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

PMRA Submission Number 2006-2445 EPA MRID Number 46801709

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: 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.

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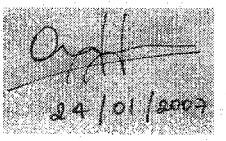
Final Reviewer: Olga Braga **Signature:**
DEH Reviewer **Date:**



Company Code: BCZ
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CITATION: Fliege, R. 2004. [Phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-AE 0317309: aerobic soil metabolism in a loamy sand soil of US origin under laboratory conditions at 25°C. Unpublished study performed, sponsored and submitted by Bayer CropScience, GmbH, Frankfurt, Germany.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 02/011 and Report No.: MEF-386/03. Experimental start date June 24, 2002, and termination date July 31, 2003 (p. 6). Final report issued June 22, 2004.

EXECUTIVE SUMMARY

The biotransformation of [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-labeled (5-hydroxy-1,3-dimethylpyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone (pyrasulfotole, AE 0317309) was studied in a loamy sand soil (pH 5.6-6.2, organic carbon 1.2%) from North Carolina for 358 days under aerobic conditions in darkness at 25 ± 1°C and 75% of 1/3 bar soil moisture. [^{14}C]Pyrasulfotole was applied at a rate of 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 CO_2 (soda lime) and volatile organics (paraffin oil-coated glass wool). A single flask per test substance was taken for analysis after 0, 2, 4, 7, 10, 14, 21, 30, 39, 50, 65, 80, 100, 120, 168, 259 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 and LC/MS/MS-ESI 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 101.1 ± 1.2% (range 97.5-103.3%) of the applied, with no significant losses of total applied radioactivity over the 358-day incubations for either label. [^{14}C]Pyrasulfotole dissipation followed a biphasic pattern decreasing quickly from 96.4-97.5% of the applied at day 0 posttreatment to 53.8-54.8% at 4 days and was 40.0-40.7% at 7 days, then dissipation significantly slowed with [^{14}C]pyrasulfotole comprising 20.2-22.8% at study termination. The reviewer-calculated **linear half-life** was 240 days (r^2 = 0.4428) and the **nonlinear half-life** was 69 days (r^2 = 0.441). Based on a 2-compartment nonlinear regression model the **DT_{50} and DT_{90}** estimates were 5.8 and 749 days, respectively (r^2 = 0.977). The **observed DT_{50}** and **DT_{90}** values were 4-7 days and >358 days, respectively.

2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555) was a major transformation product in phenyl-label treated soil detected at a maximum 12.2% of the applied at 7 days posttreatment and was 4.2% at study termination. No minor transformation products were identified for either label. Unidentified [^{14}C]residues were detected at maximum totals of 13.8-14.0%, with the residues comprised of a single HPLC component (designated "largest single

unknown") detected at ≤3.9% of the applied, an HPLC "region" of unresolved residues found (via TLC) to consist of at least twelve individual components each ≤2.5%, and the remaining a total of other minor HPLC components (up to six to nine) detected at ≤4.9%. Extractable [^{14}C]residues decreased from 98.1-99.3% of the applied at day 0 to 36.2-38.5% at 358 days. Non-extractable [^{14}C]residues increased from 1.7-1.9% at day 0 to maximums of 49.7-50.1% at 100-120 days and were 43.2-44.8% at 358 days. Organic matter fractionation of 4-, 30- and 259-day extracted soil found 3.4-5.7%, 12.5-27.4% and 9.0-19.8% of the applied associated with the humin, fulvic acids and humic acids, respectively. At study termination, volatilized $^{14}CO_2$ totaled 17.3%-18.6% of the applied, while volatile [^{14}C]organic compounds were ≤0.4% at any sampling interval.

Under **sterile** (autoclaved soil, both labels) conditions, parent pyrasulfotole comprised 94.8-95.4% of the applied at 120 days (final interval), with AE B197555 in phenyl-label treated soil detected at ≤3.2% at any interval. At study termination, extractable and nonextractable [^{14}C]residues were 95.6-99.3% and 2.7-3.5% of the applied, respectively, with volatilized $^{14}CO_2$ and volatile [^{14}C]organic compounds ≤0.2%. During the 120-day incubations, recoveries of material balance ranged from 99.4 to 103.8% 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 numerous unidentified minor compounds, with rapid formation of bound soil residues and moderate levels of mineralization to CO_2 over time. 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 dissipation of a second application of [^{14}C]pyrasulfotole made at 80 days following the initial application was found to yield degradate and total residue profiles comparable to those found in the definitive study. The results indicated that the test soil still contained viable microbial populations when the second application was made suggesting that the biphasic dissipation of pyrasulfotole evidenced in the definitive study was not due to a lack of microbial viability.

In a supplementary experiment, the potential mobility of pyrasulfotole decreased with time from moderately mobile (K_{oc} values of 276-357) at 50 days posttreatment to slightly mobile (K_{oc} values of 2,090-2,183) at 358 days, as measured by the FAO classification scheme. The study author proposed that the biphasic dissipation of pyrasulfotole may have been due to increased soil adsorption which reduced the availability of pyrasulfotole to microbial degradation.

In a supplementary experiment, there were no significant differences in the degradate and total residue profiles between soil samples from the definitive study and those in which the soil moisture content was increased to 45% of maximum water holding capacity (16.8% soil moisture as compared to 6.8% soil moisture at 75% of 1/3 bar).

In a supplementary experiment, pyrasulfotole and its transformation products remained stable in soil extracts stored frozen up to 266-345 days.

Results Synopsis:

Test system used: Loamy sand from North Carolina.

Linear half-life:	240 days (r^2 = 0.4428).
Non-linear half-life:	69 days (r^2 = (0.4409).
Non-linear, 2-compartment DT_{50}:	5.8 days (r^2 = 0.977).
Non-linear, 2 compartment DT_{90}:	747 days (r^2 = 0.977).
Observed DT_{50}:	4-7 days.
Observed DT_{90}:	>358 days.

Note: Linear and non-linear first-order half-life models do not adequately fit bi-phasic transformation pattern.

Major transformation products:

2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555, maximum 12.2% of applied).

CO_2 (maximum 17.3-18.6% of applied).

Minor transformation products:

No minor transformation products were identified.

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

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-^{14}C] and [pyrazole-3-^{14}C]pyrasulfotole (Figure 1, p. 87).

Chemical Structure: See DER Attachment 1.

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

Description:		Technical; pale, yellow solid (p. 23).
Purity:	Radiochemical purity:	>97% (Figure 7, p. 96; Appendix 3, p. 119).
	Batch No.	SEL/1006 (p. 23).
	Analytical purity:	>99% (NMR; Appendix 3, p. 119).
	Specific activity:	191,400 dpm/µg (31.33 mCi/mmol, 3.19 MBq/mg).
	Location of the radiolabel:	Uniformly on phenyl ring.

[Pyrazole-3-^{14}C]pyrasulfotole

Description:		Technical; white solid (p. 24).
Purity:	Radiochemical purity:	>99% (Figure 7, p. 96; Appendix 4, p. 120).
	Batch No.	SEL/1009 (p. 24).
	Analytical purity:	100% (HPLC), 90% (NMR, unadjusted for mol. wt.; Appendix 4, p. 120).
	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.

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 pyrasulfatole chemistry review of Submission 2006-2445.

2. Soil Characteristics

Table 1: Description of soil collection and storage.

Description		Details
Geographic location		Field (grassland) located at former Aventis CropScience Research Farm, Pikeville, North Carolina.
Coordinates	Latitude:	N 35° 29.303'
	Longitude:	W 78° 02.421'
Collection date		May 21, 2002
Pesticide use history at the collection site		No pesticide applications for at least prior 10 years.
Collection procedures		Sampled from field with a shovel into a bucket (no further description).
Sampling depth		*ca.* 0- to 8-inch depth, with grass cover removed (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		34 days based on collection date (above) and the date of application on June 24, 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. 63; Appendix 2, p. 118 of the study report.

