

US EPA ARCHIVE DOCUMENT

Data Evaluation Report on the terrestrial field dissipation of pyrasulfotole (AE 0317309)

PMRA Submission Number 2006-2445

EPA MRID Number 46801716

Data Requirement: PMRA Data Code: 8.3.2
 EPA DP Barcode: D328639
 OECD Data Point: IIA 7.3, IIA 7.3.1, IIA 7.3.2, IIA 7.3.3
 IIIA 9.2.1, IIIA 9.2.2, IIIA 9.2.3
 EPA Guideline: §164-1

Test material: AE 0317309

End Use Product name: AE 0317309 02 SE06 A103
Formulation type: Suspo-emulsion

Concentration of a.i.: 4.32%

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)cc2S(C)(=O)=O.
CS(=O)(=O)c1c(ccc(c1)C(F)F)C(=O)c1c(n(nc1C)C)O.

Primary Reviewer: Dan Hunt
 Cambridge Environmental

Signature:
Date: 6/14/06

Secondary Reviewer: Joan Harlin
 Cambridge Environmental

Signature:
Date: 6/14/06

QC/QA Manager: Joan Gaidos
 Cambridge Environmental

Signature:
Date: 6/14/06

Final Reviewer: Marietta Echeverria
 EPA Reviewer

Signature: *Marietta Echeverria*
Date: 11/28/07

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Final Reviewer: JD Whall (Officer # 1268)
PMRA Reviewer

Signature: 

Date: 5/16/07

Final Reviewer: Olga Braga
DEH Reviewer

Signature: 

Date: 04/01/2007

Company Code
Active Code
Use Site Category
EPA PC Code: 000692

CITATION: Lenz, M. 2006. Terrestrial field dissipation of AE 0317309 in Kansas soil, 2004. Unpublished study performed by Bayer CropScience, Stilwell, KS; AGVISE Laboratories, Northwood, ND; and Diamond Ag Research, Inc., Larned, KS; and submitted by Bayer CropScience, Research Triangle Park, NC. Study No: MEAIY008. Experiment initiation June 24, 2004 and completion January 13, 2006 (p. 13). Final report issued February 28, 2006.

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EXECUTIVE SUMMARY

Soil dissipation/accumulation of pyrasulfotole [(5-hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α -trifluoro-2-mesyl-*p*-tolyl)methanone] under US field conditions was conducted in three replicate bare plots and three replicate cropped plots (wheat) of loam soil in Kansas. The experiment was carried out in accordance with the USEPA Pesticide Assessment Guidelines Subdivision N, §164-1 and the Canadian PMRA data code DACO 8.3.2, and in compliance with the USEPA FIFRA (40 CFR, Part 160) GLP standards. Pyrasulfotole was broadcast once with the end-use product AE 0317309 02 SE06 A103 (50 g a.i./L pyrasulfotole), at a target rate of 0.055 kg a.i./ha (0.049 lb a.i./A) to 78 x 6.5 m replicate plots. Application to the crop occurred at the 1 leaf to 4 tiller stage; the height of the wheat at the time of application was 5-7.5 cm. The proposed label rate was reported as 0.050 kg a.i./ha (0.045 lb a.i./A). Total water input during the 526-day study period was 58.67 inches or 147% of the 30-year average precipitation. A control plot was located 15 m from the treated plots.

The application rate was verified for both plots using both solvent saturation pads (6 pads for each treatment) and pans containing control soil (3 pans for each treatment) that were placed in the treated plots prior to the test application. Mean recovery of pyrasulfotole from the pads placed in the bare plot was equivalent to an application rate of 64.91 g a.i./ha or a reviewer-calculated 118% of the 55 g a.i./ha target. Mean recovery of pyrasulfotole from the pads placed in the cropped plot was equivalent to an application rate of 64.72 g a.i./ha or a reviewer-calculated 118% of the target rate. Mean recovery of pyrasulfotole plus the transformation product AE B197555 from the pans was equivalent to an application rate of 45.88 g a.i./ha for the bare plot and 42.39 g a.i./ha for the cropped plot, which corresponds to 83.4% and 77.1% of the target rate, respectively. Field spikes to determine the stability of the parent and transformation products during transport and storage were not prepared.

Soil samples were collected from the bare and cropped plots at 0, 1, 4, 7, 14, 27, 58, 127, 166, 257, 348, and 526 days posttreatment to a depth of 0-122 cm (excluding day-0 samples). Samples were extracted using an Accelerated Solvent Extractor with acetonitrile:water (65:35, v:v) at 100°C and 1500 psi pressure. An aliquot of the extraction solvent was cleaned up using a RP-102 SPE cartridge and analyzed for pyrasulfotole and the transformation product AE B197555 (2-(methylsulfonyl)-4-(trifluoromethyl) benzoic acid) by LC/MS/MS. The LOD and LOQ were 0.1 $\mu\text{g}/\text{kg}$ and 0.5 $\mu\text{g}/\text{kg}$, respectively, for both analytes. Soil samples were stored frozen for up to 561 days prior to analysis.

