

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Data Requirement: PMRA Data Code: 8.2.3.4.2
 EPA DP Barcode: D328639
 OECD Data Point: IIA 7.2.3
 EPA Guideline: 162-1

Test material:

Common name: Pyrasulfotole.

Chemical name:

IUPAC name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α -trifluoro-2-mesyl-*p*-tolyl)methanone.

(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

CAS name: (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl]-4(trifluoromethyl)phenyl]methanone.

Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].

CAS No: 365400-11-9.

Synonyms: AE 0317309; K-1196; K-1267.

SMILES string: FC1CC(C(C1)C(=O)C1C(N(C1)C)O)S(=O)(=O)C(F)F (ISIS v2.3/Universal SMILES).

No EPI Suite, v3.12 SMILES String found as of 6/7/06.

Cc1nn(C)c(O)c1C(=O)c2ccc(C(F)(F)F)cc2S(C)(=O)=O.

CS(=O)(=O)c1c(ccc(c1)C(F)(F)F)C(=O)c1c(n(nc1C)C)O.

Primary Reviewer: Lynne Binari
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Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

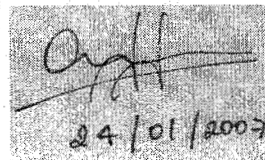
PMRA Reviewer

Date:

**Final Reviewer: Olga Braga
DEH Reviewer**

Signature:

Date:



Handwritten signature of Olga Braga and the date 24/01/2007.

Company Code: BCZ
Active Code: PSA
Use Site Category: 13,14
EPA PC Code: 000692

CITATION: Fliege, R. 2004. [Phenyl-U-¹⁴C]- and [pyrazole-3-¹⁴C]-AE 0317309: aerobic soil metabolism in a silt loam soil of US origin under laboratory conditions at 25°C. Unpublished study performed, sponsored and submitted by Bayer CropScience, GmbH, Frankfurt, Germany. BCS Study No.: CB 02/012 and Report No.: MEF-387/03. Experimental start date July 2, 2002, and termination date July 4, 2003 (p. 6). Final report issued June 22, 2004.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

EXECUTIVE SUMMARY

The biotransformation of [phenyl-U-¹⁴C]- and [pyrazole-3-¹⁴C]-labeled (5-hydroxy-1,3-dimethylpyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone (pyrasulfotole, AE 0317309) was studied in a silt loam soil (pH 7.0-7.3, organic carbon 4.7%) from North Dakota for 358 days under aerobic conditions in darkness at 25 ± 1°C and 75% of 1/3 bar soil moisture. [¹⁴C]Pyrasulfotole was applied at a rate of 0.13-0.14 mg a.i./kg (equivalent to 0.1 kg a.i./ha). This study was conducted in accordance with USEPA Subdivision N Guideline §162-1, and in compliance with OECD Principles of GLP [C(97)186/Final] (1997). The test system consisted of 300-mL Erlenmeyer flasks, each fitted with an air-permeable, solid-phase trap for the collection of CO₂ (soda lime) and volatile organics (paraffin oil-coated glass wool). A single flask per test substance was taken for analysis after 0, 3, 7, 14, 21, 30, 41, 50/51, 65, 80, 100, 120, 155, 190, 251 and 358 days of incubation. Soil samples were extracted using an Accelerated Solvent Extraction (ASE) system, which conducted two-phase ["mild" (40°C, 100 bar) and "aggravated" (100°C, 100 bar) conditions], automated, multi-step extractions with acetonitrile:water (2:1, v:v) as the extraction solvent. The subsequent "mild" and "aggravated" extracts were separately concentrated via rotary evaporation (40°C, under vacuum) for reverse-phase HPLC analysis. Three reference standards, in addition to parent pyrasulfotole, were available for identification purposes (see Table 5 below), with one transformation product, 2-methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555), identified via HPLC against reference standard. The identification was confirmed using normal-phase, one-dimensional TLC against reference standard.

Incubation temperature averaged 25.1 ± 0.6°C during the 358-day study. No supporting records were provided to establish that aerobicity and soil moisture were maintained throughout the study.

For both labels, overall recovery of material balance averaged 99.1 ± 2.2% (range 90.8-102.8%) of the applied, with no consistent pattern of decline in recoveries for either label. Dissipation of [¹⁴C]pyrasulfotole was biphasic with a steady decline during the initial 2 months posttreatment, decreasing from 94.3-97.1% of the applied at day 0 to 47.2-50.0% at 65 days, then dissipation slowed with [¹⁴C]pyrasulfotole comprising 22.0-24.9% at study termination. The reviewer-calculated **linear half-life** for both radiolabels was 161 days ($r^2 = 0.8227$) and the **nonlinear half-life** was 95 days ($r^2 = 0.9144$). The reviewer-calculated **DT₅₀** and **DT₉₀** estimates based on a 2-compartment nonlinear model were 63 and 1424 days, respectively ($r^2 = 0.998$). The **Observed DT₅₀** and **DT₉₀** and values were 50-65 days and >358 days, respectively.

No major nonvolatile transformation products were detected for either label. 2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555) was a minor transformation product in phenyl-label treated soil detected at a maximum 3.8% of the applied; no other minor products were identified for either label. Unidentified [¹⁴C]residues, consisting of up to five to six components, were detected at maximum totals of 6.1-6.5%. Extractable [¹⁴C]residues decreased from 99.0-99.7% of the applied at day 0 to 26.6-29.3% at 358 days. Nonextractable [¹⁴C]residues increased from

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

0.4-1.1% at day 0 to maximums of 31.3-35.2% at 155-190 days and were 30.1-30.7% at 358 days. Organic matter fractionation of 30-, 100- and 251-day extracted soil found 8.1-14.2%, 5.0-8.5% and 5.4-13.2% of the applied associated with the humin, fulvic acids and humic acids, respectively. At study termination, volatilized $^{14}\text{CO}_2$ totaled 33.5-40.5% of the applied, while volatile [^{14}C]organic compounds were <0.1% at all intervals.

Under **sterile** (autoclaved soil, both labels) conditions, parent pyrasulfotole comprised 93.6-94.2% of the applied at 120 days (final interval), with AE B197555 in phenyl-label treated soil detected at a maximum 3.7% at study termination. At 120 days, extractable and nonextractable [^{14}C]residues were 93.6-97.9% and 3.8-5.2% of the applied, respectively, with volatilized $^{14}\text{CO}_2$ and volatile [^{14}C]organic compounds $\leq 0.4\%$. During the 120-day incubations, recoveries of material balance ranged from 98.6-103.1% of the applied.

A transformation pathway was provided by the study author that was consistent with the products detected. Transformation of pyrasulfotole involves cleavage of the phenyl and pyrazole moieties to yield the benzoic acid derivative, 2-methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555) [found in phenyl moiety only], plus several unidentified minor compounds, with steady formation of bound soil residues and mineralization to CO_2 . Based on the lack of transformation occurring in the sterilized controls, the breakdown of pyrasulfotole appears to be controlled by microbial processes.

In a supplementary experiment, the potential mobility of pyrasulfotole in the silt loam soil at 1 year posttreatment was classified as mobile (K_{oc} value of 88), as measured by the FAO classification scheme.

In a supplementary experiment, pyrasulfotole and its transformation products remained stable in soil extracts stored frozen up to 209-326 days.

Results Synopsis:

Test system used: Silt loam from North Dakota.

Linear half-life:	161 days ($r^2 = 0.8227$).
Non-linear half-life:	95 days ($r^2 = 0.9144$).
Non-linear, 2 compartment DT_{50} :	63 days ($r^2 = 0.998$).
Non-linear, 2 compartment DT_{90} :	1424 days ($r^2 = 0.998$).
Observed DT_{50} :	50-65 days.
Observed DT_{90} :	>358 days.

Major transformation products:

CO_2 (maximum 33.5-40.5% of applied).

Minor transformation products:

2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555, maximum 3.8% of applied).

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Study Acceptability: This study is classified as **acceptable**. No significant deviations from good scientific practices were noted.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with USEPA Subdivision N Guideline §162-1 and PMRA Environmental Chemistry and Fate Guidelines for Registration of Pesticides in Canada, Section C1: Biotransformation, Soil (Laboratory) - Degradation Pathways and Persistence (1987, p. 6). No significant deviations from the objectives of Subdivision N guidelines were noted.

COMPLIANCE: This study was conducted in compliance with OECD Principles of GLP [C(97)186/Final] (1997, p. 3). Signed and dated Data Confidentiality, GLP and Quality Assurance statements and a Certification of Authenticity were provided (pp. 2-5).

A. MATERIALS:

1. Test Materials

[Phenyl-U-¹⁴C] and [pyrazole-3-¹⁴C]pyrasulfotole (Figure 1, p. 79).

Chemical Structure:

See DER Attachment 1.

[Phenyl-U-¹⁴C]pyrasulfotole

Description:

Technical; pale, yellow solid (p. 23).

Purity: Radiochemical purity:

>97% (Figure 6, p. 87; Appendix 3, p. 107).

Lot/Batch No.

SEL/1006.

Analytical purity:

>99% (NMR; Appendix 3, p. 107).

Specific activity:

191,400 dpm/μg (31.33 mCi/mmol, 3.19 MBq/mg).

Location of the radiolabel:

Uniformly on phenyl ring.

