Data Evaluation Repot on the photolysis of pyrasulfotole (AE 0317309) on soil

PMRA Submission Number 2006-2445 EPA MRID Number 46801707

Data Requirement: PMRA Data Code: 8.2.3.3.1
EPA DP Barcode: D328639
OECD Data Point:
EPA Guideline: 161-3

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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CITATION: Arthur, E.L., J. Shepherd, and A.R. Dominic. 2004. [Pyrazole-3-^{14}C] AE0317309: phototransformation on soil. Unpublished study performed by Bayer CropScience, Stilwell, KS, and sponsored and submitted by Bayer CropScience, Research Triangle Park, NC. Bayer Study No.: A9082101. Bayer Report No.: 200638. Experiment started May 6, 2003, and completed September 9, 2003 (p. 6). Final report issued April 5, 2004.

EXECUTIVE SUMMARY

The phototransformation of [pyrazole-3-^{14}C]-labeled (5-hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-*p*-tolyl)methanone (pyrasulfotole, AE 0317309; radiochemical purity 100.0%), at 0.51 mg/kg (equivalent to 75 g a.i./ha), was studied on silt loam soil [pH 7.4, organic matter 7.1%] from North Dakota that was irradiated continuously using a UV-filtered xenon lamp for 9 days at 25 ± 0.1°C. The intensity of the lamp was 680 W/m^2, and 7.0 hours of irradiation with the artificial light was reported to be equivalent to 1 solar day in late June in Phoenix, Arizona. This experiment was conducted in accordance with USEPA Subdivision N §161-3 guidelines and in compliance with USEPA GLP standards. The test system consisted of quartz glass jar-like vessels (4 cm diameter x 3 cm height) containing treated moistened soil (3 g dry weight) that were covered with quartz glass plates and placed on a cooling tray within the irradiation apparatus. Samples serving as dark controls were wrapped in aluminum foil and maintained in a darkened incubator. Volatiles were not collected. Duplicate irradiated and dark control samples were collected at 0, 1, 3, 6 and 9 days posttreatment. The soil samples were extracted two times with methanol:water (8:2, v:v) and methanol:water (7:3, v:v) using an accelerated solvent extractor (ASE), extractions were done under pressure (1,500 psi) at 100°C. The extracts were analyzed for total radioactivity using LSC, and portions of the extracted soil were analyzed for unextracted residues using LSC following combustion. The extracts were analyzed for specific [^{14}C]compounds using HPLC. Pyrasulfotole was identified by comparison to the HPLC retention time of the test substance and by LC/EIS-MS. There was no attempt to identify transformation products.

The temperature of the irradiation chamber and dark incubator averaged 25.3 ± 0.1°C; no supporting data were provided. Soil moisture was maintained at 75% of 1/3 bar. The soil was viable at study start; viability was not determined at any other interval.

Overall [^{14}C]residue recoveries averaged 99.2 ± 4.7% (range 91.6-106.9%) of the applied in the irradiated samples and 100.4 ± 4.1% (range 91.9-106.9%) in the dark controls. Recoveries were significantly higher (average 106.4% of the applied) at time 0 than at 1 through 9 days posttreatment in both the irradiated and dark controls; there was no pattern of loss of material from the samples between 1 and 9 days.

[^{14}C]Pyrasulfotole decreased from an average of 104.2% of the applied at time 0 to 87.2% in the irradiated samples and 89.9% in the dark controls at study termination (9 days posttreatment). Concentrations were variable and were affected by overall recoveries of [^{14}C]residues; [^{14}C]pyrasulfotole comprised 97.9% of the recovered at time 0 and 90.0% and 93.6% in the irradiated and dark controls, respectively, at 9 days posttreatment. No major transformation products were isolated from either the irradiated or dark control soils. No minor transformation products, which averaged ≤1.0% of the applied, were identified in either the irradiated or dark control soils. Extractable [^{14}C]residues decreased from an average of 104.2% of the applied at time 0 to 88.2% in the irradiated samples and 90.5% in the dark controls at 9 days posttreatment. Nonextractable [^{14}C]residues increased from 2.2% of the applied at time 0 to 8.6% in the irradiated samples and 5.5% in the dark controls. Volatiles were not collected.

