(4-2-2004)

Data Evaluation Report on the phototransformation of penoxsulam in water

PMRA Submission Number {.....} EPA MRID Number 45834801

Data Requirement: PMRA Data Code:
EPA DP Barcode: D288160
OECD Data Point:
EPA Guideline: 161-2

Test material:
Common name: Penoxsulam
Chemical names:
IUPAC: 6-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy-s-triazolo[1,5-c]pyrimidin-2-yl)-α,α,α-trifluoro-o-toluenesulfonamide;
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 : 2-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide
CAS No: 219714-96-2
Synonyms: XDE-638
SMILES string: n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F

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EXECUTIVE SUMMARY

The aqueous phototransformation of [triazolopyrimidine-2- ^{14}C]- labeled and [phenyl-U- ^{14}C]-labeled 3-(2,2-difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-α,α,α-trifluorotoluene-2-sulfonamide (penoxsulam; XDE-638) were studied at 25 ± 2°C in sterile aqueous phosphate buffer (0.68 M; pH 7) and natural water (lake water from Letcombe, England; pH 7.8) for 28 days at a nominal concentration of 0.15 µg a.i./mL (equivalent to the maximum application rate of 150 g/ha at 10 cm deep of current practical use) under continuous irradiation using a UV-filtered xenon arc lamp (290-800 nm). Using an actinometer, it was estimated that the intensity of the xenon lamp was approximately 1.3x greater than average summer sunlight at 40°N. The wavelength distribution was similar to natural sunlight at summer solstice. The guidance used to design the study was not identified. The study was in compliance with OECD Principles of Good Laboratory Practice.

For irradiated samples, quartz glass tubes (24 mL volume; 200 mm x 10 mm i.d.) containing 22 mL of the treated test solution test solution were placed in a circulating water-cooled bath within a SUNTEST CPS+ system. For the dark controls, borosilicate glass tubes (24 mL volume; 200 mm x 10 mm i.d.) containing 22 mL of treated test solution were stored in a temperature-controlled incubator. No volatile traps were present in the definitive study. The [^{14}C-triazolopyrimidine]-labeled samples were collected after 0, 0.5, 1, 1.4, 3, 7, 14, and 28 days. The [^{14}C-phenyl]-labeled samples were collected after 0, 0.167, 0.33, 0.5, 1, 1.5, 3, 7, 14, and 28 days. Single samples were collected at each sampling interval and were analyzed directly by LSC and HPLC. Identification of penoxsulam and its [^{14}C]transformation products was done by co-chromatography with unlabeled reference standards on one or two of the three HPLC systems. Further identification of isolated compounds was done with positive and negative ion electrospray ESI-LC/MS analysis. Attempts were made to isolate polar degradates and identify polar compounds comprising >10% of the applied. Volatiles were not measured in the definitive study, but were in a supplementary study using the phenyl label.

Sterile Buffer solution: Total [^{14}C]residue recovery from the [^{14}C-triazolopyrimidine]-labeled buffer samples decreased from 100% to 96.0% of the applied (mean 99.2 ± 1.4%) during irradiation and ranged from 99.8% to 102% (mean 101.0 ± 1.0%) with no pattern of decline in the corresponding dark control. Total [^{14}C]residue recovery from the [^{14}C-phenyl]-labeled buffer samples decreased from 100% to 78.8% of the applied (mean 94.3 ± 7.2%) during irradiation and ranged from 98.6% to 103% (mean 99.9 ± 1.3%) with no pattern of decline in the corresponding dark controls.

In the irradiated samples, [^{14}C-triazolopyrimidine]penoxsulam decreased from 100.0% of the applied at time 0 to 17.3% at 1.0 day, and was not detected at and after 1.4 days. Major transformation products were 5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl-sulfamic acid (TPSA), which was a maximum 48.1% of the applied at 1.4 days posttreatment and was not detected at 28 days and 5,8-dimthoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-amine(2-amino TP), which

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was a maximum 18.2% at 1.0 days and was not detected at and after 14 days. Minor identified transformation products were 8-methoxy-[1,2,4]triazolo[1,5-c]pyrimidin-5-ol-2-amine (5-OH, 2-amino TP) at a maximum 9.0% of the applied (14 days) and methyl,5-[[[2(2,2-difluoroethoxy)6-(trifluoromethyl)phenyl] sulphonyl]amino],1H-1,2,4-triazole-3-carboxylic acid (BSTCA-methyl) at a maximum 1.2% (0.5 days). Six distinct HPLC peaks, each a maximum of 5.1-7.7% of the applied, were not identified. At least nine polar compounds totaled a maximum of 84.6% of the applied at 28 days posttreatment. 2-Amino TCA (2-amino-1,2,4-triazole carboxylic acid) was the only polar degradate comprising >10% of the applied.

[^{14}C-Phenyl]penoxsulam decreased from 100.0% of the applied at time 0 to 26.7% at 1.0 days to 0.0% at 3.0 days. The only major transformation product was 2-(2,2-difluoroethoxy)-5-(trifluoromethyl)benzenesulphonic acid (BSA), which was a maximum 36.1% of the applied at 1.5 days posttreatment and was not detected at and after 14 days. Minor transformation products, each at a maximum of 5.1-7.0% of the applied, were methyl,5[[[2(2,2-difluoroethoxy)6-(trifluoromethyl)phenyl]sulphonyl]amino],1H-1,2,4-triazole-3-carboxylic acid (BSTCA), BSTCA-methyl, and 3-(2,2-difluoroethoxy)-2-hydroxybenzoic acid (di-FESA). At least 17 polar compounds totaled a maximum of 85.7% of the applied at 14 days posttreatment and were 78.8% at 28 days. No polar compounds comprised >10% of the applied..

In the corresponding dark controls for both labels, [^{14}C]penoxsulam was reported to be stable during the 28 days of incubation. Quantitative data were not provided. No major or minor transformation products were identified. Volatiles were not measured in the definitive study.

Natural water: Total [^{14}C]residue recovery from the [^{14}C-triazolopyrimidine]-labeled natural water samples decreased from 100% to 87.8% of the applied (mean 96.0 ± 3.7%) during irradiation and decreased from 100 to 96.8% of the applied (mean 98.7 ± 1.0%) in the corresponding dark control.

Total [^{14}C]residue recovery from the [^{14}C-phenyl]-labeled natural water samples decreased from 100 to 73.6-74.1% of the applied (mean 89.7 ± 10.5%) during irradiation, and ranged from 96.6% to 100.0% (mean 98.3 ± 0.9%) with no clear pattern of loss in the dark control.

In the irradiated samples, [^{14}C-triazolopyrimidine]penoxsulam decreased from 100.0% of the applied at time 0 to 6.8% at 1.0 day posttreatment and was not detected at and after 3 days. Major transformation products were TPSA, which was a maximum 56.0% of the applied at 1 day posttreatment and was not detected at and after 14 days. 5-OH, 2-Amino TP, which was a maximum 23.4% at 14 days and 16.9% at 28 days. 2-Amino TP, which was a maximum 17.8% at 3 days and was not detected at and after 7 days. The only minor identified transformation product was BSTCA-methyl at a maximum 4.4% of the applied (1 day). Two distinct HPLC peaks, at maximums of 3.6 and 7.4% of the applied, were not identified, and polar compounds totaled a maximum of 71.7% of the applied at 14 days posttreatment.

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[^{14}C-Phenyl]penoxsulam decreased from 100.0% of the applied at time 0 to 43.0% at 1.0 day and was not detected at and after 3.0 days. The only major transformation product was BSA, which was a maximum 33.5% of the applied at 1.5 days posttreatment and was not detected at and after 7 days. Minor transformation products, each at a maximum of 7.2-7.6% of the applied, were BSTCA, BSTCA-methyl, and di-FESA. Polar compounds totaled a maximum of 74.1% of the applied at 28 days posttreatment.

In the corresponding dark controls for both labels, [^{14}C]penoxsulam was reported to be stable during the 28 days of incubation. Quantitative data were not provided. No major or minor transformation products were identified. Volatiles were not measured in the definitive study.

Based on first-order linear regression analysis (Excel 2000) and using data points through the first nondetect, the half-life of penoxsulam (combined labels) is 0.51 days in sterile buffer solution and 0.39 days in natural water, based on the *continuous irradiation* used in the study. Since no degradation occurred in the dark control, the **phototransformation half-lives** are approximately 0.5 and 0.4 days, respectively. The artificial light was determined to be approximately 1.3x stronger than average summer sunlight at 40°N. Therefore the **predicted environmental phototransformation half-life** in both the buffer solution and natural water is slightly less than 1.5 day.

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.

A transformation pathway was proposed by the study authors. The proposed transformation pathway involved two major route of degradation and one minor route of degradation. The two major routes of degradation involved the cleavage of the sulfonamide group at different sites. The 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.

The more favored proposed major route of degradation involved the sulfur-nitrogen cleavage of the sulfonamide group, generating 2-amino TP and BSA. 2-amino TP degraded via demethylation to (5-OH, 2-amino TP), which further degraded to multiple polar degradates including 2-amino TCA. BSA degraded to multiple polar degradates and carbon dioxide. The less favored major route of degradation involved the sulfur-phenyl cleavage of the sulfonamide group, generating TPSA and the phenyl moiety. TPSA degraded to 2-amino TP, which then followed the degradation pathway which was described above. The phenyl moiety could not be detected. However, its degradation product, di-FESA, was identified in the primary [^{14}C-Ph]penoxsulam experiment. Di-FESA further degraded to multiple polar degradates and carbon dioxide.

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The minor proposed route of degradation involved the opening of the pyrimidine ring, generating BSTCA methyl. BSTCA methyl degraded to BSTCA via ester hydrolysis. BSTCA further degraded to multiple polar degradates and carbon dioxide.

It was proposed that while the initial cleavage of the less favored major route of degradation occurred via direct photolysis, the subsequent degradation of TPSA to 2-amino TP occurred via indirect photolysis.

Results Synopsis:

Test medium: 0.69M sodium phosphate buffer at pH 7
Source of irradiation: Xenon lamp
Half-life/irradiated (0-3 days data): 1.5 days (based on 12 hour light/dark cycle; $r^2 = 0.91$)
Half-life/dark control: Stable
Major transformation products/irradiated:
TPSA; (5,8-dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidin-2-yl-sulfamic acid)
2-Amino TP; (5,8-dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidine-2-amine)
BSA; (2-(2,2-difluoroethoxy)-5-(trifluoromethyl) benzenesulphonic acid)
2-Amino-1,2,4-triazole carboxylic acid; (2-amino TCA)
Major transformation products/dark control:
None
Minor transformation products/irradiated:
BSTCA methyl; (methyl 5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-3-carboxylic acid)
BSTCA; (5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-3-carboxylic acid)
Di-FESA; (3-(2,2-difluoroethoxy)-2-hydroxybenzoic acid)
5-OH, 2-Amino TP; (8-methoxy-[1,2,4]triazolo[1,5-c]pyrimidin-5-ol-2-amine)
Minor transformation products/dark:
None

Test medium: Lake water.
Source of irradiation: Xenon lamp.
Half-life/ irradiated (0-3 day data): 1.5 days (based on 12 hour light/dark cycle; $r^2 = 0.68$).
Half-life/dark control: Stable
Major transformation products/irradiated:
TPSA; (5,8-dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidin-2-yl-sulfamic acid)
2-Amino TP; (5,8-dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidine-2-amine)
5-OH, 2-Amino TP; (8-methoxy-[1,2,4]triazolo[1,5-c]pyrimidin-5-ol-2-amine)
BSA; (2-(2,2-difluoroethoxy)-5-(trifluoromethyl) benzenesulphonic acid)
2-Amino-1,2,4-triazole carboxylic acid; (2-amino TCA)
Major transformation products/dark control:
None

Minor transformation products:
BSTCA methyl; (methyl 5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-3-carboxylic acid)
BSTCA; (5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-3-carboxylic acid)
Di-FESA; (3-(2,2-difluoroethoxy)-2-hydroxybenzoic acid)
Minor transformation products/dark control:
None

Study Acceptability: This study is classified supplemental. This study cannot be used to fulfill the aqueous photolysis guideline for penoxsulam because material balances in the phenyl-labeled experiment was incomplete (total [^{14}C]residue recovery from the [^{14}C-phenyl]-labeled buffer samples decreased to 78.8% of the applied radioactivity). The portion of this study using natural water does not fulfill requirements because the CO_2 data are contradictory.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: The guidelines used to design the study were not identified. No significant deviations from USEPA Pesticide Assessment Guidelines, Subdivision N §161-2 guidelines were noted in the portion of the study conducted using the sterile buffer solution.

COMPLIANCE: This study was conducted in compliance with OECD Principles of Good Laboratory Practice (p.3a). Signed and dated GLP Compliance, Quality Assurance, and No Data Confidentiality statements were provided (pp.2-4). No Certificate of Authenticity statement was provided.