In the bare test plot, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 19.80 ppb or 63.9% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 31 $\mu\text{g}/\text{kg}$). Pyrasulfotole decreased to 11.20 ppb by 7 days, 6.54 ppb by 14 days, 1.36 ppb by 58 days, and was last detected above the LOQ at 0.69 ppb at 257 days posttreatment. Pyrasulfotole was detected at levels below the LOQ in the 15-30 cm soil depth, and was not detected below 30 cm. The major transformation product **AE B197555** was detected in the 0-15 cm soil depth at a maximum concentration of 6.15 ppb at 4 days (which is equivalent to 8.31 ppb parent equivalents or 26.8% of the theoretical applied

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pyrasulfotole based on the target application rate), then decreased to 3.25 ppb by 14 days, was below the LOQ by 58 days, and was not detected by 257 days posttreatment. AE B197555 was not detected below the 0-15 cm soil depth at any sampling intervals.

In the cropped test plot, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 20.85 ppb or 71.9% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 29 µg/kg). Pyrasulfotole increased to a maximum of 22.75 ppb by 1 day, then decreased to 10.31 ppb by 14 days, 5.62 ppb by 27 days, 1.67 ppb by 58 days, and was last detected above the LOQ at 0.62 ppb at 348 days posttreatment. Pyrasulfotole was detected in the 15-30 cm soil depth at 0.52-0.73 ppb at 14, 58, 127, and 166 days, and was not detected above the LOQ at any other sampling intervals or at lower depths. The major transformation product **AE B197555** was detected in the 0-15 cm soil depth at a maximum of 6.03 ppb at 7 days (which is equivalent to 8.15 ppb parent equivalents or 28.1% of the theoretical applied pyrasulfotole based on the target application rate), then decreased to 1.42-1.82 ppb by 14-27 days, was below the LOQ by 58 days, and was not detected by 526 days posttreatment. AE B197555 was not detected below the 0-15 cm soil depth with one exception. The study author-calculated half-life value for AE B197555 was 5 days.

Under field conditions in the bare test plot, pyrasulfotole had a reviewer-calculated half-life value of 87.7 days in soil ($r^2 = 0.6814$; based on all available replicate data in the top 15 cm soil layer, using linear regression and the equation $t_{1/2} = \ln 2 / k$, where k is the rate constant); however, dissipation was bi-phasic with a more rapid decline phase occurring through the 58-day sampling interval. The reviewer-calculated half-life based on 0-58 day data in the top 15 cm soil layer was 14.9 days ($r^2 = 0.9250$). The reviewer-calculated DT_{50} and DT_{90} values for pyrasulfotole in the whole soil column using a double first order regression model were 8.9 and 45 days, respectively ($r^2 = 0.97$). Reviewer calculated DT_{50} and DT_{90} values for the strongly bi-phasic dissipation pattern of AE B197555 residues in the whole soil column were 17 and 45 days following initial application, respectively ($r^2 = 0.87$). In the bare test plot, residue carryover (i.e., percentage of the total amount of parent material in the whole soil column relative to Day 0 concentrations) was 4.5% at the beginning of the following growing season (i.e., at 257 days post treatment), and 0.9% at the end of the study (i.e., 526 days post treatment).

Under field conditions in the cropped test plot, pyrasulfotole had a reviewer-calculated half-life value of 86.6 days in soil ($r^2 = 0.7074$; based on all available replicate data in the top 15 cm soil layer, using linear regression and the equation $t_{1/2} = \ln 2 / k$, where k is the rate constant); however, dissipation was bi-phasic with a more rapid decline phase occurring through the 58-day sampling interval. The reviewer-calculated half-life based on 0-58 day data in the top 15 cm soil layer was 15.4 days ($r^2 = 0.9637$). The registrant-calculated DT_{90} value was 94 days for pyrasulfotole (DFOP model). In the cropped test plot, residue carryover (i.e., percentage of the total amount of parent material in the whole soil column relative to Day 0 concentrations) was 7.2% at the beginning of the following growing season (i.e., at 257 days post treatment), and 4.9% at the end of the study (i.e., 526 days post treatment).

The major route of dissipation of pyrasulfotole under terrestrial field conditions in both test plots was transformation.

RESULTS SYNOPSIS

Bare plot

Location/soil type: Larned, KS/Loam (0-45 cm) over sandy loam (60-122 cm).

Half-life: 87.7 days ($r^2 = 0.6814$; based on all replicate detections in the top 15 cm soil layer; reviewer-calculated).

14.9 days ($r^2 = 0.9250$; based on 0-58 day data in the top 15 cm soil layer; reviewer-calculated).

DT₅₀: 8.9 days ($r^2 = 0.97$; DFOP model for residues in whole soil column; reviewer-calculated).

DT₉₀: 45 days ($r^2 = 0.97$; DFOP model for residues in whole soil column; reviewer-calculated).

Major transformation products detected: AE B197555.

DT₅₀: 17 days ($r^2 = 0.87$; DFOP model for residues in whole soil column; reviewer-calculated).

DT₉₀: 45 days ($r^2 = 0.87$; DFOP model for residues in whole soil column; reviewer-calculated).

Dissipation routes: Transformation.

Carryover to following growing season : 4.5%

Cropped plot

Location/soil type: Larned, KS/Loam (0-30 cm) over clay loam (30-75 cm).

Half-life: 86.6 days ($r^2 = 0.7074$; based on all replicate detections in the top 15 cm soil layer; reviewer-calculated).

15.4 days ($r^2 = 0.9637$; based on 0-58 day data in the top 15 cm soil layer; reviewer-calculated).

DT₉₀: 94 days (registrant-calculated).