Based on first order linear regression analysis (Excel 2000), pyrasulfotole dissipated with half-lives of 32.5 days in the irradiated samples (continuous irradiation) and 64.2 days in the dark controls. The half-lives are of uncertain value because they are extrapolated well beyond the duration of the study, between replicate variability at some intervals is *ca.* 5% of the applied, and the calculations are based on the assumption that degradation follows a linear pattern. The **phototransformation half-life** for pyrasulfotole, determined using the equation

(Ln 2) ÷ [(Ln 2/dark control half-life) - (Ln 2/irradiated half-life)],

was 66 days based on the continuous irradiation used in the study. The study author stated that 7.0 hours of continuous irradiation with the artificial light was equivalent to 1 day of natural sunlight in Phoenix, Arizona (33.26° N latitude) and that 5.21 hours of continuous irradiation was equivalent to 1 day of natural sunlight in Edmonton, Alberta (53.33°N latitude). Therefore, the **environmental phototransformation half-life** is expected to be *ca.* 227 days in Phoenix, AZ and *ca.* 304 days in Edmonton, AB.

A transformation pathway was not proposed by the study author. A transformation pathway could not be developed because pyrasulfotole was relatively stable to photolysis under the conditions of this study.

In a supplementary study using a low organic loamy sand soil [pH 4.6, organic carbon 1.2%] from North Carolina, [^{14}C]pyrasulfotole decreased from an average 99.3% of the applied at time 0 to 80.6% in the irradiated samples and 92.1% in the dark controls at 9 days posttreatment. No major transformation products were isolated and no minor transformation products were identified. Based on three sampling intervals, the study author estimated an environmental phototransformation half-life of 173 solar days for the Phoenix location. Therefore, photolysis on soil surfaces does not appear to be a significant transformation pathway for AE 0317309 in soils with either low or high organic content.

Results Synopsis

Loamy sand	Half-life (days)	Transformation products	
		Major	**Minor**
Irradiated	32.5	None.	---
Dark	64.2	None.	---
Environmental phototransformation half-life: *ca.* 227 days at Phoenix, AZ (33.26°N latitude), or *ca.* 304 days at Edmonton, AB (53.33°N latitude).			

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 the USEPA Pesticide Assessment Guidelines, Subdivision N §161-3 and PMRA DACO Number 8.2.3.3.1 (pp. 1, 15).

COMPLIANCE: This study was conducted in compliance with USEPA FIFRA GLP Standards (40 CFR Part 160; p. 3). Signed and dated Data Confidentiality, GLP, Quality Assurance, and Certificate of Authenticity statements were provided (pp. 2-5).

A. MATERIALS:

1. Test Material [Pyrazole-3-^{14}C]pyrasulfotole (p. 16).

Chemical Structure: See DER Attachment 1.

Description: Technical grade (p. 16).

Purity: Radiochemical purity: 100.0% (p. 16, Figure 1, p. 41).
Vial No.: C-930.
Analytical purity: Not reported.
Specific activity: 54.2 mCi/mMole.
Location of the radiolabel: Labeled on the 3-carbon of the pyrazole ring.

Storage conditions of test chemicals: The test substance was stored frozen in acetonitrile (p. 16).

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: Field information and handling procedures.

Information	Details
Geographic location	Grand Forks, North Dakota. (Latitude N 47° 42.619, Longitude W 097° 35.831)
Pesticide use history at the collection site	None.
Collection procedures	Collected from a wooded area adjacent to a field. The soil was thawed and collected using a spade and placed in 5 gallon buckets. The buckets were then sealed.
Sampling depth (cm)	0-15
Storage conditions	Stored under alfalfa cover in a greenhouse.
Storage length	73 days.
Soil preparation	Soil was air dried and the cover vegetation was removed followed by sieving (2 mm). Soil was acclimated to study temperature prior to use.

Data obtained from p. 17, Table 2, p. 34 and Appendix 2, p. 63 in the study report.

Table 2: Properties of the soil.