Table 2: Properties of the soil.

Property		Details
Soil texture		Loamy sand.
% Sand (0.05-2.0 mm)		77
% Silt (0.002-0.05 mm)		22
% Clay (<0.002 mm)		1
pH	in water (1:1):	6.2
	in $CaCl_2$ (1:1):	5.6
Organic carbon (%)		1.2
Organic matter (%)[1]		2.1
CEC (meq/100g)		5.8
Moisture at 1/3 bar (%)		9.0
Maximum water holding capacity (%)		37.3
Bulk density, disturbed (g/cm^3)		1.40
Microbial biomass (mg/100 g dry wt. soil)[2]		23.9 ± 2.8
Microbial plate counts (CFU/g dry wt. soil)[2]	Aerobic bacteria:	5,000,000
	Aerobic spore forming bacteria:	1,000,000
	Yeasts and molds:	20,000
	Actinomycetes:	60,000
Soil taxonomic classification (USDA)		Fine-loamy, siliceous, subactive, thermic, Aquic Paleudults.
Soil series		Goldsboro.
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. 63-64 of the study report.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: None reported.

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 *ca.* 1 month prior to use.	
Soil (g/replicate)		80 g dry wt.	
Application rates (mg a.i./kg & equiv. kg a.i./ha)	Nominal	0.133 mg a.i./kg[1]	
	Actual	0.137 mg a.i./kg for [phenyl-U-^{14}C]-label. 0.143 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, *ca.* 30 minutes) three times at 1- to 2-day intervals during the 10-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 0.3% based on soil weight [500 µL of acetone:deionized, autoclave sterilized water (1:1, v:v) test solution in 80 g dry wt. soil].	
Test material	Volume of the test solution used/treatment:	500 µL/80 g soil (dry wt).	
	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.	
Any indication of the test material adsorbing to the walls of the test apparatus?		Not indicated.	
Microbial plate counts of the sterile controls		Initial[2]	Final (65 days)[3]
	Aerobic bacteria:	<100	<100

Parameter		Both labels	
(CFU/g dry wt. soil)	Aerobic spore forming bacteria:	<100	<100
	Yeasts and molds:	n.d.[4]	200
	Actinomycetes:	n.d.	<100
Microbial plate counts of treated (CFU/g dry wt. soil)		Initial[2]	Final (358 days)[3]
	Aerobic bacteria:	5,000,000	6,000,000
	Aerobic spore forming bacteria:	1,000,000	700,000
	Yeasts and molds:	20,000	40,000
	Actinomycetes:	60,000	1,000,000
Microbial biomass of treated soil (mg/100 g dry wt. soil)		Initial[2]	Final (365 days)[3]
		23.9 ± 2.8	9.3 ± 0.6
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		The test systems were prepared and acclimatized to study conditions for 10 days prior to treatment.	

1 Assuming a soil incorporation depth of 5 cm and bulk density of 1.5 g/cm^3,the test application rate of 0.133 mg a.i./kg converts to the proposed application rate of 100 g a.i./acre (p. 22).
2 Determined at study initiation using untreated soil (Tables 2-3, pp. 64-65).
3 Determined using soil treated with unlabeled pyrasulfotole at 0.134 mg a.i./kg (p. 29; Tables 2-3, pp. 64-65).
4 Not detected.
Data obtained from pp. 19, 21-22, 26-30; Tables 2-4, pp. 64-66; Figure 6, p. 95 of the study report.

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: Second dose experiments. At 80 days posttreatment, reserve, nonsterile, treated samples (one per label) received, respective to label, a second application of [phenyl-U-^{14}C]- or [pyrazole-3-^{14}C]-pyrasulfotole at 0.14 mg a.i./kg (p. 32; Appendix 9, p. 65). Application and incubation of the second dose treated samples were conducted as described above. These samples were taken for analysis 20 days after the second application (100 days post-initial treatment).

Determination of adsorption of aged pyrasulfotole residues. Nonsterile, treated, reserve samples (one per label) were taken at 50 and 358 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 (p. 33). The soil:solution slurry was agitated via magnetic stirring for 24 hours, then the pH was determined and soil and solution were separated by centrifugation (speed, interval not reported). Two to three additional calcium chloride extractions were conducted as described above with solution volumes *ca.* 50-60 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. Extracts, extracted soil and trapping solutions were analyzed for total radioactivity using LSC. Extracts were concentrated and analyzed by HPLC as described below.

Increased soil moisture experiments. At 57 days posttreatment, the soil moisture of nonsterile, treated, reserve samples (one per label) was adjusted to 45% of maximum water holding capacity; 16.8% soil moisture as compared to 6.8% soil moisture at 75% of 1/3 bar (p. 33). These samples were taken for analysis at 65 days posttreatment and analyzed in the same manner as the definitive study soil samples.

5. Sampling:

Table 4: Sampling details.

Criteria		**Both labels**
Sampling intervals (posttreatment)	Sterile controls	4, 10, 21, 65 and 120 days.
	Nonsterile treated	0 (*ca.* 30 minutes), 2, 4, 7, 10, 14, 21, 30, 39, 50, 65, 80, 100, 120, 168, 259 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 65 days.
Moisture content:		Flask weights were monitored at *ca.* 2- to 4-week intervals. Soil moisture adjustments occurred twenty-six times over the 1-year incubations.
Redox potential, other:		None determined.

Criteria	Both labels
Sample storage before analysis	**Soil samples** were extracted the day of collection, except for 30-day samples which were extracted after 1 day of frozen storage.
	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.
	Extracted soil (air-dried, milled) was stored frozen until combustion analysis, which was reported as typically occurring within two months after extraction.
	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.
Other details, if any	None.

Data obtained from pp. 30-32; Table 2, p. 64; Table 5, p. 67 of the study report.

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods: Diatomaceous earth (10 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. 34; Figure 8, p. 97). 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, 37). Pooled extracts were concentrated via rotary evaporation (40°C, under vacuum), with final volumes of *ca.* 5.0-7.6 mL and 6.5 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. 35).

Total ^{14}C measurement: Total ^{14}C residues were determined by summing the concentrations of residues measured in the soil extracts, extracted soil and volatile trapping materials (p. 43).

Determination of nonextractable residues: Extracted soil was air-dried, then homogenized to a powder using a planetary mill (Retsch; p. 36; Appendix 1, p. 117). Six aliquots (*ca.* 0.5 g) were analyzed for total radioactivity by LSC following combustion (p. 37).

Acid extraction. Aliquots (*ca.* 25 g) of 4- and 30-day extracted soil (both labels) were further extracted with 1M hydrochloric acid (volume not reported) for 24 hours (p. 36). Extract was separated from soil by centrifugation (speed, interval not reported), and aliquots were analyzed for total radioactivity by LSC.

Organic matter fractionation. Aliquots (*ca.* 20-25 g) of 4-, 30- and 259-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; pp. 36-37; Figure 10, p. 99). 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 concentrated hydrochloric acid (conc. HCl), stored overnight at *ca.* 4-6°C, and 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. [^{14}C]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. 36).

To recover radioactivity (presumably, $^{14}CO_2$) 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 (pp. 35-36; Figure 9, p. 98). Released $^{14}CO_2$ 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. 36-37).