[Pyrazole-3-¹⁴C]pyrasulfotole

Description:

Technical; white solid (p. 24).

Purity: Radiochemical purity:

≥98% (Figure 6, p. 87; Appendix 4, p. 108).

Lot/Batch No.

SEL/1009.

Analytical purity:

100% (HPLC), 90% (NMR, unadjusted for mol. wt.; Appendix 4, p. 108).

Specific activity:

330,600 dpm/μg (54.18 mCi/mmol, 5.51 MBq/mg).

Location of the radiolabel:

At 3-C position on pyrazole ring.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Storage conditions of test chemicals:

The test substances were dissolved in acetonitrile, then stored in darkness in a freezer (temperature not reported; pp. 23-24).

Physico-chemical properties of pyrasulfotole:

Parameter	Value	Comment
Molecular weight	362.3 g/mol	
Water Solubility (g/L) at 20°C	4.2 at pH 4 69.1 at pH 7 49.0 at pH 9	Very soluble
Vapor Pressure/Volatility	2.7×10^{-7} Pa at 20°C 6.8×10^{-7} Pa at 25°C	Non-volatile
UV Absorption	water $\lambda_{\max} = 264$ 0.1M HCl $\lambda_{\max} = 241$ 0.1M NaOH $\lambda_{\max} = 216$	Not likely to undergo photolysis.
Pka	4.2 ± 0.15	
log K _{ow} at 23°C	0.276 at pH 4 -1.362 at pH 7 -1.58 at pH 9	Not likely to bioaccumulate
Stability of compound at room temperature, if provided		No significant degradation over 12 months at ambient temperatures.

Data obtained from pyrasulfotole chemistry review of Submission 2006-2445.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

2. Soil Characteristics

Table 1: Description of soil collection and storage.

Description		Details
Geographic location		A wooded area adjacent to a field located in Grand Forks County, North Dakota.
Coordinates	Latitude:	N 47° 42.619'
	Longitude:	W 97° 35.831'
Collection date		April 23, 2002.
Pesticide use history at the collection site		Site has never received any pesticide (plant protection agent) applications.
Collection procedures		Sampled from a field with a shovel into a bucket (no further description).
Sampling depth		ca. 0- to 6-inch depth (soil horizon A).
Storage conditions		Soil transported to test facility in an air-permeable, plastic bag at ambient temperature. At test facility, after sieving and mixing, the soil was stored aerated, in a ventilated plastic bag, and moist at ca. 4°C until use.
Storage length		70 days based on collection date (above) and the date of application on July 2, 2002.
Soil preparation		Large debris (stones, plant material) was removed and the soil moisture partially reduced at ambient temperature prior to sieving (2-mm). After sieving, the soil was mixed (method not reported) to yield a homogenous batch.

Data obtained from pp. 6, 26; Table 1, p. 58; Appendix 2, p. 106 of the study report.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Table 2: Properties of the soil.

Property		Details
Soil texture		Silt loam.
% Sand (0.05-2.0 mm)		29
% Silt (0.002-0.05 mm)		54
% Clay (<0.002 mm)		17
pH	In water (1:1):	7.3
	In CaCl ₂ (1:1):	7.0
Organic carbon (%)		4.7
Organic matter (%) ¹		8.1
CEC (meq/100g)		26.0
Moisture at 1/3 bar (%)		45.5
Maximum water holding capacity (%)		86.0
Bulk density, disturbed (g/cm ³)		0.86
Microbial biomass (mg/100 g dry wt. soil) ²		113.6 ± 5.8
Microbial plate counts (CFU/g dry wt. soil) ²	Aerobic bacteria:	5,000,000
	Aerobic spore forming bacteria:	1,000,000
	Yeasts and molds:	10,000
	Actinomycetes:	10,000
Soil taxonomic classification (USDA)		Fine-silty, mixed, cumulic udic Haploborolls.
Soil series		LaDelle.
Sol mapping unit		Not reported.

1 As presented reported in the study report, organic matter (%) = organic carbon (%) x 1.724.

2 At study initiation.

Data obtained from Tables 1-2, pp. 58-59 of the study report.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: No preliminary experiments were reported.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

2. Experimental conditions:

Table 3: Experimental design.

Parameter		Both labels
Duration of the test		358 days.
Soil condition: (Air dried/fresh)		Fresh; soil stored aerated, moist <i>ca.</i> 2 months prior to use. The test systems were prepared and acclimatized to study conditions for 11-12 days prior to treatment.
Soil (g/replicate)		50 g dry wt.
Application rates (mg a.i./kg & equiv. kg a.i./ha)	Nominal	0.133 mg a.i./kg (equivalent to 0.1 kg a.i./ha). ¹
	Actual	0.129 mg a.i./kg for [phenyl-U- ¹⁴ C]-label. 0.136 mg a.i./kg for [pyrazole-3- ¹⁴ C]-label.
Control conditions, if used		Sterile controls were used. Prior to treatment, additional soil samples were prepared in the same manner as the nonsterile samples, but sterilized by autoclaving (121°C, <i>ca.</i> 30 minutes) three times at 1- to 2-day intervals during the 11-12-day pre-incubation period.
No. of Replications	Controls, if used	Seven treated sterile controls were prepared for each label. This allowed for a single replicate/label at each sampling interval, plus reserves.
	Treatment	Twenty-two treated nonsterile soil samples were prepared for each label. This allowed for a single replicate/label at each sampling interval, plus reserves.
Test apparatus	Type/material/volume	300-mL Erlenmeyer flask fitted with an air-permeable, solid-phase, volatiles trap.
	Details of traps for CO ₂ and organic volatiles, if any	Glass wool, coated with paraffin oil to trap organic volatiles (one layer). Soda lime pellets to trap CO ₂ (two, 5-g layers separated by untreated glass wool). The soda lime pellets contained a carbon dioxide indicator dye to prevent CO ₂ saturation.
If no traps were used, is the system closed/open?		Volatiles traps were used.
Identity and concentration of co-solvent		Acetone; final concentration 1.0% based on soil weight [500 µL of acetone:deionized, autoclave sterilized water (1:1, v:v) test solution in 50 g dry wt. soil].
Test material	Volume of the test solution used/treatment:	500 µL
	Application method (eg: mixed/not mixed):	Applied dropwise to soil surface using a microliter pipette, after which soil flask was gently shaken to incorporate test material and allow solvent evaporation.
	Is the co-solvent evaporated?	Yes.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Parameter		Both labels	
Any indication of the test material adsorbing to the walls of the test apparatus?		Not indicated.	
Microbial plate counts of the sterile controls (CFU/g dry wt. soil)		Initial ²	Final (80 days) ³
	Aerobic bacteria:	n.d. ⁴	40,000,000
	Aerobic spore forming bacteria:	n.d.	20,000,000
	Yeasts and molds:	n.d.	5
	Actinomycetes:	n.d.	<10,000
Microbial plate counts of treated (CFU/g dry wt. soil)		Initial ²	Final (365 days) ³
	Aerobic bacteria:	5,000,000	9,000,000
	Aerobic spore forming bacteria:	1,000,000	5,000,000
	Yeasts and molds:	10,000	50,000
	Actinomycetes:	10,000	7,000,000
Microbial biomass of treated soil (mg/100 g dry wt. soil)		Initial ²	Final (357 days) ³
		113.6 ± 5.8	72.9 ± 10.4
Experimental conditions:	Temperature (°C):	25°C; maintained in a temperature-controlled incubation chamber.	
	Continuous darkness (Yes/No):	Yes.	
	Moisture content:	75 ± 10% of 1/3 bar water holding capacity.	
	Moisture maintenance method:	Gravimetric; initial weight of each soil flask maintained with addition of sterile, deionized water as needed.	
Other details, if any		None.	

1 Assuming a soil incorporation depth of 5 cm and bulk density of 1.5 g/cm³, the test application rates of 0.13-0.14 mg a.i./kg are equivalent to 100 g a.i./acre (p. 22).

2 Determined at study initiation using untreated soil (Tables 2-3, pp. 59-60).

3 Determined using soil treated with unlabeled pyrasulfotole at 0.135 mg a.i./kg (p. 29; Tables 2-3, pp. 59-60).

4 Not detected.

Data obtained from pp. 22, 27-30; Tables 2-4, pp. 59-61; Figure 5, p. 86 of the study report.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

3. Aerobic conditions: Soil samples were incubated under static conditions in a flask fitted with an air-permeable, solid-phase (soda lime, glass wool, paraffin oil-coated glass wool) volatiles trap that allowed for the passive exchange of air (pp. 27, 30). No determinations, such as redox potentials, were made to verify that aerobic conditions were maintained.

4. Supplementary experiments: Determination of adsorption of aged pyrasulfotole residues. Nonsterile, treated, reserve samples (one per label) were taken at 363 days posttreatment (p. 32). Calcium chloride (0.01M) solution was added to yield a soil:solution ratio of 1:1, taking into account soil moisture content. The soil:solution slurry was agitated via a plate vibrator for 24 hours, then the pH was determined and soil and solution were separated by centrifugation (speed, interval not reported). Two additional calcium chloride extractions were conducted as described above with solution volumes *ca.* 50-70 mL and stirring for 30-60 minutes. Aqueous extracted soil was further extracted with acetonitrile:water (2:1, v:v) using the accelerated solvent extraction method as described below for the definitive study soil samples (p. 33). Extracts, extracted soil and trapping solutions were analyzed for total radioactivity using LSC. Extracts were concentrated and analyzed by HPLC as described below.