Property	Details
Soil texture	Silt loam
% Sand	19
% Silt	62
% Clay	19
pH ($CaCl_2$)	7.4
Organic carbon (%)	4.1
Organic matter (%)	7.1
CEC (meq/100g)	26.0
Moisture at 1/3 bar (%)	46.2
Bulk density (g/cm^3)	0.90
Biomass (mg microbial C/kg)	1397
Soil taxonomic classification	Fine-silty, mixed Cumulic Udic Haploborolls.
Sol mapping unit (for EPA)	Unit 46

Data were obtained from Table 2, p. 34 in the study report.

3. Details of light source

Table 3: Artificial light source

Property	Details
Nature of light source	Xenon arc lamp (Heraeus, Atlas Suntest unit)
Emission wavelength spectrum	290-750 W/m^2.
Light intensity	680 W/m^2.
Filters used	Suprax filter.
Relationship to natural sunlight	The wavelength distribution of the artificial light was comparable to that of natural sunlight. Based on the intensity of the lamp, 7.0 hours of artificial light were reported to be equivalent to 1 day of summer sunlight (June 23, 1988) in New River near Phoenix, Arizona (33.26 N). A comparison of the artificial light to sunlight is presented in Figure 5, p. 47.

Data obtained from p. 18, and Figures 4- 5, pp. 46-47 in the study report.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary Study: A preliminary study (not described) determined that volatiles would not be generated (p. 19). Therefore, a volatile trapping system was not used in this study.

2. Experimental Conditions

Table 4: Experimental Parameters

Parameters		Pyrasulfotole
Duration of the study		9 days.
Test concentrations (mg a.i./kg) Nominal: Measured:		 Not reported. 0.51, equivalent to 75 g a.i./ha
Dark controls used (Yes/No)		Yes.
Replication	Dark	Two samples were collected at each interval.
	Irradiated	Two samples were collected at each interval.
Co-solvent, if any:		Acetonitrile.
Application	Volume used/treatment:	140 µL of 10.98 µg a.i./mL in 3 g soil (dry wt equivalent).
	Method of application:	The solution was applied uniformly over the soil surface using a Hamilton syringe.
	Is the co-solvent evaporated?	Yes.
Test apparatus (Type/Material/Volume)		Quartz glass jar-like vessels (4 cm diameter x 3 cm height) containing treated moistened soil (3 g dry weight, 3-5 mm depth) were covered with quartz glass plates. A side-arm in each vessel was sealed with a ground glass stopper. Samples to be irradiated were placed on a cooling plate within the irradiation apparatus. Samples serving as dark controls were wrapped in aluminum foil and maintained in an incubator.
Details of traps for volatile compounds, if any		Volatiles were not collected.
If no traps were used, is the test system closed/open		Closed.
Is there any indication of the test material adsorbing to the walls of the test apparatus?		No.
Experimental Conditions Temperature; Duration of light/darkness: Moisture content: Moisture maintenance method		 25 ± 0.1°C Continuous. 75% of 1/3 bar. Samples were weighed at each sampling interval.
Other details, if any		None.

Data obtained from pp. 19-21, Table 3, p. 35, and Figures 2-3, pp. 44-45, in the study report.

3. Supplementary experiments: To ensure adequate concentrations for identification of transformation products, three additional samples were treated at a rate 10x that used in the definitive study and incubated as described (p. 20).

In order to determine if the rate of degradation was correlated with soil organic matter content, an additional photodegradation in soil study was conducted using a loamy sand soil [pH 4.6, organic carbon 1.2%] from North Carolina (p. 30, Appendix 13, pp. 81-83). The description of the study methods was very brief, and it could not be determined if the study design was identical to that used in the definitive study. The soil was treated at a rate of 75 g a.i./ha and irradiated continuously using a UV-filtered xenon lamp (intensity 680 W/m^2) for up to 216 hours.

4. Sampling:

Table 5: Sampling details

Observations		Details
Sampling intervals for the parent/transformation products	Irradiated	0, 1, 3, 6, and 9 days.
	Dark	0, 1, 3, 6, and 9 days.
Sampling method		Duplicate vessels were collected from the irradiated and dark controls at each intervals.
Method of sampling volatile compounds, if any		Volatiles were not collected.
Sampling intervals/times for: Sterility check Moisture content		The soil samples were not sterile. Samples were weighed at each sampling interval and remoistened if necessary.
Sample storage before analysis, if any		Soil was extracted on the day of collection and analyzed within 24 hours of extraction. Soil extracts were stored frozen (*ca.* -24°C) when not in use.
Other observation, if any:		None.