The confirm the presence of $^{14}CO_2$, 18% HCl (75 mL) was added dropwise, under the same conditions (70°C, 90 minutes) as described above, to an aliquot (25 mL) of 2-aminoethanol:methanol solution containing radioactivity released from the 358-day soda lime samples (both labels; p. 43; Figure 9, p. 98). Released radioactivity was then purged through 10M potassium hydroxide (KOH) trapping solution, with aliquots subsequently analyzed for total radioactivity by LSC to establish recovery of the sample radioactivity; 102.8% and 103.7% of sample activity recovered for [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-label treated samples, respectively (p. 43; Table 3, p. 65). An aliquot (5 mL) of the KOH solution was 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, and 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 four gradient mobile phases (each described below), injection volume 150-300 µL, flow rate 1.0 mL/minute, UV detector (254 or 280 nm), and Berthold LB 507B or LB 509 radioactivity detector equipped with either a 400-µL yttrium or glass flow-through cell (pp. 38-40). Column recoveries of selected chromatogram runs were monitored through the collection and LSC analysis of bulk column eluates, with the average recovery of seven runs (four [phenyl-U-^{14}C]- and three [pyrazole-3-^{14}C]-label) reported as 97.5% (p. 39); individual column recoveries were not provided. The following gradient mobile phases were employed for sample extracts:

Gradient 2 a/b/c combining (A) either (a) 0.02M aqueous ammonium formate adjusted to pH 2 with formic acid, (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. 40)]. This mobile was used with 0- to 80-day extract samples.

Gradient 3 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. 40)]. This mobile phase was used with 100- to 358-day extract samples.

Parent [^{14}C]pyrasulfotole was identified by co-chromatography with and comparison to the retention time of unlabeled reference standard (pp. 38, 42; Table 6, p. 68; Figure 2, p. 89; Figures 11-12, pp. 100-101; Appendix 11, p. 128).

To confirm results from HPLC analyses, selected extracts were analyzed using one-dimensional TLC on normal-phase plates (silica gel 60 F_{254}, Merck) developed with toluene:ethanol:25% aqueous ammonia (6:5:1, v:v:v, SS-1; p. 41). Following development, areas of radioactivity were detected using a phosphorimaging system (BAS-2500; pp. 41-42). Parent [^{14}C]pyrasulfotole was identified by co-chromatography with unlabeled reference standard which was visualized under UV light (254 nm; p. 41; Table 6, p. 68; Figure 13, p. 102). 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. 35).

Identifications were also confirmed by LC/MS/MS under the following conditions: reverse-phase HPLC conditions comparable to Gradient 2c substituting formic acid for sulfuric acid in eluent A, injection volume 200 µL, 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. 42). Identifications of [^{14}C]pyrasulfotole in sample extracts were made against labeled test substances (p. 42; Figures 3-4, pp. 90-93; Figure 15, p. 104). Aliquots of 4-day "mild" extracts (both labels) were concentrated under a nitrogen stream for this analysis (p. 35).

Identification and quantification of transformation products: Transformation products were separated, quantified and identified using HPLC, TLC and LC/MS/MS as described for the parent compound (pp. 38-42; Table 6, p. 68; Figure 2, p. 89; Figure 5, p. 94; Figures 11-14, pp. 100-103).

In an attempt to further characterize an unresolved "region" of [^{14}C]residues (both labels) that was consistently detected during HPLC analyses, the fractions of interest were collected, concentrated to near dryness under a nitrogen stream, with the resulting residues reconstituted in acetonitrile:water (1:1, v:v; pp. 42-43; Tables 15-16, pp. 77-78; Figure 16A, p. 105). Concentrated "region" samples were analyzed by one-dimensional TLC as described above and also using following solvent system: toluene:ethanol:25% aqueous ammonia (3:5:1, v:v:v, SS-2; p. 41; Figures 16B-17D, pp. 105-106).

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. 88 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.* 0.5% and 0.3% of the applied for [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-label treated samples, respectively, corresponding to <0.001 ppm parent equivalents (pp. 48-49, 51). For TLC analyses, the LOQ

was reported as equivalent to *ca.* 0.2% and 0.1% of the applied for [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-label treated samples, respectively, corresponding to significantly below 0.001 ppm (pp. 49, 51). 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. 48).

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: Incubation temperature averaged 25.06 ± 0.6°C during the 358-day study (p. 50; Table 23, p. 86). 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 with averages of 23.9-22.2 mg/g soil at 0 and 129 days posttreatment, respectively, then decreased to 9.3 mg/100 g soil at 365 days (Table 2, p. 64). Microbial populations of aerobic bacteria, aerobic spore forming bacteria and yeast/molds did not significantly change over the 358-day incubations, while actinomycetes populations increased 50-fold between 121 and 358 days (Table 2, p. 64).

Microbial plate count analyses of sterile, treated (unlabeled pyrasulfotole) soil found no significant levels of aerobic bacteria, aerobic spore forming bacteria, yeasts/molds or actinomycetes through 65 days of incubation (Table 2, p. 64). The lack of transformation of [^{14}C]pyrasulfotole in [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-pyrasulfotole treated sterile soil, indicates that sterility was maintained in those samples (Table 14, p. 76).

B. MATERIAL BALANCE: Overall recovery (both labels) of radiolabeled material averaged 101.1 ± 1.2% (range 97.5-103.3%, n = 34) of the applied, with no significant losses of total applied radioactivity over the 358-day incubations for either label (DER Attachment 2, Reviewer's Comment No. 1). For each label, recoveries averaged (n = 17) 101.3 ± 1.0% (range 99.2-103.3%) of the applied in [phenyl-^{14}C]-label treated soil and 100.9 ± 1.2% (range 97.5-102.9%) in [pyrazole-3-^{14}C]-label treated soil.

In sterile soil, overall recovery averaged (n = 5) 102.1 ± 1.3% (range 99.9-103.8%) and 100.7 ± 1.1% (range 99.4-102.3%) for the [phenyl-U-^{14}C]- and [pyrazole-3^{14}C]-pyrasulfotole treated soils, respectively (DER Attachment 2).

Table 6. Biotransformation of [phenyl-U-^{14}C]pyrasulfotole (AE 0317309), expressed as percentage of applied radioactivity (n = 1), in North Carolina loamy sand soil under aerobic conditions.

Compound	Sampling times (days)																
	0	**2**	**4**	**7**	**10**	**14**	**21**	**30**	**39**	**50**	**65**	**80**	**100**	**120**	**168**	**259**	**358**
Pyrasulfotole	96.4	80.1	53.8	40.0	37.2	38.3	36.2	35.3	32.4	28.7	26.7	26.2	25.2	23.8	23.0	20.9	20.2
AE B197555[1]	2.3	5.7	11.9	12.2	7.5	5.6	5.4	3.3	3.2	1.9	2.5	1.8	2.9	2.6	3.2	3.6	4.2
Unidentified [^{14}C][2]	0.6	2.4	6.0	9.1	11.4	8.9	8.9	8.0	9.1	10.9	12.6	12.2	11.6	12.1	13.3	12.6	14.1
Extractable residues	99.3	88.2	71.6	61.3	56.1	52.8	50.5	46.6	44.8	41.5	41.8	40.3	39.6	38.5	39.5	37.1	38.5
Nonextractable residues	1.7	12.6	28.8	39.5	42.6	44.7	46.9	48.0	49.0	49.3	47.7	47.3	50.1	49.5	47.9	47.4	43.2
CO_2	---	0.1	0.1	0.9	2.7	4.0	6.0	7.4	8.5	9.5	11.9	11.8	12.1	14.2	14.7	16.2	17.3
Volatile organics	---	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	0.1	<0.1	<0.1	0.4	0.1	<0.1	0.1	0.2
Total recovery	101.0	100.8	100.5	101.7	101.3	101.5	103.3	102.0	102.3	100.4	101.5	99.4	102.1	102.4	102.2	100.9	99.2

1 2-Methylsulfonyl-4-trifluoromethylbenzoic acid (Figure 1, p. 88).

