Input Parameters

Variable	Value	Justification for Use
Aircraft boom length	70%	Based on information contained in the label
Drop Size	Fine to medium , medium, and medium/coarse sprays were considered	Three drop sizes were considered to account for the range of possible scenarios
Non-volatile rate of spray material	1.74 lb/A	Sum of non-volatiles in the formulation plus the crop oil concentrate, based on the maximum label rate of application
Active rate of spray material	0.0446 lbs a.i./A	Maximum application rate of penoxsulam
Spray volume rate	10 gallons/A	Specified in the label

Table F-6. Results of AgDRIFT Tier II Modeling for Aerial Application of Penoxsulam

Species	Test Type	Distance Required to Dissipate Spray Drift to NOAEC/EC_{25} Levels (feet)		
		Fine to Medium Spray (NOAEC/EC_{25})	Medium Spray (NOAEC/EC_{25})	Medium to Coarse Spray (NOAEC/EC_{25})
Onion (Monocot)	SE	>1,000* / 371	787 / 276	466 / 200
Sugarbeet (Dicot)	SE	341 / 141	259 / 108	187 / 66
Ryegrass (Monocot)	VV	>1,000* / 13	787 / 10	466 / 7

Soybean (Dicot)	VV	341 / 115	259 / 79	187 / 52

* The maximum dissipation distance from the edge of the field in the Tier II aerial model is 1000 feet.

Similar to the Tier I model, the results of the Tier II aerial AgDRIFT modeling show that a buffer distance of greater than 1,000 feet is required to dissipate spray drift to no effect levels for monocots under worst case conditions of fine to medium spray drift. The dissipation distance for monocot plant species decreases from >1,000 feet to <787 feet, based on the use of a medium to coarse droplet size. Dissipation distances for no effects to dicots are 341 feet for fine to medium sprays and <259 feet for medium to coarse sprays.

Tier III Aerial Modeling

Tier III aerial spray drift estimates were modeled for fine to medium spray no effect levels for monocots because the dissipation distance can be extended beyond the 1,000 foot limit seen in the Tier I and Tier II models. All input parameters for the Tier III model were identical to those entered into the Tier II model. Based on these inputs, **the distance required to dissipate aerial spray drift to NOAEC levels for monocots is 1,385 feet.**

Phytotoxicity and Downwind Distance

Distances downwind from application areas at which a particular tested plant species would exhibit a toxic effect level were estimated using the AgDRIFT model and registrant-submitted phytotoxicity data (458311-16, Schwab, 2001) for penoxsulam. EC_{25} values (for seedling emergence and vegetative vigor shoot weight) of the tested species were used with the slope of the dose-response relationship for each species to calculate EC_{10} to EC_{90} effect levels. Plant species with high (steep) slopes show large increases in toxicity from small increases in exposure, whereas species with low (shallow) slopes show small increases in toxicity from relatively large increases in exposure. A log normal toxicity distribution is assumed. Effects values were entered into an Excel spreadsheet assuming Tier I AgDRIFT (Version 2.01) deposition distance results and the maximum penoxsulam application rate (0.0446 lb a.i./A).

The effect levels (EC_{10} to EC_{90}) for all 10 test terrestrial plant species were compared to estimated environmental concentrations resulting from spray drift to display the distances to which a particular effect level is expected to occur. For example, the height of the bar associated with an effect of 10% is the downwind distance at which spray deposition is expected to be equal to the EC_{10} toxicity level. The height of the bar associated with an effect of 90% is the downwind distance at which spray deposition is expected to be equal to the EC_{90} toxicity level. The downwind distance from the application site is shown on the vertical axis, and plant species and percent effects values are shown on the horizontal axes.

Ground Application

The ground application model conditions assume a 10 mph wind. Figures F-1 and F-2 illustrate the potential seedling germination effects to nontarget plants downwind from a single ground application (0.0446 lb ai/A or 50 g ai/ha) of penoxsulam, based on upper-bound (high boom, fine spray) and lower bound (low boom, medium/coarse spray) deposition distances, respectively. Figures F-3 and F-4 illustrate the potential vegetative vigor effects to nontarget plants downwind from a single application of penoxsulam, based on upper-bound (high boom, fine spray) and lower bound (low boom, medium/coarse spray) deposition distances, respectively. Although Figures F-1 through F-4 show effects levels, they do not show distances at which plants are likely to be killed outright. When plants are tested by pesticide companies for efficacy, a 70% effect level is generally considered to be a threshold for lethal effects to a health weed (Pallett, 2003). Therefore, the EC_{70} effect level is used to provide an estimate of when non-target plants are expected to have a high likelihood of rapid death, similar to the desired effect for weed species. In general, ground applications using high boom and fine sprays are expected to produce higher drift levels than low boom and medium/coarse sprays, resulting in greater phytotoxicity at greater downwind distances.

The results of the seedling emergence toxicity test show that six out of the ten plants tested exhibit no adverse effects when exposed to maximum application rates of penoxsulam. Reduction in shoot weight was observed in only one monocot (onion) and three dicots (kale, sugarbeet, and tomato). Under the highest ground boom drift conditions (4 foot boom and fine spray; Figure F-1), four plant species (onion, kale sugarbeet, and tomato) would be expected to be killed in the area that stretches from 3 to 13 feet downwind of the treated field. Under the same conditions of high boom and fine spray, these 4 species are expected to be affected at the EC_{10} level at distances of <70 feet for kale, sugarbeet, and tomato and approximately 415 feet for onion. Under the lowest ground boom drift conditions (2 foot boom and medium/coarse spray; Figure F-2), onion, kale, sugarbeet, and tomatoes would be expected to be killed in the area that stretches only 2 feet downwind of the treated field. Tested species, under similar low boom and medium/coarse spray, would be expected to be affected at the EC_{10} level at 10 feet (sugarbeet, kale, and tomato) and 66 feet (onion).

The results of the vegetative vigor toxicity test show that two out of the ten plants tested, including corn and wheat, show no adverse effects when exposed to maximum application rates of penoxsulam. The most sensitive endpoint for the vegetative vigor test is shoot weight. Reduction in shoot weight was observed as the most sensitive endpoint in only one monocot (ryegrass) and five dicots (kale, soybean, sugarbeet, tomato, and cucumber). Under the highest ground boom drift conditions (4 foot boom and fine spray; Figure F-3), three plant species (soybean, sugarbeet, and kale) be expected to be killed in the area that stretches from 5 to 20 feet downwind of the treated field. Under the same conditions of high boom and fine spray, these 3 species are expected to be affected at the EC_{10} level at distances of 26 to 46 feet. In addition, test species including ryegrass and tomato would also be affected at the EC_{10} level at respective distances of 171 and 46 feet. Under the lowest ground boom drift conditions (2 foot boom and

medium/coarse spray; Figure F-4), sugarbeet, soybean, and kale would be expected to be killed in the area that stretches only < 3 feet downwind of the treated field. Tested species, under similar low boom and medium/coarse spray, would be expected to be affected at the EC_{10} level at < 7 feet. Ryegrass and tomato would also be expected to be affected at the EC_{10} level at distances of 20 and 5 feet, respectively.

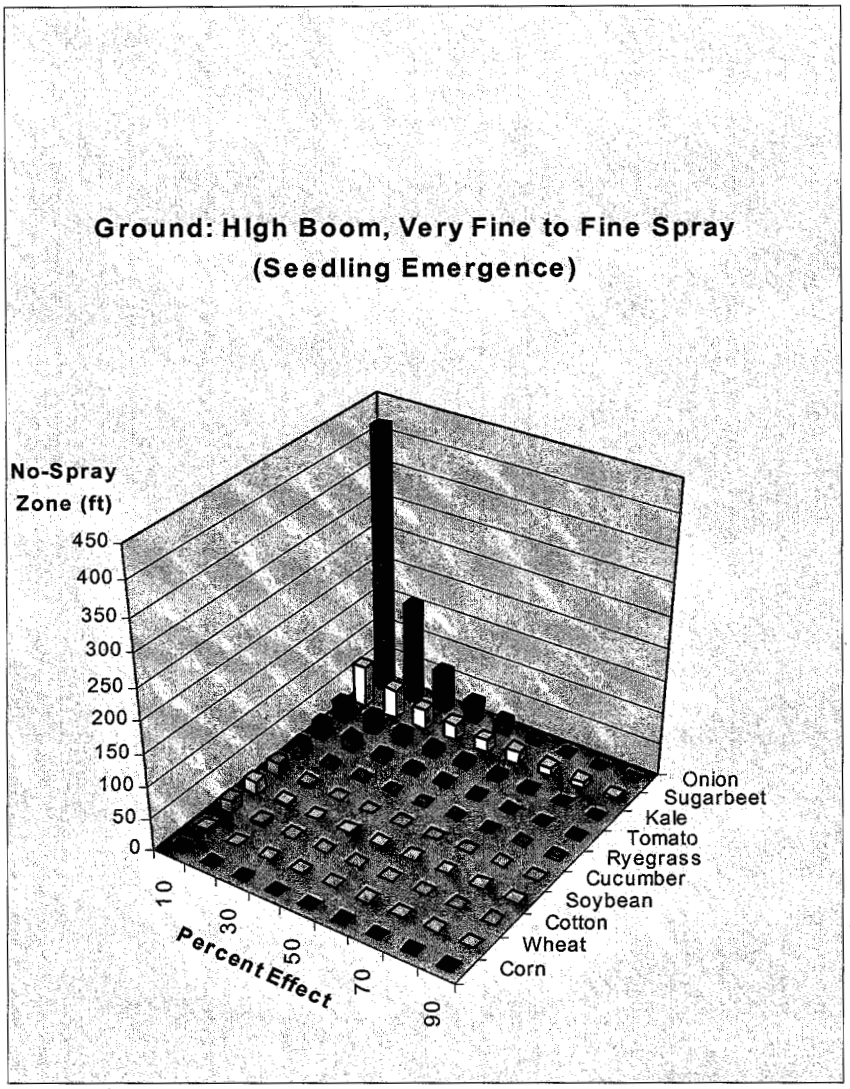


Figure F-1. Predicted **seedling emergence phytotoxicity** levels and associated downwind distances from a **ground boom** application conducted with a **fine spray** in an approximate 10 mph wind with a **4 foot release height** at an application rate of 0.0446 lbs penoxsulam per acre.