Data obtained from pp. 21, 27 and Table 4, p. 36 in the study report.

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods: The soil was transferred to an Accelerated Solvent Extractor (ASE) cell (11 mL volume) and extracted once with methanol:water (8:2, v:v) and once with methanol:water (7:3, v:v); each extraction was done at 100°C and 1500 psi pressure (pp. 22-23, Figure 6, p. 48). The extracts were combined, and aliquots (3 x 0.1 mL) were analyzed using LSC. The extracts were then transferred to a boiling flask (250-300 mL) and concentrated to 4-11 mL using rotary evaporation at 39°C. Half of the concentrate was stored frozen, the remainder was transferred to pear-shaped flasks (50 mL) and further concentrated by rotary evaporation as described until almost dry (1-2 mL). The resulting residues were diluted with methanol and analyzed using LSC and HPLC.

Nonextractable residue determination: The extracted soils were air-dried and portions were analyzed for nonextractable [^{14}C]residues using LSC following combustion (p. 23).

Volatile residue determination: Volatiles were not collected.

Total ^{14}C measurement: Total [^{14}C]residues were determined by summing the concentrations of [^{14}C]residues measured in the soil extracts and the extracted soil (p. 25).

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

Identification and quantification of parent compound: Aliquots of the sample extracts were analyzed for pyrasulfotole using HPLC under the following conditions (p. 23): Phenomenex Columbus C8 column (150 x 4.6 mm, 5 Φm), gradient mobile phase consisting of (A) 0.1% TFA in water and (B) methanol [percent A:B (v:v), 0-5 minutes 90:10; 20:25 minutes, 0:100, 35 minutes, 90:10]; flow rate 1.5 mL/minute; and UV (254 nm) and radioactive flow detection. [^{14}C]Pyrasulfotole was identified by comparison to the HPLC retention time of the test substance (Rt 18.0 minutes; p. 15; Figures 7-8; pp. 49-51). HPLC recoveries (0- and 3-day samples) ranged from 101-116% of the injected sample (p. 27).

The identification of pyrasulfotole was confirmed using LC/ESI/MS in the negative mode (p. 24; Figure 2, p. 43; Figure 9, p. 52)

Identification and quantification of transformation products: Transformation products were separated and quantified as described above. No attempt was made to identify transformation products (p. 29).

Detection limits (LOD, LOQ) for the parent: For the HPLC radiodetector, the Limit of Quantitation was 300 dpm or 1.0% of the applied (p. 26). For LSC, the Limit of Detection was 0.124% of the applied for the soil extracts and 0.05% for the combusted soil (Appendices 6-7, pp. 73-74).

Detection limits (LOD, LOQ) for the transformation: The LOD and LOQs for transformation products were the same as for the parent.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The temperature of the irradiation chamber and dark incubator averaged 25.3 ± 0.1°C; no supporting data were provided (p. 27). Soil moisture was maintained at 75% of 1/3 bar. The soil was viable at study start; viability was not determined at any other interval.

B. MASS BALANCE: Overall [^{14}C]residue recoveries averaged 99.2 ± 4.7% (range 91.6-106.9%) of the applied in the irradiated samples and 100.4 ± 4.1% (range 91.9-106.9%) in the dark controls (Tables 5-6, pp. 37-38). Recoveries were significantly higher (average 106.4% of the applied) at time 0 than at 1 through 9 days posttreatment in both the irradiated and dark controls; there was no pattern of loss of material from the samples between 1 and 9 days.

Table 6: Phototransformation of [^{14}C]pyrasulfotole, expressed as percentage of the applied radioactivity (mean ± s.d., n = 2), on silt loam soil.