2 Summation of a single HPLC component (designated "largest single unknown") comprising ≤3.4% of the applied, an HPLC "region" of unresolved residues found via TLC to consist of at least twelve individual components each ≤1.4%, and the remaining a total of other minor HPLC components (up to six to nine) comprising ≤4.9% (p. 54; Table 15, p. 77; Figures 16-17, pp. 105-106).

Data obtained from p. 54; Table 10, p. 72; Figure 1, p. 88 of the study report and DER Attachment 2.

Table 7. Biotransformation of [pyrazole-3-^{14}C]pyrasulfotole (AE 0317309), expressed as percentage of applied radioactivity (n = 1), in North Carolina loamy sand soil under aerobic conditions.

Compound	Sampling times (days)																
	0	**2**	**4**	**7**	**10**	**14**	**21**	**30**	**39**	**50**	**65**	**80**	**100**	**120**	**168**	**259**	**358**
Pyrasulfotole	97.5	82.1	54.8	40.7	36.3	36.7	33.5	32.0	29.2	29.9	27.8	27.2	26.3	25.5	23.5	21.6	22.8
Unidentified [^{14}C][1]	0.6	3.7	9.2	10.2	12.7	10.8	12.4	12.2	10.5	11.3	12.7	13.0	12.1	13.1	12.9	13.8	13.3
Extractable residues	98.1	85.8	64.0	50.9	49.0	47.4	45.9	44.2	39.8	41.2	40.5	40.2	38.4	38.6	36.4	35.4	36.2
Nonextractable residues	1.9	14.2	34.0	46.2	47.5	48.2	49.6	49.2	48.2	49.0	48.5	47.8	48.6	49.7	49.7	48.2	44.8
CO_2	---	0.9	2.0	3.9	5.1	6.1	7.4	8.5	9.6	10.2	12.7	12.6	13.3	14.3	15.6	17.2	18.6
Volatile organics	---	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	0.2	<0.1	<0.1	<0.1	0.1	<0.1	0.3
Total recovery	99.9	100.0	100.1	101.0	101.6	101.7	102.9	101.8	97.5	100.5	101.9	100.6	100.3	102.6	101.9	100.8	99.9

1 Summation of a single HPLC component (designated "largest single unknown") comprising ≤3.9% of the applied, an HPLC "region" of unresolved residues found via TLC to consist of at least twelve individual components each ≤2.5%, and the remaining a total of other minor HPLC components (up to seven) comprising ≤4.4% (p. 54; Table 16, p. 78; Figures 16-17, pp. 105-106).
Data obtained from p. 54; Table 12, p. 74 of the study report and DER Attachment 2.

C. TRANSFORMATION OF PARENT COMPOUND: [^{14}C]Pyrasulfotole (both labels) initially dissipated quickly in the loamy sand soil decreasing from 96.4-97.5% of the applied at day 0 posttreatment to 53.8-54.8% at 4 days and was 40.0-40.7% at 7 days; thereafter, dissipation significantly slowed with [^{14}C]pyrasulfotole comprising 20.2-22.8% at study termination (Table 10, p. 72; Table 12, p. 74).

In sterile soil, [^{14}C]pyrasulfotole (both labels) comprised 94.8-95.4% of the applied at 120 days posttreatment (final interval; Table 14, p. 76).

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 11.04 days (r^2 = 0.777; p. 57; Figure 25, p. 114).

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 240 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 5.8 and 749 days, respectively. The observed DT_{50} value for pyrasulfotole was in the 4-7 day range and the observed DT_{90} was >358 days.

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

Compound	Half-life (days)	Regression equation	r^2	DT50 (days)	DT90[2] (days)
[phenyl-U-^{14}C]pyrasulfotole (AE 0317309)					
Linear/natural log[1]	226	y = -0.0031x + 3.7689	0.4838	--	--
Nonlinear/normal[1]	67.3	y=58.9*exp(-0.0103*x)	0.4745	--	--
Nonlinear/normal	--	y=67.9*exp(-0.25*x)+34.6*exp(-0.0019*x)	0.975	5.8	653
Observed DT50/90	--	--	--	4-7	>358
[pyrazole-3-^{14}C]pyrasulfotole (AE 0317309)					
Linear/natural log[1]	255	y = -0.0027x + 3.7493	0.4028	--	--
Nonlinear/normal[1]	71.5	y=58.0*exp(-0.0097*x)	0.4084	--	--
Nonlinear/normal	--	y=70.8*exp(-0.23*x)+32.0*exp(-0.0013*x)	0.981	5.9	895
Observed DT50/90	--	--	--	4-7	>358
[^{14}C]pyrasulfotole (AE 0317309) – both radiolabels combined					
Linear/natural log[1]	240	y = -0.0029x + 3.7590	0.4428	--	--
Nonlinear/normal[1]	68.6	y=58.6*exp(-0.0101*x)	0.4409	--	--
Nonlinear/normal	--	y=69.0*exp(-0.24*x)+33.1*exp(-0.0016*x)	0.977	5.8	747
Observed DT50/90	--	--	--	4-7	>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 all extrapolated as observed DT90s were all >358 days; at final sampling interval, [14C]pyrasulfotole comprised 20.2-22.8% of the applied (Table 10, p. 72; Table 12, p. 74).

In sterile soil, observed DT50 values of [^{14}C]pyrasulfotole were >120 days (Table 14, p. 76).

TRANSFORMATION PRODUCTS: One major transformation product, 2-methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555), was identified in [phenyl-U-^{14}C]-label treated soil (pp. 55-56; Figure 5, p. 94; Figures 13-14, pp. 102-103). No minor products were identified for either label.

In [phenyl-U-^{14}C]-pyrasulfotole treated soil, AE B197555 was detected at a maximum 12.2% of the applied at 7 days, decreased to 5.4-5.6% at 14-21 days and was 4.2% at 358 days (Table 10, p. 72). Unidentified [^{14}C]residues were detected at a maximum 14.1% at 358 days, with the residues comprised of a single HPLC component (designated "largest single unknown") detected at ≤3.4% of the applied, an HPLC "region" of unresolved residues found via TLC to consist of at least twelve individual components each ≤1.4%, and the remaining a total of other minor HPLC

components (up to six to nine) detected at ≤4.9% (p. 54; Table 10, p. 72; Table 15, p. 77; Figures 16-17, pp. 105-106; DER Attachment 2).

In [pyrazole-3-^{14}C]-pyrasulfotole treated soil, unidentified [^{14}C]residues were detected at a maximum 13.8% at 259 days and were 13.3% at 358 days, with the residues comprised of a single HPLC component ("largest single unknown") detected at ≤3.9% of the applied, an HPLC "region" of unresolved residues found via TLC to consist of at least twelve individual components each ≤2.5%, and the remaining a total of other minor HPLC components (up to seven) detected at ≤4.4% (p. 54; Table 12, p. 74; Table 16, p. 78; Figures 16-17, pp. 105-106).

In sterile soil (both labels), AE B197555 was detected at a maximum 3.2% of the applied and unidentified [^{14}C]residues were ≤0.8% at any interval (Table 14, p. 76).

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: In [phenyl-U-^{14}C]-pyrasulfotole treated soil, extractable [^{14}C]residues decreased from 99.3% of the applied at day 0 to 50.5% at 21 days and were 37.1-38.5% at 259-358 days (Table 10, p. 72). Nonextractable [^{14}C]residues quickly increased from 1.7% at day 0 to 39.5% at 7 days, then gradually increased to 50.1% at 100 days and were 43.2% at 358 days. Acid extraction of 4- and 30-day extracted soil only released an additional 1.0-2.3% of the applied nonextractable [^{14}C]residues (p. 55; Table 21, p. 84). Organic matter fractionation of 4-, 30- and 259-day extracted soil found 3.4-4.4%, 15.0-27.4% and 9.0-14.8% of the applied associated with the humin, fulvic acids and humic acids, respectively (Table 21, p. 84).