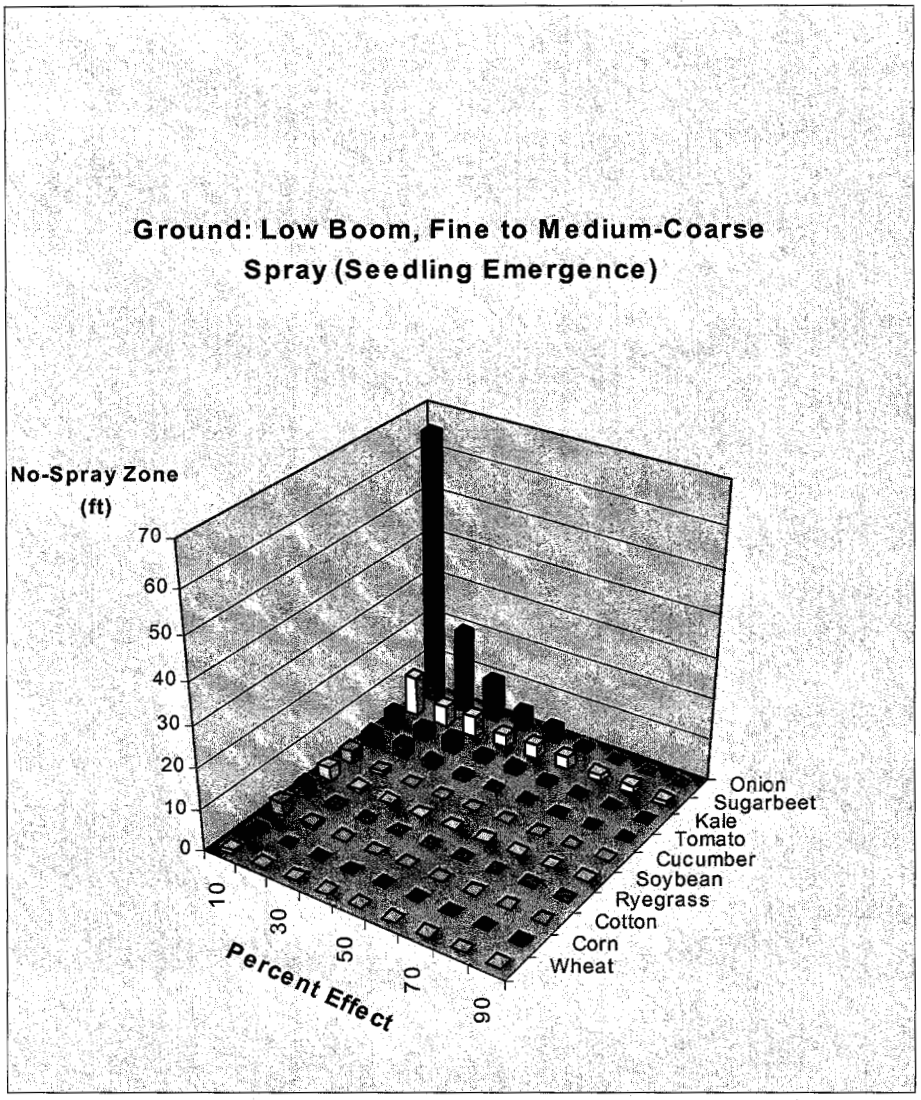


Figure F-2. Predicted **seedling emergence phytotoxicity** levels and associated downwind distances from a **ground boom** application conducted with a **medium/coarse spray** in an approximate 10 mph wind with a **2 foot release height** at an application rate of 0.0446 lbs penoxsulam per acre.

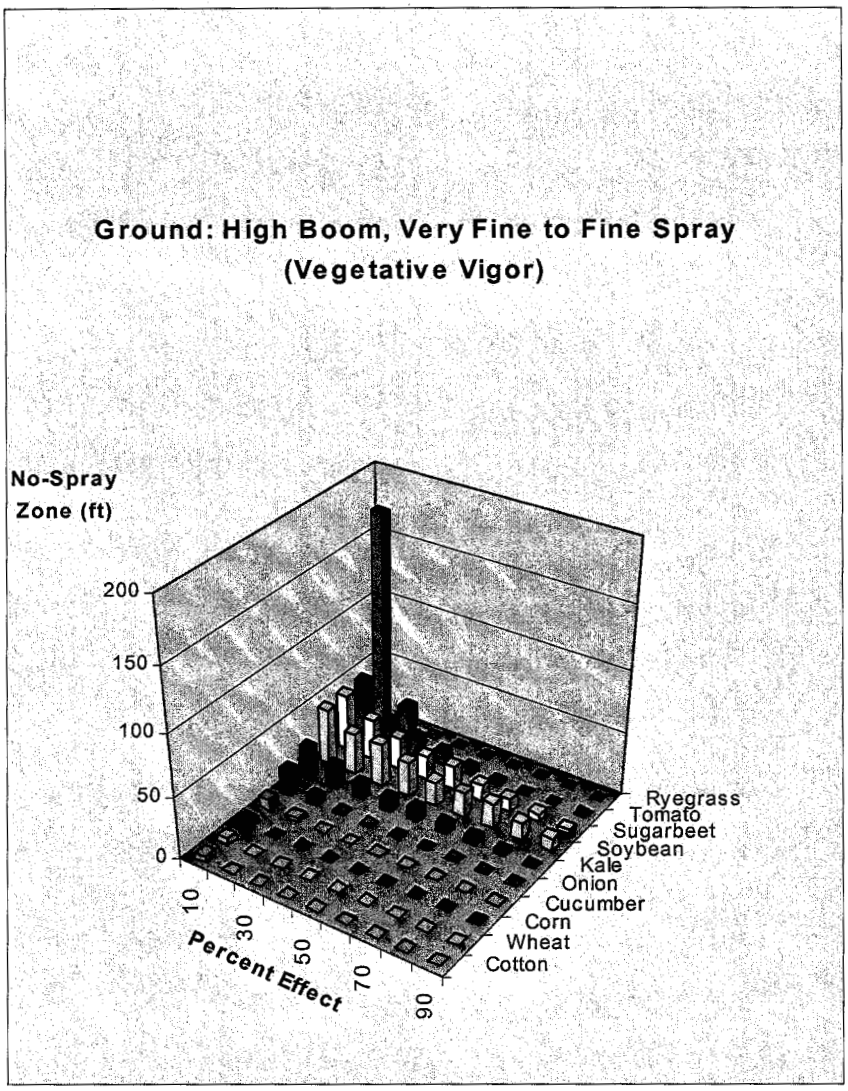


Figure F-3. Predicted **vegetative vigor phytotoxicity** levels and associated downwind distances from a **ground boom** application conducted with a **fine spray** in an approximate 10 mph wind with a **4 foot release height** at an application rate of 0.0446 lbs penoxsulam per acre.

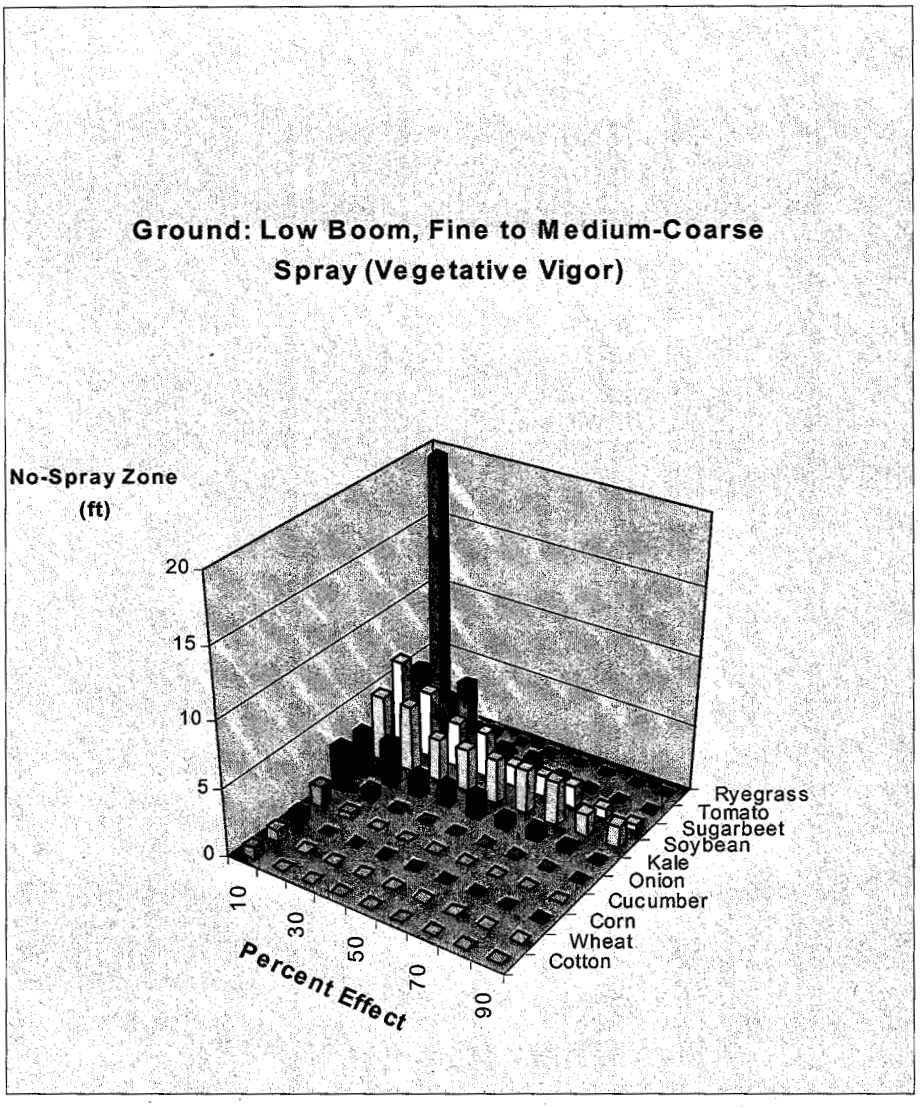


Figure F-4. Predicted **vegetative vigor phytotoxicity** levels and associated downwind distances from a **ground boom** application conducted with a **medium/coarse spray** in an approximate 10 mph wind with a **2 foot release height** at an application rate of 0.0446 lbs penoxsulam per acre.