Major transformation products detected: AE B197555.

Dissipation routes: Transformation.

Carryover to following growing season : 7.2%

Study Acceptability: This study is classified **acceptable**. No significant deviations from good scientific practices or Subdivision N Guidelines were noted.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED:

The study was conducted according to USEPA Pesticide Assessment Guidelines Subdivision N, §164-1 and Canadian PMRA data code DACO No.8.3.2 (p. 13). There were no deviations from guideline §164-1.

COMPLIANCE:

The study was conducted in compliance with USEPA FIFRA (40 CFR Part 160) Good Laboratory Practice standards (p. 14). Signed and dated Data Confidentiality, GLP compliance, Quality Assurance,

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and Certification of Authenticity statements were provided (pp. 2-5).

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A. MATERIALS:

1. Test Material Pyrasulfotole.

Chemical Structure of the active ingredient(s): See DER Attachment 1.

Description: Formulation: Suspo-emulsion (p. 14).

Storage conditions of test chemicals: The test substance was stored in the dark under ambient conditions (8.6-29.9°C; p. 14).

Physico-chemical properties of the active ingredient(s):

Parameter	Value	Comment
Chemical formula	C ₁₄ H ₁₃ F ₃ N ₂ O ₄ S	
Molecular mass	362.3242	
Water Solubility	Bi-distilled water: 2.3 g/L pH 4: 4.2 g/L pH 7: 69.1 g/L pH 9: 49.0 g/L	At 20°C
Vapor Pressure/Volatility	2.7x10 ⁻⁷ Pa 6.8x10 ⁻⁷ Pa 4.8x10 ⁻⁵ Pa	At 20°C At 25°C At 50°C
UV Absorption	264 nm: 11127 L/mol*cm 306 nm: 5925 L/mol*cm	In water
Pka	4.2	
K _{ow} /log K _{ow}	pH 4: 1.89/0.276 pH 7: 0.043/-1.362 pH 9: 0.026/-1.580	At 23°C
Stability of compound at room temperature, if provided	Stable in solid state (ambient temperature); stable in aqueous solution at pH 5, 7, and 9 (25°C); no significant degradation in aqueous solution under continuous irradiation.	

Data were obtained from Tables 2 and 11, pp. 28 and 39 of the study report.

2. Test site: The test site was located in Larned, Kansas on a loam soil (0-30 cm; Tables 1 and 5, pp. 27 and 31). The site was located in the market region for the product (p. 15). No hardpan or confining layer was found in the test site. A three-year crop and pesticide use history for the test site is reported below in Table 2.

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Table 1: Geographic location, site description and climatic data at the study site.

Details		Kansas
Geographic coordinates	Latitude	39.1054
	Longitude	-99.05 58
	Province/State	Kansas
	Country	USA
	Ecoregion	9.4
Slope Gradient		1-2%
Depth to ground water (m)		>3 m
Distance from weather station used for climatic measurements		On-site station
Indicate whether the meteorological conditions before starting or during the study were within 30 year normal levels (Yes/No). If no, provide details.		Total water input (rainfall plus irrigation) during the 526-day study period was 58.67 inches or 147% of the 30-year average precipitation.

Data were obtained from p. 15; Table 3, p. 29; and Appendix 4, Table 1, p. 107 of the study report.

Table 2: Site usage and management history for the previous three years.

Use	Year	Kansas
Crops grown	Previous year	Alfalfa
	2 years previous	Alfalfa
	3 years previous	Alfalfa
Pesticides used	Previous year	Treflan, Roundup Ultra, 2,4-D LVE 6, Mustang Max, Furadan 4F, and Gramoxone Max
	2 years previous	Trifluralin and Mustang
	3 years previous	Trifluralin and Mustang
Fertilizers used	Previous year	Not reported
	2 years previous	Not reported
	3 years previous	Not reported
Cultivation methods, if provided (eg., Tillage)	Previous year	Tillage
	2 years previous	Tillage
	3 years previous	Tillage

Data were obtained from Table 4, p. 30 of the study report.

* The test plots were cultivated with a tractor and field cultivator and 20 tons/A of raw manure were applied prior to the test application (p. 16).

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3. Soils:

Table 3a: Properties of the soil in the bare test plot.

Property	Depth (cm)							
	0-15	15-30	30-45	45-60	60-75	75-90	90-105	105-122
Textural classification	Loam	Loam	Loam	Sandy clay loam	Sandy loam	Sandy loam	Sandy loam	Sandy loam
%sand	47	45	47	53	63	64	63	57
%silt	34	36	30	24	18	19	20	26
%clay	19	19	23	23	19	17	17	17
pH (1:1 soil:water)	7.5	7.7	8.3	8.7	8.8	9.0	9.2	9.2
Organic matter (%)	2.3	1.4	0.8	0.4	0.2	0.1	0.1	0.1
Total organic carbon (%)	1.3	0.8	0.5	0.2	0.1	0.06	0.06	0.06
CEC (meq/100 g)	15.9	15.9	18.9	19.3	17.1	15.7	15.3	14.7
Bulk density (g/cm ³)	1.20	1.21	1.24	1.19	1.26	1.26	1.32	1.32
Moisture at 1/3 atm (%)	20.0	19.0	21.9	24.8	23.2	22.4	22.1	21.7
Taxonomic classification (e.g., ferro-humic podzol)	Soil Series: Farnum Sub Order: Ustolls Soil Order: Mollisols Great Group: Argiustolls Mineralogy: Mixed Taxonomic classification: Fine-loamy, mixed, superactive, mesic Pachic Argiustolls							
Soil mapping unit	Typical pedon: Farnum loam, on a east facing, convex, 1% slope in a cultivated field at an elevation of 1650 ft. Ap - 0 to 5 inches, A - 5 to 15 inches, Bt1 - 15 to 21 inches, Bt2 - 21 to 24 inches, Bt3 - 34 to 48 inches							

Data were obtained from Table 5, p. 31 of the study report. Organic carbon was calculated by the reviewer from percent organic matter (% o.c. = % o.m. x 0.58). The particle distribution of the soil is presented graphically in Appendix 5, p. 125 of the study report.