In [pyrazole-3-^{14}C]-pyrasulfotole treated soil , extractable [^{14}C]residues decreased from 98.1% at day 0 to 50.9% at 7 days and were 35.4-36.2% at 259-358 days (Table 12, p. 74). Nonextractable [^{14}C]residues quickly increased from 1.9% at day 0 to 46.2% at 7 days, then were 47.5-49.7% at 10-259 days and 44.8% at 358 days. Acid extraction of 4- and 30-day extracted soil only released an additional 1.2-2.7% of the applied nonextractable [^{14}C]residues (p. 55; Table 21, p. 84). Organic matter fractionation of 4-, 30- and 259-day extracted soil found 4.6-5.7%, 12.5-21.9% and 15.0-19.8% of the applied associated with the humin, fulvic acids and humic acids, respectively (Table 21, p. 84).

In sterile soil (both labels), extractable and nonextractable [^{14}C]residues were 95.6-99.3% and 2.7-3.5% of the applied, respectively, at 120 days (Table 14, p. 76).

VOLATILIZATION: At study termination (358 days), volatilized $^{14}CO_2$ comprised 17.3% and 18.6% of the applied for the [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-label treated soils, respectively, while volatile [^{14}C]organic compounds were ≤0.4% (both labels) at any sampling interval (Table 10, p. 72; Table 12, p. 74). There appeared to be a short lag phase of *ca.* 4 days in $^{14}CO_2$ formation from the [phenyl-U-^{14}C]-label treated soil as compared to the [pyrazole-3-^{14}C]-label (p. 53). Barium chloride precipitation confirmed the presence of $^{14}CO_2$ in 358-day volatiles trap samples (both labels, >99.9% of sample radioactivity; p. 43).

For sterile soil (both labels), volatilized $^{14}CO_2$ and volatile [^{14}C]organic compounds were ≤0.2% at all sampling intervals (Table 14, p. 76).

TRANSFORMATION PATHWAY: The study author provided a transformation pathway that was consistent with the products detected in this study (p. 58; Figure 26, p. 115). 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 with the phenyl moiety only], plus numerous unidentified minor compounds, with rapid formation of bound soil residues and moderate levels of mineralization to CO_2 over time.

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	$C_9H_7F_3O_4S$	268.2	CS(=O)(=O)c1cc(C(F)(F)F)ccc1C(=O)O
		CAS:	Benzoic acid, 2-methylsulfonyl)-4-(trifluoromethyl)			

1 Identification confirmed using LC/MS/MS against reference standard (p. 56; Figure 5, p. 94; Figure 14, p. 103). Data obtained from Figure 1, p. 88 of the study report.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: Second dose experiments. At 80 days posttreatment, reserve, nonsterile, treated soil samples (one per label) received a second application, respective to label, of [phenyl-U-^{14}C]- or [pyrazole-3-^{14}C]-pyrasulfotole, then were incubated for 20 days and taken for analysis at 100 days post-initial treatment (p. 59). Results from analysis of the double-treated ("supplemental") soil samples were compared to the single-treated ("regular") 20-, 80- and 100-day samples. Following subtraction of "regular" 100-day soil results from the "supplemental" 100s-day results, parent [^{14}C]pyrasulfotole comprised 39.8-45.5% of the applied, AE B197555 was 9.9%, extractable and nonextractable [^{14}C]residues were 55.4-62.0% and 34.3-38.4%, respectively, and volatilized $^{14}CO_2$ totaled 4.2-6.3% (Table 18, pp. 80-81). These results are comparable to the "regular" 20-day soil samples indicating that the test soil still contained viable microbial populations when the second application occurred at 80 days post-initial treatment. The results also indirectly indicate that the distinct reduction in the dissipation rate of pyrasulfotole that occurred after 7 days posttreatment in the definitive study was not due to a lack of microbial viability.

Determination of adsorption of aged pyrasulfotole residues. Nonsterile, treated, reserve samples (one per label) were taken at 50 and 358 days posttreatment and analyzed for the distribution of parent pyrasulfotole between the aqueous phase (calcium chloride solution) and soil (acetonitrile:water plus reflux extracts). [^{14}C]Pyrasulfotole (both labels) comprised 8.1% and 15.3-17.6% of the applied in the aqueous phase and soil, respectively, at 50 days and was 1.8-2.2% and 17.6-18.2%, respectively, at 358 days (Table 19, p. 82). Calculated K_d values were 3.3-4.3 and 25.1-26.2 at 50 and 358 days, respectively, with corresponding K_{oc} values of 276-357 and 2,090-2,183, respectively. Based on the FAO classification scheme, the potential

mobility of pyrasulfotole in the loamy sand soil decreased from moderate mobility (K_{oc} 100-1,000) at 50 days posttreatment to slight mobility (K_{oc} 1,000-10,000) at 358 days. The study author proposed that the biphasic dissipation of pyrasulfotole may have been due to increased soil adsorption which reduced the availability of pyrasulfotole to microbial degradation (p. 59).

Increased soil moisture experiments. At 57 days posttreatment, the soil moisture of nonsterile, treated, reserve samples (one per label) was adjusted to 45% of maximum water holding capacity (16.8% soil moisture as compared to 6.8% soil moisture at 75% of 1/3 bar); an increase in soil moisture of *ca.* 2.5-fold (p. 60). The "moisture augmented" soil samples were taken and analyzed at 65 days posttreatment, with the results compared to the "regular" 65-day samples from the definitive study (Table 20, p. 83). There were no significant differences in the results between the "regular" and "moisture augmented" soil samples.

Storage stability. HPLC re-analysis found no significant quantitative differences in the chromatographic profiles of selected 0- to 50-day soil extracts after 266-345 days of frozen storage (p. 58; Table 22, p. 85).

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 23% of the parent still being present at 358 days, having declined very slowly from 7 days after treatment, where 40% was present.

2. The provided supplementary experiments (to investigate the bi-phasic decline of pyrasulfotole in the test soil and the degradation when a second dose of pyrasulfotole were added to aged soil) are not considered robust due to the low sample numbers per experiment. Two data points per experiment is not statistically significant to draw conclusions of chemical's fate and behaviour in a soil (such as Koc values). Therefore, the conclusions made about pyrasulfotole's mobility in soil are not reliable and very different from the other soil metabolism studies ([phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-AE 0317309: aerobic soil metabolism in a silt loam soil of US origin under laboratory conditions at 25°C, MRID 46801710).

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 12% AR), CO_2 (maximum of 18.6% AR), and non-extractable residues (maximum of 50.1%

AR), but adds to the conclusion that residues of pyrasulfotole were found up to 358 days (maximum of 22.8% AR).

4. In the second dose experiment, the study author concluded that "sampling and comparative analysis at day 100 (i.e. 20 days after second dosing) showed degradation of the additional dose to be similar to the degradation of the initial dose observed in the regular test system at day 21". The following comments are about this experiment:

The microbial biomass determination results indicated appropriate microbial soil activity at the start of the study (day 0) and at day 129 after application (23.9 and 22.2 mg biomass carbon per 100 g soil), however, at the end of the incubation period (day 365) a decrease of ~ 60% in soil microbial activity was observed (9.3 mg biomass carbon per 100 g soil).

The degradation of the second pyrasulfotole dose was similar to the degradation of the initial dose because biomass activity was similar to that of day 100. If the second dose was done when the microbial biomass began to decrease, the degradation rate might be very different than the observed in this experiment.

5. 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. 69-72; Table 12, p. 74; Tables 14-16, pp. 76-78) were verified by the primary reviewer and, with a few exceptions, there was consistent agreement (within ± 0.1% of applied) between the study author's reported values and those determined by the primary reviewer (DER Attachment 2). The only exception of note was the material balance for the [pyrazole-3-^{14}C]-label at 2 days posttreatment was reported as 100.0%, when the result is actually 100.9%; it appears 0.9% of applied as $^{14}CO_2$ was not included in the summation (Table 8, p. 70).