Aerial Application

For aerial application of penoxsulam, Tier I aerial AgDRIFT modeling input parameters (i.e., 10 mph wind and a 10 foot release height) were assumed. Figures F-5 and F-6 illustrate the potential seedling germination effects to nontarget plants downwind from a single aerial application (0.0446 lb ai/A or 50 g ai/ha) of penoxsulam, based on upper-bound (fine to medium spray) and lower bound (medium to coarse spray) deposition distances, respectively. Figures F-7 and F-8 illustrate the potential vegetative vigor effects to nontarget plants downwind from a single aerial application of penoxsulam, based on upper-bound (fine to medium spray) and lower bound (medium to coarse spray) deposition distances, respectively. In general, fine to medium sprays are expected to produce higher drift levels than medium to coarse sprays, resulting in greater phytotoxicity at greater downwind distances.

Under the highest drift conditions (fine to medium spray; Figure F-5), only sugarbeet would be expected to be killed from seedling germination effects (i.e., EC_{70}) in the area that stretches 98 feet downwind of the treated field. Under the lowest aerial drift conditions (medium to coarse spray; Figure F-6), sugarbeet would be expected to be killed in the area that stretches 26 feet downwind of the treated field. Under conditions of fine to medium spray, species expected to be affected at the seedling emergence EC_{10} level at distances of >1,000 feet include onion and sugarbeet. In addition, kale, tomato, and ryegrass would be expected to be affected at the EC_{10} level at distances of approximately 164 to 505 feet. Tested species, under aerial application of medium to coarse spray, would be expected to be affected at the EC_{10} level at >1,000 feet (onion) and <282 feet (sugarbeet, kale, tomato, ryegrass).

Under the highest aerial drift conditions (fine to medium spray; Figure F-7), three plant species (soybean, sugarbeet, and kale) would be expected to be killed via foliar exposure in the area that stretches from 7 to 164 feet downwind of the treated field. Under the same conditions of fine to medium spray, these 3 species are expected to be affected at the EC_{10} level at distances of 308 to 761 feet. In addition, test species including ryegrass and tomato would also be affected at the EC_{10} level at respective distances of >1,000 and 636 feet. Under the lowest aerial drift conditions (medium to coarse spray; Figure F-8), sugarbeet, soybean, and kale would be expected to be killed in the area that stretches only < 59 feet downwind of the treated field. Tested species, under similar medium to coarse spray, would be expected to be affected at the EC_{10} level at < 177 feet. Ryegrass and tomato would also be expected to be affected at the EC_{10} level at distances of 971 and 171 feet, respectively.

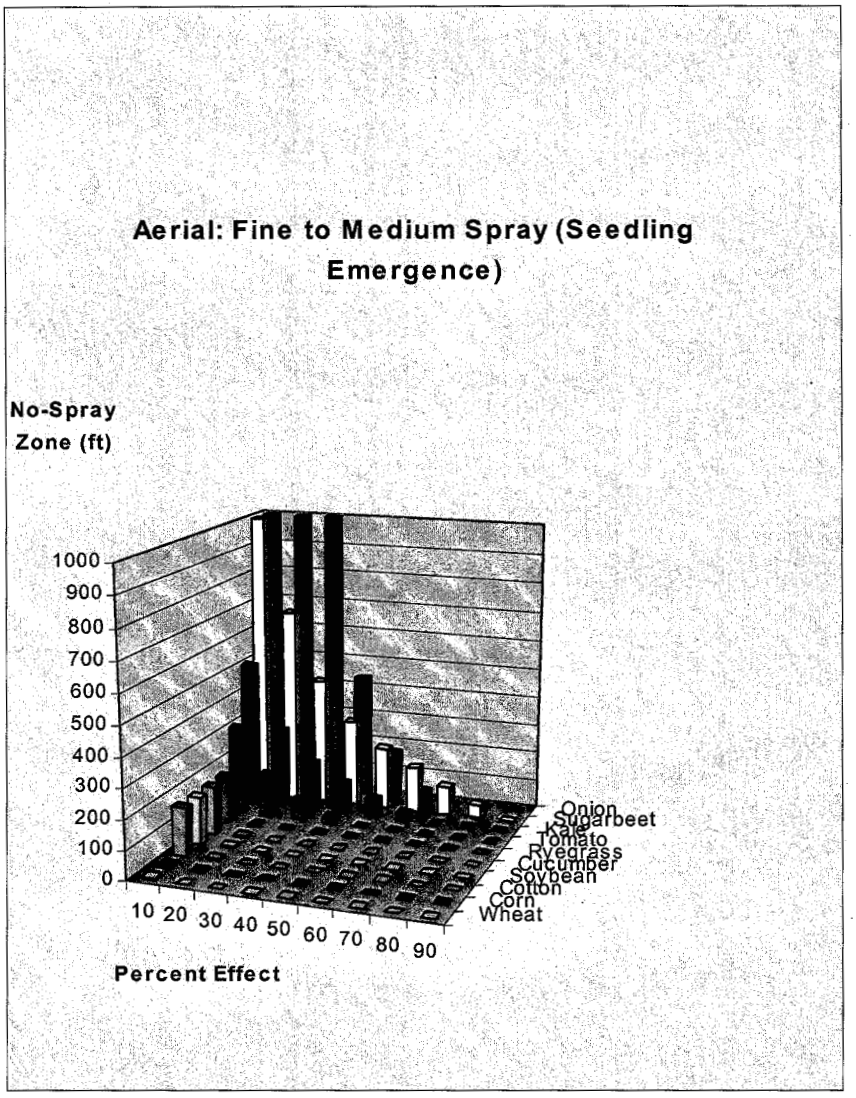


Figure F-5. Predicted **seedling emergence phytotoxicity** levels and associated downwind distances from an **aerial** application conducted with a **fine to medium spray** in an approximate 10 mph wind with a 10 foot release height at an application rate of 0.0446 lbs penoxsulam per acre.

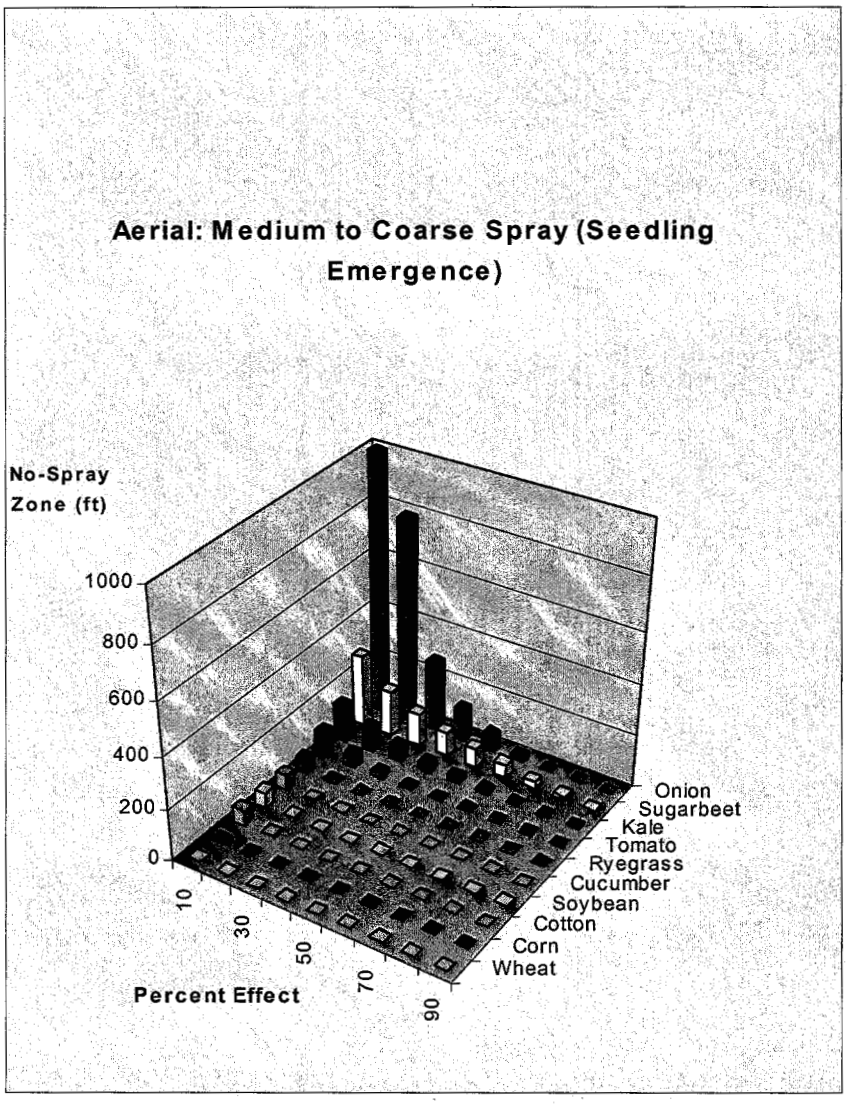


Figure F-6. Predicted **seedling emergence phytotoxicity** levels and associated downwind distances from an **aerial** application conducted with a **medium to coarse spray** in an approximate 10 mph wind with a 10 foot release height at an application rate of 0.0446 lbs penoxsulam per acre.