5. Sampling:

Table 4: Sampling details.

Criteria		Both labels
Sampling intervals (posttreatment)	Sterile controls	7, 21, 41, 80 and 120 days.
	Nonsterile treated	0 (<i>ca.</i> 30 minutes), 3, 7, 14, 21, 30, 41, 50/51 ¹ , 65, 80, 100, 120, 155, 190, 251 and 358 days.
Sampling method		A single treated sample per label at each interval.
Method of collection of CO ₂ and organic volatile compounds		Volatiles traps were collected at each sampling interval.
Sampling intervals/times for:		
Sterility check, if sterile controls are used:		0, 21 and 80 days.
Moisture content:		Flask weights were monitored at <i>ca.</i> 2- to 4-week intervals. Soil moisture adjustments occurred twenty-six times over the 1-year incubations.
Redox potential, other:		None determined.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Criteria	Both labels
Sample storage before analysis	<p>Soil samples were extracted the day of collection.</p> <p>Soil extracts were analyzed by HPLC within a few days of preparation; however, specific extraction and analysis dates were not reported. Extracts were stored frozen when not in use.</p> <p>Extracted soil (air-dried, milled) was stored frozen until combustion analysis, which was reported as typically occurring within two months after extraction.</p> <p>Volatiles traps were wrapped in aluminum foil and stored at room temperature until analysis, which was reported as typically occurring within two months after collection.</p>
Other details, if any	None reported.

1 The 50-day [phenyl-U-¹⁴C]-label treated soil sample was replaced with a nonsterile, phenyl-label treated, reserve, soil sample taken at 51 days posttreatment (Table 5, p. 62).
 Data obtained from pp. 30-32; Table 2, p. 59; Table 5, p. 62 of the study report.

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods: Diatomaceous earth (7 g, Bulk Isolute HM-N sorbent) was added to the soil sample, which was then mixed and transferred to a 100-mL extraction cell of an Accelerated Solvent Extraction (ASE) system (Model ASE 300, Dionex; p. 33; Figure 7, p. 88). The test flask was rinsed with acetonitrile (up to 5 mL) and the rinsate added to the soil mixture. Two-phase ("mild" and "aggravated" conditions), automated, multi-step extractions were conducted using acetonitrile:water (2:1, v:v) as the extraction solvent. For "mild" conditions, the soil was extracted at 40°C, *ca.* 100 bar cell pressure and 5-minute cycle times, with the final extraction yield generally ≤2% of the applied radioactivity. Ten "mild" extraction cycles were usually run with partial solvent renewal at each cycle and final extract pool volumes of 500-550 mL per sample. For the subsequent "aggravated" conditions, the extracted soil was further extracted at 100°C, *ca.* 100 bar cell pressure and 15-minute cycle times until the extraction yield was typically ≤2% of the applied. In general, three "aggravated" cycles were run with final extract pool volumes of 200 mL. Triplicate aliquots (volume not specified) of individual extracts were analyzed for total radioactivity using LSC, then respective "mild" extracts and "aggravated" extracts were combined (pp. 34, 36). Pooled extracts were concentrated via rotary evaporation (40°C, under vacuum), with final volumes of *ca.* 4-10 mL and 7 mL for the "mild" and "aggravated" extract samples, respectively (p. 34). Aliquots (volume not reported) of the concentrated extracts were centrifuged (speed, interval not reported) prior to HPLC analysis (p. 34).

Total ¹⁴C measurement: Total ¹⁴C residues were determined by summing the concentrations of residues measured in the soil extracts, extracted soil and volatile trapping materials (p. 45).

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Determination of nonextractable residues: Extracted soil was air-dried, then homogenized to a powder using a planetary mill (Retsch; p. 35; Appendix 1, p. 105). Six aliquots (*ca.* 0.5 g) were analyzed for total radioactivity by LSC following combustion (p. 36).

Organic matter fractionation. Aliquots (*ca.* 20-25 g) of 30-, 100- and 251-day extracted soil (both labels) were further extracted for 24 hours via magnetic stirrer (continuous) with 0.5M sodium hydroxide (NaOH, 50 mL), with the resulting extract separated from soil by centrifugation (speed, interval not reported; p. 35; Figure 9, p. 90). The supernatant was decanted, then the remaining pellet was washed twice with 0.5M NaOH (10 mL); washes were separated from the soil via centrifugation. All NaOH supernatants were combined, acidified to pH 1 with concentrated hydrochloric acid (conc. HCl), stored overnight at *ca.* 4-6°C, then the resulting precipitate (humic acids) was removed by centrifugation. The supernatant was decanted and the remaining precipitate washed twice with conc. HCl (2 mL); washes were separated from the precipitate via centrifugation. All HCl supernatants (fulvic acids) were combined and analyzed for total radioactivity using LSC. The remaining precipitate (humic acids) was dissolved in 1M NaOH and analyzed using LSC. [¹⁴C]Residues remaining in the extracted soil (humin) were analyzed by LSC following combustion.

Determination of volatile residues: The paraffin-coated glass wool was combined with scintillation fluid and analyzed directly for total radioactivity by LSC (p. 35).

To recover radioactivity (presumably, ¹⁴CO₂) from the soda lime, 18% (w:w) HCl (50 mL) was applied dropwise to the soda lime with heating to 70°C for *ca.* 90 minutes (p. 35; Figure 8, p. 89). Released ¹⁴CO₂ was purged (air, flow rate not specified) through 2-aminoethanol:methanol (2:1, v:v) trapping solution, with triplicate aliquots (volume not specified) of the trapping solution analyzed for total radioactivity by LSC (pp. 35-36).

To confirm the presence of ¹⁴CO₂, volatile [¹⁴C]residues were released and recovered, as described above, from 358-day soda lime samples, except the released volatile residues were trapped in 10M potassium hydroxide (KOH) solution instead of 2-aminoethanol:methanol (p. 41). Aliquots of the KOH solution were analyzed for total radioactivity by LSC. An aliquot (5 mL) of the KOH solution was then combined with 1M aqueous sodium carbonate (2 mL) and 1M aqueous barium chloride (5 mL). The test solution was mixed via magnetic stirrer for 15 minutes, allowed to stand at room temperature for 15 minutes, then centrifuged until complete sedimentation of the precipitate occurred. Aliquots of the resulting supernatant were analyzed for total radioactivity by LSC.

Derivatization method, if used: None was reported.

Identification and quantification of parent compound: Concentrated extract samples were analyzed by reverse-phase HPLC under the following conditions: Phenomenex Luna C18(2) (4.6 x 250 mm, 5 µm) column, one of three gradient mobile phases (each described below), injection volume generally 200 µL, flow rate 1.0 mL/minute, UV detector (254 or 280 nm), and Berthold

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

LB 507B or LB 509 radioactivity detector equipped with either a 400- μ L yttrium or glass flow-through cell (pp. 37-39). Column recoveries of selected chromatogram runs were monitored through the collection and LSC analysis of bulk column eluates, with the average recovery of two runs (one per label) reported as 97.6% (p. 37); individual column recoveries were not provided. The following gradient mobile phases were employed for sample extracts:

Gradient 1 b/c combining (A) either (b) 0.02M aqueous ammonium formate adjusted to pH 2 with trifluoroacetic acid, or (c) water adjusted to pH 2 with sulfuric acid and (B) acetonitrile [percent A:B at 0-5 min. 90:10 (v:v), 40 min. 75:25, 45 min. 70:30, 55 min. 60:40, 60 min. 40:60, 65-70 min. 5:95, 75-80 min. 90:10 (p. 38)]. This mobile was used with all extract samples, except 251-day samples (p. 39).

Gradient 2 combining (A) water adjusted to pH 2 with sulfuric acid and (B) acetonitrile [percent A:B at 0-5 min. 90:10 (v:v), 25 min. 70:30, 35 min. 60:40, 55-65 min. 5:95, 70-75 min. 90:10 (p. 39)]. This mobile phase was used with 251-day extract samples.

Parent [14 C]pyrasulfotole was identified by co-chromatography with and comparison to the retention time of unlabeled reference standard (pp. 37, 40, 53; Table 6, p. 63; Figure 2, p. 81; Figures 10-11, pp. 91-92; Appendix 10, p. 115).

To confirm results from HPLC analyses, selected extracts were analyzed using one-dimensional TLC on normal-phase plates (silica gel 60 F₂₅₄, Merck) developed with toluene:ethanol:25% aqueous ammonia (6:5:1, v:v:v; pp. 39-40). Following development, areas of radioactivity were detected using a phosphorimaging system (BAS-2500). Parent [14 C]pyrasulfotole was identified by co-chromatography with unlabeled reference standard which was visualized under UV light (254 nm; p. 40, 53; Table 6, p. 63; Figure 12, p. 93). For the TLC analyses, soil extracts were used as prepared for HPLC analysis, as described above, or aliquots were taken to near-dryness under a nitrogen stream, with the residues re-dissolved in acetonitrile:water (1:1,v:v; p. 34).