6. The test application rate of 0.14 mg a.i./kg used in this study was based on the highest proposed maximum seasonal field application rate of 100 g a.i./ha (0.089 lb a.i./acre; pp. 19, 21-22; Table 4, p. 66). 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).

7. 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.

8. Observed DT50 values for total residues.

Test substance	Parent +nonvolatile [^{14}C]products[1]	Total [^{14}C]residues[2]
[Phenyl-U-^{14}C]-pyrasulfotole	*ca.* 21 days	>358 days
[Pyrazole-3-^{14}C]-pyrasulfotole	7-10 days	>358 days

1 Parent pyrasulfotole plus identified/unidentified [^{14}C]transformation products.
2 All [^{14}C]residues other than volatilized $^{14}CO_2$.
Data obtained from DER Attachment 2.

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.

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: Structures of Parent Compound and Transformation Products

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

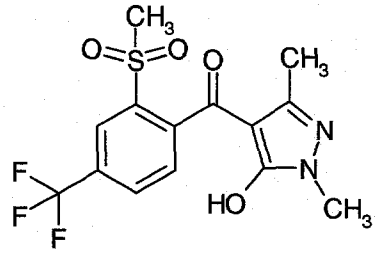
IUPAC Name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-*p*-tolyl)methanone.
(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

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].

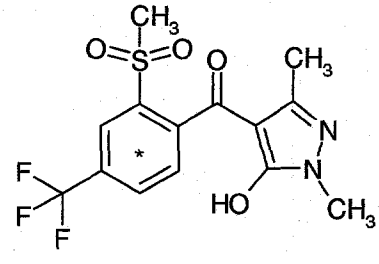
CAS Number: 365400-11-9.

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



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

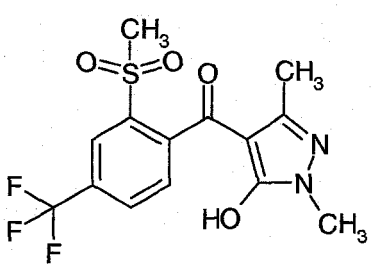


^{14}C = Position of radiolabel.

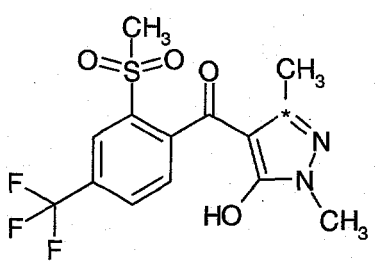
Pyrasulfotole [AE 0317309; K-1196; K-1267]

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-^{14}C]pyrasulfotole



^{14}C = Position of radiolabel.

Identified Compounds

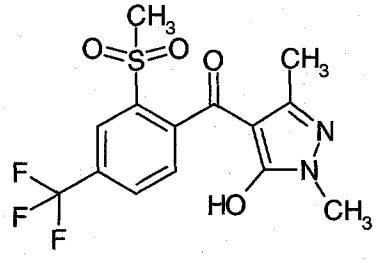
Pyrasulfotole [AE 0317309; K-1196; K-1267]

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].

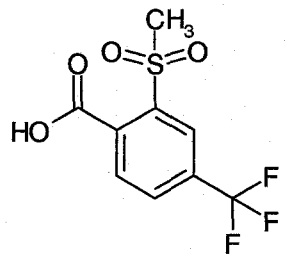
CAS Number: 365400-11-9.

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.



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

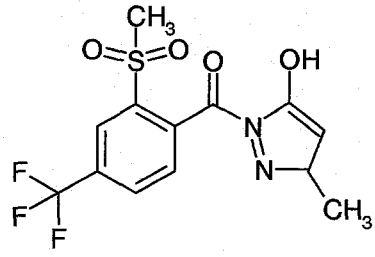
IUPAC Name: Not reported.
CAS Name: Not reported.
CAS Number: Not reported.

O=C=O

Unidentified Reference Compounds

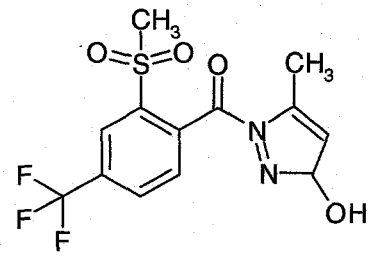
AE 1898321

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: 46801709
Guideline: 162-1

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

North Carolina loamy sand

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

Half-life (days)	67.3
R squared	0.4745

[Pyrazole-3-^{14}C]-label

Half-life (days)	71.5
R squared	0.4084

Both labels

Half-life (days)	68.6
R squared	0.4409

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801709
Guideline: 162-1

Aerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Determination of overall mean recoveries of radioactivity.
[Phenyl-U-^{14}C]-label/nonsterile

	Soil		Volatiles		Material	Study reported
	Total Ext	Nonext	CO_2	Organic vol.	balance	material balance
Day	% AR	% AR	% AR	% AR	% AR	% AR
0	99.3	1.7			101.0	101.0
2	88.2	12.6	0.1		100.9	100.8
4	71.6	28.8	0.1		100.5	100.5
7	61.3	39.5	0.9		101.7	101.7
10	56.1	42.6	2.7		101.4	101.3
14	52.8	44.7	4.0		101.5	101.5
21	50.5	46.9	6.0		103.4	103.3
30	46.6	48.0	7.4		102.0	102.0
39	44.8	49.0	8.5		102.3	102.3
50	41.5	49.3	9.5	0.1	100.4	100.4
65	41.8	47.7	11.9		101.4	101.5
80	40.3	47.3	11.8		99.4	99.4
100	39.6	50.1	12.1	0.4	102.2	102.1
120	38.5	49.5	14.2	0.1	102.3	102.4
168	39.5	47.9	14.7		102.1	102.2
259	37.1	47.4	16.2	0.1	100.8	100.9
358	38.5	43.2	17.3	0.2	99.2	99.2
				Mean	101.3	101.3
				std dev.	1.0	1.0
				maximum	103.4	103.3
				minimum	99.2	99.2
				n =	17	17

Results from Table 7, p. 69 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: 46801709
Guideline: 162-1

Aerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Determination of overall mean recoveries of radioactivity.
[Pyrazole-3-^{14}C]-label/nonsterile

	Soil		Volatiles		Material balance	Study reported material balance
	Total Ext	Nonext	CO_2	Organic vol.		
Day	% AR	% AR	% AR	% AR	% AR	% AR
0	98.1	1.9			100.0	99.9
2	85.8	14.2	0.9		100.9	100.0
4	64.0	34.0	2.0		100.0	100.1
7	50.9	46.2	3.9		101.0	101.0
10	49.0	47.5	5.1		101.6	101.6
14	47.4	48.2	6.1		101.7	101.7
21	45.9	49.6	7.4		102.9	102.9
30	44.2	49.2	8.5		101.9	101.8
39	39.8	48.2	9.6		97.6	97.5
50	41.2	49.0	10.2		100.4	100.5
65	40.5	48.5	12.7	0.2	101.9	101.9
80	40.2	47.8	12.6		100.6	100.6
100	38.4	48.6	13.3		100.3	100.3
120	38.6	49.7	14.3		102.6	102.6
168	36.4	49.7	15.6	0.1	101.8	101.9
259	35.4	48.2	17.2		100.8	100.8
358	36.2	44.8	18.6	0.3	99.9	99.9
				Mean	100.9	100.9
				std dev.	1.2	1.2
				maximum	102.9	102.9
				minimum	97.6	97.5
				n =	17	17
				Mean Phe+Pyr	101.1	101.1
				std dev.	1.1	1.2
				n =	34	34

Results from Table 8, p. 70 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: 46801709
Guideline: 162-1

Aerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Determination of overall mean recoveries of radioactivity.
[Phenyl-U-^{14}C]-label/sterile

	Soil		Volatiles		Material balance	Study reported material balance
	Total Ext	Nonext	CO_2	Organic vol.		
Day	% AR	% AR	% AR	% AR	% AR	% AR
4	99.1	0.7			99.8	99.9
10	101.9	1.0			102.9	102.9
21	102.3	1.4			103.7	103.8
65	100.0	2.1			102.1	102.1
120	99.3	2.7			102.0	102.0
				Mean	102.1	102.1
				std dev.	1.3	1.3
				Maximum	103.7	103.8
				Minimum	99.8	99.9
				n =	5	5

[Pyrazole-3-^{14}C]-label/nonsterile

	Soil		Volatiles		Material balance	Study reported material balance
	Total Ext	Nonext	CO_2	Organic vol.		
Day	% AR	% AR	% AR	% AR	% AR	% AR
4	100.3	0.9			101.2	101.2
10	99.9	1.2			101.1	101.1
21	100.3	2.0			102.3	102.3
65	96.1	3.0	0.2		99.3	99.4
120	95.6	3.5	0.2		99.3	99.4
				Mean	100.6	100.7
				std dev.	1.2	1.1
				Maximum	102.3	102.3
				Minimum	99.3	99.4
				n =	5	5
				Mean Phe+Pyr	101.4	101.4
				std dev.	1.4	1.4
				n =	10	10

Results from Table 9, p. 71 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: 46801709
Guideline: 162-1

Aerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil. Determination of total unidentified [^{14}C]residues following HPLC analysis.

Day	[Phenyl-U-14C]-label/nonsterile					
	Pyrasulfotole	AE B197555	Single Unk	"Region"	Others	Total Unided
	% AR	% AR	% AR	% AR	% AR	% AR
0	96.4	2.3	0.0	0.6	0.0	0.6
2	80.1	5.7	0.3	2.1	0.0	2.4
4	53.8	11.8	0.6	5.2	0.2	6.0
7	40.0	12.2	1.6	6.5	1.0	9.1
10	37.1	7.5	2.1	7.4	1.9	11.4
14	38.3	5.6	1.5	5.9	1.6	9.0
21	36.2	5.4	1.8	7.0	0.0	8.8
30	35.2	3.3	0.7	6.6	0.8	8.1
39	32.4	3.2	1.0	7.1	1.0	9.1
50	28.7	1.9	2.1	7.7	1.2	11.0
65	26.7	2.5	2.2	7.8	2.7	12.7
80	26.2	1.9	2.1	7.4	2.9	12.4
100	25.1	2.9	3.3	6.3	2.0	11.6
120	23.8	2.7	3.4	5.5	3.2	12.1
168	23.0	3.2	3.4	6.5	3.5	13.4
259	21.0	3.5	3.4	6.1	3.0	12.5
358	20.2	4.2	3.3	5.9	4.8	14.0

Day	[Pyrazole-3-14C]-label/nonsterile				
	Pyrasulfotole	Single Unk	"Region"	Others	Total Unided
	% AR	% AR	% AR	% AR	% AR
0	97.4	0.6	0.0	0.0	0.6
2	82.1	0.6	2.7	0.4	3.7
4	54.8	1.4	7.7	0.0	9.1
7	40.7	1.6	7.9	0.8	10.3
10	36.3	1.8	8.0	2.7	12.5
14	36.7	1.4	7.0	2.3	10.7
21	33.4	1.5	7.4	3.5	12.4
30	32.0	1.4	7.2	3.5	12.1
39	29.3	1.2	6.6	2.7	10.5
50	29.9	2.5	6.0	2.7	11.2
65	27.8	2.4	6.8	3.6	12.8
80	27.2	2.1	6.6	4.2	12.9
100	26.3	3.3	4.9	3.9	12.1
120	25.4	3.4	5.4	4.4	13.2
168	23.5	3.4	5.1	4.4	12.9
259	21.6	3.9	5.6	4.3	13.8
358	22.9	3.7	5.4	4.3	13.4

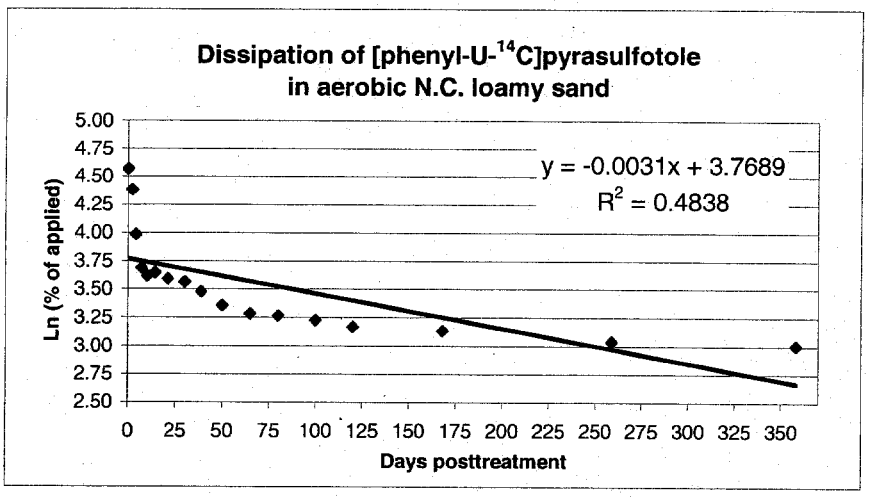
Results from Tables 15-16, pp. 77-78 of the study report.

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801709
Guideline: 162-1

Aerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Half-life determination
[Phenyl-U-^{14}C]-label/nonsterile
Half-life (days) 226 (0- to 358-day data)

Days Posttreatment	Pyrasulfotole (% of Applied)	Ln (% applied)
0	96.4	4.568506202
2	80.1	4.383275854
4	53.8	3.985273467
7	40.0	3.688879454
10	37.2	3.616308761
14	38.3	3.645449896
21	36.2	3.589059119
30	35.3	3.563882964
39	32.4	3.478158423
50	28.7	3.356897123
65	26.7	3.284663565
80	26.2	3.265759411
100	25.2	3.226843995
120	23.8	3.169685581
168	23.0	3.135494216
259	20.9	3.039749159
358	20.2	3.005682604

Data obtained from Table 10, p. 72 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.695551676
R Square	0.483792133
Adjusted R Square	0.449378276
Standard Error	0.32766435
Observations	17

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	1.509328696	1.5093	14.05806163	0.0019333
Residual	15	1.610458899	0.1074		
Total	16	3.119787595			

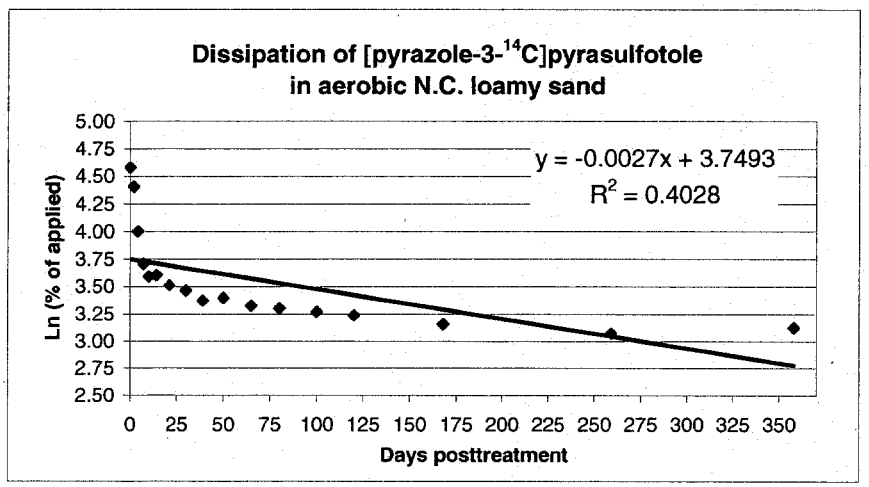
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.76889338	0.101921472	36.978	3.75558E-16	3.5516528	3.986134	3.551652772	3.98613399
X Variable 1	-0.003065273	0.000817535	-3.749	0.001933292	-0.004808	-0.0013227	-0.00480781	-0.00132274