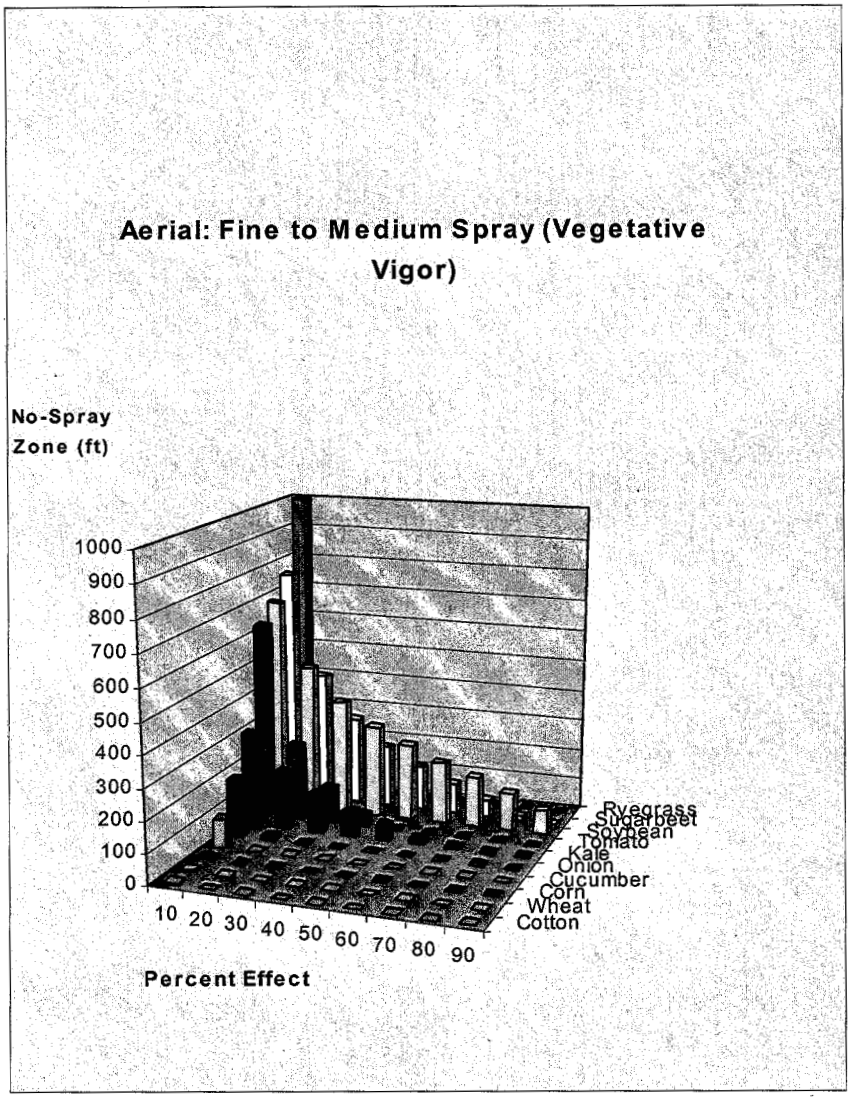


Figure F-7. Predicted **vegetative vigor phytotoxicity** levels and associated downwind distances from an **aerial** application conducted with a **fine to medium spray** in an approximate 10 mph wind with a 10 foot release height at an application rate of 0.0446 lbs penoxsulam per acre.

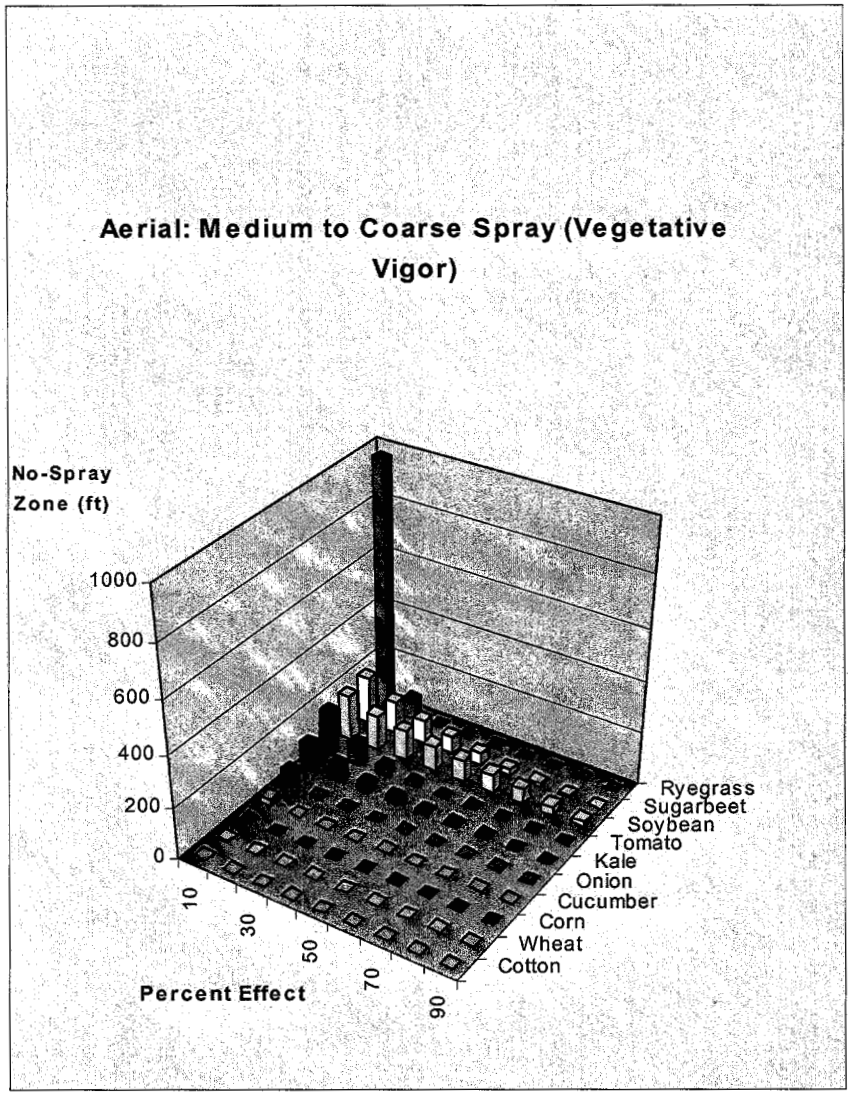


Figure F-8. Predicted **vegetative vigor phytotoxicity** levels and associated downwind distances from an **aerial** application conducted with a **medium to coarse spray** in an approximate 10 mph wind with a 10 foot release height at an application rate of 0.0446 lbs penoxsulam per acre.

Labeling

The results of this analysis suggest that mandatory product labeling that places restrictions on droplet size and potentially flight speed for aerial applications and droplet size and boom height for ground boom application may reduce risks associated with penoxsulam applications. Any resulting label language should identify ASAE S-572 as the droplet sizing standard.

Uncertainites

There are a number of uncertainties associated with the assessment of potential effects of penoxsulam spray drift to plants. It may be possible to further refine this assessment with additional information addressing the following uncertainties:

- The representativeness of tested species for non-target plant species in penoxsulam use areas. It is possible that woody and other perennial plant species may be exposed to spray drift in penoxsulam use areas near rice fields; however, their sensitivity to penoxsulam is uncertain. Toxicity data on a wider range of plants could be used to reduce uncertainty related to the potential effects of penoxsulam on perennial and woody species at field edges and downwind of treated fields.

- The adequacy of laboratory spraying treatments in representing spray drift far from field boundaries. Plants in laboratory studies are exposed to herbicide in volumes of carrier that are adequate to cover the test plants. Plants exposed to spray drift downwind of field boundaries would contact the same amount of herbicides tested in the laboratory, but in much lower volumes of carrier. Plants are exposed to spray drift far away from the field edge in discrete spots where droplets impact the plant foliage, whereas plants are covered with a diffuse coating in lab studies. The effect of small concentrated exposures relative to diffuse exposure is uncertain. Data on the effect of exposure volume on phytotoxicity could be used to refine effect level estimates.

References

Pallett, K. Efficacy testing processes n Industry: relevance for NTTP assessment. Efficacy Data Workshop. August 20, 2003. Office of Pesticide Programs, Crystal City, Arlington, VA.

Schwab. D. 2001. Effects of XDE-638 on the Emergence and Vegetative Vigor of Non-Target Terrestrial Plants (Tier II). Unpublished study performed by ABC Laboratories, Inc., Columbia, Missouri. Laboratory Study No. 46089. Study submitted by Dow AgroSciences LLC, Indianapolis, In.

Appendix G Summary of Endangered / Threatened Species Assessment

Dow AgroSciences (hereafter referred to as Dow) completed an assessment of potential effects on Federally listed threatened and endangered species from the use of penoxsulam in U.S. rice (Dow AgroSciences LLC, 2004). The report was intended to support EPA's review process by providing an evaluation of potential risks for adverse effects to Federally listed threatened and endangered species related to the proposed use of penoxsulam in rice. In addition, risk mitigation measures were proposed where potential risks to threatened and endangered species exceed EPA's Levels of Concern (LOCs). As part of this effort, Dow completed a Tier I ecological risk assessment and species-specific endangered/threatened species assessment.

The results of the ecological risk assessment were used to select taxa of threatened and endangered species for further evaluation. Consistent with its activity as a herbicide, the results of the Dow Tier I risk assessment concluded that penoxsulam exceeds LOCs for non-target aquatic and terrestrial plants.

Dow used the Information Management System (IMS) developed by the FIFRA Endangered Species Task Force (FESTF) to identify those U.S. rice-producing counties where Federally listed threatened and endangered plant species also occur. For counties where overlap in rice production and endangered species occurred, Geographical Information System (GIS) technology was used to produce cartographic maps that provide detailed spatial information on the proximity of the species' habitat to rice production.

The results of the county-level overlap of rice production with taxa of concern show that there are a total of 33 dicot and 7 monocot Federally listed threatened and endangered plant species that occur in counties where rice is grown. However, none of the species included in this list are aquatic non-vascular or aquatic vascular plants. Consequently, further analysis was limited to endangered terrestrial plants.

Dow's list of threatened and endangered plant species that occur in rice-producing counties are listed in Table G-1. This list is identical to the endangered species list presented in Appendix G-2 of EPA's ecological risk assessment for penoxsulam, with the exception of several additional endangered species that were added to Dow's list for counties in California as a result of information available from NatureServe and the California Department of Fish and Game Natural Diversity Data Base (CNDDB). In addition, a larger number of counties were included in the endangered species assessment for Missouri. All adjustments to EPA's county-level occurrence data are designated with footnotes in Table G-1.