Identifications were also confirmed by LC/MS/MS under the following conditions: reverse-phase HPLC conditions comparable to Gradient 1c substituting formic acid for sulfuric acid in eluent A, injection volume 200 μ L, Micromass Quattro LC triple quadrupole MS, electrospray ionization (ESI) in positive and/or negative modes, UV detector (wavelength not specified), and Berthold LB 509 radioactivity detector (p. 40). Identifications of [14 C]pyrasulfotole in sample extracts were made against labeled test substances (pp. 40-41, 53; Figures 3-4, pp. 82-85; Figure 13, p. 94). Aliquots of 30-day "mild" extracts (both labels) were concentrated under a nitrogen stream for this analysis (p. 34).

Identification and quantification of transformation products: Transformation products were separated, quantified and identified using HPLC and TLC as described for the parent compound (pp. 37-41, 53; Table 6, p. 63; Figure 2, p. 81; Figures 10-12, pp. 91-93).

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Table 5: Reference compounds available for identifying transformation products of pyrasulfotole (AE 0317309).

Applicant codes	Chemical Name	Purity ¹
AE B197555, RPA 203328	IUPAC: 2-Methylsulfonyl-4-trifluoromethylbenzoic acid	99.6%
	CAS: Benzoic acid, 2-methylsulfonyl-4-(trifluoromethyl)	
AE 1898321 ²	IUPAC: 3-Methyl-1-[2-(methylsulfonyl)-4-(trifluoromethyl)benzoyl]-1H-pyrazol-5-ol	99.3%
	CAS: Not available.	
AE 1898322 ²	IUPAC: 5-Methyl-1-[2-(methylsulfonyl)-4-(trifluoromethyl)benzoyl]-1H-pyrazol-3-ol	99.3%
	CAS: Not available.	

¹ Purity w/w unless otherwise designated.

² AE 1898321 and AE 1898322 are structural isomers, with one of the compounds accidentally used as a reference standard due to an incorrect initial structure assignment. The compound was used only as a chromatographic marker (p. 25).

Data obtained from p. 25; Figure 1, p. 80 of the study report.

Detection limits (LOD, LOQ) for the parent compound and transformation products: For HPLC analyses, the LOQ (limit of quantitation) was reported as equivalent to *ca.* 1.0% and 0.5% of the applied for [phenyl-U-¹⁴C]- and [pyrazole-3-¹⁴C]-label treated samples, respectively, corresponding to ≤ 0.001 ppm parent equivalents (pp. 46-47, p. 49). For TLC analyses, the LOQ was reported as equivalent to *ca.* 0.4% and 0.2% of the applied for [phenyl-U-¹⁴C]- and [pyrazole-3-¹⁴C]-label treated samples, respectively, corresponding to < 0.001 ppm (pp. 47, 49). For LSC analyses (both labels), the LOQ was reported as $< 0.1\%$ for liquid (soil extracts, trapping solutions) and solid (soil combustions) samples, which corresponded to ≤ 0.0001 ppm (p. 46).

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: Incubation temperature averaged $25.06 \pm 0.6^\circ\text{C}$ during the 358-day study (p. 48; Table 21, p. 78). No supporting records were provided to establish that aerobicity and soil moisture were maintained throughout the study.

In nonsterile, treated (unlabeled pyrasulfotole) soil, microbial biomass remained constant at 0-121 days posttreatment with averages of 113.6-123.6 mg/100 g soil, then decreased to 72.9 mg/100 g soil at 357 days (Table 2, p. 59). Microbial populations of aerobic bacteria, aerobic spore forming bacteria and yeasts/molds were relatively stable during the 1-year study, while actinomycetes populations increased 350-fold between 121 and 365 days (Table 2, p. 59).

Microbial plate count analyses of sterile, treated (unlabeled pyrasulfotole) soil found no significant levels of aerobic bacteria, aerobic spore forming bacteria, yeasts/molds, or

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

actinomycetes through 21 days of incubation; however, significant levels ($20-40 \times 10^6$ CFU/g soil) of aerobic bacteria and aerobic spore forming bacteria were present in sterile, treated soil taken at 80 days posttreatment (Table 2, p. 64).

B. MATERIAL BALANCE: Overall recovery (both labels) of radiolabeled material averaged $99.1 \pm 2.2\%$ (range 90.8-102.8%, $n = 32$) of the applied, with no consistent pattern of decline in recoveries for either label (DER Attachment 2, Reviewer's Comment No. 1). For each label, recoveries averaged ($n = 16$) $98.9 \pm 1.7\%$ (range 93.3-100.5%) of the applied in [phenyl- ^{14}C]-label treated soil and $99.4 \pm 2.5\%$ (range 90.8-102.8%) in [pyrazole-3- ^{14}C]-label treated soil.

In sterile soil, overall recovery averaged ($n = 5$) $101.5 \pm 1.6\%$ (range 98.6-103.1%) and $100.0 \pm 0.7\%$ (range 98.9-100.9%) for the [phenyl-U- ^{14}C]- and [pyrazole-3- ^{14}C]-pyrasulfotole treated soils, respectively (DER Attachment 2).

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Table 6. Biotransformation of [phenyl-U-¹⁴C]pyrasulfotole (AE 0317309), expressed as percentage of applied radioactivity (n = 1), in North Dakota silt loam soil under aerobic conditions.¹

Compound	Sampling times (days)															
	0	3	7	14	21	30	41	51	65	80	100	120	155	190	251	358
Pyrasulfotole	94.3	91.7	85.1	76.0	73.0	66.8	58.3	52.2	50.0	43.5	39.8	34.2	29.0	28.3	25.6	24.9
AE B197555 ¹	2.6	3.1	2.9	3.6	2.8	3.8	1.7	2.0	1.9	2.6	2.1	1.0	1.8	1.4	2.1	1.0
Unidentified [¹⁴ C] ²	2.8	1.0	2.7	4.6	2.7	1.7	1.9	2.6	1.9	3.2	3.0	1.6	6.5	5.2	4.3	3.5
Extractable residues	99.7	95.8	90.7	84.2	78.4	72.3	61.9	56.8	53.8	49.3	44.9	36.8	37.3	35.0	31.9	29.3
Nonextractable residues	0.4	3.5	7.6	12.0	15.1	18.3	22.4	25.2	26.3	28.4	29.8	30.2	30.5	31.3	30.9	30.1
CO ₂	---	0.3	1.4	4.3	6.9	9.7	13.6	16.3	19.0	22.3	24.9	26.4	30.0	32.3	34.7	40.5
Volatile organics	---	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Total recovery	100.1	99.4	99.6	100.5	100.4	100.3	97.9	98.4	99.1	99.9	99.7	93.3	97.7	98.6	97.5	99.9

¹ 2-Methylsulfonyl-4-trifluoromethylbenzoic acid (Figure 1, p. 80).

² Summation of a single HPLC component (designated "largest single unknown") comprising ≤2.7% of the applied, plus other minor HPLC components totaling ≤5.0% (p. 51; Table 15, p. 72).

Data obtained from p. 51; Table 10, p. 67; Figure 1, p. 80 of the study report.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Table 7. Biotransformation of [pyrazole-3-¹⁴C]pyrasulfotole (AE 0317309), expressed as percentage of applied radioactivity (n = 1), in North Dakota silt loam soil under aerobic conditions.

Compound	Sampling times (days)															
	0	3	7	14	21	30	41	50	65	80	100	120	155	190	251	358
Pyrasulfotole	97.1	93.3	85.7	80.0	73.6	68.8	59.0	53.0	47.2	41.1	38.0	35.1	29.6	27.5	24.7	22.0
Unidentified [¹⁴ C] ¹	1.9	1.7	2.8	2.8	3.1	3.7	3.4	3.5	4.6	4.9	4.8	3.8	6.1	5.5	5.6	4.6
Extractable residues	99.0	95.0	88.6	82.8	76.7	72.5	62.3	56.5	51.7	46.0	42.8	38.9	35.7	32.9	30.2	26.6
Nonextractable residues	1.1	5.3	10.1	14.6	18.0	21.6	25.6	28.1	30.8	32.0	33.5	34.4	35.2	34.4	34.5	30.7
CO ₂	---	1.0	2.2	4.2	6.3	8.7	11.9	14.1	17.7	20.6	23.6	25.5	28.8	31.2	33.8	33.5
Volatile organics	---	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Total recovery	100.1	100.3	101.0	101.6	101.0	102.8	99.9	98.8	100.3	98.6	99.9	98.7	99.7	98.4	98.5	90.8

¹ Summation of a single HPLC component ("largest single unknown") comprising ≤2.5% of the applied, plus other minor HPLC components totaling ≤4.0% (p. 52; Table 16, p. 73).

Data obtained from p. 52; Table 12, p. 69 of the study report.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

C. TRANSFORMATION OF PARENT COMPOUND: [^{14}C]Pyrasulfotole (both labels) steadily dissipated in the silt loam soil during the initial 2 months posttreatment decreasing from 94.3-97.1% of the applied at day 0 to 47.2-50.0% at 65 days, thereafter dissipation slowed with [^{14}C]pyrasulfotole comprising 22.0-24.9% at study termination (Table 10, p. 67; Table 12, p. 69).

In sterile soil, [^{14}C]pyrasulfotole (both labels) comprised 93.6-94.2% of the applied at 120 days posttreatment (final interval; Table 14, p. 71).

HALF-LIFE/DT50/DT90: Based on single-compartment, first order regression analysis (Microsoft Excel 97 Solver) and using the mean [^{14}C]pyrasulfotole (both labels) detected at each sampling interval, the study author calculated a half-life of 72 days ($r^2 = 0.976$; pp. 53-54; Figure 21, p. 102).