A. MATERIALS

1. Test Materials [Triazolopyrimidine-2- ^{14}C]- and [phenyl-U- ^{14}C]penoxsulam (p.12).

Chemical Structure: See Attachment 2.

Description: Not reported.

Purity:
Triazolopyrimidine label
Radiochemical purity: >99% (p.12)
Batch No. INV1456 (Indianapolis); INV99/6 (Letcombe).
Analytical purity: Not reported.
Specific activity: 28.9 mCi/mmole (1069.3 MBq/mmol).

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Location of the radiolabel: 2-Carbon in the triazolopyrimidine (TP) ring.

Phenyl label

Radiochemical purity: 98.4% (p.12)
Batch No. INV1475 (Indianapolis); INV99/5 (Letcombe).
Analytical purity: Not reported.
Specific activity: 24.6 mCi/mmole (910.2 MBq/mmol).
Location of the radiolabel: Uniformly on the phenyl (Ph) ring.

Storage conditions of test chemicals:

The test chemicals were stored at <-16°C (p.12).

Physico-chemical properties of penoxsulam.

Parameter	Values	Comments
Water solubility	44 ppm at pH 3.17; 6 ppm at pH 1.25.	
Molecular Weight	483 g/mole	
Molecular Formula	$C_{16}H_{14}F_5N_5O_5S$	
Density	Not reported.	
Vapor pressure	20°C: 1.87×10^{-16} mmHg. 25°C: 7.16×10^{-16} mmHg.	
UV absorption	220-290 nm	
pK_a	4.37	
K_{ow}/log K_{ow}	Not reported.	
Log K_{oc}:	Not reported.	
Stability of compound at room temperature	Not reported.	

Data obtained from p.12 of this MIRD, pp.12, 45 of MRID 45830721, and p.21 of MRID 45830723

2a. Buffer Solution: The following buffer solution was prepared with analytical grade reagents and HPLC grade solvents:

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Table 1a: Description of buffer solution.

pH	Type and final molarity of buffer	Composition
7[a]	0.68M Sodium phosphate buffer[b]	A 1 L solution of sodium dihydrogen orthophosphate (31.2 g/L) and disodium hydrogen orthophosphate (71.6 g/L) was prepared using distilled water.

Data obtained from p.13 of the study report.

a The buffer solution is reported to have been pH 7. However, the study report does not indicate that the pH of the solution was ever measured.

b The molarity of buffer solution was not reported. A molarity of 0.68M provided was calculated using the data provided in the MRID.

2b. Natural Water:

Table 1b: Description of natural water.

Parameter	Details
Location of collection	Brook-fed lake at Dow AgroSciences Letcombe laboratory test facility; Letcombe, U. K.
Date of collection	Not reported.
Depth of collection	20-30 cm.
Length of storage	Not reported.
Storage conditions	Not reported.
pH	7.8
Alkalinity	242 mg HCO_3/L
Organic Carbon	Not reported
Oxidizability	<0.5 mg/L
Other Details	Filtered through a 0.2 micron filter prior to addition of test substance.

Data obtained from p.13, Appendix 2, p.62 of the study report.

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3. Details of light source:

Table 2: Artificial light source.

Property	Details
Type of photoreactor used:	SUNTEST CPS+ system (from Atlas Material Testing Technology.
Type of lamp used:	Xenon lamp.
Emission wavelength spectrum:	290-800 nm.
Light intensity:	6.62 W/m^2 at 400 nm. An illustration of light intensity as a function of wavelength (280-340 nm) was provided in Appendix 4, Figure A, p.71 of the study report.
Filters used:	UV filter (< 290 nm), calibrated with the Xenocal UV light sensor.
Relationship to natural sunlight:	The wavelength distribution of the xenon lamp was similar to natural sunlight at summer solstice. The intensity of the xenon lamp was measured using an actinometer and was reported to be similar to natural summer sunlight at 40 °N latitude. The calculated ratio of artificial light to summer sunlight was 1.3:1.

Data obtained from pp.14, 17, 20; Appendix 4, pp.65-67.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: The study author referenced the results from two additional experiments. An outdoor probe photolysis study performed using the Letcombe Brook water, and a hydrolysis study in aqueous pH 5-9 buffer solutions (p.11).

2. Experimental conditions:

Table 3: Experimental design.

Parameter		Details
Duration of the test:		28 days (continuous irradiation).
Application rate: Nominal		0.15 µg/mL
Measured		[^{14}C-TP]penoxsulam: 0.15 µg/mL [^{14}C-Ph]penoxsulam: 0.17 µg/mL
Dark controls used (Yes/No):		Yes.
Replications	Dark controls:	None. Only one sample was collected at each interval.
	Irradiated:	None. Only one sample was collected for each label, at each interval.

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Parameter		Details
Preparation of the test medium:	Volume used/ treatment:	A 800 µL aliquot of the [^{14}C]penoxsulam stock solution was transferred with a micro-pipette to 1000 mL of both the sterile pH 7 buffer solution and the natural water. Aliquots (22 mL) of these bulk treatment solutions were transferred to individual test tubes.
	Method of sterilization:	The buffer solution was autoclaved for 20 minutes prior to addition of test compound. The natural water was filtered through a 0.2 µm filter prior to use.
	Co-solvent, if any:	None. The test substance was prepared as a stock solution using the buffer solution and natural water.
Test apparatus (Type/material/ volume):	Dark controls:	24 mL borosilicate glass tubes (200 mm x 10 mm i.d.) were filled with 22 mL of the test solution and stored in a temperature controlled incubator.
	Irradiated:	24 mL quartz glass tubes (200 mm x 10 mm i.d.) were filled with 22 mL of the test solution, sealed with Teflon-lined screw caps, and placed in the photolysis apparatus. The [^{14}C-TP]penoxsulam and [^{14}C-Ph]penoxsulam experiments were not performed concurrently.
Details of traps for CO_2 and organic volatiles, if any:	Dark controls:	Volatiles were not trapped.
	Irradiated:	Volatiles were not trapped in the definitive experiment. Volatiles were trapped in a supplementary experiment using only the phenyl label.
If no traps were used, is the system closed/open?		Closed.
Any indication of the test material adsorbing to the walls of the test apparatus?		Not reported.
Experimental conditions.	Temperature (°C):	25 ± 2°C
	Duration of light/ darkness:	Samples were continuously irradiated.
Other details, if any:		None

Data obtained from pp.13-15, 17, and 20-22.

3. Supplementary experiments:

Measurement of $^{14}CO_2$/Volatiles: After 28 days of continuous irradiation, the pH 7 buffer and natural water solutions with [^{14}C-Ph]penoxsulam demonstrated a loss of 21.2% and 25.9% applied radioactivity, respectively (Table 1a, p.30). Therefore, a separate experiment was performed in order to determine if this loss of applied radioactivity was due to the generation of organic and/or inorganic volatiles (p.16).

Photolytic vessels (one per system) with two side arms were placed under the xenon lamp. Three traps were attached sequentially to one side arm of each photolysis vessel (listed from closest to furthest from the photolysis vessel: silica gel trap, coconut charcoal trap, and 2M NaOH trap (50 mL). A gas scrubber of 2M NaOH was placed on the other side arm of each photolysis vessel. The traps and gas scrubber were not under the xenon lamp. During the experiment, air was pumped through the system at a rate of 172-174 mL/minute. For each system (unspecified number of systems), the air flowed through the gas scrubber and photolysis vessel to the three volatile traps. The system was illustrated on page16 of the study report.

In order to quantify the organic and inorganic volatiles which were generated, the NaOH and charcoal traps were collected and measured by LSC (p.15). The measurement of the silica gel trap media was not experimentally reported. The media of the 2M sodium hydroxide traps were measured for volatiles. The presence of CO_2 in NaOH traps was confirmed using barium chloride precipitation. The charcoal traps were extracted with two 10 mL aliquots of cold carbon disulfide. After extraction, aliquots of the carbon disulfide extracts were measured for $^{14}CO_2$ by LSC.

Actinometry: The intensity of the artificial light was measured using chemical actinometers composed of *p*-nitroacetophenone (PNAP; 1 x 10^{-5} M) and pyridine (pyr; 1 x 10^{-5} M) in deionized, sterile water (p.18; Appendix 4, pp.64-78). The incubation conditions were the same for the actinometer samples as for the [^{14}C]penoxsulam samples (Table II, p.66). The samples were analyzed by HPLC, which was calibrated with PNAP. The half-life of PNAP was calculated for the experimental conditions and compared to the half-life at normal sunlight intensity at 40 °N latitude for summer.

Generation of additional [^{14}C]residues for identification: Because a number of transformation products were not identified using HPLC, additional material was generated for use in MS analyses. Natural water samples were treated at a rate of 9.4 µg/mL with [triazolopyrimidine-^{14}C]- or [phenyl-^{14}C]penoxsulam (62x the normal application rate), transferred into the quartz vessels, and irradiated as described for 8 days (p.17). Additional samples were prepared in HPLC grade water and incubated as described for 21 days. Samples were analyzed using LC-MS. The study author stated that high-dose samples were not prepared using the phosphate buffer solution because the phosphate interfered with the LC-MS interface being used.

4. Sampling:

Table 4: Sampling details.

Parameters	Details
Sampling intervals:	Triazolopyrimidine label: 0, 0.5, 1, 1.4, 3, 7, 14, and 28 days. Phenyl label: 0, 0.167, 0.33, 0.5, 1, 1.5, 3, 7, 14, and 28 days.
Sampling method:	Entire samples (one) were removed and analyzed at each sampling interval.
Method of collection of volatile compounds, if any:	Volatiles were not measured in the definitive study. A supplementary study using the phenyl label was provided.
Sampling intervals/times for: Sterility check: pH measurement:	The pH 7 buffer solution was checked before application of test compound and at every sampling interval. The natural water samples were not checked for sterility. Not reported.
Sample storage before analysis:	Samples were not stored prior to LSC and HPLC analysis. Samples were stored refrigerated before LC/MS analysis.
Other observations, if any:	Freeze-drying samples caused an insoluble precipitate to form.

Data obtained from pp.13, 14, 17, 21, and 22 of the study report.

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods, if used: No manipulation of the test samples was reported.

Volatile residue determination: Volatiles were not measured in the definitive study.

Total ^{14}C measurement: Total ^{14}C in the test solutions was determined using LSC. Volatiles were not measured.

Derivatization method, if used: A derivatization method was not employed.

Identification and quantification of the parent: Analyses of [^{14}C]penoxsulam residues in the test solutions were performed using three different HPLC systems: YMC ODS-AQ, Hypercarb, and Intersil ODS3. Only the YMC ODS-AQ system was used for identification of the parent (p.15). The reversed-phase HPLC instrument was equipped with a Varian 9010 pump, a Waters auto sampler (Model 717), a Varian 9050 UV detector (set to 255 nm), and a Packard Radiomatic 515TR solid flow cell detector (p.15). For the YMC ODS-AQ HPLC system, the conditions were the following: YMC ODS-AQ column, 5 µm, (250 x 4.6 mm i.d.), temperature, 35°C, gradient mobile phase consisting of water:acetic acid 100:2 (A) and acetonitrile:acetic acid 100:2 (B) [percent A:B (v:v), 0 to 5 minutes 95:5, 30 to 35 minutes 10:90, and 40 to 50 minutes 95:5], and 1 mL/minute flow rate (Appendix 3, p.63).

[^{14}C]Penoxsulam was identified by co-chromatography in the YMC ODS-AQ HPLC system with the non-radiolabeled penoxsulam reference standard. 1000 µL aliquots (unspecified number) were measured of each pH 7 buffer and natural water photodegradation sample (irradiated and dark, p.21).

Further confirmation of [^{14}C]penoxsulam was reported by positive and negative ion electrospray LC/MS analysis. The LC/MS instrument conditions were as followings: Finnigan TSQ700 triple sector quadrupole mass spectrometer (Thermoquest Ltd, Paradise, Hemel Hempstead, Hertfordshire, U.K.), YMC ODS-AQ column, 5 µm, (250 x 4.6 mm i.d.), column temperature, ambient, capillary temperature, 260°C, ESI spray voltage, *ca* 4.5 kV, gradient mobile phase consisting of water with 0.1% formic acid (A) and acetonitrile with 0.1% formic acid (B) [percent A:B (v:v), 0 to 10 minutes 95:5, 10 to 30 minutes 95:5 to 10:90, 30 to 35 minutes 10:90, 35 to 40 minutes 10:90 to 95:5, and 40 to 50 minutes 95:5], and 1 mL/minute flow rate (Appendix 5, p.2 of 106). The specific samples from which [^{14}C]penoxsulam was isolated for LC/MS from the natural water ID test solution was not reported. Appendix 5 of the study report contained all relevant raw data, LC/MS spectra. However, the titles of the spectra did not clearly indicate which sample produced the data. Samples were also analyzed with the LC/MS using the Hypercarb column and conditions, and a GC-MS. However, these analyses were inconclusive (Appendix 5, p.3 of 106). Additionally, the trifluoroacidic acid in the Hypercarb conditions caused the ion current to be too high in the LC/MS instrument (p.15).