Federally listed threatened and endangered terrestrial plant species occur in rice-producing counties as follows: 6 Arkansas counties; 13 California counties, 5 Missouri counties; 3 Mississippi counties; and 2 Texas counties. Federally listed threatened and endangered plants were not found to occur in any of the rice-producing counties (parishes) in Louisiana; therefore,

no further analysis was required for this state.

In order to make effects determinations for endangered species/county combinations, analyses were conducted to determine the proximity of these plants relative to rice fields. A "no effects" determination is made if listed species do not co-occur or are located within 1,400 feet (based on EFED's buffer distance for aerial application of penoxsulam; see Appendix D) of rice crops. For county-species combinations that exceed the Agency's endangered species levels of concern, Dow proposes the use of appropriate protective measures to allow a "Not Likely to Adversely Affect" determination. These measures include use of the granular formulation of penoxsulam to essentially eliminate drift, or the use of spray buffers when applying the liquid formulation of penoxsulam with aerial or ground equipment. The proposed spray buffer distances for aerial and ground application of penoxsulam are 1,400 feet and 300 feet, respectively (see Appendix D). A summary of the effects determination by state, county and species is provided in Table G-3. Effects determinations based on listed species proximity analysis are discussed for each state and sub-county below.

In general, there was greater certainty and precision in the spatial analysis conducted for California than for the other rice-producing states, due to the availability of more detailed cropping and element occurrence (EO) data. EO data for listed species included in the Dow assessment had not been obtained for the states of Arkansas, Mississippi, Missouri, or Texas at the time the analyses were conducted. According to Dow, use of EO data for additional analyses in these states might enable a "No Effect" determination in at least some of the instances where this determination could not be made.

Arkansas

Six counties in Arkansas produce rice where threatened and endangered plants occur. According to Dow, an inquiry requesting EO location data was not answered by the Arkansas Natural Heritage Inventory. Therefore, the NatureServe database was queried to provide information on USGS hydrologic units and habitat descriptions for the EOs. Of the six county-species combinations for Arkansas, two counties including Drew and Yell yielded an effects finding of "No Effect" because listed species are not located in areas suitable for rice production. The remaining counties, including Clay, Jackson, Lawrence, and Woodruff, include listed species that overlap areas suitable for rice crops. In the absence of more detailed EO data, protections may be needed in these counties to protect pondberry. Therefore, the effects determination for listed species (pondberry) in these counties is "Not Likely to Adversely Affect" if protections are in place. If no protections are in place, then levels of concern are exceeded for pondberry.

Missouri

As previously mentioned, species/county combinations for Missouri were modified to include additional counties based on NatureServe database records. In addition to Butler, Dunklin, and Ripley Counties, additional listed species were also determined to be present in Mississippi and Wayne Counties, where rice is grown. Of the five county-species combinations for Missouri, effects determinations for Mississippi and Wayne counties were classified as "No Effect"

because listed species are not co-located with rice crops. Detailed examination of the GIS maps for Butler, Dunklin, and Ripley Counties revealed that listed species occurred in locations with distinctive in-field berms used for water management of rice culture. Therefore, combinations for these counties are classified as "Not Likely to Adversely Affect" if protections are in place. If no protections are in place, then levels of concern are exceeded for endangered plant species in these counties.

Mississippi

Pondberry is found in three Mississippi counties including Bolivar, Sharkey, and Sunflower. According to the USFWS recovery plan for this species, the populations of pondberry in Sharkey County are entirely within the Delta National Forest, and thus are protected by programmatic means. Pondberry populations in Bolivar and Sunflower Counties are on private land. Therefore, the effects determination for pondberry in Sharkey County is "No Effect." In the absence of more detailed information, the effects determination for pondberry in Bolivar and Sunflower Counties is "Not Likely to Adversely Affect" if protections are in place. If no protections are in place, then levels of concern are exceeded for pondberry in these counties.

Texas

The Texas Prairie dawn-flower is found in Fort Bend and Harris Counties in Texas where rice production also occurs. According to Dow, an inquiry requesting detailed EO location data from the Texas Natural Heritage Inventory was not answered. Agricultural areas in Fort Bend and Western Harris Counties are located near Buffalo Bayou. Information from the Texas Parks and Wildlife Department indicates that many occurrences of Texas Prairie dawn flower have been observed in the Barker and Addicks Reservoir areas. These reservoirs are large flood control basins for Buffalo Bayou; therefore, rice fields near Buffalo Bayou may require protection for the Texas Prairie dawn flower. The effects determination for Western Harris and Fort Bend Counties is "Not Likely to Adversely Affect" if protections are in place. If no protections are in place in Western Harris and Fort Bend Counties, then levels of concern are exceeded for the Texas Prairie dawn-flower. In Eastern Harris County, the effects determination is "No Effect" because the sparsely vegetated habitat necessary for the Texas Prairie dawn-flower is not present. West of the city of Houston, there appears to be agricultural areas interspersed with grasslands, which could provide habitat for the Texas Prairie dawn-flower. It is unknown if these agricultural areas are used to produce rice; however, if they are, protections may be needed. Therefore, levels of concern for the Texas Prairie dawn-flower are exceeded if no protections are in place. If protections are in place, the effects determination for this portion of Harris County is "Not Likely to Adversely Affect."

California

As previously mentioned, the California endangered species assessment was conducted with a high degree of certainty and precision (as opposed to the other states) due to the availability of more detailed cropping and EO location data. The California Department of Fish and Game Natural Diversity Data Base (CNDDB), a product of the California Natural Heritage Program,

was linked with GIS layers to provide spatially-referenced point EO data. Within 13 counties that grow rice in California, 79 county-species combinations were identified. Of the 13 identified counties, "No Effect" determinations were made for 8 counties (Alameda, Fresno, Madera, Merced, Placer, Sacramento, San Joaquin, and Tehama) because listed species are not located in proximity (i.e., greater than 1,400 feet) to rice crops. Effects determinations for the remaining five counties (Butte, Colusa, Glenn, Stanislaus, and Yolo) are discussed below.

In Butte County, occurrences of endangered species in the southern part of the county are close to, and in some cases, adjacent to rice fields. Protections may be necessary for Butte County meadowfoam, Green's tuctoria, Hoover's spruge, and hairy orcutt grass in the southern half of Butte County. These species are all located within 180 feet of rice fields; therefore, proposed buffer distances of 1,400 feet for aerial application and 300 feet for ground application of penoxsulam would not be protective of these species. Slender orcutt grass is over 5,450 ft from the nearest rice field. Levels of concern are exceeded for the occurrences of Butte County meadowfoam, Green's tuctoria, Hoover's spruge, and Hairy orcutt grass in Butte County; with appropriate protections the determination is "Not Likely to Adversely Affect." Because these listed species are located within the proposed buffer zones for both ground and aerial application of penoxsulam, appropriate protections in Butte County would include restrictions on all liquid applications of penoxsulam. The determination for Slender orcutt grass is "No effect."

Species under consideration in Colusa County include Palmate-bracted bird's beak and Colusa grass. Habitat for these two species is found within the Develan and Colusa National Wildlife Refuges. As a protected area, programmatic management programs should be in place for these wildlife refuges. If not, protections may be needed. Therefore, the effects determination for these endangered plant species is "Not Likely to Adversely Affect" if programmatic management practices are in place; if not, then levels of concern for these species are exceeded.

Rice is grown extensively in Glenn County along the Sacramento River. The EOs are confined to the Sacramento National Wildlife Refuge. Because the wildlife refuge is a protected area, programmatic management practices should be in place. If not, protections may be needed for listed species. The effects determination for Hoover's spurge, Palmate-Bracted Bird's-Beak, and Hairy Orcutt Grass are"Not Likely to Adversely Affect" if programmatic management or protections are in place. If programmatic management or protections are not in place, then levels of concern for these listed species are exceeded.

In Stanislaus County, rice is grown in three small areas. The spatial join distance between Greene's Tuctoria and rice fields is 163 meters (535 feet), indicating that some protections (i.e., restrictions on aerial application of penoxsulam) may be needed for this species. The effects finding for Greene's Tuctoria is "Not Likely to Affect" if protections are in effect. If no protections are in place, then levels of concern for Greene's Tuctoria are exceeded. Greene's Tuctoria is located within the proposed 1,400 foot buffer distance required for aerial application of penoxsulam; therefore, this type of application is not recommended in Stanislaus County. For other listed species in the county, the effects finding is "No Effect."

In Yolo County, the rice producing areas are in the center and eastern parts of the county. The

closest EO of Palmate-bracted Bird's-Beak is approximately 370 meters (1,214 feet) from the nearest rice field. Therefore, in Yolo County, the effects determination for Palmate-bracted Bird's-Beak is " Not Likely to Affect" with protections (i.e., restrictions on aerial application of penoxsulam). With no protections, levels of concern for Palmate-bracted Bird's-Beak are exceeded. Palmate-bracted Bird's-Beak is located within the proposed 1,400 foot buffer distance required for aerial application of penoxsulam; therefore, this type of application is not recommended in Yolo County. The effects determination for Colusa grass and Crampton's tuctoria is "No Effect."