Reviewer-calculated estimates (see DER Attachment 2): Based on first order regression analysis (Excel 2000; all sampling intervals), the linear half-life for both radiolabels combined was 161 days (Table 8). Based on a 2-compartment, 4-parameter nonlinear regression model (SigmaPlot v 8) the DT_{50} and DT_{90} estimates for both radiolabels combined were 63 and 1424 days, respectively (Table 8; DER Attachment 2). The observed DT_{50} value for combined pyrasulfotole labels was in the 50-65 day range and the observed DT_{90} was >358 days.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Half-lives/DT50/DT90 for pyrasulfotole (AE 0317309) in US silt loam aerobic soil.

Compound	Half-life (days)	Regression equation	r ²	DT50 ² (days)	DT90 (days)
[Phenyl-U-¹⁴C]-pyrasulfotole					
Linear/natural log ¹	168	y = -0.0041x + 4.2852	0.8105	--	--
Nonlinear/normal ¹	99.0	y = 85.9*exp(-0.007*x)	0.9094	--	--
Nonlinear/normal	--	y = 69.0019*exp(-0.018*x) + 30.1849*exp(-0.004*x)	0.998	67	2762
Observed DT50/DT90		--	--	ca. 65	>358
[Pyrazole-3-¹⁴C]-pyrasulfotole					
Linear/natural log ¹	156	y = -0.0045x + 4.3065	0.8358	--	--
Nonlinear/normal ¹	91.2	y = 88.6*exp(-0.0076*x)	0.9204	--	--
Nonlinear/normal		y = 66.534*exp(-0.020*x) + 32.835*exp(-0.0011*x)	0.998	62	1081
Observed DT50/DT90		--	--	50-65	>358
Both labels					
Linear/natural log ¹	161	y = -0.0043x + 4.2958	0.8227	--	--
Nonlinear/normal ¹	95.0	y = 87.2*exp(-0.0073*x)	0.9144		
Nonlinear/normal		y = 66.6209*exp(-0.019*x) + 31.2395*exp(-0.0008*x)	0.998	63	1424
Observed DT50/DT90		--	--	50-65	>358

¹ Determined by the primary reviewer using Excel 2000 (linear) and Sigmaplot v 8.0 (nonlinear) and individual sample data obtained from Tables 5a-5b, p. 46 of the study report (DER Attachment 2).

² non-linear DT90s were extrapolated as observed DT90s were all >358 days; at final sampling interval, [¹⁴C]pyrasulfotole comprised 22.0-24.9% of the applied (Table 10, p. 67; Table 12, p. 69).

In sterile soil, observed DT50 values of [¹⁴C]pyrasulfotole were >120 days (Table 14, p. 71).

TRANSFORMATION PRODUCTS: No major nonvolatile transformation products were detected for either label. One minor product, 2-methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555), was identified in [phenyl-U-¹⁴C]-label treated soil via HPLC and TLC; sufficient levels were not present to confirm the identification with LC/MS/MS (pp. 41, 51-53; Figure 2, p. 81; Figure 10, p. 91; Figure 12, p. 93).

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

In [phenyl-U-¹⁴C]-pyrasulfotole treated soil, AE B197555 was detected at a maximum 3.8% of the applied at 30 days and was 1.0% at 358 days (Table 10, p. 67). Unidentified [¹⁴C]residues, consisting of up to five components, were detected at a maximum total 6.5% at 155 days, and were 3.5% at 358 days (p. 51; Table 10, p. 67).

In [pyrazole-3-¹⁴C]-pyrasulfotole treated soil, unidentified [¹⁴C]residues, consisting of up to six components, were detected at a maximum total 6.1% at 155 days, and were 4.6% at 358 days (p. 52; Table 12, p. 69).

In sterile soil (both labels), AE B197555 was detected at a maximum 3.7% of the applied and unidentified [¹⁴C]residues were ≤1.1% at any interval (Table 14, p. 71).

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: In [phenyl-U-¹⁴C]-pyrasulfotole treated soil, extractable [¹⁴C]residues decreased from 99.7% of the applied at day 0 to 49.3% at 80 days and were 29.3% at 358 days (Table 10, p. 67). Nonextractable [¹⁴C]residues gradually increased from 0.4% at day 0 to 31.3% at 190 days and were 30.1% at 358 days. Organic matter fractionation of 30-, 100- and 251-day extracted soil found 8.1-14.2%, 5.0-8.5% and 5.4-11.7% of the applied associated with the humin, fulvic acids and humic acids, respectively (Table 19, p. 76).

In [pyrazole-3-¹⁴C]-pyrasulfotole treated soil, extractable [¹⁴C]residues decreased from 99.0% at day 0 to 51.7% at 65 days and were 26.6% at 358 days (Table 12, p. 69). Nonextractable [¹⁴C]residues increased from 1.1% at day 0 to 35.2% at 155 days and were 30.7% at 358 days. Organic matter fractionation of 30-, 100- and 251-day extracted soil found 10.5-14.0%, 4.7-8.0% and 6.1-13.2% of the applied associated with the humin, fulvic acids and humic acids, respectively (Table 19, p. 76).

In sterile soil (both labels), extractable and nonextractable [¹⁴C]residues were 93.6-97.9% and 3.8-5.2% of the applied, respectively, at 120 days (Table 14, p. 71).

VOLATILIZATION: At study termination (358 days), volatilized ¹⁴CO₂ comprised 40.5% and 33.5% of the applied for the [phenyl-U-¹⁴C]- and [pyrazole-3-¹⁴C]-label treated soils, respectively, while volatile [¹⁴C]organic compounds were <0.1% (both labels) at all sampling intervals (Table 10, p. 67; Table 12, p. 69). Barium chloride precipitation confirmed the presence of ¹⁴CO₂ in 358-day volatiles trap samples (both labels, ≥99.7% of sample radioactivity; p. 41).

For sterile soil (both labels), volatilized ¹⁴CO₂ totaled ≤0.4% at 120 days and volatile [¹⁴C]organic compounds were <0.1% at all sampling intervals (Table 14, p. 71).

TRANSFORMATION PATHWAY: The study author provided a transformation pathway that was consistent with the products detected in this study (pp. 54-55; Figure 29, p. 103).

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Transformation of pyrasulfotole involves hydrolytic cleavage of the phenyl and pyrazole moieties to yield the benzoic acid derivative, 2-methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555), plus several unidentified minor compounds, with steady formation of bound soil residues and mineralization to CO₂.

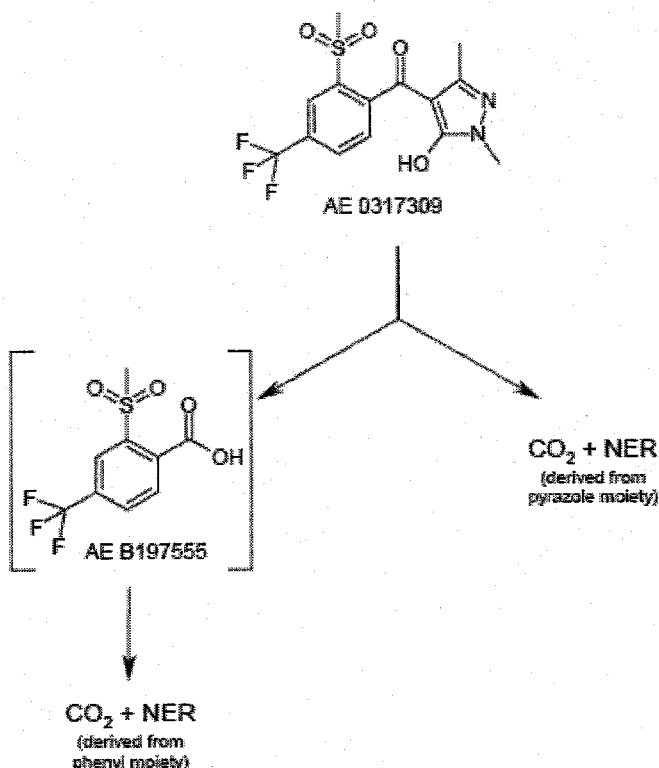


Table 8: Chemical names and CAS numbers for the transformation products of pyrasulfotole.¹

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	MW (g/mol)	Smiles String
AE B197555, RPA 203328	142994-06-07	IUPAC: 2-methylsulfonyl-4-trifluoromethylbenzoic acid	C ₉ H ₇ F ₃ O ₄ S	268.2	CS(=O)(=O)c1cc(C(F)(F)F)ccc1C(=O)O
		CAS: benzoic acid, 2-methylsulfonyl-4-(trifluoromethyl)			

¹ Identification made via reverse-phase HPLC and normal-phase, one-dimensional TLC co-chromatography with reference standard (p. 53); however, supporting co-elution chromatograms (UV) were not provided for review. Data obtained from Figure 1, p. 80 of the study report.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: Determination of adsorption of aged pyrasulfotole residues. Nonsterile, treated, reserve samples (one per label) were taken at 363 days posttreatment and analyzed for the distribution of parent pyrasulfotole between the aqueous phase (calcium chloride solution) and soil (acetonitrile:water plus reflux extracts).