The parent was quantified by measuring the distribution of radioactivity in the HPLC data and expressing it in percent of applied radioactivity recovered in the total sample (p.21).

Identification and quantification of transformation products: Analyses of [^{14}C]penoxsulam residues in the test solutions were performed using three different HPLC systems: YMC ODS-AQ, Hypercarb, and Intersil ODS3. The YMC ODS-AQ system was used for separation of the parent from its non-polar and polar degradates. The Hypercarb and Intersil ODS3 systems were used to separate the polar degradates. All three HPLC systems were employed to quantify all transformation products (p.15)

The reversed-phase HPLC instrument was equipped with a Varian 9010 pump, a Waters auto sampler (Model 717), a Varian 9050 UV detector (set to 255 nm), and a Packard Radiomatic 515TR solid flow cell detector (p.15)

For the YMC ODS-AQ HPLC system, the conditions were the following: YMC ODS-AQ column, 5 µm, (250 x 4.6 mm i.d.), temperature, 35°C, gradient mobile phase consisting of water:acetic acid 100:2 (A) and acetonitrile:acetic acid 100:2 (B) [percent A:B (v:v), 0 to 30 minutes 95:5, 30 to 40 minutes 10:90, and 40 to 50 minutes 95:5], and 1 mL/minute flow rate (Appendix 3, p.63).

For the Hypercarb HPLC system, the conditions were the following: Hypercarb column, 5 µm (75 x 4.6 mm i.d.), temperature, ambient, gradient mobile phase consisting of water:trifluoroacetic acid

100:1 (A) and acetonitrile:trifluoroacetic acid 100:1 (B) [percent A:B (v:v), 0 to 20 minutes 100:0, 20 to 40 minutes 0:100, and 40 to 45 minutes 100:0], and 1 mL/minute flow rate (Appendix 3, p.63).

For the Intersil ODS3 HPLC system, the conditions were the following: Intersil ODS3 column, 5 µm (250 x 4.6 mm i.d.), temperature, 35°C, gradient mobile phase consisting of water:acetic acid 100:2 (A) and acetonitrile:acetic acid 100:2 (B) [percent A:B (v:v), 0 to 30 minutes 95:5, 30 to 40 minutes 10:90, and 40 to 50 minutes 95:5], and 1 mL/minute flow rate (Appendix 3, p.63). The following reference standards were co-chromatographed on the HPLC systems and analyzed for comparison: TPSA (5,8-dimethoxy[1,2,4]triazolo-[1,5-*c*]pyrimidin-2-yl-sulfamic acid), 2-amino TP (5,8-dimethoxy[1,2,4]triazolo-[1,5-*c*]pyrimidine-2-amine), BSA (2-(2,2-difluoroethoxy)-5-(trifluoromethyl) benzenesulphonic acid), 5-OH, 2-amino TP (8-methoxy[1,2,4]triazolo-[1,5-*c*]pyrimidin-5-ol-2-amine), BSTCA-methyl (methyl 5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-3-carboxylic acid), BSTCA (5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-3-carboxylic acid), 2-amino TCA (2-amino-1,3,4-triazole-5-carboxylic acid), and 2-amino triazole (2-amino-1,3,4-triazole; Appendix 1, pp.60-61). The co-chromatography of each degradation product and its reference standard was established in two HPLC systems when possible (p.15).

Further confirmation of the transformation products by LC/MS was completed, using the same conditions as those for the parent. The reference standards for the identification of degradation products by LC/MS analysis were the following: 5-Hydroxy XDE-638, Hydroxyphenyl XDE-638, TPSA, 2-amino TP, BSA, (5-OH, 2-amino TP), BSTCA-methyl, and BSTCA (Appendix 5, Table 1, p.5 of 106).

The quantification of the transformation products was the same as of the parent.

The study authors stated that the parent did not degrade in the dark controls. No quantitative data were provided (p.22).

Detection limits (LOD, LOQ) for the parent: Detection limits for the LSC and HPLC were not reported.

Detection limits (LOD, LOQ) for the transformation products: Detection limits for the LSC and HPLC were not reported.

II. RESULTS AND DISCUSSION:

A. TEST CONDITIONS: The incubation temperatures were reportedly maintained at 25 ± 2°C. However, supporting data were provided only for [^{14}C-TP]penoxsulam experiment conducted beginning June 24th (p.14; Figure 2, p.35). The pH ranges for the pH 7 buffer were not reported. The sterility of the buffer solution was checked prior to treatment and at each sampling interval. Results were not reported (p.13).

B. MATERIAL BALANCE: Total [^{14}C]residue recovery in the test solutions of the [^{14}C-TP]penoxsulam experiment at 25°C ranged from 96.0% to 100.0% of the applied (mean 99.2 ± 1.4%) for the irradiated samples of the sterile pH 7 buffer, from 99.8% to 102.0% of the applied (mean 101.0 ± 1.0%) for the dark controls of the sterile pH 7 buffer, from 87.8% to 100.0% of the applied (mean 96.0 ± 3.7%) for irradiated samples of the natural water, and from 96.8% to 100.0% of the applied (mean 98.7 ± 1.0%) for dark controls of the natural water (Table 1a, p.30). The study authors proposed that low recovery of applied radioactivity (87.8%) in the irradiated samples of the natural water test solution at 28 days was due to generation of volatiles or adsorption of degradation products to the glass vessel (p.21).

Total [^{14}C]residue recovery in the test solutions of the [^{14}C-Ph]penoxsulam experiment at 25°C ranged from 78.8% to 100.0% of the applied (mean 94.3 ± 7.2%) for the irradiated samples of the sterile pH 7 buffer, from 98.6% to 103.0% of the applied (mean 99.9 ± 1.3%) for the dark controls of the sterile pH 7 buffer, from 74.1% to 100.0% of the applied (mean 89.7 ± 10.5%) for irradiated samples of the natural water, and from 96.6% to 100.0% of the applied (mean 98.3 ± 0.9%) for dark controls samples of the natural water (Table 1a, p.30).

Table 5a: Phototransformation of [^{14}C-thiazolopyrimidine]penoxsulam in pH 7 phosphate buffer, expressed as a percentage of the applied radioactivity.*

Compound		Sampling intervals (days)							
		0	0.5	1	1.4	3	7	14	28
XDE-638 (Penoxsulam)	Irradiated	100.0	35.7	17.3	0.0	0.0	0.0	0.0	0.0
	Dark	It was reported that no degradation occurred in the dark control. Quantitative data were not provided.							
Polars	Irradiated	0.0	0.0	0.0	22.0	23.7	36.4	62.7	84.6
5-OH, 2-amino TP	Irradiated	0.0	0.0	0.0	2.6	7.5	7.4	9.0	5.3
M1a	Irradiated	0.0	0.0	0.0	0.0	3.7	4.0	5.1	2.1
M2	Irradiated	0.0	0.0	0.0	0.0	5.3	6.6	0.0	4.0
M3	Irradiated	0.0	0.0	0.0	0.0	2.9	5.6	3.9	0.0
TPSA	Irradiated	0.0	47.7	53.0	48.1	36.5	26.4	17.6	0.0
M5	Irradiated	0.0	0.0	7.7	3.4	4.8	3.0	0.0	0.0
2-amino TP	Irradiated	0.0	9.2	18.2	16.0	10.4	5.8	0.0	0.0
M7	Irradiated	0.0	6.4	3.6	5.2	0.0	0.0	0.0	0.0
M8	Irradiated	0.0	0.0	0.0	2.9	5.4	4.4	0.0	0.0
BSTCA-methyl	Irradiated	0.0	1.2	0.0	0.0	0.0	0.0	0.0	0.0
Volatiles		Volatiles were not measured.							
Total % recovery:	Irradiated	100	100.2	99.8	100.2	100.2	99.6	98.3	96.0
	Dark	100	102	99.8	101	102	101	102	100

* Data were obtained from Table 1a, p.30 and Table 2, p.32. Only one sample was collected at each sampling interval.

Table 5b: Phototransformation of [^{14}C-phenyl]penoxsulam in sterile pH 7 buffer, expressed as a percentage of the applied radioactivity.*

Compound		Sampling intervals (days)									
		0	0.167	0.33	0.5	1	1.5	3	7	14	28
Penoxsulam (XDE-638)	Irradiated	100.0	87.5	75.1	60.5	26.7	12.2	0.0	0.0	0.0	0.0
	Dark	It was reported that no degradation occurred in the dark control. Quantitative data were not provided.									
Polars	Irradiated	0.0	0.0	0.0	0.0	25.6	31.6	58.7	84.9	85.7	78.8
BSA	Irradiated	0.0	11.0	16.6	26.3	35.8	36.1	32.0	4.7	0.0	0.0
BSTCA	Irradiated	0.0	0.0	2.8	7.0	4.8	3.9	3.5	0.0	0.0	0.0
BSTCA-methyl	Irradiated	0.0	0.0	5.2	5.0	6.3	6.8	2.1	0.0	0.0	0.0
Di-FESA	Irradiated	0.0	0.0	0.0	0.0	0.0	5.1	0.0	0.0	0.0	0.0
Volatiles	Irradiated	Volatiles not measured.									
Total % recovery:	Irradiated	100	98.5	99.7	98.8	99.1	95.7	96.3	89.9	85.7	78.8
	Dark	100	99.2	99.2	99.5	98.6	99.1	99.0	101	99.9	103

*Data obtained from Table 3, p.33 and Table 1a, p.30 of the study report. Only one sample was collected at each sampling interval.

Table 5c: Phototransformation of [^{14}C-thiazolopyrimidine]penoxsulam in natural water, expressed as a percentage of the applied radioactivity.*

Compound		Sampling intervals (days)							
		0	0.5	1	1.4	3	7	14	28
Penoxsulam (XDE-638)	Irradiated	100.0	42.8	6.8	3.2	0.0	0.0	0.0	0.0
	Dark	It was reported that no degradation occurred in the dark control. Quantitative data were not provided.							
Polars	Irradiated	0.0	0.0	12.8	18.9	32.0	63.9	71.7	70.9
5-OH, 2-amino TP	Irradiated	0.0	0.0	0.0	0.0	10.4	11.0	23.4	16.9
M1b	Irradiated	0.0	0.0	0.0	0.0	7.4	3.9	0.0	0.0
TPSA	Irradiated	0.0	33.7	56.0	55.4	30.7	9.1	0.0	0.0
2-amino TP	Irradiated	0.0	13.7	15.1	17.4	17.8	0.0	0.0	0.0
M8a	Irradiated	0.0	3.6	0.0	0.0	0.0	0.0	0.0	0.0
BSTCA-methyl	Irradiated	0.0	4.1	4.4	2.6	0.0	0.0	0.0	0.0
Volatiles	Irradiated	Volatiles were not measured.							
Total % recovery:	Irradiated	100	98.0	95.1	97.6	98.5	95.7	95.1	87.8
	Dark	100	99.2	98.5	98.4	98.2	100	98.6	96.8

*Data obtained from Table 1a, p.30, and Table 2, p.32. Only one sample was collected at each sampling interval.

Table 5d: Phototransformation of [^{14}C-phenyl]penoxsulam in natural water, expressed as a percentage of the applied radioactivity.*

Compound		Sampling intervals (days)									
		0	0.167	0.33	0.5	1	1.5	3	7	14	28
Penoxsulam (XDE-638)	Irradiated	100	90	71.2	64.5	43	13.7	0	0	0	0
	Dark	It was reported that no degradation occurred in the dark control. Quantitative data were not provided.									
Polars	Irradiated	0	0	0	0	0	32.6	65.9	78.8	73.6	74.1
BSA	Irradiated	0	4	11.6	20.3	30.2	33.5	21.1	0	0	0
BSTCA	Irradiated	0	0	2.7	3.8	7.2	7	0	0	0	0
BSTCA-methyl	Irradiated	0	0	4.3	3.7	7.6	4.1	0	0	0	0
Di-FESA	Irradiated	0	4.2	7.8	5.3	7.6	2.7	0	0	0	0
Volatiles	Irradiated	Volatiles not measured.									
Total % recovery:	Irradiated	100	98.2	97.6	97.7	95.7	93.7	87.0	78.8	73.6	74.1
	Dark	100	98.8	97.9	98.2	97.3	96.6	98.2	98.7	98.4	98.4

*Data obtained from Table 1a, p.30, and Table 3, p.33. Only one sample was collected at each sampling interval.