Compound		Sampling times (days)				
		0	1	3	6	9
Pyrasulfotole	Irradiated	104.2 ± 0.5	96.3 ± 5.4	90.6 ± 1.2	86.6 ± 4.6	87.2 ± 0.8
	Dark		93.2 ± 0.2	95.8 ± 2.0	95.3 ± 3.1	89.9 ± 4.5
Unknown A	Irradiated	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	1.0 ± 0.1	2.1, 0.0
	Dark		0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0
Unknown B	Irradiated	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0
	Dark		0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0, 1.1
Extractable residues	Irradiated	104.2 ± 0.5	96.3 ± 5.4	90.6 ± 1.2	87.6 ± 4.7	88.2 ± 2.3
	Dark		93.2 ± 0.2	95.8 ± 2.0	95.3 ± 3.1	90.5 ± 5.3
Nonextractable residues	Irradiated	2.2 ± 0.1	4.8 ± 0.2	6.5 ± 0.2	7.1 ± 0.4	8.6 ± 0.9
	Dark		4.1 ± 0.3	5.1 ± 0.3	6.2 ± 0.2	5.5 ± 0.6
CO_2	Irradiated	Volatiles were not collected.				
	Dark					
Volatile organics	Irradiated	Volatiles were not collected.				
	Dark					
Total recovery	Irradiated	106.4 ± 0.6	101.1 ± 5.6	97.1 ± 1.4	94.7 ± 4.4	96.8 ± 1.4
	Dark		97.2 ± 0.1	100.9 ± 1.7	101.5 ± 3.2	96.0 ± 5.9

Data obtained from Table 7, p. 39 and Appendices 8-9, pp. 75-76 in the study report. Means and standard deviations were calculated by the study authors.

C. TRANSFORMATION OF PARENT COMPOUND: [^{14}C]Pyrasulfotole decreased from an average of 104.2% of the applied at time 0 to 87.2% in the irradiated samples and 89.9% in the dark controls at study termination (9 days posttreatment; Table 7, p. 39; Appendices 8-9, pp. 75-76). Concentrations were variable and were affected by overall recoveries of [^{14}C]residues; [^{14}C]pyrasulfotole comprised 97.9% of the recovered at time 0 and 90.0% and 93.6% in the irradiated and dark controls, respectively, at 9 days posttreatment.

HALF-LIFE/DT50/DT90: Based on first order linear regression analysis (Excel 2000), pyrasulfotole dissipated with half-lives of 32.5 days in the irradiated samples (continuous irradiation) and 64.2 days in the dark controls (DER Attachment 2). The half-lives are of uncertain value because they are extrapolated well beyond the duration of the study, replicate variability at some intervals is *ca.* 5% of the applied, and the calculations are based on the assumption that degradation follows a linear pattern.

Half-lives/DT50/DT90

Treatment	First order linear			DT50[1] (days)	DT90[1] (days)
	Half-life (days)	Regression equation	r^2		
Irradiated	32.5	y = -0.0213x + 4.6602	0.8762	90	1,027
Dark	64.2	y = -0.0108x + 4.6008	0.4513	---	---

Calculated by the reviewer using data obtained from Appendices 8-9, pp. 75-76 in the study report (DER Attachment 2).

1 Phototransformation DT values based on the least-squared line of best fit calculated by the study author using averaged data and GraphPad PRISM software (pp. 25-26, 29; Figure 16, p. 59).

The **phototransformation half-life** for pyrasulfotole, determined using the equation

(Ln 2) ÷ [(Ln 2/dark control half-life) - (Ln 2/irradiated half-life)],

was 66 days based on the continuous irradiation used in the study. The study author stated that 7.0 hours of continuous irradiation with the artificial light was equivalent to 1 day of natural sunlight in Phoenix, Arizona (33.26° N latitude; p. 18; Appendix 3, p. 64). Therefore, the **environmental phototransformation half-life** is expected to be *ca.* 227 days. Assuming that 5.21 hours of continuous irradiation with the artificial light was equivalent to 1 day of natural light in Edmonton, Alberta (53.33°N latitude; Appendix 3, p. 64), the environmental phototransformation half-life is expected to be ~304 days for this representative Canadian use area.

TRANSFORMATION PRODUCTS: No major transformation products were isolated from either the irradiated or dark control soils (Table 7, p. 39). No minor transformation products were identified in either the irradiated or dark control soils. Two unidentified HPLC peaks ("Unknown A" and "Unknown B") were isolated at average concentrations of ≤1.0% of the applied (Appendices 8-9, pp. 75-76).

Table 7: Chemical names and CAS numbers for the transformation products of pyrasulfotole.

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	MW (g/mol)	Smiles String
No transformation products were identified.					