Table G-1. Federally Listed Threatened and Endangered Plant Species in U.S. Rice-Producing Counties - Listed by State and County					
State	**County**	**No. of Species**	**Taxa**	**Scientific Name**	**Common Name**
Arkansas	Clay	1	Dicot	*Lindera melissifolia*	Pondberry
	Drew	1	Dicot	*Geocarpon minium*	– (None)
	Jackson	1	Dicot	*Lindera melissifolia*	Pondberry
	Lawrence	1	Dicot	*Lindera melissifolia*	Pondberry
	Woodruff	1	Dicot	*Lindera melissifolia*	Pondberry
	Yell	1	Dicot	*Ptiliminum nodosum*	Harperella
Missouri	Butler	1	Dicot	*Lindera melissifolia*	Pondberry
	Dunklin	2	Dicot	*Boltonia decurrens*	aster, Decurrent false[1]
			Dicot	*Trifolium stoloniferum*	clover, Running
	Ripley	1	Dicot	*Lindera melissifolia*	Pondberry
	Mississippi	1	Dicot	*Boltonia decurrens*	aster, Decurrent false[1]
	Wayne	1	Dicot	*Trifolium stoloniferum*	clover, Running[2]
Mississippi	Bolviar	1	Dicot	*Lindera melissifolia*	Pondberry
		1	Dicot	*Lindera melissifolia*	Pondberry
		1	Dicot	*Lindera melissifolia*	Pondberry
Texas	Fort Bend	1	Dicot	*Hymenoxys texana*	dawn-flower, Texas (also called Prairie Dawn)
	Harris	1	Dicot	*Hymenoxys texana*	dawn-flower, Texas
California	Alameda	12	Dicot	*Cordylanthus palmatus*	bird's beak, Palmatebracted
			Dicot	*Clarkia franciscana*	clarkia, Presidio
			Dicot	*Dudleya setchellii*	dudleya, Santa Clara Valley
			Dicot	*Amsinckia grandiflora*	fiddleneck, Large-flowered
			Dicot	*Lasthenia conjugens*	goldfields, Contra Costa
			Dicot	*Arctostaphylos pallida*	manzanita, Pallid
			Dicot	*Naverretia leucocephala* spp. *pauciflora*	navarretia, Few-flowered

California (cont.)	Alameda (cont.)		Dicot	*Naverretia leucocephala* spp. *plieantha*	navarretia, Many-flowered
			Dicot	*Parvisedum leiocarpum*	stonecrop, Lake County[3]
			Dicot	*Chorizanthe robusta* var. *robusta*	robust spineflower[4]
			Dicot	*Suaeda californica*	California seablite
			Dicot	*Holocarpha macradenia*	Santa Cruz tarplant[5]
	Butte	5	Dicot	*Limnanthes floccose*	meadowfoam, Butte County
			Dicot	*Chamaesyce hooveri*	spurge, Hoover's
			Mono-cot	*Tuctoria greenei*	tuctoria, Greene's
			Mono-cot	*Orcuttia pilosa*	hairy orcutt grass
			Mono-cot	*Orcuttia tenuis*	slender orcutt grass
	Colusa	2	Dicot	*Cordylanthus palmatus*	bird's beak, Palmatebracted
			Mono-cot	*Neostapfia colusana*	Colusa grass
	Fresno	14	Dicot	*Cordylanthus palmatus*	bird's beak, Palmatebracted
			Dicot	*Sidalcea keckii*	checker-mallow, Keck's
			Dicot	*Dudleya setchellii*	dudleya, Santa Clara Valley
			Dicot	*Caulanthus californicus*	jewelflower, California
			Dicot	*Castilleja campestris* spp. *succulenta*	owl's-clover, Fleshy
			Dicot	*Calyptridium pulchellum*	pussypaws, Mariposa
			Dicot	*Pseudobahia bahiifolia*	sunburst, Hartweg's golden
			Dicot	*Pseudobahia peirsonii*	sunburst, San Joaquin adobe
			Dicot	*Eriastrum hooveri*	wooly-star, Hoover's
			Dicot	*Monolopia (=Lembertia congdonii)*	wooly-threads, San Joaquin

California (cont.)	Fresno (cont.)		Mono-cot	*Orcuttia inaequalis*	San Joaquin Valley orcutt grass
			Dicot	*Camissonia benitensis*	San Benito evening-primrose
			Dicot	*Botrychium lineare*	slender moonwort
			Mono-cot	*Tuctoria greenei*	Greene's tuctoria
	Glenn	3	Dicot	*Chamaesyce hooveri*	spurge, Hoover's
			Mono-cot	*Orcuttia pilosa*	grass, Hairy Orcutt
			Dicot	*Cordylanthus palmatus*	bird's beak, Palmatebracted
	Madera	9	Dicot	*Cordylanthus palmatus*	bird's beak, Palmatebracted
			Dicot	*Lupinus tidestromii*	lupine, Clover
			Dicot	*Castilleja campestris* spp. *succulenta*	owl's-clover, Fleshy
			Dicot	*Calyptridium pulchellum*	pussypaws, Mariposa
			Dicot	*Pseudobahia bahiifolia*	sunburst, Hartweg's golden
			Dicot	*Pseudobahia peirsonii*	sunburst, San Joaquin adobe
			Mono-cot	*Orcuttia pilosa*	grass, Hairy Orcutt
			Mono-cot	*Tuctoria greenei*	Greene's tuctoria
			Mono-cot	*Orcuttia inaequalis*	San Joaquin Valley orcutt grass
	Merced	7	Dicot	*Castilleja campestris* spp. *succulenta*	owl's-clover, Fleshy
			Mono-cot	*Neostapfia colusana*	grass, Colusa
			Mono-cot	*Orcuttia pilosa*	grass, Hairy Orcutt
			Mono-cot	*Tuctoria greenei*	Greene's tuctoria
			Dicot	*Pseudobahia bahiifolia*	sunburst, Hartweg's golden

California (cont.)	Merced (cont.)		Dicot	*Chamaesyce hooveri*	spurge, Hoover's
			Mono-cot	*Orcuttia inaequalis*	San Joaquin Valley orcutt grass
	Placer	2	Dicot	*Berberis (=Mahonia) sonnei*	barberry, Truckee
			Dicot	*Rorippa subumbellata*	Cress, Tahoe yellow
	Sacramento	3	Dicot	*Oenothera deltoids* spp. *howellii*	evening-primrose, Antioch Dunes
			Mono-cot	*Orcuttia viscida*	grass, Sacramento Orcutt
			Mono-cot	*Orcuttia tenuis*	grass, Slender Orcutt
			Mono-cot	*Erigonum apricum var. apricum*	Lone buckwheat
	San Joaquin	4	Dicot	*Cordylanthus palmatus*	bird's beak, Palmatebracted
			Dicot	*Amsinckia grandifloria*	fiddleneck, Large-flowered
			Mono-cot	*Tuctoria greenei*	Greene's tuctoria
			Dicot	*Castilleja campestris* spp. *succulenta*	owl's-clover, Fleshy
	Stanislaus	6	Dicot	*Castilleja campestris* spp. *succulenta*	owl's-clover, Fleshy
			Dicot	*Chamaesyce hooveri*	spurge, Hoover's
			Dicot	*Pseudobahia bahiifolia*	sunburst, Hartweg's golden
			Dicot	*Pseudobahia peirsonii*	sunburst, San Joaquin adobe
			Mono-cot	*Neostapfia colusana*	grass, Colusa
			Mono-cot	*Orcuttia pilosa*	grass, Hairy Orcutt
			Mono-cot	*Tuctoria greenei*	Greene's tuctoria
			Mono-cot	*Orcuttia inaequalis*	San Joaquin Valley orcutt grass

California (cont.)	Stanislaus (cont.)		Dicot	*Atriplex coronata var. notatior*	San Jacinto Valley crownscale
	Tehama	5	Dicot	*Limnanthes floccose*	meadowfoam, Butte County
			Dicot	*Chamaesyce hooveri*	spurge, Hoover's
			Mono-cot	*Orcuttia pilosa*	grass, Hairy Orcutt
			Mono-cot	*Orcuttia tenuis*	grass, Slender Orcutt
			Mono-cot	*Tuctoria greenei*	Greene's tuctoria
	Yolo	2	Dicot	*Cordylanthus palmatus*	bird's beak, Palmatebracted
			Mono-cot	*Neostapfia colusana*	grass, Colusa
			Mono-cot	*Tuctoria mucronata*	Crampton's tuctoria or Solano grass

[1] In U.S. EPA Endangered Species Protection Program (ESPP) database, but not in NatureServe database; therefore, not evaluated in this assessment.
[2] Not in ESPP database, but in NatureServe database; therefore, evaluated in this assessment.
[3] In ESSP database, not in California Department of Fish and Game Natural Diversity Database (CNDDB); therefore, not evaluated in this assessment.
[4] Not in ESSP database, in CNDDB database; therefore, evaluated in this assessment.
[5] Not in ESSP database, listed in CNDDB database as extirpated; therefore, not evaluated in this assessment.