C. TRANSFORMATION OF PARENT COMPOUND: [^{14}C]Penoxsulam degraded very rapidly via photolysis in sterile pH 7 buffer and natural water at 25 °C. In all irradiated samples, no parent was present in solution after 3 days (Tables 2 and 3, pp.32, 33). [^{14}C]Penoxsulam did not degrade in the dark controls indicating that hydrolysis was not a significant route of degradation (p.29).

[^{14}C-TP]Penoxsulam (irradiated): In the sterile pH 7 buffer solution, [^{14}C-TP]penoxsulam decreased from 100.0% of the applied radioactivity at time 0 to 17.3% at 1.0 days to 0.0% at 1.4 days (Table 2, p.32). In the natural water solution, [^{14}C-TP]penoxsulam decreased from 100.0% of the applied radioactivity at time 0 to 6.8% at 1.0 days to 0.0% at 3.0 days (Table 2, p.32).

[^{14}C-Ph]penoxsulam (irradiated): In the sterile pH 7 buffer solution, [^{14}C-Ph]penoxsulam decreased from 100.0% of the applied radioactivity at time 0 to 26.7% at 1.0 days to 0.0% at 3.0 days (Table 3, p.33). In the natural water solution, [^{14}C-Ph]penoxsulam decreased from 100.0% of the applied radioactivity at time 0 to 43.0% at 1.0 days to 0.0% at 3.0 days (Table 3, p.33).

[^{14}C-TP]penoxsulam and [^{14}C-Ph]penoxsulam (dark controls): The study authors stated that penoxsulam did not degrade in the dark controls (p.22). No quantitative data were provided.

HALF-LIVES: Based on first-order linear regression analysis (Excel 2000) and using data through the first non-detect (<3 days), the calculated **half-life** of penoxsulam (combined labels) was 1.5 days in sterile buffer solution and 1.3 days in natural water, based on a 12 hour light/dark cycle, and normal solar radiant intensity at 40° latitude. Penoxsulam was stable in the dark controls.

The study authors calculated rates of degradation, DT50s, and DT90s for the parent and three of the major transformation products for the sterile pH 7 buffer and natural water solutions of the [^{14}C-TP]penoxsulam experiments in terms of days of continuous irradiation using the ModelMaker software from Cherwell Scientific. The study authors stated that they did not calculate rates of degradation DT50s, or DT90s for the [^{14}C-Ph]penoxsulam experiments because the route of degradation could not be followed clearly from the parent through the transformation products. (p.28; Figure 16, pp.58-59)

Half-lives *Not Corrected* for 12 Hour Light/Dark Cycle and 40° Latitude*

Test system	First order linear			DT50 (days)	DT90 (days)
	Half-life (not corrected)	Regression equation	r^2		
Triazolopyrimidine label					
Sterile pH 7 Buffer	0.40 days	y = -1.7545x + 4.5542	0.9900	0.332	1.1
Natural Water	0.27 days	y = -2.5929x +4.7403	0.9774	0.369	1.22
Phenyl label					
Sterile pH 7 Buffer	0.54 days	y = -1.2723x + 4.6726	0.9892	ND	ND
Natural Water	0.68 days	y = -1.0242x + 4.6725	0.9584	ND	ND
Combined labels					
Sterile pH 7 Buffer	0.51 days	y = -1.3582x + 4.6005	0.9063	ND	ND
Natural Water	0.39 days	y = -1.7874x + 4.7329	0.6816	ND	ND

*Half-lives were calculated using data points through the final detection of the parent. Data were obtained from Table 2, p.32 and Table 3, p.33 of the study report. DT50s and DT90s were determined by the study authors for the [^{14}C-TP]penoxsulam experiment only (p.28).

Since no degradation was reported to have occurred in the dark control, the **phototransformation half-lives** were approximately 1.0 and 0.8 days, respectively, based on **continuous irradiation** or a 12-hour light/dark cycle. The artificial light was approximately **1.3x stronger** than average summer sunlight at 40°N (calculated using data in Appendix 4, pp.64, 65). Therefore, the **predicted environmental phototransformation half-life** of penoxsulam in both the buffer solution and natural water is **1.5 days.**

TRANSFORMATION PRODUCTS: The study authors stated that penoxsulam did not degrade in the dark controls. No quantitative data were provided (p.22).

In the irradiated samples, more than 20 distinct transformation products were isolated. Of these, four major degradation products (17-56% of applied radioactivity), two minor degradation products (approximately 7% of applied radioactivity), and two polar degradation products (<10% and 17.5% of applied radioactivity) were identified by co-chromatography with reference standards and by LC/MS analysis (pp.23-25).

Four Major Degradation Products [TPSA, 2-amino TP, (5-OH, 2-amino TP), and BSA]: TPSA, 2-amino TP, and (5-OH, 2-amino TP) were only detected in the [^{14}C-TP]penoxsulam experiment, whereas, BSA was only detected in the [^{14}C-Ph]penoxsulam experiment (Table 2 and 3, pp.32-33). TPSA increased from 0.0% of the applied radioactivity at time 0 to 53.0% at 1.0 days, then decreased to 0.0% at 28 days posttreatment in the sterile pH 7 buffer solution. Similarly, TPSA increased from 0.0% of the applied radioactivity at time 0 to 56.0% at 1.0 days, then decreased to 0.0% at 28 days posttreatment in the natural water solution. 2-amino TP increased from 0.0% of the applied radioactivity at time 0 to 18.2% at 1.0 days, then decreased to 0.0% at 28 days posttreatment in the sterile pH 7 buffer solution. Similarly, 2-amino TP increased from 0.0% of the applied radioactivity at time 0 to 17.8% at 3.0 days, then decreased to 0.0% at 28 days posttreatment in the natural water solution. (5-OH, 2-amino TP) increased from 0.0% of the applied radioactivity at time 0 to 9.0% at 14 days, then decreased to 5.3% at 28 days posttreatment in the sterile pH 7 buffer solution. Similarly, (5-OH, 2-amino TP) increased from 0.0% of the applied radioactivity at time 0 to 23.4% at 14 days, then decreased to 16.9% at 28 days posttreatment in the natural water solution. BSA increased from 0.0% of the applied radioactivity at time 0 to 36.1% at 1.5 days, then decreased to 0.0% at 28 days posttreatment in the sterile pH 7 buffer solution. Similarly, BSA increased from 0.0% of the applied radioactivity at time 0 to 33.5% at 1.5 days, then decreased to 0.0% at 28 days posttreatment in the natural water solution (Table 2 and 3, pp.32-33).

Two Minor Degradation Products [BSTCA methyl and BSTCA]: BSTCA methyl was detected in both the [^{14}C-TP]penoxsulam and [^{14}C-Ph]penoxsulam experiments, whereas, BSTCA was only detected in the [^{14}C-Ph]penoxsulam experiment (Table 2 and 3, pp.32-33). In the [^{14}C-TP]penoxsulam sterile pH 7 buffer experiment, BSTCA methyl was only detected once at 1.2% of applied radioactivity at 0.5 days posttreatment. In the [^{14}C-TP]penoxsulam natural water experiment, BSTCA methyl increased from 0.0% of applied radioactivity at time 0 to 4.4% at 1.0 days, then decreased to 0.0% at 28 days posttreatment. In the [^{14}C-Ph]penoxsulam sterile pH 7 buffer experiment, BSTCA methyl increased from 0.0% of applied radioactivity at time 0 to 6.8% at 1.5 days, then decreased to 0.0% at 28 days posttreatment. Similarly, in the [^{14}C-Ph]penoxsulam natural water experiment, BSTCA methyl increased from 0.0% of applied radioactivity at time 0 to 7.6% at 1.0 days, then decreased to 0.0% at 28 days posttreatment. BSTCA increased from 0.0% of applied radioactivity at time 0 to 7.0% at 0.5 days, then decreased to 0.0% at 28 days posttreatment. Similarly, BSTCA increased from 0.0% of applied radioactivity at time 0 to 7.2% at 1.0 days, then decreased to 0.0% at 28 days posttreatment.

Two Polar Degradation Products [2-amino TCA and 2-amino triazole]: In the [^{14}C-TP]penoxsulam experiment, the Polars increased from 0.0% of applied radioactivity at time 0 to 84.6% and 70.9% at 28 days posttreatment in the sterile pH 7 buffer and natural water experiments, respectively (Table 2 and 3, p.32-33). In the [^{14}C-Ph]penoxsulam experiment, the Polars increased from 0.0% of applied radioactivity at time 0 to 78.8% and 74.1% at 28 days posttreatment in the sterile pH 7 buffer and natural water experiments, respectively.

The Polars of the [^{14}C-TP]penoxsulam experiment were determined to be composed of more than 15 distinct components, and the Polars of the [^{14}C-Ph]penoxsulam experiment were determined to be composed of approximately 17 distinct components. However, after multiple resolutions were performed, the study authors determined that only one distinct compound of the Polars was present above 10% of applied radioactivity. The compound was identified as 2-amino TCA, present at 17.5% of applied radioactivity at 28 days posttreatment in the [^{14}C-TP]penoxsulam experiment. Additionally, 2-amino triazole was identified in [^{14}C-TP]penoxsulam experiment, present in less than 10% of applied radioactivity at 28 days posttreatment (pp.25-26; Figures 8, p.49; Figure 10, p.51; Figure 12, p.53).

Table 6: Chemical names for the transformation products of penoxsulam.

Applicant's Code Name	CAS Number	Chemical Names	Chemical formula	Molecular weight (g/mol)	Smiles string
2-Amino TP		5,8-Dimethoxy[1,2,4]triazolo-[1,5-*c*]pyrimidin-2-amine		195	
TPSA		5,8-Dimethoxy[1,2,4]triazolo-[1,5-*c*]pyrimidine-2-yl-sulfamic acid		275	
BSA		2-(2,2-Difluoroethoxy)-6-(trifluoromethyl) benzenesulphonic acid		306	
5-OH, 2-Amino TP		8-Methoxy[1,2,4]triazolo-[1,5-*c*]pyrimidin-5-ol-2-amine		181	
BSTCA		5-[[[2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-3-carboxylic acid		416	
BSTCA-methyl		Methyl 5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-3-carboxylic acid		430	
2-Amino TCA		2-Amino-1,3,4-triazole-5-carboxylic acid		128	
2-Amino triazole		2-Amino-1,3,4-triazole		84	
di-FESA		3-(2,2-Difluoroethoxy)-2-hydroxybenzoic acid			

Chemical names and information obtained from pp.22-24, and Appendix 1, pp.60-61.

VOLATILIZATION: Volatiles were not measured. See the Supplementary Experiments section of the Data Evaluation Report.

TRANSFORMATION PATHWAY: A transformation pathway was proposed by the study authors (pp.10, 26, 27; Figure 15, p.57). The proposed transformation pathway involved two major routes of degradation and one minor route of degradation. The 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.

The more favored proposed major route of degradation involved the sulfur-nitrogen cleavage of the sulfonamide group, generating 2-amino TP and BSA. 2-amino TP degraded via demethylation to (5-OH, 2-amino TP), which further degraded to multiple polar degradates including 2-amino TCA. BSA degraded to multiple polar degradates and carbon dioxide. In the ID solution experiments,

another intermediate degradation product was seen for 2-amino TP. However, it was not detected in the primary [^{14}C-TP]penoxsulam experiment.

The less favored proposed major route of degradation involved the sulfur-phenyl cleavage of the sulfonamide group, generating TPSA and the phenyl moiety. TPSA degraded to 2-amino TP, which then followed the degradation pathway which was described above. The phenyl moiety could not be detected in the ID solution experiments. However, its degradation product, di-FESA, was identified in the primary [^{14}C-Ph]penoxsulam experiment. Di-FESA further degraded to multiple polar degradates and carbon dioxide.

The minor route of degradation involved the opening of the pyrimidine ring, generating BSTCA methyl. BSTCA methyl degraded to BSTCA via ester hydrolysis. BSTCA further degraded to multiple polar degradates and carbon dioxide. Due to the low amounts (<10% of applied radioactivity) of BSTCA methyl and BSTCA which were detected in the [^{14}C-TP]penoxsulam and [^{14}C-Ph]penoxsulam experiments, the study authors did not consider this proposed minor route a significant degradation pathway for the parent, XDE-638.

By comparing the sterile pH 7 buffer experiments to the natural water experiments, the study authors proposed that, while the initial cleavage of the less favored major route of degradation occurred via direct photolysis, the subsequent degradation of TPSA to 2-amino TP occurred via indirect photolysis. The study authors did not comment on the other transformation reactions in their pathway.

D. SUPPLEMENTARY EXPERIMENT-RESULTS:

Measurement of $^{14}CO_2$/Volatiles: For the pH 7 buffer and natural water solutions with [^{14}C-Ph]penoxsulam, the results of the volatile trapping and measuring indicated that $^{14}CO_2$ was the only significant volatile generated. The results of the supplementary study were provided in the following tables (Table 1b and 1c, p.31).