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: Extractable [^{14}C]residues decreased from an average of 104.2% of the applied at time 0 to 88.2% in the irradiated samples and 90.5% in the dark controls at 9 days posttreatment (Table 7, p. 39). Nonextractable [^{14}C]residues increased from 2.2% of the applied at time 0 to 8.6% in the irradiated samples and 5.5% in the dark controls.

VOLATIZATION: Volatiles were not collected.

TRANSFORMATION PATHWAY: A transformation pathway was not proposed by the study author. A transformation pathway could not be developed because pyrasulfotole was relatively stable to photolysis under the conditions of this study.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: Results from the analysis of the high dose samples is incorporated into the discussion of the definitive experiment.

In the low organic soil, overall [^{14}C]residue recoveries averaged 95.2 ± 4.7% (decreasing from 99.2% to 90.0%) from the irradiated soil and 97.9 ± 1.1% (range 97.1-99.2%) from the dark controls (Appendix 13, pp. 81-82). [^{14}C]Pyrasulfotole decreased from an average 99.3% of the applied at time 0 to 80.6% in the irradiated samples and 92.1% in the dark controls at 9 days posttreatment. No major transformation products were isolated and no minor transformation products were identified. The study author estimated a phototransformation DT50 of 173 solar days.

Table 8: Phototransformation of [^{14}C]pyrasulfotole, expressed as percentage of the applied radioactivity (n = 1 or 2), on loamy sand soil.

Compound		**Sampling times (days)**		
		0	5	9
Pyrasulfotole	Irradiated	99.3	88.8	80.6
	Dark		91.8	92.1
Unknown A	Irradiated	0.0, 1.2	1.7	1.2
	Dark		0.6	0.5
Unknown B	Irradiated	0.0	1.7	0.0
	Dark		2.5	2.0
Extractable residues	Irradiated	98.4	92.2	81.8
	Dark		94.9	94.6
Nonextractable residues	Irradiated	0.8	4.2	8.2
	Dark		2.6	2.4
CO_2	Irradiated	Volatiles were not collected.		
	Dark			
Volatile organics	Irradiated	Volatiles were not collected.		
	Dark			
Total recovery	Irradiated	99.2	96.4	90.0
	Dark		97.5	97.1

Data obtained from Appendix 13, Tables 2-3, pp. 84-85 in the study report. Means, when n = 2, calculated by the study author.

III. STUDY DEFICIENCIES

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

IV. REVIEWER'S COMMENTS

1. The reviewers agree with the conclusions made by the study author that AE 0317309 was not readily photodegraded in the study, and no major transformation products were formed in the study.
2. The wavelength distribution of the artificial light was comparable to that of natural sunlight. Based on the intensity of the lamp, 7.0 hours of artificial light were reported to be equivalent to 1 day of summer sunlight (June 23, 1988) in New River near Phoenix, Arizona (33.26 N). Therefore, 9 experimental days is equivalent to 30.0 environmental days.
3. The Retention Time of Unknown A is less than 2 minutes and expresses as a broad peak, which suggests that it may be actually be a mixture of polar compounds (Figure 13, p. 56).
4. Although reference compounds were identified (Figure 1, pp. 41-42), it was stated that "reference standards were not utilized because no significant degradation was observed…" (p. 16).
5. The time 0 sample extracts were reanalyzed after 30 days of frozen storage (p. 21). Pyrasulfotole was stable during storage (Figure 17, p. 60).

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 161-3. Photolysis studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.

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

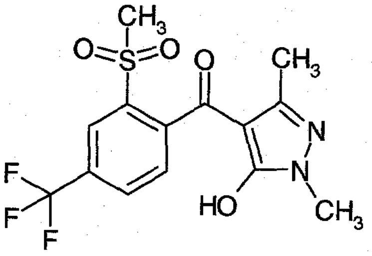
3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

Attachment 1: Structures of Parent Compound and Transformation Products

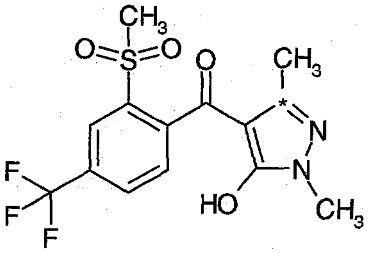
Pyrasulfotole [AE 0317309; K-1196; K-1267]

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



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

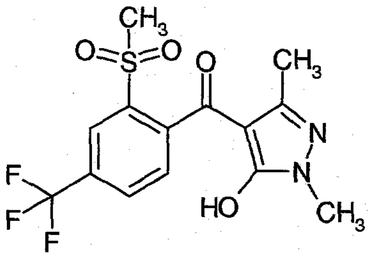


^{14}C = Position of radiolabel.