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Table 3b: Properties of the soil in the cropped test plot.

Property	Depth (cm)							
	0-15	15-30	30-45	45-60	60-75	75-90	90-105	105-122
Textural classification	Loam	Loam	Clay loam	Clay loam	Clay loam	Loam	Sandy clay loam	Sandy clay loam
%sand	49	45	39	39	36	41	51	49
%silt	34	34	32	32	35	32	24	25
%clay	17	21	29	29	29	27	25	26
pH (1:1 soil:water)	7.6	7.8	7.8	8.0	8.3	8.5	8.6	8.7
Organic matter (%)	1.9	1.5	0.9	0.6	0.3	0.3	0.2	0.2
Total organic carbon (%)	1.1	0.9	0.5	0.3	0.2	0.2	0.1	0.1
CEC (meq/100 g)	14.5	18.0	22.7	22.3	21.9	20.6	19.9	20.5
Bulk density (g/cm ³)	1.26	1.28	1.20	1.20	1.25	1.34	1.27	1.28
Moisture at 1/3 atm (%)	19.5	20.8	26.6	26.7	27.2	25.6	25.5	25.3
Taxonomic classification (e.g., ferro-humic podzol)	Soil Series: Farnum Sub Order: Ustolls Soil Order: Mollisols Great Group: Argiustolls Mineralogy: Mixed Taxonomic classification: Fine-loamy, mixed, superactive, mesic Pachic Argiustolls							
Soil mapping unit	Typical pedon: Farnum loam, on a east facing, convex, 1% slope in a cultivated field at an elevation of 1650 ft. Ap - 0 to 5 inches, A - 5 to 15 inches, Bt1 - 15 to 21 inches, Bt2 - 21 to 34 inches, Bt3 - 34 to 48 inches							

Data were obtained from Table 5, p. 31 of the study report. Organic carbon was calculated by the reviewer from percent organic matter (% o.c. = % o.m. x 0.58). The particle distribution of the soil is presented graphically in Appendix 5, p. 125 of the study report.

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B. EXPERIMENTAL DESIGN:

1. Experimental design:

Table 4: Experimental design.

Details		Bare plot	Cropped plot
Duration of study		526 days	526 days
Uncropped (bare) or cropped		Bare	Cropped
Control used (Yes/No)		Yes	No
No. of replications	Controls	One	N/A
	Treatments	Three	Three
Plot size (L x W m)	Controls	9 x 6.5 m	N/A
	Treatments	78 x 6.5 m	78 x 6.5 m
Distance between control plot and treated plot		15 m	N/A
Distance between treated plots		3 m	3 m
Application rate(s) used (g a.i./ha)		55 g a.i./ha	55 g a.i./ha
Was the maximum label rate per ha used in study? (Yes/No)		110% of the proposed label rate	110% of the proposed label rate
Number of applications		One	One
Application Date(s) (dd mm yyyy)		24/06/2004	24/06/2004
For multiple applications, application rate at Day 0 and at each application time (mg a.i./kg soil)		0.031 mg a.i./kg soil ¹	0.029 mg a.i./kg soil ¹
Application method (eg., spraying, broadcast etc.)		Liquid broadcast spray	Liquid broadcast spray
Type of spray equipment, if used		A 3-point sprayer #1715 equipped with #XBR80 02 flat fan nozzles spaced 15 inches apart and set at 15 inches above the ground	A 3-point sprayer #1715 equipped with #XBR80 02 flat fan nozzles spaced 15 inches apart and set at 15 inches above the ground
Total volume of spray solution applied/plot OR total amount broadcasted/plot		193.9 L/ha	193.9 L/ha
Identification and volume of carrier (e.g., water), if used		Water	Water
Name and concentration of co-solvents, adjuvants and/or surfactants, if used		None	None
Indicate whether the following monthly reports were submitted:			
Precipitation:		Yes	Yes
Average minimum and maximum air temperature:		Yes	Yes
Average minimum and maximum soil temperature:		Yes	Yes
Average annual frost-free periods:		No	No