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

[¹⁴C]Pyrasulfotole (both labels) comprised 9.4-9.9% and 16.2-18.9% of the applied in the aqueous phase and soil, respectively (Table 18, p. 75). Calculated K_d and corresponding K_{oc} values were 4.1 and 88, respectively, indicating the potential mobility of pyrasulfotole at 1 year posttreatment in the silt loam soil was mobile (K_{oc} 10-100), based on the FAO mobility classification scheme.

Storage stability. HPLC re-analysis found no significant quantitative differences in the chromatographic profiles of selected 0- to 100-day soil extracts after 209-326 days of frozen storage (p. 55; Table 20, p. 77).

III. STUDY DEFICIENCIES

No significant deviations from good scientific practices or Subdivision N guidelines were noted.

IV. REVIEWERS' COMMENTS

1. The approach used by the study author underestimate the persistence shown in this study, with up to 25% of the parent still being present at 358 days, having declined very slowly from 65 days after treatment, where 50% was present.
2. The provided supplementary experiment (to investigate the increase in soil adsorption) is not considered robust due to the low sample numbers per experiment. Two data points are not statistically significant to draw conclusions of the chemical's fate and behaviour in a soil. Therefore, the conclusions made about pyrasulfotole's mobility in soil are not reliable and very different from the other soil metabolism studies ([phenyl-U-¹⁴C]- and [pyrazole-3-¹⁴C]- AE 0317309: aerobic soil metabolism in loamy sand soil of US origin under laboratory conditions at 25°C, MRID 46801709).
3. The reviewers agree with the study author's conclusion that pyrasulfotole is degradable in microbially active soil under aerobic conditions producing a main metabolite (a maximum of 3.8% AR), CO₂ (maximum of 40.5% AR), and non-extractable residues (maximum of 35.2% AR), but adds to the conclusion that residues of pyrasulfotole were found up to 358 days (maximum of 24.9% AR).

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

4. Mean results and standard deviations presented in this review were determined by the primary reviewer using Microsoft Excel 2000 (9.0.2720) software (DER Attachment 2). Standard deviations were determined using the "biased" or "n" method which determines the standard deviation of the entire sample population. Mean material balances, standard deviations and summations reported by the study author (Tables 7-10, pp. 64-67; Table 12, p. 69; Tables 14-16, pp. 71-73) were verified by the primary reviewer and, with a few exceptions, there was consistent agreement (within $\pm 0.1\%$ of applied) between the study author's reported values and those determined by the primary reviewer (DER Attachment 2).
5. The test application rates of 0.13-0.14 mg a.i./kg used in this study were based on the highest proposed maximum seasonal field application rate of 100 g a.i./ha (0.089 lb a.i./acre; pp. 19, 22; Table 4, p. 61). Assuming a soil incorporation depth of 5 cm and bulk density of 1.5 g/cm³, the 100 g a.i./ha field rate converts to a test application rate of 0.133 mg a.i./kg (p. 22).
6. The study authors assert that the non-extractable residues are assumed to originate from substantial assimilation of degradates into the soil matrix since the sterilized soil control test system showed virtually no degradation and marginal formation of non-extractable residues.
7. Observed DT50 values for total residues.

Test substance	Parent +nonvolatile [¹⁴ C]products ¹	Total [¹⁴ C]residues ²
[Phenyl-U- ¹⁴ C]-pyrasulfotole	65-80 days	>358 days
[Pyrazole-3- ¹⁴ C]-pyrasulfotole	65-80 days	>358 days

¹ Parent pyrasulfotole plus identified/unidentified [¹⁴C]transformation products.

² All [¹⁴C]residues other than volatilized ¹⁴CO₂.

Data obtained from DER Attachment 2.

8. Total recovery on day 358 for the pyrazole-14C labeled soil (90.8%) was lower than typical recoveries throughout the study. AE 0317309 radioactivity levels however, were in keeping with the general pattern of decline for both radiolabels. The estimation of DT50 for the pyrazole-14C label is therefore expected to be adequate.
9. Sterility was lost in the sterile controls, however this does not affect the validity of the study or estimates of parent transformation rates in non-sterile soil.

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 162-1, Aerobic Soil Metabolism Studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

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.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Attachment 1: Structures of Parent Compound and Transformation Products

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Pyrasulfotole [AE 0317309; K-1196; K-1267]

IUPAC Name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α -trifluoro-2-mesyl-*p*-tolyl)methanone.

(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

CAS Name: (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl]-4-(trifluoromethyl)phenyl]methanone.

Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].

CAS Number: 365400-11-9.

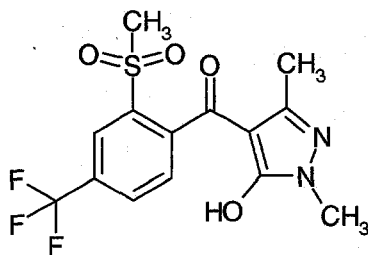
SMILES String: FC(c1cc(c(cc1)C(=O)c1c(n(nc1C)C)O)S(=O)(=O)C(F)F (ISIS v2.3/Universal SMILES).

No EPI Suite, v3.12 SMILES String found as of 6/7/06.

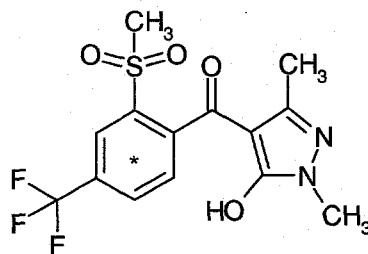
Cc1nn(C)c(O)c1C(=O)c2ccc(C(F)F)cc2S(C)(=O)=O.

CS(=O)(=O)c1c(ccc(c1)C(F)F)C(=O)c1c(n(nc1C)C)O.

Unlabeled



[Phenyl-U-¹⁴C]pyrasulfotole



¹⁴C = Position of radiolabel.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Pyrasulfotole [AE 0317309; K-1196; K-1267]

IUPAC Name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α -trifluoro-2-mesyl-*p*-tolyl)methanone.

(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

CAS Name: (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl]-4-(trifluoromethyl)phenyl]methanone.

Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].

CAS Number: 365400-11-9.

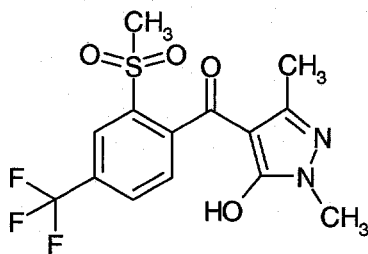
SMILES String: FC(c1cc(c(cc1)C(=O)c1c(n(nc1C)C)O)S(=O)(=O)C(F)F (ISIS v2.3/Universal SMILES).

No EPI Suite, v3.12 SMILES String found as of 6/7/06.

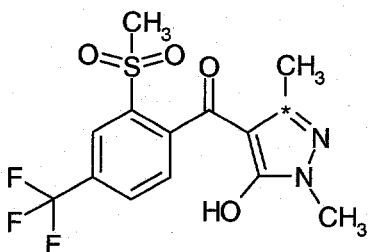
Cc1nn(C)c(O)c1C(=O)c2ccc(C(F)(F)F)cc2S(C)(=O)=O.

CS(=O)(=O)c1c(ccc(c1)C(F)(F)F)C(=O)c1c(n(nc1C)C)O.

Unlabeled



[Pyrazole-3-¹⁴C]pyrasulfotole



¹⁴C = Position of radiolabel.

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Identified Compounds

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Pyrasulfotole [AE 0317309; K-1196; K-1267]

IUPAC Name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α -trifluoro-2-mesyl-*p*-tolyl)methanone.

(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

CAS Name: (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl]-4(trifluoromethyl)phenyl]methanone.

Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].

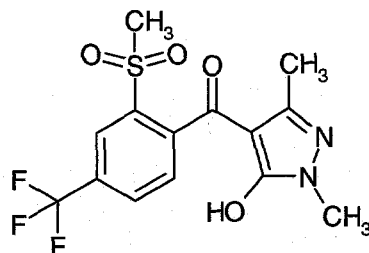
CAS Number: 365400-11-9.

SMILES String: FC(c1cc(c(cc1)C(=O)c1c(n(nc1C)C)O)S(=O)(=O)C(F)F (ISIS v2.3/Universal SMILES).

No EPI Suite, v3.12 SMILES String found as of 6/7/06.

Cc1nn(C)c(O)c1C(=O)c2ccc(C(F)(F)F)cc2S(C)(=O)=O.

CS(=O)(=O)c1c(ccc(c1)C(F)(F)F)C(=O)c1c(n(nc1C)C)O.



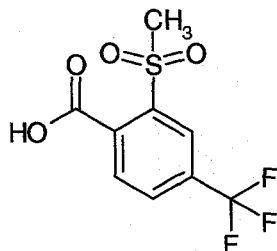
Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

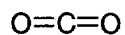
RPA 203328 [AE B197555-benzoic acid; AE B197555; K-1198; K-1367]

IUPAC Name: 2-Mesyl-4-trifluoromethylbenzoic acid.
CAS Name: Benzoic acid, 2-(methylsulfonyl)-4-(trifluoromethyl)-.
CAS Number: 142994-06-7.
SMILES String: O=C(c1ccc(cc1S(=O)(=O)C)C(F)(F)F)O (ISIS v2.3/Universal SMILES).
No EPI Suite, v3.12 SMILES String found as of 6/7/06.
CS(=O)(=O)c1cc(C(F)(F)F)ccc1C(=O)O.
CS(=O)(=O)c1cc(ccc1C(=O)O)C(F)(F)F.