Identified Compounds

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

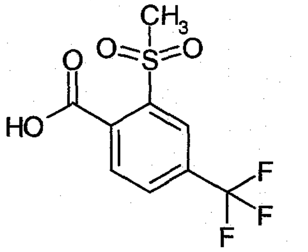
IUPAC Name:	(5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-*p*-tolyl)methanone. (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.
CAS Name:	(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl)-4(trifluoromethyl)phenyl]methanone. Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)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.



Unidentified Reference Compounds

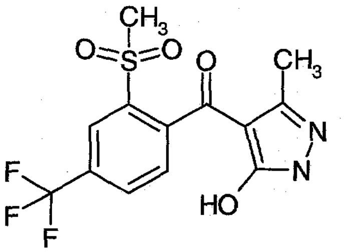
RPA 203328 [AE B197555-benzoic acid; AE B197555; K-1198; K-1367]

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.



AE 1073910 [AE 0317309 N-Desmethyl; K-1385; K-1197]

IUPAC Name: (5-Hydroxy-3-methyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methanone.
CAS Name: Methanone, (5-hydroxy-3-methyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].
CAS Number: Not reported.
SMILES String: O=C(C2=C(O)NN=C2C)C1=C(S(=O)(C)=O)C=C(C(F)(F)F)C=C1.
CS(=O)(=O)c1cc(ccc1C(=O)c1c([nH]nc1C)O)C(F)(F)F.



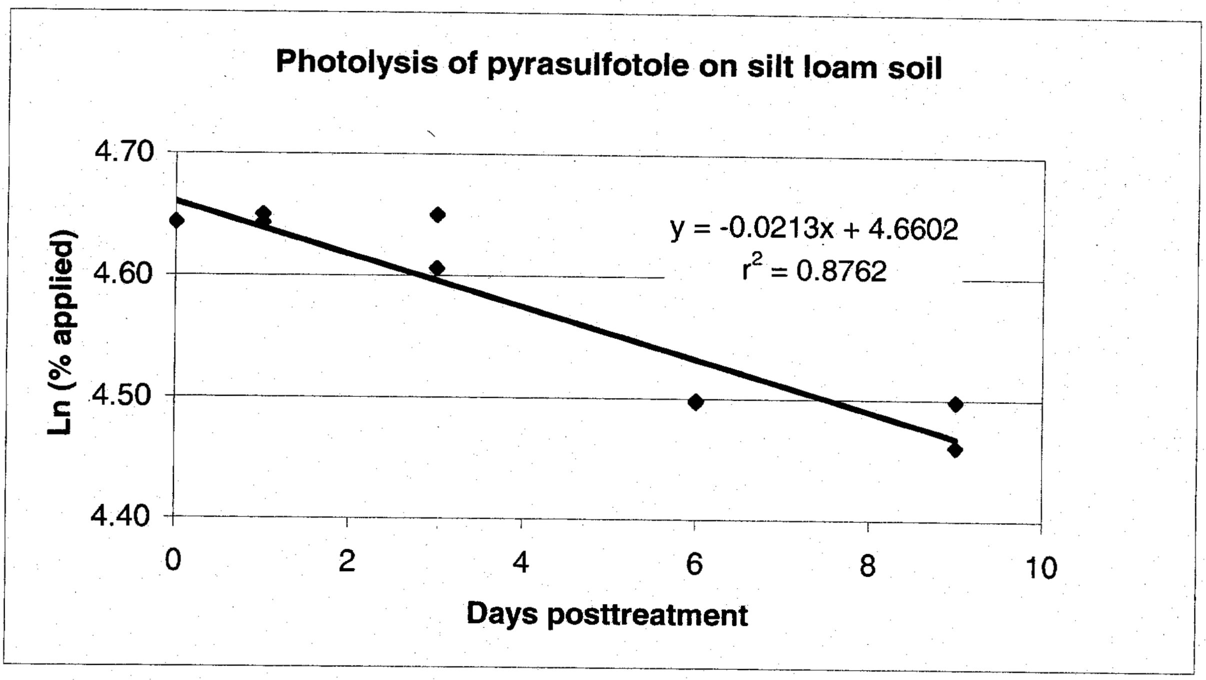
Chemical: Pyrasulfotole
PC Code: 000692
MRID: 46801707
Guideline: 161-3