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Details		Bare plot	Cropped plot
Indicate whether the Pan evaporation data were submitted		No	No
Meteorological conditions during application	Cloud cover	75%	75%
	Temperature (EC)	29.4	29.4
	Humidity	76%	76%
	Sunlight (hr)	Not reported	Not reported
Pesticides used during study:			
Name of product/a.i concentration: Amount applied:		Headline, 9 fl oz/A; Puma, 0.67 pt/A; 2,4-D LVE, 1.3 lb a.i./A; Mirage, 1.2 lb a.i./A; RoundUp Weather Max, 1.125 lb a.i./A; Glyphos X-tra, 1 lb a.i./A or 1 qt/A; Glystar Plus, 1.5 lb a.i./A; 2,4-D Lov Vol Ester, 1.0 lb a.i./A; Landmaster BW, 0.63 lb a.i./A; 2,4-D Amine, 0.24 lb a.i./A; Baythroid, 0.04 lb a.i./A; Trifluralin 4 EC, 2.1 lb a.i./A ²	Headline, 9 fl oz/A; Puma, 0.67 pt/A; 2,4-D LVE, 1.3 lb a.i./A; Mirage, 1.2 lb a.i./A; RoundUp Weather Max, 1.125 lb a.i./A; Glyphos X-tra, 1 lb a.i./A or 1 qt/A; Glystar Plus, 1.5 lb a.i./A; 2,4-D Lov Vol Ester, 1.0 lb a.i./A; Landmaster BW, 0.63 lb a.i./A; 2,4-D Amine, 0.24 lb a.i./A; Baythroid, 0.04 lb a.i./A; Trifluralin 4 EC, 2.1 lb a.i./A ²
Application method:		Broadcast	Broadcast
Supplemental irrigation used (Yes/No)		Yes	Yes
If yes, provide the following details:			
No. of irrigation:		15	15
Interval between irrigation:		2-76 days	2-76 days
Amount of water added each time:		0.37-0.96 inches	0.37-0.96 inches
Method of irrigation:		Overhead sprinkler	Overhead sprinkler
Indicate whether water received through rainfall + irrigation equals the 30 year average rainfall (Yes/No)		Yes	Yes
Were the application concentrations verified?		Yes	Yes
Were field spikes used?		No	No
Good agricultural practices followed (Yes or No)		Yes	Yes
Indicate if any abnormal climatic events occurred during the study (eg., drought, heavy rainfall, flooding, storm etc.)		None	None

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Details	Bare plot	Cropped plot
If cropped plots are used, provide the following details: Plant - Common name/variety: Details of planting: Crop maintenance:	N/A	Jagger wheat Lot No. D06168 Planted March 14, 2004 at a rate of 70 pounds seed per acre at 1.5 inch depth with a John Deere Grain Drill and on March 14, 2005 at 215 pounds seed per acre at 1.5 inch depth with Hege No-till drill. Raw manure applied at 20 tons/A prior to application
Volatilization included in the study (Yes/No)	No	No
Leaching included in the study (Yes/No)	Yes	Yes
Run off included in the study (Yes/No)	No	No

Data were obtained from pp. 15-17; Table 6, pp. 33-34; Appendix 4, Tables 1-2, pp. 107-108; and Appendix 5, Table 2, pp. 113-124 of the study report.

1 Reviewer-calculated for the 0-15 cm soil depth based on one application at 0.049 lb a.i./A and a site-specific bulk density of 1.20 g/cm³ for the bare plot, and one application at 0.049 lb a.i./A and a site-specific bulk density of 1.26 g/cm³ for the cropped plot.

2 It was not specified which plot received the maintenance pesticides or if both plots received all applications.

2. Application Verification: To verify the application rate, one pair of solvent saturation pads (13.7 cm x 22 cm) was placed in individual aluminum pans (17.5 cm x 23.5 cm) that were then placed in each of the three replicate bare plots and three replicate cropped test plots (p. 16). Following application, the saturation pans and pads were collected, grouped by pairs, and stored frozen prior to analysis. The pads were extracted with acetonitrile:water (65:35, v:v) by shaking for two hours (p. 17). The extract was diluted to volume with acetonitrile:0.1% acetic acid in water (10:90, v:v), filtered using an Acrodisc 0.45-mm syringe filter, and analyzed for pyrasulfotole by LC/MS/MS.

In addition, an aluminum pan (25.4 x 38.1 cm) containing a layer of sieved, air-dried control soil was placed into each of the three replicate plots of the bare and cropped test plots prior to application (p. 16). Following application, the soil from the pans was transferred to a plastic bag and stored frozen until analysis. The soil was extracted using an Accelerated Solvent Extractor with acetonitrile:water (65:35, v:v) at 100°C and 1500 psi pressure (p. 18). Following dilution with acetonitrile, the extract was concentrated by evaporation, cleaned up using a RP-102 SPE cartridge, diluted to 5 mL with 0.1% acetic acid in water:acetonitrile (90:10, v:v), and analyzed for pyrasulfotole and AE B197555 by LC/MS/MS.

3. Field Spiking: Field spikes to determine the stability of the parent and transformation products during transport and storage were not prepared.

4. Volatilization: Volatilization was not measured.

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5. Leaching: Fifteen cores were taken from the bare and cropped plots at -7, 0, 1, 4, 7, 14, 27, 58, 127, 166, 257, 348, and 526 days posttreatment to a depth of 122 cm (excluding day-0 samples which were collected to a depth of 15 cm) to determine the mobility of the test substance in the soil profile (p. 16 and Table 7, p. 35).

6. Run off: Run off was not studied.

7. Supplementary Study: An on-going storage stability study is currently being conducted using soil collected from the test site and fortified with pyrasulfotole and the transformation product AE B197555 (p. 17; Appendix 10, p. 189). Soil samples were fortified with pyrasulfotole and AE B197555 at 0.010 ppm; results through 10 months of storage were reported.