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801709
Guideline: 162-1

Aerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Half-life determination
[Pyrazole-3-^{14}C]-label/nonsterile
Half-life (days) 255 (0- to 358-day data)

	Pyrasulfotole	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	97.5	4.579852378
2	82.1	4.407938016
4	54.8	4.003690194
7	40.7	3.706228092
10	36.3	3.591817741
14	36.7	3.602776755
21	33.5	3.511545439
30	32.0	3.465735903
39	29.2	3.374168709
50	29.9	3.39785848
65	27.8	3.325036021
80	27.2	3.303216973
100	26.3	3.269568939
120	25.5	3.238678452
168	23.5	3.157000421
259	21.6	3.072693315
358	22.8	3.126760536

Data obtained from Table 12, p. 74 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.634655846
R Square	0.402788043
Adjusted R Square	0.362973913
Standard Error	0.342120284
Observations	17

ANOVA

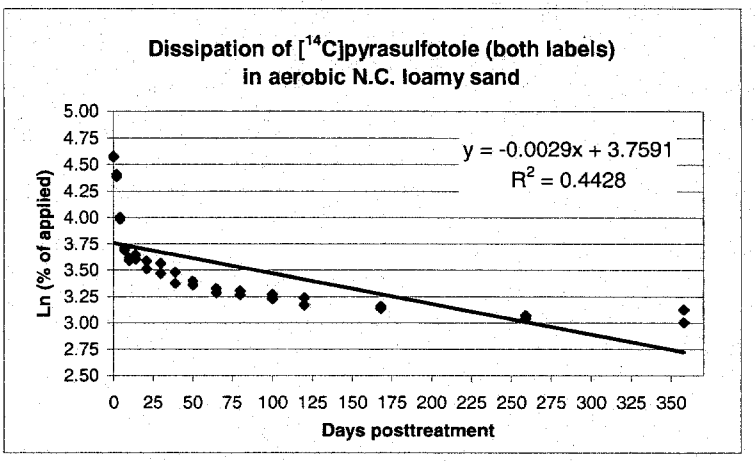
	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	1.184123453	1.1841	10.1167108	0.0062045
Residual	15	1.75569433	0.117		
Total	16	2.939817783			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.74926004	0.106418055	35.231	7.70134E-16	3.5224352	3.9760849	3.522435186	3.97608489
X Variable 1	-0.002715037	0.000853603	-3.181	0.00620446	-0.004534	-0.0008956	-0.00453445	-0.00089562

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801709
Guideline: 162-1

Aerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Half-life determination
[Phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-labels/nonsterile
Half-life (days) 240 (0- to 358-day data)

	Pyrasulfotole	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	96.4	4.568506202
0	97.5	4.579852378
2	80.1	4.383275854
2	82.1	4.407938016
4	53.8	3.985273467
4	54.8	4.003690194
7	40.0	3.688879454
7	40.7	3.706228092
10	37.2	3.616308761
10	36.3	3.591817741
14	38.3	3.645449896
14	36.7	3.602776755
21	36.2	3.589059119
21	33.5	3.511545439
30	35.3	3.563882964
30	32.0	3.465735903
39	32.4	3.478158423
39	29.2	3.374168709
50	28.7	3.356897123
50	29.9	3.39785848
65	26.7	3.284663565
65	27.8	3.325036021
80	26.2	3.265759411
80	27.2	3.303216973
100	25.2	3.226843995
100	26.3	3.269568939
120	23.8	3.169685581
120	25.5	3.238678452
168	23.0	3.135494216
168	23.5	3.157000421
259	20.9	3.039749159
259	21.6	3.072693315
358	20.2	3.005682604
358	22.8	3.126760536



Data obtained from Table 10, p. 72; Table 12, p. 74 of the study report.

SUMMARY OUTPUT

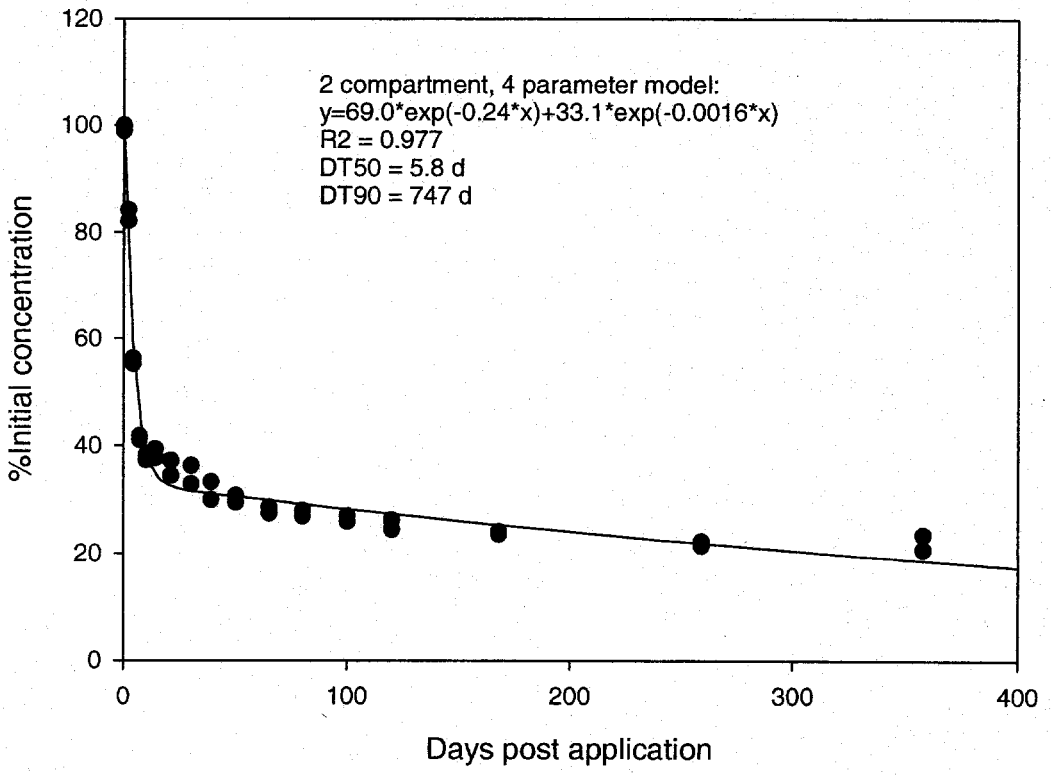
Regression Statistics	
Multiple R	0.665454894
R Square	0.442830215
Adjusted R Square	0.42541866
Standard Error	0.324832179
Observations	34

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	2.683599856	2.6836	25.43312163	1.753E-05
Residual	32	3.376510231	0.1055		
Total	33	6.060110087			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.75907671	0.071446431	52.614	1.19024E-32	3.6135452	3.9046082	3.613545215	3.9046082
X Variable 1	-0.002890155	0.000573088	-5.043	1.75302E-05	-0.004057	-0.0017228	-0.0040575	-0.00172281

[^{14}C]Pyrasulfotole dissipation in aerobic N.C. loamy sand (combined radiolabels): nonlinear regression (MRID 46801709, Sub. No. 2006-2445)



[Pyrazole-U-^{14}C]pyrasulfotole in aerobic N.C. loamy sand: nonlinear regression (MRID 46801709, Sub. No. 2006-2445)