Carbon Dioxide

IUPAC Name: Not reported.
CAS Name: Not reported.
CAS Number: Not reported.



Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

Unidentified Reference Compounds

Data Evaluation Report on the aerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445

EPA MRID Number 46801710

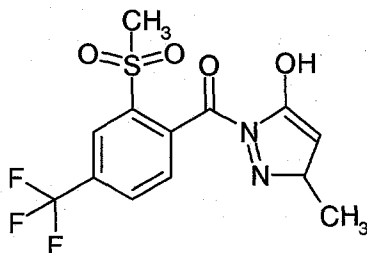
AE 1898321

IUPAC Name: 3-Methyl-1-[2-(methylsulfonyl)-4-(trifluoromethyl)benzoyl]-1H-pyrazol-5-ol.

CAS Name: Not reported.

CAS Number: Not reported.

SMILES String: Cc2cc(O)n(C(=O)c1ccc(C(F)(F)F)cc1S(C)(=O)=O)n2.



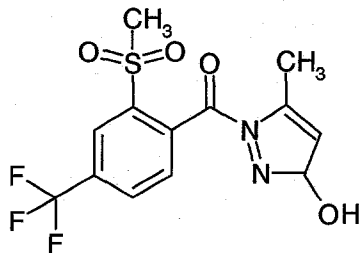
AE 1898322

IUPAC Name: 5-Methyl-1-[2-(methylsulfonyl)-4-(trifluoromethyl)benzoyl]-1H-pyrazol-3-ol.

CAS Name: Not reported.

CAS Number: Not reported.

SMILES String: Cc1cc(O)nn1C(=O)c2ccc(C(F)(F)F)cc2S(C)(=O)=O.



Chemical: Pyrasulfotole (AE 0317309)

PC: 000692

MRID: 46801710

Guideline: 162-1

Nonlinear half-lives (exponential decay/single, 2 parameter)

North Dakota silt loam

[Phenyl-U-¹⁴C]-label

Half-life (days) 99.0

R squared 0.9094

[Pyrazole-3-¹⁴C]-label

Half-life (days) 91.2

R squared 0.9204

Both labels

Half-life (days) 95.0

R squared 0.9144

Chemical: Pyrasulfotole (AE 0317309)

PC: 000692

MRID: 46801710

Guideline: 162-1

Aerobic metabolism of [¹⁴C]pyrasulfotole in a North Dakota silt loam soil.

Determination of overall mean recoveries of radioactivity.

[Phenyl-U-¹⁴C]-label/nonsterile

Day	Soil		Volatiles		Material balance	Study reported material balance
	Total Ext	Nonext	CO ₂	Organic vol.		
	% AR	% AR	% AR	% AR	% AR	% AR
0	99.7	0.4			100.1	100.1
3	95.8	3.5	0.3		99.6	99.4
7	90.7	7.6	1.4		99.7	99.6
14	84.2	12.0	4.3		100.5	100.5
21	78.4	15.1	6.9		100.4	100.4
30	72.3	18.3	9.7		100.3	100.3
41	61.9	22.4	13.6		97.9	97.9
51	56.8	25.2	16.3		98.3	98.4
65	53.8	26.3	19.0		99.1	99.1
80	49.3	28.4	22.3		100.0	99.9
100	44.9	29.8	24.9		99.6	99.7
120	36.8	30.2	26.4		93.4	93.3
155	37.3	30.5	30.0		97.8	97.7
190	35.0	31.3	32.3		98.6	98.6
251	31.9	30.9	34.7		97.5	97.5
358	29.3	30.1	40.5		99.9	99.9
			Mean		98.9	98.9
			std dev.		1.7	1.7
			maximum		100.5	100.5
			minimum		93.4	93.3
			n =		16	16

Results from Table 7, p. 64 of the study report.

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Pyrasulfotole (AE 0317309)

PC: 000692

MRID: 46801710

Guideline: 162-1

Aerobic metabolism of [¹⁴C]pyrasulfotole in a North Dakota silt loam soil.

Determination of overall mean recoveries of radioactivity.

[Pyrazole-3-¹⁴C]-label/nonsterile

Day	Soil		Volatiles		Material	Study reported
	Total Ext	Nonext	CO ₂	Organic vol.	balance	material balance
	% AR	% AR	% AR	% AR	% AR	% AR
0	99.0	1.1			100.1	100.1
3	95.0	5.3	1.0		101.3	100.3
7	88.6	10.1	2.2		100.9	101.0
14	82.8	14.6	4.2		101.6	101.6
21	76.7	18.0	6.3		101.0	101.0
30	72.5	21.6	8.7		102.8	102.8
41	62.3	25.6	11.9		99.8	99.9
50	56.5	28.1	14.1		98.7	98.8
65	51.7	30.8	17.7		100.2	100.3
80	46.0	32.0	20.6		98.6	98.6
100	42.8	33.5	23.6		99.9	99.9
120	38.9	34.4	25.5		98.8	98.7
155	35.7	35.2	28.8		99.7	99.7
190	32.9	34.4	31.2		98.5	98.4
251	30.2	34.5	33.8		98.5	98.5
358	26.6	30.7	33.5		90.8	90.8
			Mean		99.5	99.4
			std dev.		2.5	2.5
			maximum		102.8	102.8
			minimum		90.8	90.8
			n =		16	16
			Mean Phe+Pyr		99.2	99.1
			std dev.		2.2	2.2
			n =		32	32

Results from Table 8, p. 65 of the study report.

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Pyrasulfotole (AE 0317309)

PC: 000692

MRID: 46801710

Guideline: 162-1

Aerobic metabolism of [¹⁴C]pyrasulfotole in a North Dakota silt loam soil.

Determination of overall mean recoveries of radioactivity.

[Phenyl-U-¹⁴C]-label/sterile

Day	Soil		Volatiles		Material balance % AR	Study reported material balance % AR
	Total Ext	Nonext	CO ₂	Organic vol.		
	% AR	% AR	% AR	% AR		
7	101.5	1.2			102.7	102.8
21	101.1	2.0			103.1	103.1
41	96.0	2.6			98.6	98.6
80	98.0	3.2			101.2	101.3
120	97.9	3.8			101.7	101.7
Mean					101.5	101.5
std dev.					1.6	1.6
Maximum					103.1	103.1
Minimum					98.6	98.6
n =					5	5

[Pyrazole-3-¹⁴C]-label/nonsterile

Day	Soil		Volatiles		Material balance % AR	Study reported material balance % AR
	Total Ext	Nonext	CO ₂	Organic vol.		
	% AR	% AR	% AR	% AR		
7	97.8	2.1			99.9	100.0
21	97.6	3.0			100.6	100.6
41	97.1	3.7	0.1		100.9	100.9
80	94.1	4.5	0.3		98.9	98.9
120	93.6	5.2	0.4		99.2	99.4
Mean					99.9	100.0
std dev.					0.8	0.7
Maximum					100.9	100.9
Minimum					98.9	98.9
n =					5	5
Mean Phe+Pyr					100.7	100.7
std dev.					1.5	1.5
n =					10	10

Results from Table 9, p. 66 of the study report.

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Pyrasulfotole (AE 0317309)

PC: 000692

MRID: 46801710

Guideline: 162-1

**Aerobic metabolism of [¹⁴C]pyrasulfotole in a North Dakota silt loam soil.
Determination of total unidentified [¹⁴C]residues following HPLC analysis.**

Day	[Phenyl-U-14C]-label/nonsterile				
	Pyrasulfotole	AE B197555	Single Unk	Others	Total Unided
	% AR	% AR	% AR	% AR	% AR
0	94.3	2.6	1.3	1.5	2.8
3	91.8	3.1	1.0	0.0	1.0
7	85.2	2.9	2.7	0.0	2.7
14	76.0	3.7	1.8	2.7	4.5
21	72.9	2.8	1.4	1.3	2.7
30	66.8	3.8	0.9	0.8	1.7
41	58.3	1.7	0.8	1.2	2.0
51	52.2	2.0	1.3	1.4	2.7
65	49.9	1.9	0.8	1.1	1.9
80	43.5	2.5	1.1	2.1	3.2
100	39.8	2.1	1.0	2.1	3.1
120	34.2	1.0	1.1	0.4	1.5
155	29.1	1.8	1.5	5.0	6.5
190	28.2	1.5	1.2	4.0	5.2
251	25.5	2.1	1.9	2.3	4.2
358	24.8	1.0	1.4	2.1	3.5

Day	[Pyrazole-3-14C]-label/nonsterile			
	Pyrasulfotole	Single Unk	Others	Total Unided
	% AR	% AR	% AR	% AR
0	97.1	1.4	0.5	1.9
3	93.3	1.0	0.7	1.7
7	85.7	1.4	1.4	2.8
14	80.0	2.0	0.9	2.9
21	73.6	2.0	1.1	3.1
30	68.8	2.0	1.6	3.6
41	58.9	1.8	1.6	3.4
50	53.0	1.6	1.9	3.5
65	47.2	2.0	2.7	4.7
80	41.1	2.5	2.5	5.0
100	38.0	2.0	2.9	4.9
120	35.1	2.1	1.7	3.8
155	29.6	2.1	4.0	6.1
190	27.5	1.5	4.0	5.5
251	24.7	1.6	3.9	5.5
358	22.1	1.7	2.9	4.6

Results from Tables 15-16, pp. 72-73 of the study report.