Irradiated

Half life (days): 32.5

Days	% applied	Ln (% applied)
0	103.9	4.6434
0	104.6	4.6434
1	100.1	4.6501
1	92.5	4.6434
3	89.8	4.6501
3	91.5	4.6062
6	83.3	4.4976
6	89.9	4.4987
9	87.8	4.4987
9	86.6	4.4613

Data obtained from Appendix 8, p. 75 of the study report.



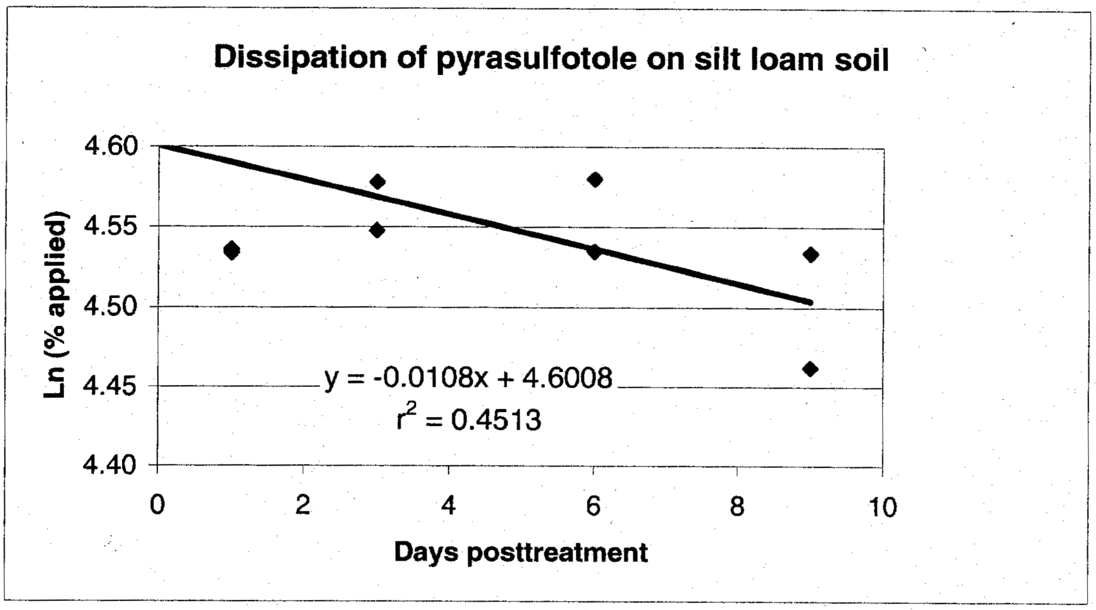
Chemical: Pyrasulfotole
PC Code: 000692
MRID: 46801707
Guideline: 161-3

Dark

Half life (days): 64.2

Days	% applied	Ln (% applied)
0	103.9	4.6434
0	104.6	4.6501
1	93.3	4.5358
1	93.1	4.5337
3	94.4	4.5475
3	97.3	4.5778
6	97.5	4.5799
6	93.2	4.5347
9	86.7	4.4625
9	93.1	4.5337

Data obtained from Appendix 9, p. 76 of the study report.



Chemical: Pyrasulfotole
PC Code: 000692
MRID: 46801707
Guideline: 161-3

Irradiated

Half life (days): 32.5

Days	% applied	Ln (% applied)
0	103.9	4.6434
0	104.6	4.6434
1	100.1	4.6501
1	92.5	4.6434
3	89.8	4.6501
3	91.5	4.6062
6	83.3	4.4976
6	89.9	4.4987
9	87.8	4.4987
9	86.6	4.4613

Data obtained from Appendix 8, p. 75 of the study report.