Sterile pH 7 Buffer

Days	Aqueous Phase	Acetone Rinse	CO_2 Trap	Organic Trap	Total*
0	100	0	0	0	100
7	89.5	0	10.8	0	100.3
14	79.1	0.2	9.7	0	89.0

*Note: Data obtained from Table 1b, p.31 in the study report with the exception of the Total value for day 14.

Natural Water

Days	Aqueous Phase	Acetone Rinse	CO_2 Trap	Organic Trap	Total*
0	100	0	0	0	100
7	87.1	0	4.7	0	91.8
14	80.8	3.0	7.0	0	90.8

*Note: Data obtained from Table 1c, p.31 in the study report with the exception of the Total value for day 14.

Actinometry: The experimental half-life of *p*-nitroacetophenone (PNAP; 1 x 10^{-5} M) and pyridine (pyr; 1 x 10^{-5} M) in deionized, sterile water was calculated as 5.85 days (p.18; Appendix 4, pp.64-78). The predicted half-life of *p*-nitroacetophenone (PNAP; 1x10^{-5} M) and pyridine (pyr; 1 x 10^{-2} M) in deionized, sterile water at normal sunlight intensity at 40 °N latitude for summer was 7.80 days, based on the quantum yield of the actinometer. The difference in the predicted and experimental half-lives for the actinometer indicated that the xenon lamp intensity of the SUNTEST CPS+ system was slightly higher than the natural sunlight intensity at 40 °N latitude in summer.

III. STUDY DEFICIENCIES:

1. The mass balance for the experiment conducted with buffer solution and [^{14}C-Ph]penoxsulam decreased to 85.7% of the applied at 14 days posttreatment and 78.8% at 28 days (Table 1a, p.30). A corresponding supplementary study attempted to demonstrate that the missing material was CO_2, but failed to characterize any other residue at any sampling interval (Table 1b, p.31).

2. The mass balance for the experiments conducted with natural water and [^{14}C-Ph]penoxsulam decreased to 87.0% of the applied at 3 days posttreatment and 74.1% at 28 days (Table 1a, p.30). A corresponding supplementary study attempted to demonstrate that the missing material was CO_2, but failed to characterize any other residue at any sampling interval (Table 1c, p.31).

3. The phosphate buffer appeared to be too concentrated (calculated as 0.69 M from data on p.13). However, since no interactions between the test substance and the buffer were noted in the dark controls, the concentration of the buffer did not have a significant impact on the study results.

4. The study author did not quantify the ratio of the intensity of artificial light to sunlight, but reported that the intensity of the artificial light was "slightly higher" than the predicted intensity of summer sunlight at 40°N latitude (Appendix 4, p.65). The study author also reported that the half-life of the actinometer solution was 5.85 days under artificial light and was predicted to be 7.80 days under summer sunlight at 40°N latitude, which was determined by the reviewer to be a ratio of 1.3:1 (Appendix 4, pp.64, 65). This ratio was used by the reviewer to estimate the environmental half-life of penoxsulam. However, since the experiments with the two label were

conducted approximately 1 month apart and since the intensity of xenon lamps decreases with use, it is not certain that the 1.3:1 ratio is valid for both experiments.

IV. REVIEWER'S COMMENTS:

1. An unacceptable material balance in one study can not be adequately corrected by a running a supplemental study measuring only the combined residues of parent and degradation products.

2. The concentration of [^{14}C-TP] and [^{14}C-Ph]penoxsulam stock solutions and the solubility of penoxsulam in buffered water was not provided.

3. The period of irradiation time for the natural water and pure HPLC water ID solutions was unclear. In Section 2.9 entitled, Preparation of the metabolites for identification, it was stated that the natural water ID solutions were "left under a xenon light source for 8 days" and the pure HPLC water ID solutions were "left under a xenon light source for up to 21 days" (p.17). However, in Section 4.4 entitled, Identification of degradation products, it was indicated that the analysis of the natural water solution was completed "after 21 days exposure to natural light" (p.22). It was unclear why the reported exposure period was different, and why the time period was reported as natural light. No additional report of the time period of exposure for the pure HPLC water was present in this section. No data figure or table clearly indicated results from the ID experiments. Therefore, the reviewer could not determine the length of exposure for the ID samples by supplied data figures and tables.

4. The temperature for the definite study was reported as 25 ± 2°C (pp.14, 20). However, the temperature range of the study was reported as 24-26°C "for both the TP-labeled and Ph-labeled experiments" in the study text (p.20) and as 24-26°C for the photolysis chamber (irradiated samples) and 24-25°C for the incubator (dark controls) in Figure 2 (p.35).

5. The structures which were provided in the degradation scheme (p.10; Figure 15, p.57) and Appendix 1 (pp.60-61) were of poor quality.

6. The Limits of Quantification and Detection were not reported for the LSC or the HPLC systems (p.15).

7. The study authors calculated rates of degradation, DT50s and DT90s for the parent and three of the major transformation products for the sterile pH 7 buffer and natural water solutions of the [^{14}C-TP]penoxsulam experiments in terms of days of continuous irradiation using the ModelMaker software from Cherwell Scientific. For the sterile buffer solutions, the calculated rate constants for degradation of penoxsulam, TPSA, 2-amino TP, and BSA were 2.09 days^{-1}, 0.148 days^{-1}, 1.19 days^{-1}, and 0.743 days^{-1}, respectively. For the natural water, the calculated

rate constants for degradation of penoxsulam-638, TPSA, 2-amino TP, and BSA were 1.88 days^{-1}, 0.343 days^{-1}, 1.14 days^{-1}, and 1.02 days^{-1}, respectively.

The calculated DT50s for degradation of TPSA, 2-amino TP, and BSA in the buffer solution were 4.68 days, 0.582 days, and 0.933 days, respectively, and in the natural water were 2.02 days, 0.608 days, and 0.680 days, respectively. The study authors calculated DT90s for degradation of TPSA, 2-amino TP, and BSA in the sterile buffer were 15.6 days, 1.93 days, and 3.10 days, respectively, and in the natural water were 6.71 days, 2.02 days, and 2.26 days, respectively

8. The study authors did not calculate rates of degradation, DT50s, or DT90s for the [^{14}C-Ph]penoxsulam experiments because the route of degradation could not be followed clearly from the parent through the transformation products (p.28; Figure 16, pp.58-59).

9. Several of the calculated total % recovery values for Tables 2 and 3 (pp.32-33), which was summarized in Tables 5a-5d of the Data Evaluation Report, differed slightly from the corresponding total % recovery mean values from the study report.

10. The spectrum for Figure 62: Mass Spectrum of XDE-638 Photoproduct, Molecular Mass 290 (P-Label) in Appendix 5 was missing. Except for the figure title, the header and the footer, page 78 of 106 is completely blank.

11. The study report contained multiple typographical errors. The entire sentence, "2-amino TP further degrades to give 5-OH, 2-amino TP before undergoing further degradation to give smaller polar metabolites including 3-amino TCA.", was repeated in the first and third paragraphs without apparent reason on p.27. This repeated sentence on p.27 also contained the error of calling the 2-amino TCA degradate, 3-amino TCA. The same error was made again in the third paragraph on p.25. The reviewer assumed that the sentence, "Degradation of XDE-638 proceeded more slowly at the increased rate", was meant to read, "Degradation of XDE-638 proceeded more slowly at the increased concentration" (p.22). "Triazolo" was incorrectly spelled "triazaolo" in the name of XDE-638 which was listed in Appendix 1 and the name of (5-OH, 2-amino TP) which was listed in Appendix 1 and in the Identification of degradation products, section 4.4.4 (pp.60-61; p.24). In Appendix 1, the chemical name of BSA was given as "2-(2,2-difluoroethoxy)-5-(trifluoromethyl) benzenesulphonic acid" instead of "2-(2,2-difluoroethoxy)-6-(trifluoromethyl) benzenesulphonic acid", BSTCA was given as "5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphonyl]amino],1H-1,2,4-triazole-3-carboxylic acid" instead of "3-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphonyl]amino],1H-1,2,4-triazole-5-carboxylic acid", and BSTCA-methyl was given as "methyl 5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphonyl]amino],1H-1,2,4-triazole-3-carboxylic acid" instead of "methyl 3-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphonyl]amino],1H-1,2,4-triazole-5-carboxylic acid"(p.60). Additionally, in Figures 4a and 4b, the fourth HPLC chromatogram on pp.37 and 39 were

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mistitled with respect to time. The two chromatograms were entitled with the time, "T = 1.5 days". However, only a 1.4 days time interval was written in the experimental protocol for the [^{14}C-TP]penoxsulam experiments (p.14).

12. The chemical names which were provided by the study authors for TPSA and 2-amino TP were inconsistent in the study report. In Appendix 1 (p.60), TPSA was listed as "5,8-dimethoxy[1,2,4]triazolo-[1,5-*c*]pyrimidin-2-yl)-sulfamic acid". However, in the Identification of degradation products, section 4.4.2 (p.23), it was listed as "5,8-dimethoxy[1,2,4]triazolo-[1,5-*c*]pyrimidine-2-sulfamic acid". Similarly, in Appendix 1 (p.60), 2-amino TP was listed as "5,8-dimethoxy[1,2,4]triazolo-[1,5-*c*]pyrimidin-2-amine". However, in the Identification of degradation products, section 4.4.2 (p.23), it was listed as "5,8-dimethoxy[1,2,4]triazolo-[1,5-*c*]pyrimidine-2-amine". Additionally, the chemical name of TPSA which was listed in Appendix 1 contained an unnecessary unclosed parentheses.

13. The study report was badly organized. Many page and figure numbers were incorrectly reported in the text and table of contents. Some examples are the following: the LC/MS analysis was reportedly presented in Appendix 6, instead of Appendix 5, on p.25. The degradation pathway was reportedly illustrated in Figure 19, instead of Figure 15, on p.26, and in the table of contents, no page number was correct for any item after and including Figure 14 (p.7).

14. An aqueous storage stability study (MRID 45830803) indicated that penoxsulam did not significantly degrade after 130 days of refrigerated storage (average recovery 100.7% of applied) or 221 days of frozen storage (average recovery 96.0%), while recoveries of 5-OH-XDE-638 and BSTCA after 284 days of refrigerated storage averaged 99.7% and 90.7%, respectively (Tables 2-3, pp.28-35 in MRID 45830803), BSTCA-methyl and 5,8-diOH were not tested.

15. Beginning on page 10, many of the chemical structures drawn in the study report were, at best, only partially legible.

V. REFERENCES:

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 161-2. Photolysis studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.

2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.

3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

Attachment 1

Excel Spreadsheets

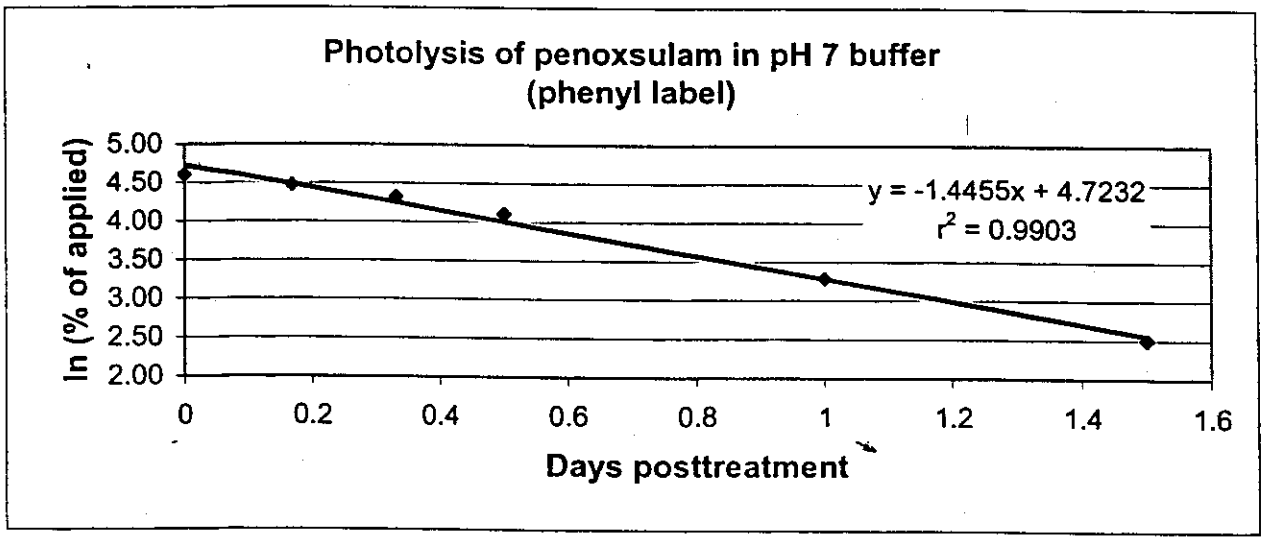
Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Sterile pH 7 buffer, 25°C
Phenyl label

Half-life (days): 0.48

Days Posttreatment	Penoxsulam (% of applied)	ln (% of applied)
0	100.0	4.6052
0.167	87.5	4.4716
0.33	75.1	4.3188
0.5	60.5	4.1026
1	26.7	3.2847
1.5	12.2	2.5014
3	0.0	
7	0.0	
14	0.0	
28	0.0	

Data obtained from Table 3, p. 33 of the study report.