8. Sampling:

Table 5: Soil sampling.

Details	Bare plot	Cropped plot
Method of sampling (random or systematic)	Random	Random
Sampling intervals	-7, 0, 1, 4, 7, 14, 27, 58, 127, 166, 257, 348, and 526 days	-7, 0, 1, 4, 7, 14, 27, 58, 127, 166, 257, 348, and 526 days
Method of soil collection (eg., cores)	Cores	Cores
Sampling depth	122 cm, except for day-0 samples which were collected to a depth of 15 cm.	122 cm, except for day-0 samples which were collected to a depth of 15 cm.
Number of cores collected per plot	5 per replicate plot (15 total)	5 per replicate plot (15 total)
Number of segments per core	Eight	Eight
Length of soil segments (after sectioning)	15 cm	15 cm
Core diameter	5.7 cm	5.7 cm
Method of sample processing, if any	Samples were composited by replicate plot and depth. Composited samples were milled with dry ice by a hammer mill and mixed using a bucket mixer with inner paddle blades.	Samples were composited by replicate plot and depth. Composited samples were milled with dry ice by a hammer mill and mixed using a bucket mixer with inner paddle blades.
Storage conditions	Frozen	Frozen
Storage length (days)	561 days	561 days

Data were obtained from p. 17 and Table 7, p. 35 of the study report.

9. Analytical Procedures:

Number of soil samples analysed per treatment or composite sample: Not reported.

Extraction, clean up and concentration of soil samples: Samples (5-20 g) were extracted using an Accelerated Solvent Extractor with acetonitrile:water (65:35, v:v) at 100°C and 1500 psi

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pressure (p. 18; Appendix 3, pp. 64-67 and 104). An aliquot of the extract was concentrated, cleaned up using a RP-102 SPE cartridge, and diluted to 5 mL with 0.1% acetic acid:acetonitrile (90:10, v:v).

Identification and quantification of parent compound: Extracts were fortified with an isotopic internal standard containing pyrasulfotole-d₃, and analyzed for pyrasulfotole by LC/MS/MS (Phenomenex Prodigy 5 μ C8 50 x 2.00 mm column; p. 18; Appendix 3, p. 67 and Table 1, p. 71). The mobile phase for the separation was A: 0.1% acetic acid in water; B: acetonitrile:water + 0.2% formic acid (85:15, v:v); A:B, 97:3 to 7:93 to 97:3 (Appendix 3, p. 76). The retention time of pyrasulfotole was approximately 3.4 minutes.

Identification and quantification of transformation products: Extracts were fortified with an isotopic internal standard containing AE B197555-¹³C₆, and analyzed for AE B197555 by LC/MS/MS (Phenomenex Prodigy 5 μ C8 50 x 2.00 mm column; p. 18; Appendix 3, p. 67 and Table 1, p. 71). The retention time of AE B197555 was approximately 3.8 minutes.

Detection limits (LOD, LOQ) for the parent compound in soil: The LOD and LOQ were 0.1 μ g/kg and 0.5 μ g/kg, respectively (p. 18).

Detection limits (LOD, LOQ) for the transformation products in soil: The LOD and LOQ were 0.1 μ g/kg and 0.5 μ g/kg, respectively (p. 18).

II. RESULTS AND DISCUSSION

APPLICATION MONITORS: Mean recovery of pyrasulfotole from the solvent saturation pads placed in the bare plot was equivalent to an application rate of 64.91 g a.i./ha or a reviewer-calculated 118% of the 55 g a.i./ha target (Appendix 7, Table 1, p. 159). Mean recovery from the pads placed in the cropped plot was equivalent to an application rate of 64.72 g a.i./ha or a reviewer-calculated 118% of the target rate. Mean recovery of pyrasulfotole plus the transformation product AE B197555 from the pans was equivalent to an application rate of 45.88 g a.i./ha for the bare plot and 42.39 g a.i./ha for the cropped plot, which corresponds to 83.4% and 77.1% of the target rate, respectively (Appendix 7, Table 2, p. 160).

2. RECOVERY FROM FIELD SPIKES: Field spikes were not prepared.

3. MASS ACCOUNTING: A mass balance was not determined.

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Table 6a. Concentration of pyrasulfotole residues expressed as ppb in soil from the bare plot.

Compound	Soil depth (cm)	Sampling times (days)											
		0	1	4	7	14	27	58	127	166	257	348	526
Pyrasulfotole (AE 0317309)	0-15	19.80	16.94	15.00	11.20	6.54	3.15	1.36	1.08	0.73	0.69	0.37	0.13
	15-30	NS	ND	ND	ND	0.41	0.16	0.34	0.24	ND	0.21	0.19	ND
	30-45	NS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	45-60	NS					ND	ND	ND	ND	ND	ND	ND
	60-75	NS											
	75-90	NS											
	90-105	NS											
	105-120	NS											
	Total	19.80	16.94	15.00	11.20	6.96	3.31	1.70	1.32	0.73	0.90	0.56	0.13
AE B197555	0-15	0.56	2.83	6.15	6.12	3.25	2.06	0.15	0.16	0.07	ND	ND	ND
	15-30	NS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	30-45	NS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	45-60	NS					ND	ND	ND	ND	ND	ND	ND
	60-75	NS											
	75-90	NS											
	90-105	NS											
	105-120	NS											
	Total	0.56	2.83	6.15	6.12	3.25	2.06	0.15	0.16	0.07	ND	ND	ND

Residue data were obtained from Table 9, p. 37 of the study report; values are registrant-calculated means of three replicates. Total extractable and non-extractable residues were not determined. NS = No sample. ND = Not detected. Blank cell indicates sample not analyzed. Values in bold are above the LOQ.