Table G-2: Summary of Plant Species in Counties With at Least 100 Acres of Rice

Plant Species in Counties at Least 100 Acres of Rice

Crop #: 163

SPECIES	SCIENTIFIC NAME	GROUP	KNOWN	STATUS
ARKANSAS				
CLAY, AR Crop Acres: 69785				
PONDBERRY	Lindera melissifolia	PLANT	KNOWN	E
DREW, AR Crop Acres: 15008				
GEOCARPON MINIMUM	Geocarpon minimum	PLANT	KNOWN	E
JACKSON, AR Crop Acres: 84704				
PONDBERRY	Lindera melissifolia	PLANT	KNOWN	E
LAWRENCE, AR Crop Acres: 72906				
PONDBERRY	Lindera melissifolia	PLANT	KNOWN	E
WOODRUFF, AR Crop Acres: 58677				
PONDBERRY	Lindera melissifolia	PLANT	KNOWN	E
YELL, AR Crop Acres: 717				
HARPERELLA	Ptilimnium nodosum	PLANT	KNOWN	E
CALIFORNIA				
ALAMEDA, CA Crop Acres: 684				
BIRD'S-BEAK, PALMATE-BRACTED	Cordylanthes palmatus	PLANT	KNOWN	E
CLARKIA, PRESIDIO	CLARKIA FRANCISCANA	PLANT	POSSIBLE	E
DUDLEYA, SANTA CLARA VALLEY	DUDLEYA SETCHELLII	PLANT	POSSIBLE	E
FIDDLENECK, LARGE-FLOWERED	Amsinckia grandiflora	PLANT	KNOWN	E,CH
GOLDFIELDS, CONTRA COSTA	LASTHENIA CONJUGENS	PLANT	POSSIBLE	E
MANZANITA, PALLID	ARCTOSTAPHYLOS PALLIDA	PLANT	KNOWN	T
NAVARRETIA, FEW-FLOWERED	NAVARRETIA LEUCOCEPHALA SSP. PAUCIF	PLANT	POSSIBLE	E
NAVARRETIA, MANY-FLOWERED	NAVARRETIA LEUCOCEPHALA SSP. PLIEAN	PLANT	POSSIBLE	E
STONECROP, LAKE COUNTY	PARVISEDUM LEIOCARPUM	PLANT	POSSIBLE	E
BUTTE, CA Crop Acres: 102410				
MEADOWFOAM, BUTTE COUNTY	Limnanthes floccosa ssp. californica	PLANT	KNOWN	E
SPURGE, HOOVER'S	CHAMAESYCE HOOVERI	PLANT	KNOWN	T
TUCTORIA, GREEN'S	TUCTORIA GREENEI	PLANT	KNOWN	E
COLUSA, CA Crop Acres: 129974				
BIRD'S-BEAK, PALMATE-BRACTED	Cordylanthes palmatus	PLANT	KNOWN	E
FRESNO, CA Crop Acres: 4771				
ADOBE SUNBURST, SAN JOAQUIN	PSEUDOBAHIA PEIRSONII	PLANT	KNOWN	E
BIRD'S-BEAK, PALMATE-BRACTED	Cordylanthes palmatus	PLANT	KNOWN	E
CHECKER-MALLOW, KECK'S	SIDALCEA KECKII	PLANT	KNOWN	E
DUDLEYA, SANTA CLARA VALLEY	DUDLEYA SETCHELLII	PLANT	POSSIBLE	E
GOLDEN SUNBURST, HARTWEG'S	PSEUDOBAHIA BAHIIFOLIA	PLANT	KNOWN	E
JEWELFLOWER, CALIFORNIA	Caulanthus californicus	PLANT	KNOWN	E
OWL'S-CLOVER, FLESHY	CASTILLEJA CAMPESTRIS SSP. SUCCULENT	PLANT	KNOWN	E
PUSSYPAWS, MARIPOSA	CALYPTRIDIUM PULCHELLUM	PLANT	KNOWN	T
WOOLLY-STAR, HOOVER'S	ERIASTRUM HOOVERI	PLANT	KNOWN	T
WOOLLY-THREADS, SAN JOAQUIN	Lembertia congdonii	PLANT	KNOWN	E
GLENN, CA Crop Acres: 83771				
GRASS, HAIRY ORCUTT	ORCUTTIA PILOSA	PLANT	KNOWN	E
SPURGE, HOOVER'S	CHAMAESYCE HOOVERI	PLANT	KNOWN	T
MADERA, CA Crop Acres: 353				
ADOBE SUNBURST, SAN JOAQUIN	PSEUDOBAHIA PEIRSONII	PLANT	KNOWN	E
BIRD'S-BEAK, PALMATE-BRACTED	Cordylanthes palmatus	PLANT	POSSIBLE	E
GOLDEN SUNBURST, HARTWEG'S	PSEUDOBAHIA BAHIIFOLIA	PLANT	KNOWN	E
GRASS, HAIRY ORCUTT	ORCUTTIA PILOSA	PLANT	KNOWN	E
LUPINE, CLOVER	Lupinus tidestromii	PLANT	KNOWN	E

Plant Species in Counties at Least 100 Acres of Rice

Crop #: 163

SPECIES		SCIENTIFIC NAME	GROUP	KNOWN	STATUS
OWL'S-CLOVER, FLESHY		CASTILLEJA CAMPESTRIS SSP. SUCCULENT	PLANT	KNOWN	E
PUSSYPAWS, MARIPOSA		CALYPTRIDIUM PULCHELLUM	PLANT	KNOWN	T
MERCED, CA	Crop Acres: 4341				
GRASS, COLUSA		NEOSTAPFIA COLUSANA	PLANT	KNOWN	T
GRASS, HAIRY ORCUTT		ORCUTTIA PILOSA	PLANT	KNOWN	E
OWL'S-CLOVER, FLESHY		CASTILLEJA CAMPESTRIS SSP. SUCCULENT	PLANT	KNOWN	E
TUCTORIA, GREEN'S		TUCTORIA GREENEI	PLANT	KNOWN	E
PLACER, CA	Crop Acres: 16661				
BARBERRY, TRUCKEE		BERBERIS (=MAHONIA) SONNEI	PLANT	KNOWN	E
SACRAMENTO, CA	Crop Acres: 8069				
EVENING-PRIMROSE, ANTIOCH DUNES		Oenothera deltoides ssp. howellii	PLANT	KNOWN	E,CH
GRASS, SACRAMENTO ORCUTT		ORCUTTIA VISCIDA	PLANT	KNOWN	E
GRASS, SLENDER ORCUTT		ORCUTTIA TENUIS	PLANT	KNOWN	T
SAN JOAQUIN, CA	Crop Acres: 4700				
BIRD'S-BEAK, PALMATE-BRACTED		Cordylanthes palmatus	PLANT	KNOWN	E
FIDDLENECK, LARGE-FLOWERED		Amsinckia grandiflora	PLANT	KNOWN	E,CH
STANISLAUS, CA	Crop Acres: 2564				
ADOBE SUNBURST, SAN JOAQUIN		PSEUDOBAHIA PEIRSONII	PLANT	KNOWN	E
GOLDEN SUNBURST, HARTWEG'S		PSEUDOBAHIA BAHIIFOLIA	PLANT	KNOWN	E
GRASS, COLUSA		NEOSTAPFIA COLUSANA	PLANT	KNOWN	T
GRASS, HAIRY ORCUTT		ORCUTTIA PILOSA	PLANT	KNOWN	E
OWL'S-CLOVER, FLESHY		CASTILLEJA CAMPESTRIS SSP. SUCCULENT	PLANT	KNOWN	E
SPURGE, HOOVER'S		CHAMAESYCE HOOVERI	PLANT	KNOWN	T
TEHAMA, CA	Crop Acres: 723				
GRASS, HAIRY ORCUTT		ORCUTTIA PILOSA	PLANT	KNOWN	E
GRASS, SLENDER ORCUTT		ORCUTTIA TENUIS	PLANT	KNOWN	T
MEADOWFOAM, BUTTE COUNTY		Limnanthes floccosa ssp. californica	PLANT	KNOWN	E
SPURGE, HOOVER'S		CHAMAESYCE HOOVERI	PLANT	KNOWN	T
TUCTORIA, GREEN'S		TUCTORIA GREENEI	PLANT	KNOWN	E
YOLO, CA	Crop Acres: 26332				
BIRD'S-BEAK, PALMATE-BRACTED		Cordylanthes palmatus	PLANT	KNOWN	E
GRASS, COLUSA		NEOSTAPFIA COLUSANA	PLANT	KNOWN	T
MISSISSIPPI					
BOLIVAR, MS	Crop Acres: 73526				
PONDBERRY		Lindera melissifolia	PLANT	KNOWN	E
SHARKEY, MS	Crop Acres: 5520				
PONDBERRY		Lindera melissifolia	PLANT	KNOWN	E
SUNFLOWER, MS	Crop Acres: 33543				
PONDBERRY		Lindera melissifolia	PLANT	KNOWN	E
MISSOURI					
BUTLER, MO	Crop Acres: 53696				
PONDBERRY		Lindera melissifolia	PLANT	KNOWN	E
DUNKLIN, MO	Crop Acres: 3266				
CLOVER, RUNNING BUFFALO		Trifolium stoloniferum	PLANT	KNOWN	E
RIPLEY, MO	Crop Acres: 4088				
PONDBERRY		Lindera melissifolia	PLANT	KNOWN	E
TEXAS					
FORT BEND, TX	Crop Acres: 11592				
DAWN-FLOWER, TEXAS PRAIRIE (=TEXAS BIT		HYMENOXYS TEXANA	PLANT	KNOWN	E

Plant Species in Counties at Least 100 Acres of Rice

Crop #: 163

SPECIES	SCIENTIFIC NAME	GROUP	KNOWN	STATUS
HARRIS, TX Crop Acres: 7218				
DAWN-FLOWER, TEXAS PRAIRIE (=TEXAS BIT	HYMENOXYS TEXANA	PLANT	KNOWN	E

Table G-3. Summary of Effects Determinations by State, County, and Species		
State **County**	**Species**	**Effects Determination**
Arkansas		
Clay	Pondberry	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
Drew	*Geocarpon*	No Effect
Jackson	Pondberry	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
Lawrence	Pondberry	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
Woodruff	Pondberry	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
Yell	Harperella	No Effect
Missouri		
Butler	Pondberry	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
Dunklin	clover, running buffalo	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
Ripley	Pondberry	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect (No effect for HUC 11010009)
Mississippi	Aster, decurrent flase	No Effect
Wayne	clover, running buffalo	No Effect
Mississippi		
Bolivar	Pondberry	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
Sharkey	Pondberry	No Effect
Sunflower	Pondberry	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
Texas		
Fort Bend	Texas dawn-flower or Prairie dawn	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
Harris (west: 1204104)	Texas dawn-flower or Prairie dawn	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect

Harris (east: 12040104)	Texas dawn-flower or Prairie dawn	No Effect
Harris (12040102)	Texas dawn-flower or Prairie dawn	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
Harris (12040101)	Texas dawn-flower or Prairie dawn	No Effect
California		
Alameda	large-flowered fiddleneck	No Effect
	pallid manzanita	No Effect
	robust spineflower	No Effect
	Presidio clarkia palmate-bracted bird's beak	No Effect
	Santa Cruz tarplant	None - extirpated
	Contra Costa goldfields	No Effect
	California seablite	No Effect
	Few-flowered navarretia	No occurrences in Alameda County
	Many-flowered navarretia	No occurrences in Alameda County
	Lake County stonecrop	No occurrences in Alameda County
Butte	Butte County meadowfoam	No protections: Levels of Concern are Exceeded With protections: Not Likely to Adversely Affect
	Greene's tuctoria	No protections: Levels of Concern are Exceeded With protections including restrictions on all liquid applications: Not Likely to Adversely Affect
	Hoover's spurge	No protections: Levels of Concern are Exceeded With protections including restrictions on all liquid applications: Not Likely to Adversely Affect
	hairy orcutt grass	No protections: Levels of Concern are Exceeded With protections including restrictions on all liquid applications: Not Likely to Adversely Affect
	slender orcutt grass	No effect
Colusa	Bird's beak, palmatebracted	No protections or programmatic management: Levels of Concern are Exceeded With protections or programmatic management: Not Likely to Adversely Affect
	Colusa grass	No protections or programmatic management: Levels of Concern are Exceeded With protections or programmatic management: Not Likely to Adversely Affect