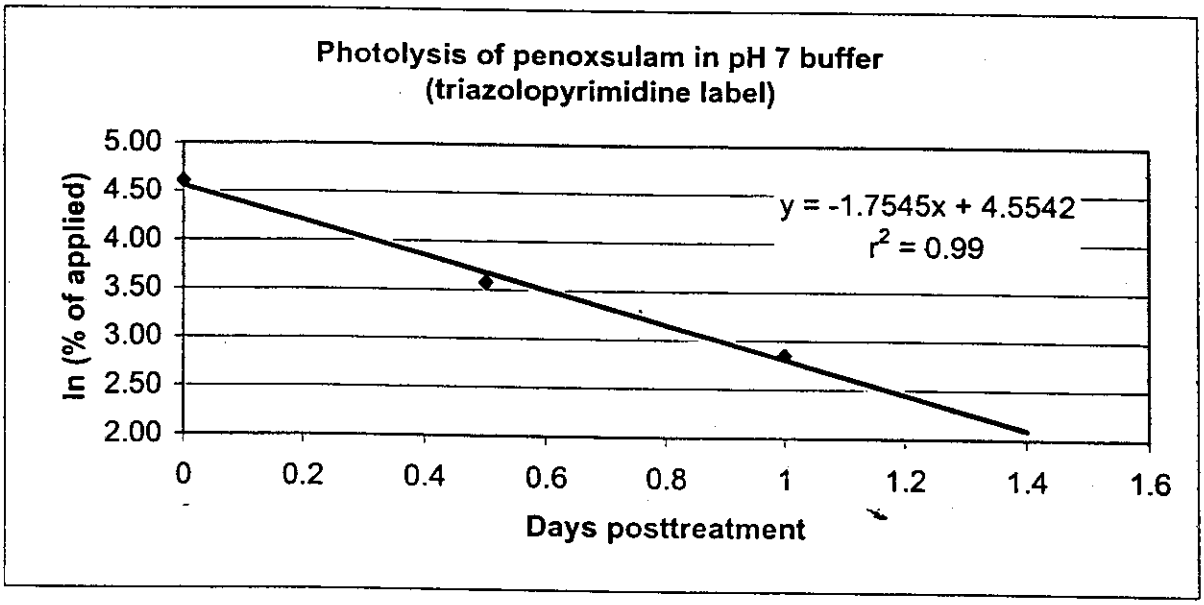
Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Sterile pH 7 Buffer, 25°C
Triazolopyrimidine label

Half-life (days): 0.40

Days Posttreatment	Penoxsulam (% of applied)	ln (% of applied)
0	100.0	4.6052
0.5	35.7	3.5752
1	17.3	2.8507
1.4	0.0	
3	0.0	
7	0.0	
14	0.0	
28	0.0	

Data obtained from Table 2, p. 32 of the study report.



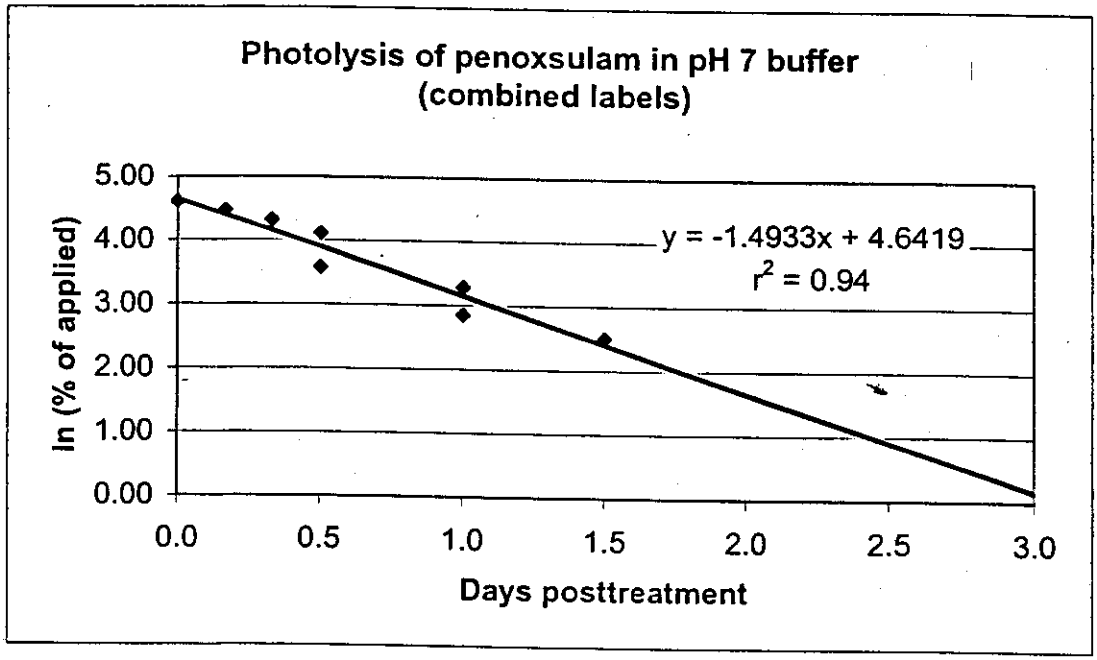
Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Sterile pH 7 buffer, 25°C
Combined data

Half-life (days): 0.46

Days Posttreatment	Penoxsulam (% of applied)	ln (% of applied)	
0	100.0	4.6052	
0.167	87.5	4.4716	
0.33	75.1	4.3188	Phenyl
0.5	60.5	4.1026	
1	26.7	3.2847	
1.5	12.2	2.5014	
3	0.0		
0	100.0	4.6052	
0.5	35.7	3.5752	
1	17.3	2.8507	Triazolopyrimidine
1.4	0.0		
3	0.0		

Data obtained from Table 2-3, pp. 32-33 of the study report.



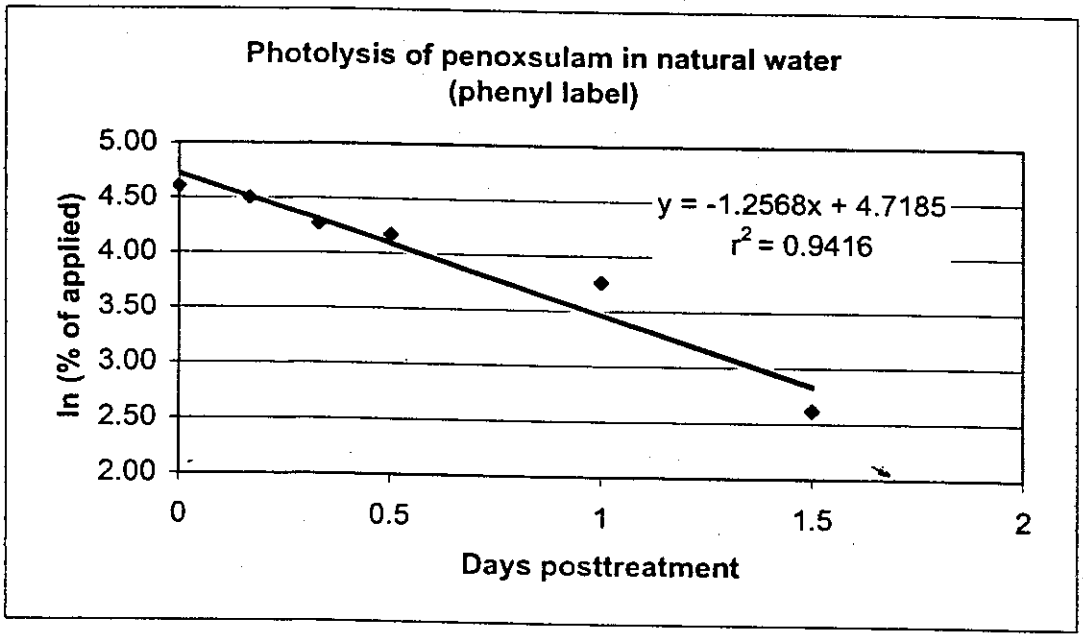
Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Natural Water, 25°C
Phenyl label

Half-life (days): 0.55

Days Posttreatment	Penoxsulam (% of applied)	ln (% of applied)
0	100.0	4.6052
0.167	90.0	4.4998
0.33	71.2	4.2655
0.5	64.5	4.1667
1	43.0	3.7612
1.5	13.7	2.6174
3	0.0	
7	0.0	
14	0.0	
28	0.0	

Data obtained from Table 3, p. 33 of the study report.



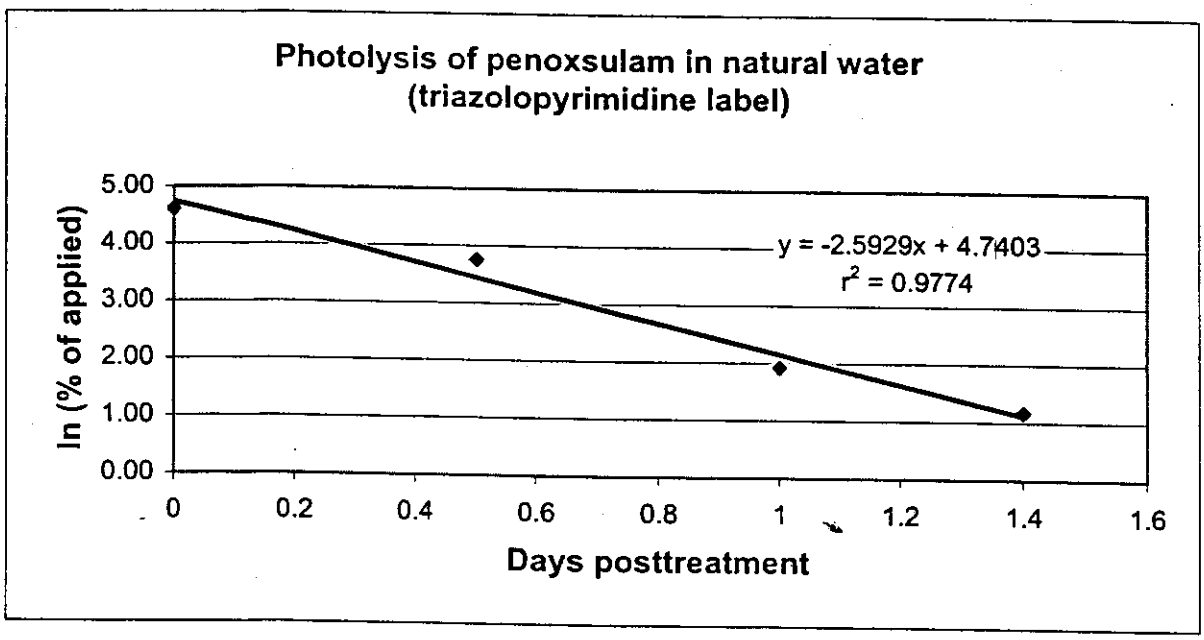
Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Natural Water, 25°C
Triazolopyrimidine label

Half-life (days): 0.27

Days Posttreatment	Penoxsulam (% of applied)	ln (% of applied)
0	100.0	4.6052
0.5	42.8	3.7565
1	6.8	1.9169
1.4	3.2	1.1632
3	0.0	
7	0.0	
14	0.0	
28	0.0	

Data obtained from Table 2, p. 32 of the study report.