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Table 6b. Concentration of pyrasulfotole residues expressed as ppb in soil from the cropped plot.

Compound	Soil depth (cm)	Sampling times (days)											
		0	1	4	7	14	27	58	127	166	257	348	526
Pyrasulfotole (AE 0317309)	0-15	20.85	22.75	18.37	15.64	10.31	5.62	1.67	1.01	0.7	0.68	0.62	0.35
	15-30	NS	0.28	ND	ND	0.63	0.48	0.71	0.73	0.52	0.42	0.41	0.22
	30-45	NS	ND	ND	ND	ND	ND	0.11	0.13	0.14	0.26	0.16	0.19
	45-60	NS	ND			ND	ND	ND	ND	ND	0.14		0.26
	60-75	NS								ND			
	75-90	NS								ND			
	90-105	NS								ND			
	105-120	NS								ND			
	Total		20.85	23.03	18.37	15.64	10.94	6.10	2.49	1.87	1.36	1.50	1.19
AE B197555	0-15	0.65	3.48	5.84	6.03	1.82	1.42	0.30	0.19	0.29	0.19	0.16	ND
	15-30	NS	ND	ND	ND	ND	ND	ND	ND	0.13	ND	ND	ND
	30-45	NS	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	45-60	NS	ND			ND	ND	ND	ND	ND	ND		ND
	60-75	NS								ND			
	75-90	NS								ND			
	90-105	NS								ND			
	105-120	NS								ND			
	Total		0.65	3.48	5.84	6.03	1.82	1.42	0.30	0.19	0.42	0.19	0.16

Residue data were obtained from Table 10, p. 38 of the study report; values are registrant-calculated means of three replicates. Total extractable and non-extractable residues were not determined. NS = No sample. ND = Not detected. Blank cell indicates sample not analyzed. Values in bold are above the LOQ.

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4. PARENT COMPOUND: In the bare test plot, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 19.80 ppb or 63.9% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 31 µg/kg; Table 9, p. 37; see footnote to DER Table 4). Pyrasulfotole decreased to 11.20 ppb by 7 days, 6.54 ppb by 14 days, 1.36 ppb by 58 days, and was last detected above the LOQ at 0.69 ppb at 257 days posttreatment. Pyrasulfotole was detected at levels below the LOQ in the 15-30 cm soil depth, and was not detected below 30 cm.

In the cropped test plot, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 20.85 ppb or 71.9% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 29 µg/kg; Table 10, p. 38; see footnote to DER Table 4). Pyrasulfotole increased to a maximum of 22.75 ppb by 1 day, then decreased to 10.31 ppb by 14 days, 5.62 ppb by 27 days, 1.67 ppb by 58 days, and was last detected above the LOQ at 0.62 ppb at 348 days posttreatment. Pyrasulfotole was detected in the 15-30 cm soil depth at 0.52-0.73 ppb at 14, 58, 127, and 166 days, and was not detected above the LOQ at any other sampling intervals. Pyrasulfotole was detected at levels below the LOQ in the 30-45 cm depth from 58 to 526 days, and in the 45-60 cm depth at 257 and 526 days posttreatment.

HALF-LIFE: Under field conditions in the bare test plot, pyrasulfotole had a reviewer-calculated half-life value of 87.7 days in soil ($r^2 = 0.6814$; based on all available replicate data, using linear regression and the equation $t_{1/2} = \ln 2 / k$, where k is the rate constant; DER Attachment 2); however, dissipation was bi-phasic, with a more rapid decline phase occurring through the 58-day sampling interval. The reviewer-calculated half-life based on 0-58 day data was 14.9 days ($r^2 = 0.9250$). The reviewer-calculated DT_{50} and DT_{90} values for pyrasulfotole using a double first order regression model were 8.9 and 45 days, respectively [$y = 17.4365 * \exp(-0.0873 * x) + 1.9234 * \exp(-0.0037 * x)$; $r^2 = 0.97$]. This estimate was somewhat shorter than the registrant-calculated DT_{90} value of 75 days for pyrasulfotole (DFOP model, p. 21).

Under field conditions in the cropped test plot, pyrasulfotole had a reviewer-calculated half-life value of 86.6 days in soil ($r^2 = 0.7074$; based on all available replicate data, using linear regression and the equation $t_{1/2} = \ln 2 / k$, where k is the rate constant; DER Attachment 2); however, dissipation was bi-phasic, with a more rapid decline phase occurring through the 58-day sampling interval. The reviewer-calculated half-life based on 0-58 day data was 15.4 days ($r^2 = 0.9637$). The registrant-calculated DT_{90} value was 94 days for pyrasulfotole (DFOP model, p. 21).