Chemical: Pyrasulfotole (AE 0317309)
 PC: 000692
 MRID: 46801710
 Guideline: 162-1

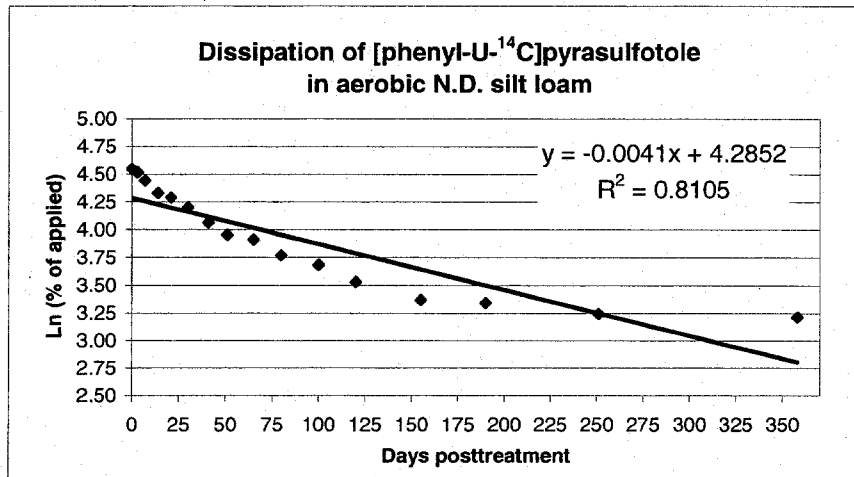
**Aerobic metabolism of [¹⁴C]pyrasulfotole in a North Dakota silt loam soil.
 Half-life determination**

[Phenyl-U-¹⁴C]-label/nonsterile

Half-life (days) 168 (0- to 358-day data)

Days Posttreatment	Pyrasulfotole	
	(% of Applied)	Ln (% applied)
0	94.3	4.54648119
3	91.7	4.518522379
7	85.1	4.443827036
14	76.0	4.33073334
21	73.0	4.290459441
30	66.8	4.201703081
41	58.3	4.065602093
51	52.2	3.955082495
65	50.0	3.912023005
80	43.5	3.772760938
100	39.8	3.683866912
120	34.2	3.532225644
155	29.0	3.36729583
190	28.3	3.342861805
251	25.6	3.242592351
358	24.9	3.214867803

Data obtained from Table 10, p. 67 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.900270729
R Square	0.810487386
Adjusted R Square	0.796950771
Standard Error	0.209740191
Observations	16

ANOVA					
	df	SS	MS	F	Sig F
Regression	1	2.633901261	2.6339	59.87371061	2.014E-06
Residual	14	0.615873265	0.044		
Total	15	3.249774526			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.28517723	0.072184202	59.364	3.18677E-18	4.1303574	4.4399971	4.130357377	4.43999708
X Variable 1	-0.004133197	0.000534156	-7.738	2.01402E-06	-0.005279	-0.0029875	-0.00527885	-0.00298755

Chemical: Pyrasulfotole (AE 0317309)
 PC: 000692
 MRID: 46801710
 Guideline: 162-1

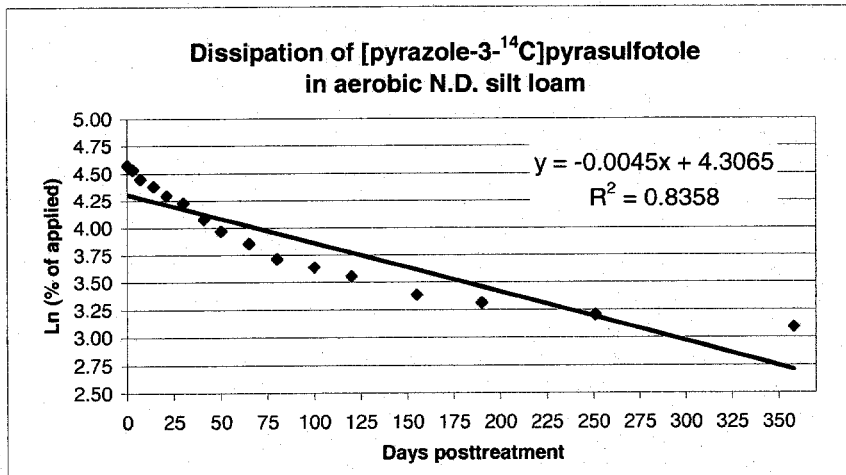
**Aerobic metabolism of [¹⁴C]pyrasulfotole in a North Dakota silt loam soil.
 Half-life determination**

[Pyrazole-3-¹⁴C]-label/nonsterile

Half-life (days) 156 (0- to 358-day data)

Days Posttreatment	Pyrasulfotole	
	(% of Applied)	Ln (% applied)
0	97.1	4.575741375
3	93.3	4.535820108
7	85.7	4.450852826
14	80.0	4.382026635
21	73.6	4.298645026
30	68.8	4.231203745
41	59.0	4.077537444
50	53.0	3.970291914
65	47.2	3.854393893
80	41.1	3.716008122
100	38.0	3.63758616
120	35.1	3.55820113
155	29.6	3.387774361
190	27.5	3.314186005
251	24.7	3.206803244
358	22.0	3.091042453

Data obtained from Table 12, p. 69 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.914226286
R Square	0.835809701
Adjusted R Square	0.824081823
Standard Error	0.207268367
Observations	16

ANOVA

	df	SS	MS	F	Sig F
Regression	1	3.061639154	3.0616	71.26691348	7.283E-07
Residual	14	0.601442466	0.043		
Total	15	3.66308162			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.306483397	0.07130159	60.398	2.50482E-18	4.1535566	4.4594102	4.15355656	4.45941023
X Variable 1	-0.004454963	0.000527716	-8.442	7.28299E-07	-0.005587	-0.0033231	-0.0055868	-0.00332312

Chemical: Pyrasulfotole (AE 0317309)

PC: 000692

MRID: 46801710

Guideline: 162-1

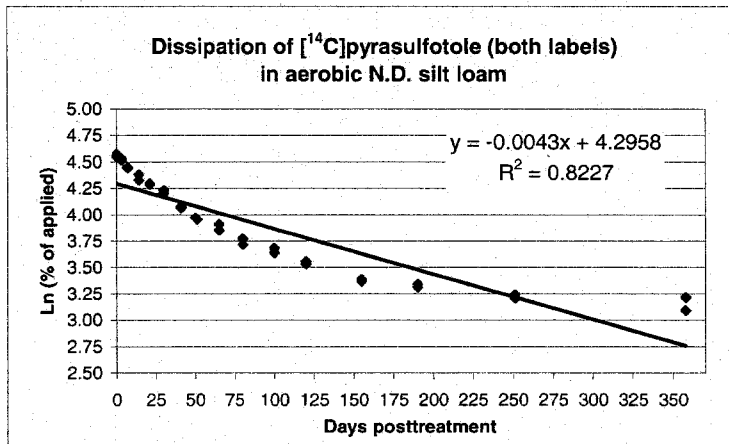
Aerobic metabolism of [¹⁴C]pyrasulfotole in a North Dakota silt loam soil.

Half-life determination

[Phenyl-U-¹⁴C]- and [pyrazole-3-¹⁴C]-labels/nonsterile

Half-life (days) 161 (0- to 358-day data)

Days Posttreatment	Pyrasulfotole	
	(% of Applied)	Ln (% applied)
0	94.3	4.54648119
0	97.1	4.575741375
3	91.7	4.518522379
3	93.3	4.535820108
7	85.1	4.443827036
7	85.7	4.450852826
14	76.0	4.33073334
14	80.0	4.382026635
21	73.0	4.290459441
21	73.6	4.298645026
30	66.8	4.201703081
30	68.8	4.231203745
41	58.3	4.065602093
41	59.0	4.077537444
51	52.2	3.955082495
50	53.0	3.970291914
65	50.0	3.912023005
65	47.2	3.854393893
80	43.5	3.772760938
80	41.1	3.716008122
100	39.8	3.683866912
100	38.0	3.63758616
120	34.2	3.532225644
120	35.1	3.55820113
155	29.0	3.36729583
155	29.6	3.387774361
190	28.3	3.342861805
190	27.5	3.314186005
251	25.6	3.242592351
251	24.7	3.206803244
358	24.9	3.214867803
358	22.0	3.091042453



Data obtained from Table 10, p. 67; Table 12, p. 69 of the study report.

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.907016993
R Square	0.822679826
Adjusted R Square	0.816769154
Standard Error	0.202145704
Observations	32

ANOVA					
	df	SS	MS	F	Sig F
Regression	1	5.687520626	5.6875	139.1854873	8.524E-13
Residual	30	1.225886564	0.0409		
Total	31	6.91340719			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.295838152	0.049182753	87.344	1.13438E-37	4.1953937	4.3962826	4.195393674	4.39628263
X Variable 1	-0.00429411	0.000363979	-11.8	8.52387E-13	-0.005037	-0.0035508	-0.00503745	-0.00355077

[¹⁴C]Pyrasulfotole (both labels) in aerobic N.D. silt loam:
nonlinear regression (MRID 46801710, Sub. No. 2006-2445)