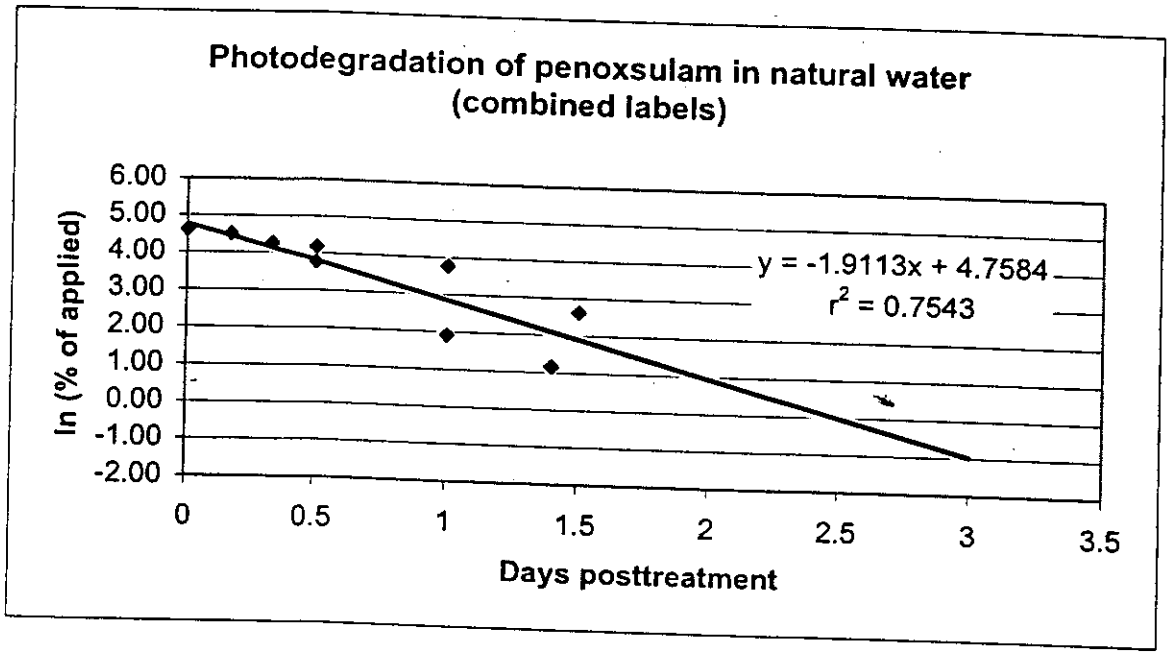
Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Natural Water, 25°C
Combined data

Half-life (days): 0.36

Days Posttreatment	Penoxsulam (% of applied)	ln (% of applied)	
0	100.0	4.6052	
0.167	90.0	4.4998	
0.33	71.2	4.2655	Phenyl
0.5	64.5	4.1667	
1	43.0	3.7612	
1.5	13.7	2.6174	
3	0.0		
0	100.0	4.6052	
0.5	42.8	3.7565	
1	6.8	1.9169	Triazolopyrimidine
1.4	3.2	1.1632	
3	0.0		

Data obtained from Table 2-3, pp. 32-33 of the study report.



Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Data obtained from Tables 1a and 3, pp. 30, 33, of MRID 45384801.

Sterile pH 7 Buffer **25°C**

[^{14}C-Ph]XDE-638 Experiment

Experimental Days	Overall Recovery (% Applied Radioactivity) Exposed	Dark
0	100.0	100.0
0.167	98.5	99.2
0.33	99.7	99.2
0.5	98.8	99.5
1	99.1	98.6
1.5*	95.7	99.1
3*	96.3	99.0
7*	89.9	101.0
14*	85.7	99.9
28*	78.8	103.0
Mean	94.3	99.9
SD	7.2	1.3

*Note: Loss of applied radioactivity in the exposed samples was due to CO_2 production.

Natural Water **25°C**

Experimental Days	Overall Recovery (% Applied Radioactivity) Exposed	Dark
0	100.0	100.0
0.167	98.2	98.8
0.33	97.6	97.9
0.5	97.8	98.2
1	95.6	97.3
1.5*	93.8	96.6
3*	87.0	98.2
7*	78.8	98.7
14*	73.6	98.4
28*	74.1	98.4
Mean	89.7	98.3
SD	10.5	0.9

*Note: Loss of applied radioactivity in the exposed samples was due to CO_2 production.

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Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Sterile pH 7 Buffer 25°C **[^{14}C-Ph]XDE-638 Experiment**

Experimental

Days	Polars	BSA	BSTCA	BSTCA-me	di-FESA	XDE-638	CO_2	Total	Total w/o CO_2
0	0.0	0.0	0.0	0.0	0.0	100.0	*	100.0	100.0
0.167	0.0	11.0	0.0	0.0	0.0	87.5	*	98.5	98.5
0.33	0.0	16.6	2.8	5.2	0.0	75.1	*	99.7	99.7
0.5	0.0	26.3	7.0	5.0	0.0	60.5	*	98.8	98.8
1	25.6	35.8	4.8	6.3	0.0	26.7	*	99.2	99.2
1.5	31.6	36.1	3.9	6.8	5.1	12.2	*	95.7	95.7
3	58.7	32.0	3.5	2.1	0.0	0.0	*	96.3	96.3
7	84.9	4.7	0.0	0.0	0.0	0.0	10.5	100.1	89.6
14	85.7	0.0	0.0	0.0	0.0	0.0	20.9	106.6	85.7
28	78.8	0.0	0.0	0.0	0.0	0.0	*	78.8	78.8

*Note: CO_2 not measured for these timepoints.

Natural Water 25°C

Experimental

Days	Polars	BSA	BSTCA	BSTCA-me	di-FESA	XDE-638	CO_2	Total	Total w/o CO_2
0	0.0	0.0	0.0	0.0	0.0	100.0	*	100.0	100.0
0.167	0.0	4.0	0.0	0.0	4.2	90.0	*	98.2	98.2
0.33	0.0	11.6	2.7	4.3	7.8	71.2	*	97.6	97.6
0.5	0.0	20.3	3.8	3.7	5.3	64.5	*	97.6	97.6
1	0.0	30.2	7.2	7.6	7.6	43.0	*	95.6	95.6
1.5	32.6	33.5	7.0	4.1	2.7	13.7	*	93.6	93.6
3	65.9	21.1	0.0	0.0	0.0	0.0	*	87.0	87.0
7	78.8	0.0	0.0	0.0	0.0	0.0	12.9	91.7	78.8
14	73.6	0.0	0.0	0.0	0.0	0.0	19.2	92.8	73.6
28	74.1	0.0	0.0	0.0	0.0	0.0	*	74.1	74.1

*Note: CO_2 not measured for these timepoints.

Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Data obtained from Tables 1a and 2, pp. 30, 32, of MRID 45384801.

Sterile pH 7 Buffer **25°C**

[^{14}C-TP]XDE-638 Experiment

Experimental Days	Overall Recovery (% Applied Radioactivity) Exposed	Dark
0	100.0	100.0
0.5	100.0	102.0
1	99.7	99.8
1.4	100.0	101.0
3	100.0	102.0
7	99.4	101.0
14	98.3	102.0
28	96.0	100.0
Mean	99.2	101.0
SD	1.4	1.0

Natural Water **25°C**

Experimental Days	Overall Recovery (% Applied Radioactivity) Exposed	Dark
0	100.0	100.0
0.5	98.0	99.2
1	95.1	98.5
1.4	97.6	98.4
3	98.5	98.2
7	95.7	100.0
14	95.1	98.6
28	87.8	96.8
Mean	96.0	98.7
SD	3.7	1.0

Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Sterile pH 7 Buffer **25°C**

Experimental Days	Polars	5-OH 2-amino TP	M1a	M2	M3	TPSA	M5	2-amino TP	M7
0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.5	0.0	0.0	0.0	0.0	0.0	47.7	0.0	9.2	6.4
1	0.0	0.0	0.0	0.0	0.0	53.0	7.7	18.2	3.6
1.4	22.0	2.6	0.0	0.0	0.0	48.1	3.4	16.0	5.2
3	23.7	7.5	3.7	5.3	2.9	36.5	4.8	10.4	0.0
7	36.4	7.4	4.0	6.6	5.6	26.4	3.0	5.8	0.0
14	62.7	9.0	5.1	0.0	3.9	17.6	0.0	0.0	0.0
28	84.6	5.3	2.1	4.0	0.0	0.0	0.0	0.0	0.0

Experimental Days	M8	BSTCA-me	XDE-638	Total
0	0.0	0.0	100.0	100.0
0.5	0.0	1.2	35.7	100.2
1	0.0	0.0	17.3	99.8
1.4	2.9	0.0	0.0	100.2
3	5.4	0.0	0.0	100.2
7	4.4	0.0	0.0	99.6
14	0.0	0.0	0.0	98.3
28	0.0	0.0	0.0	96.0

Natural Water

Experimental Days	Polars	5-OH 2-amino TP	M1b	M2	TPSA	2-amino TP	M8a	BSTCA-me	XDE-638
0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0
0.5	0.0	0.0	0.0	0.0	33.7	13.7	3.6	4.1	42.8
1	12.8	0.0	0.0	0.0	56.0	15.1	0.0	4.4	6.8
1.4	18.9	0.0	0.0	0.0	55.4	17.4	0.0	2.6	3.2
3	32.0	10.4	7.4	0.0	30.7	17.8	0.0	0.0	0.0
7	63.9	11.0	3.9	7.8	9.1	0.0	0.0	0.0	0.0
14	71.7	23.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0
28	70.9	16.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Experimental Days	Total
0	100.0
0.5	97.9
1	95.1
1.4	97.5
3	98.3
7	95.7
14	95.1
28	87.8

Chemical Name: Penoxsulam
PC Code: 119031
MRID: 45834801
Guideline No.: 161-2

Data obtained from Tables 1b and 1c, p. 31, of MRID 45384801.

Supplementary Experiment- Generation of Volatiles in [^{14}C-Ph]XDE-638 Photolysis

Sterile pH 7 Buffer

Experimental Days	Aqueous Phase	Acetone Rinse	CO_2 Trap	Organic Trap	Total
0	100.0	0.0	0.0	0.0	100.0
7	89.5	0.0	10.8	0.0	100.3
14	79.1	0.2	20.5	0.0	99.8

Natural Water

Experimental Days	Aqueous Phase	Acetone Rinse	CO_2 Trap	Organic Trap	Total
0	100.0	0.0	0.0	0.0	100.0
7	87.1	0.0	4.7	0.0	91.8
14	80.8	3.0	11.7	0.0	95.5

Attachment 2

Structures of Parent and Transformation Products

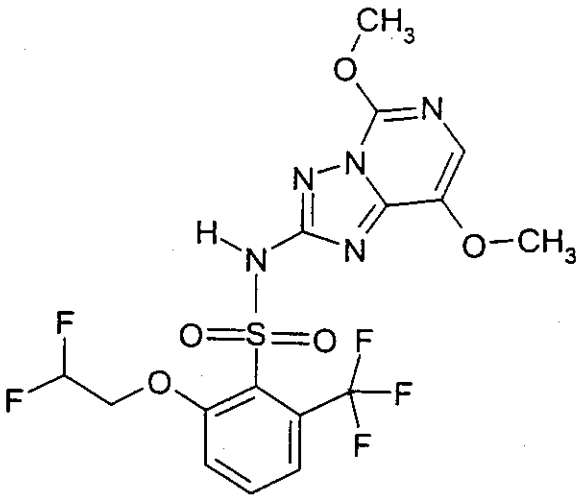
Penoxsulam

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

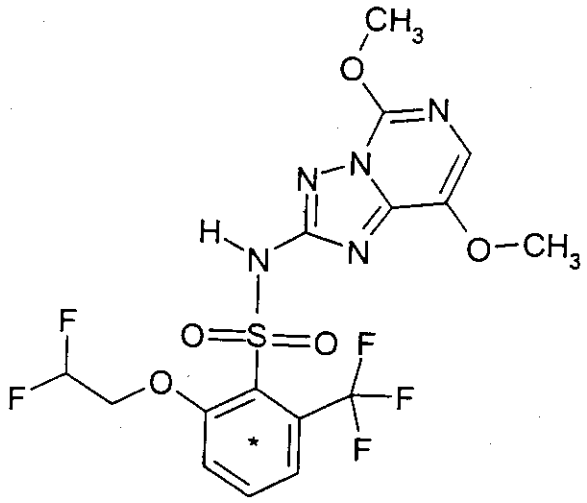
CAS name: 2-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide

CAS No: 219714-96-2

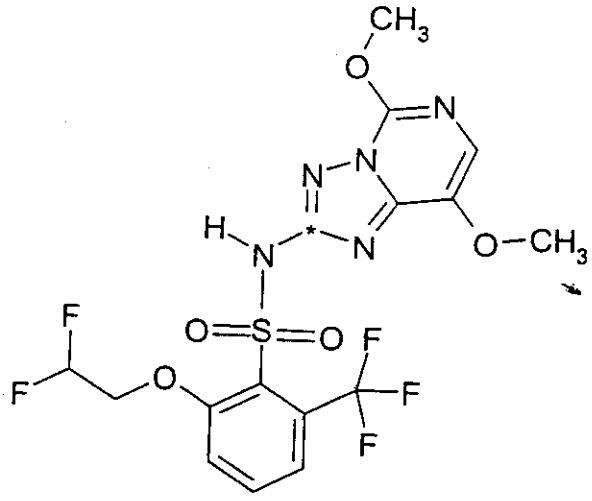
Unlabeled



[Phenyl-U-^{14}C] label



[Triazolopyrimidine-2-^{14}C] label



* Position of the radiolabel.