Fresno	Bird's beak, palmatebracted	No Effect
	Checker-mallow, Keck's	No Effect
	dudleya, Santa Clara Valley	No occurrences in Fresno County
	jewelflower, California	No Effect
	owl's-clover, fleshy (also succulent)	No Effect
	pussypaws, Mariposa	No Effect
	sunburst, Hartweg's golden	No Effect
	sunburst, San Joaquin adobe	No Effect
	woolly-star, Hoover's	No occurrences in Fresno County
	woolly-threads, San Joaquin	No Effect
	San Joaquin Valley orcutt grass	No Effect
	San Benito evening-primrose	No Effect
	slender moonwort	No Effect
	Greene's tuctoria	No Effect
Glenn	spurge, Hoover's	No protections or programmatic management: Levels of Concern are Exceeded With protections or programmatic management: Not Likely to Adversely Affect
	grass, hairy Orcutt	No protections or programmatic management: Levels of Concern are Exceeded With protections or programmatic management: Not Likely to Adversely Affect
	Bird's beak, palmatebracted	No protections or programmatic management: Levels of Concern are Exceeded With protections or programmatic management: Not Likely to Adversely Affect
Madera	Bird's beak, palmatebracted	No Effect
	lupine, clover	No occurrences in Madera County

Madera (cont.)	owl's-clover, fleshy (also succulent)	No Effect
	pussypaws, Mariposa	No Effect
	sunburst, Hartweg's golden	No Effect
	sunburst, San Joaquin adobe	No Effect
	grass, hairy Orcutt	No Effect
	Greene's tuctoria	No Effect
	San Joaquin Valley orcutt grass	No Effect
Merced	owl's-clover, fleshy	No Effect
	grass, Colusa	No Effect
	grass, hairy Orcutt	No Effect
	Greene's tuctoria	No Effect
	sunburst, Hartweg's golden	No Effect
	spurge, Hoover's	No Effect
	San Joaquin Valley orcutt grass	No Effect
Placer	Barberry, Truckee	FWS has delisted this species (68 FR 56564 56567)
	Cress, Tahoe yellow	No Effect
Sacramento	Evening-primrose, Antioch Dunes	No Effect
	grass, Sacramento Orcutt	No Effect
	grass, slender Orcutt	No Effect
	Lone buckwheat	No Effect
San Joaquin	Bird's beak, palmatebracted	No Effect
	fiddleneck, large-flowered	No Effect
	Greene's tuctoria	No Effect
	owl's clover, fleshy	No Effect
Stanislaus	owl's clover, fleshy	No Effect

Stanislaus (cont.)	spurge, Hoover's	No Effect
	sunburst, Hartweg's golden	No Effect
	sunburst, San Joaquin adobe	No Effect
	grass, Colusa	No Effect
	grass, hairy Orcutt	No Effect
	Greene's tuctoria	No protections: Levels of Concern are Exceeded With protections including restriction on aerial application: Not Likely to Adversely Affect
	San Joaquin Valley orcutt grass	No Effect
	San Jacinto Valley crownscale	No Effect
Tehama	meadowfoam, Butte County	In FESTF IMS, not in CNDDB. NatureServe listed in Butte County only. No determination needed.
	spurge, Hoover's	No Effect
	grass, hairy Orcutt	No Effect
	grass, slender Orcutt	No Effect
	Greene's tuctoria	No Effect
Yolo	Bird's beak, palmatebracted	No protections: Levels of Concern are Exceeded With protections including restriction on aerial application: Not Likely to Adversely Affect
	grass, Colusa	No Effect
	Solano grass	No Effect

Appendix H - Ecological Effects and Environmental Fate Data Requirements

Table H-1. Status of Ecological Effects Data Requirements for Penoxsulam

Guideline Number	Data Requirements	Is the Data Requirement Satisfied?	MRID	Status
71-1a	Acute avian oral, Quail	Yes	45830928	Core
	Acute Avian Oral Duck	Yes	45830929	Core
71-1(b)	Acute Avian Oral- Quail EUP GF-443	Yes	45831001	Core
71-2(a)	Avian Dietary/Quail	Yes	45831002	Supp.
71-2(b)	Avian Dietary/Duck	Yes	45831003	Supp.
71-4(a)	Avian Reproductive/Quail	Yes	45831006	Supp.
71-4(b)	Avian Reproductive/Duck	Yes	45830101	Core
72-1(a)	Acute Fish Toxicity Bluegill	Yes	45831010	Supp.
72-1(c)	Acute Fish Toxicity Rainbow Trout	Yes	45834804	Supp.
72-1(d)	Acute Fish Toxicity Bluegill EUP	Yes	45831011	Supp.
72-2(a)	Freshwater Invertebrate toxicity			
72-2(a)	Daphnid	Yes	45831012	Supp.
	Metabolic products with Daphnids			
	2-amino-TP	No	45831019	Supp.
	BSTCA	Yes	45831014	Supp.
	TPSA	No	45831018	Supp.
	BST	Yes	45831015	Supp.
	5-OH,2-amino-TP	No	45831016	Supp.
	5-hydroxy-XDE-638	Yes	45831013	Supp.
	BSA	Yes	45831017	Supp.
72-2(b)	Freshwater Invertebrate acute EUP	No	45831020	Supp.
72-3(a)	Estuarine/Marine Toxicity Fish	No	45831022	Supp.
72-3(b)	Estuarine/Marine Toxicity Mollusk	Yes	45831023	Core
72-3(c)	Estuarine/Marine Toxicity- Mysid	Yes	45831024	Core
72-4(a)	Early Life Stage Fish	Yes	45831027	Supp.
72-4(b)	Life Cycle Aquatic Invertebrate Daphnids	Yes	45831026	Core
72-4(b)	Life Cycle Aquatic Invertebrate, Mysids	No	45831028	Supp.
122-2	Aquatic Plant Growth			

Guideline Number	Data Requirements	Is the Data Requirement Satisfied?	MRID	Status
	Lemna gibba TPSA	Yes	45831109	Supp.
	Lemna gibba EUP GF-443	No	None	
	Selenastrum capricornutum TPSA	Yes	45831113	Core
	S. capricornutum 5-OH,2-amino-TP	Yes	45831114	Core
	S. capricornutum BSA	Yes	45831112	Supp.
	S. capricornutum 2-Amino-TP	Yes	45831115	Supp.
	Lemna gibba 5-OH,2-Amino-TP	Yes	45831108	Supp.
	Lemna gibba 2-Amino TP	Yes	45831111	Supp.
	Lemna gibba BSA	Yes	45831110	Supp.
123-1(a)	Seedling Emergence (Terrestrial Tier 2)			
	Onion	Yes	45831116	Core
	Sugarbeet	Yes	45831116	
123-1 (b)	Vegetative Vigor (Terrestrial Tier 2)			
	Ryegrass	Yes	45831116	Core
	Soybean	Yes	45831116	
123-2	Aquatic Plant Growth- Tier 2			
	Lemna gibba	Yes	45831120	Core
	Lemna gibba BSTCA	Yes	45831106	Core
	Lemna gibba 5-Hydroxy penoxsulam Tier 1	Yes	45831104	Core
	Lemna gibba BST	Yes	45831105	Core
123-2	*Selenastrum capricornutum*	Yes	45834805	Core
123-2	*S. capricornutum* EUP GF-443	Yes	45831107	Core
123-2	*S. capricornutum* BSTCA	Yes	45831119	Core
123-2	*S. capricornutum* BST	Yes	45831117	Core
123-2	*S. capricornutum* 5-hydroxy penoxsulam	Yes	45831118	Core
123-2	*Navicula pelliculosa*	Yes	45831121	Supp.
123-2	*Anabaena flos-aquae*	Yes	45831122	Core
123-2	*Skeletonema costatum*	Yes	45831123	Core
141-1	Honey Bee Acute Contact			

Guideline Number	Data Requirements	Is the Data Requirement Satisfied?	MRID	Status
	XDE-638	Yes	45831124	Core
	EUP	Yes	45831126	Supp.

Table H2. Status of Environmental Fate Data Requirements for Penoxsulam

Guideline #		Data Requirement	Is Data Requirement Satisfied?	MRID #'s	Study Classification
161-1	835.212	Hydrolysis	yes	458307-21	acceptable
161-2	835.224	Photodegradation in Water	yes	458348-01 458307-22	supplemental supplemental
161-3	835.241	Photodegradation on Soil	yes	458307-23	supplemental
161-4	835.237	Photodegradation in Air	not required		
162-1	835.41	Aerobic Soil Metabolism	yes	458307-24	acceptable
162-2	835.42	Anaerobic Soil Metabolism	yes		acceptable
162-3	835.44	Anaerobic Aquatic Metabolism	yes	458307-25	acceptable
162-4	835.43	Aerobic Aquatic Metabolism	yes	458307-26	acceptable
163-1	835.1240 835.1230	Leaching-Adsorption/Desorption	yes	458308-01 458308-02 458348-03	acceptable supplemental supplemental
163-2	835.141	Laboratory Volatility	not required		na
163-3	835.81	Field Volatility	not required		na
164-1	835.61	Terrestrial Field Dissipation	not required		na
164-2	835.62	Aquatic Field Dissipation	yes	458308-05 458308-04	acceptable supplemental
164-3	835.63	Forestry Dissipation	not required		na
164-4	835.64	Combination Products and Tank Mixes Dissipation	not required		na
165-4	850.173	Accumulation in Fish	no		na
165-5	850.195	Accumulation- aquatic non-target	yes	458311-01	acceptable
166-1	835.71	Ground Water- small prospective	not required		na
201-1	840.11	Droplet Size Spectrum	reserved		na
202-1	840.12	Drift Field Evaluation	reserved		na