5-OH-XDE-638

IUPAC name: 6-(2,2-Difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo-s-triazolo[1,5-c]pyrimidin-2-yl)-α,α,α-trifluoro-o-toluenesulfonamide

CAS name: 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

CAS No: NA

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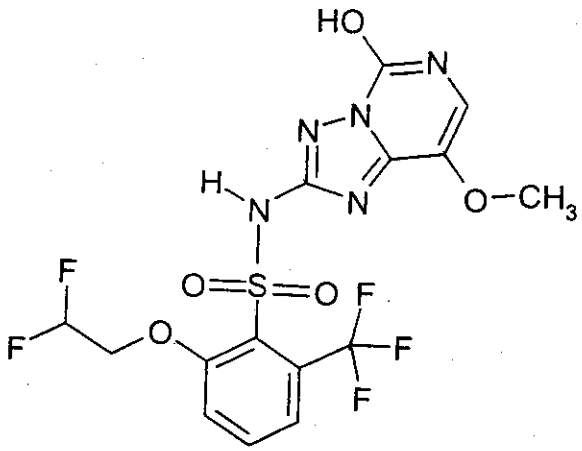
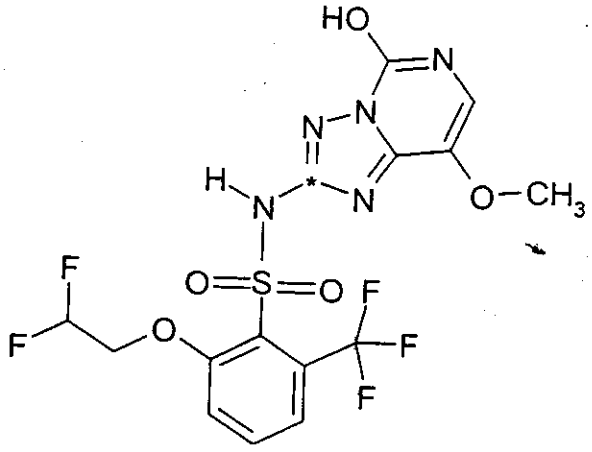


[Triazolopyrimidine-2-^{14}C] label



* Position of the radiolabel.

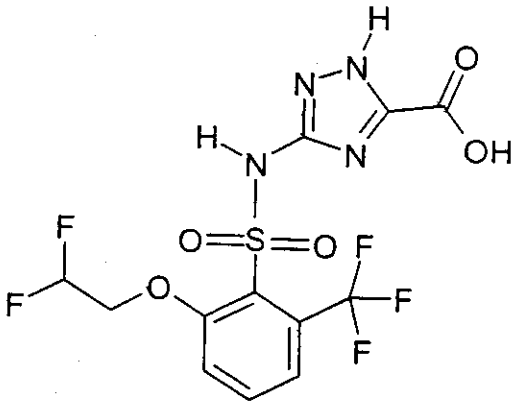
BSTCA

IUPAC name: 3-[6-(2,2-Difluoroethoxy)-α,α,α-(trifluoro-o-toluenesulfonamido]-s-triazole-5-carboxylic acid

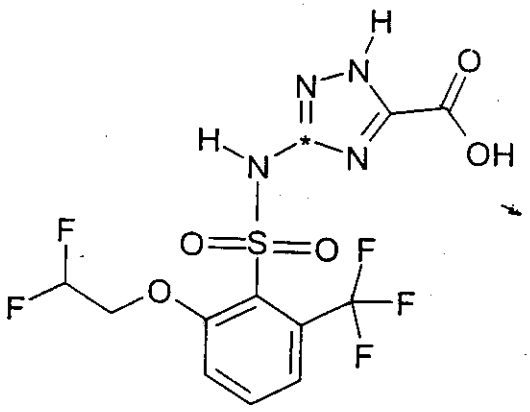
CAS name: 3-[[[2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)phenyl]-sulfonyl]amino]-1H-1,2,4-triazole-5-carboxylic acid

CAS No: NA

Unlabeled



[Triazolopyrimidine-2-^{14}C] label



* Position of the radiolabel.

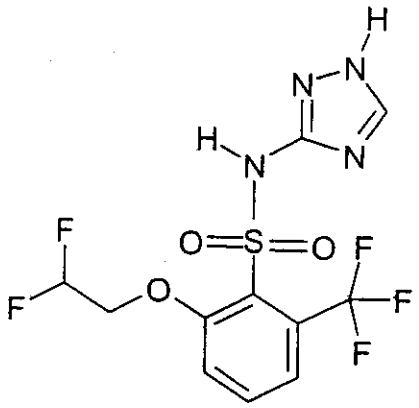
BST

IUPAC name: 6-(2,2-Difluoroethoxy)-α,α,α-trifluoro-N-s-triazol-3-yl-o-toluenesulfonamide

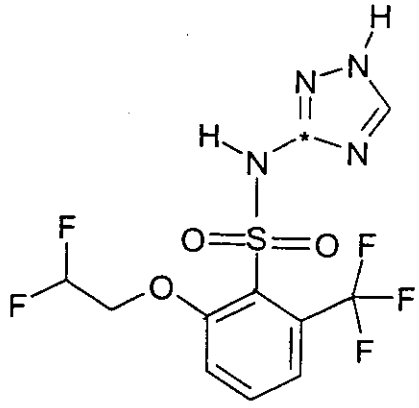
CAS name: 2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazole-3-yl-6-(trifluoromethyl)benzenesulfonamide

CAS No: NA

Unlabeled



[Triazolopyrimidine-2-^{14}C] label



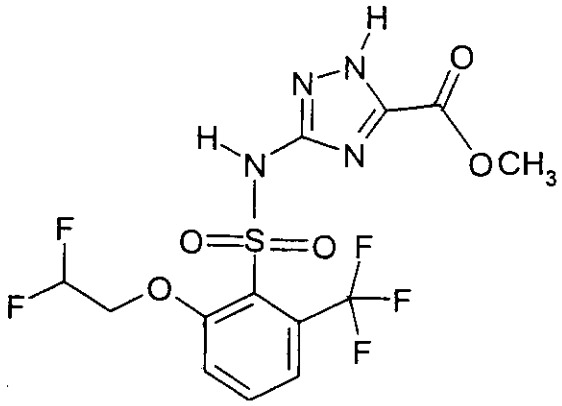
* Position of the radiolabel.

BSTCA-methyl

IUPAC name: Methyl 3-[6-(2,2-difluoroethoxy)-α,α,α-trifluoro-o-toluenesulfonamido]-s-triazole-5-carboxylate

CAS name: Methyl 3-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulfonyl]amino]-1H-1,2,4-triazole-5-carboxylate

CAS No: NA

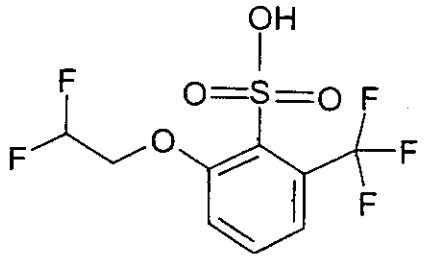


BSA

IUPAC name: 6-(2,2-Difluoroethoxy)-α,α,α-trifluoro-o-toluenesulfonic acid

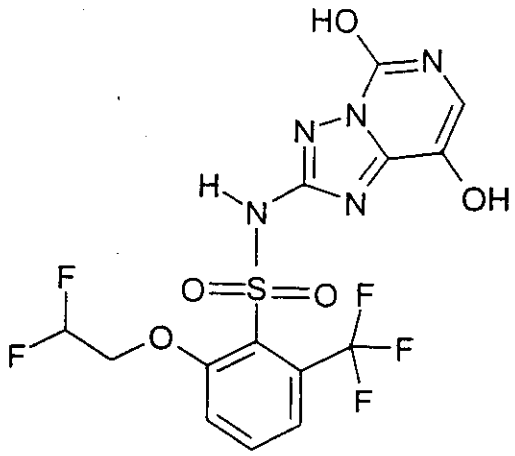
CAS name: 2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)benzenesulfonic acid

CAS No: NA



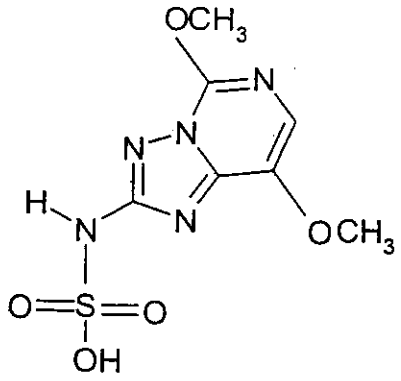
5,8-diOH

IUPAC name: NA
CAS name: 2-(2,2-Difluoroethoxy)-6-trifluoromethyl-N-(5,8-dihydroxy-[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)benzenesulfonamide
CAS No: NA



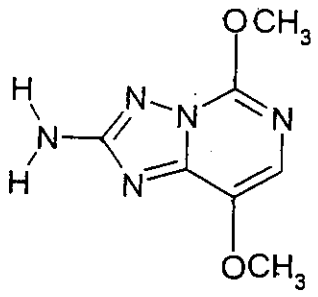
TPSA

IUPAC name: NA
CAS name: 5,8-Dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidin-2-yl-sulfamic acid
CAS No: NA



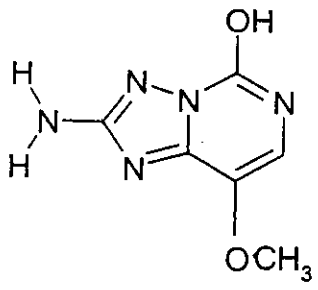
2-Amino TP

IUPAC name:	2-Amino-5,8-dimethoxy-s-triazolo[1,5-c]pyrimidine
CAS name:	5,8-Dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-amine
CAS No:	NA



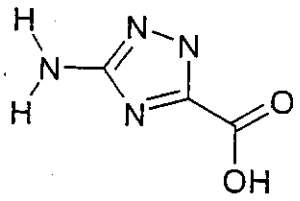
5-OH, 2-Amino TP

IUPAC name:	NA
CAS name:	8-Methoxy[1,2,4]triazolo-[1,5-c]pyrimidin-5-ol-2-amine
CAS No:	NA



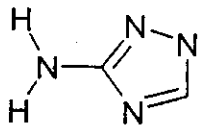
2-Amino TCA

IUPAC name: NA
CAS name: 2-Amino-1,3,4-triazole-5-carboxylic acid
CAS No: NA



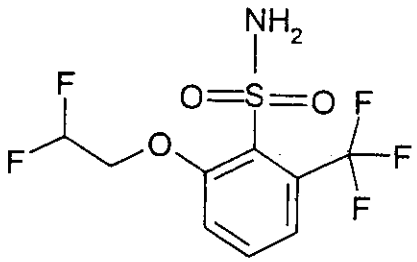
2-Amino-1,3,4-triazole

IUPAC name: NA
CAS name: 2-Amino-1,3,4-triazole
CAS No: NA



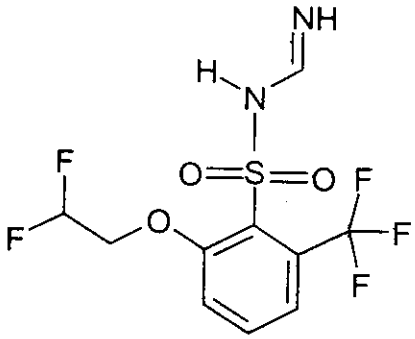
Sulfonamide

IUPAC name: 2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)-benzenesulfonamide
CAS name: 2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)-benzenesulfonamide
CAS No: NA



Sulfonylformamidine

IUPAC name: 2-(2,2-Difluoroethoxy)-N-[(E)iminomethyl-6-(trifluoromethyl)benzenesulfonamide
CAS name: 2-(2,2-Difluoroethoxy)-N-(iminomethyl-6-(trifluoromethyl)-benzenesulfonamide
CAS No: NA



Attachment 3

Transformation Pathway Presented by Registrant
Comparison of Artificial Light to Natural Sunlight

DER FOR:

MRID # 45834801

Page____ is not included in this copy.

Pages 54 through 55 are not included.

The material not included contains the following type of information:

____ Identity of product inert ingredients.

____ Identity of product impurities.

____ Description of the product manufacturing process.

____ Description of quality control procedures.

____ Identity of the source of product ingredients.

____ Sales or other commercial/financial information.

____ A draft product label.

____ The product confidential statement of formula.

____ Information about a pending registration action.

__✓__ FIFRA registration data.

____ The document is a duplicate of page(s) _____.

____ The document is not responsive to the request.

The information not included is generally considered confidential by product registrants. If you have any questions, please contact the individual who prepared the response to your request.