5. TRANSFORMATION PRODUCTS: In the bare test plot, the major transformation product AE B197555 (2-(methylsulfonyl)-4-(trifluoromethyl) benzoic acid) was initially detected in the 0-15 cm soil depth at 0.56 ppb at day 0, increased to a maximum of 6.15 ppb by 4 days (which is equivalent to 8.31 ppb parent equivalents or 26.8% of the theoretical applied pyrasulfotole based on the target application rate), then decreased to 3.25 ppb by 14 days, was below the LOQ by 58 days, and was not detected by 257 days posttreatment. AE B197555 was not detected below the 0-15 cm soil depth at any sampling intervals. The study author-calculated half-life value for AE B197555 was 6 days (p. 23). Reviewer calculated DT_{50} and DT_{90} values for the strongly bi-

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phasic dissipation pattern of AE B197555 residues in the whole soil column were 17 and 45 days following initial application, respectively [$y=22.0649 \cdot \exp(-0.0459 \cdot x) - 14.0531 \cdot \exp(-0.0415 \cdot x)$; $r^2 = 0.87$].

In the cropped test plot, the major transformation product AE B197555 was initially detected in the 0-15 cm soil depth at 0.65 ppb at day 0, increased to a maximum of 6.03 ppb by 7 days (which is equivalent to 8.15 ppb parent equivalents or 28.1% of the theoretical applied pyrasulfotole based on the target application rate), then decreased to 1.42-1.82 ppb by 14-27 days, was below the LOQ by 58 days, and was not detected by 526 days posttreatment. AE B197555 was not detected below the 0-15 cm soil depth with one exception (detected below the LOQ in the 15-30 cm layer at 166 days). The study author-calculated half-life value for AE B197555 was 5 days (p. 23).

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

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	Molecular Weight (g/mol)	Smiles String
AE B197555	142994-06-7	2-(Methylsulfonyl)-4-(trifluoromethyl) benzoic acid	C ₉ H ₇ F ₃ O ₄ S	268.2097	CS(=O)(=O)c1cc(ccc1C(=O)O)C(F)(F)F

Data were obtained from Table 11, p. 39 and Figure 1, p. 41 of the study report.

6. EXTRACTABLE AND NON-EXTRACTABLE RESIDUES: Non-extractable residues were not measured.

Table 8: Dissipation routes of pyrasulfotole under field conditions.

Route of dissipation	% of applied amount		
	Bare plot	Cropped plot	
Soil residues of pyrasulfotole at beginning of following growing season (i.e., 257 days post treatment).	4.5%	7.2%	
Accumulation (residues) in soil at study termination (i.e., 526 days post treatment)	0.9%	4.9%	
Transformation (% of transformation products) ²	26.8% (day 4)	28.1% (day 7)	
Leaching, if measured (maximum depth detected)	Pyrasulfotole	15-30 cm	45-60 cm
	AE B197555	0-15 cm	15-30 cm
Volatilization, if measured	Not measured	Not measured	
Plant uptake, if measured	N/A	Not measured	
Run off, if measured	Not measured	Not measured	
Total			

Data were obtained from Tables 9-10, pp. 37-38 of the study report. Determined by reviewer as proportion of total amount of parent material present at beginning of following growing season (i.e., Day 269 posttreatment), to the amount present in the soil at Day 0 (sum of concentrations in whole soil column).

¹ Maximum concentration of AE B197555 in the soil after converting to parent equivalents (sum of all soil depths).

N/A = Not applicable.

7. VOLATILIZATION: The concentration of applied pyrasulfotole lost through volatilization was not determined.

8. PLANT UPTAKE: N/A.

9. LEACHING: In the bare test plot, pyrasulfotole was confined to the upper 0-30 cm soil layer and AE B197555 was confined to the upper 0-15 cm soil layer for the duration of the study period (residues of parent in the 15-30 cm soil layer were below the LOQ; Table 9, p. 37). In the cropped test plot, pyrasulfotole was detected at levels above the LOQ in the 0-15 and 15-30 cm soil layers, and at levels below the LOQ in the 30-45 cm layer (from 58 to 526 days) and 45-60 cm layer (257 and 526 days; Table 10, p. 38). Residues of AE B197555 were confined to the upper 0-15 cm depth, with one exception (detected below the LOQ in the 15-30 cm layer at 166 days).

Total water input was greater than historic rainfall for the study site for the duration of the study (147% of the 30-year average). The first water input event was a rainfall of approximately 0.3 inches at 1 day posttreatment (Appendix 5, Table 2, p. 113). The test plots received 13.63 cm or 5.37 inches of water over the first 30 days of the study. Accumulated water input throughout the study period is presented graphically in Appendix 5, Figure 3, p. 126. Daily changes in soil moisture are shown in Appendix 5, Figures 4-5, pp. 128-129.

10. RUN OFF: Run off was not studied.

11. RESIDUE CARRYOVER:

Residues as a percentage of applied amount were calculated by the reviewer as the total amount of parent material present in the whole soil column relative to observed concentrations at Day 0. At the start of the following growing season (i.e., at 257 days post treatment), carryover of residues was 4.5% of the applied pyrasulfotole for the bare plot and 7.2% for the cropped plot. By the end of the study period (i.e., 526 days post treatment), 0.9 and 4.9% of the applied pyrasulfotole was present in the bare and cropped plots, respectively.

12. SUPPLEMENTARY STUDY RESULTS: Results from the on-going storage stability study indicate that pyrasulfotole and the transformation product AE B197555 were stable through 10 months of storage (Appendix 10, p. 189). Corrected recoveries of pyrasulfotole ranged from 101-111% from 0 to 10 months. Corrected recoveries of AE B197555 ranged from 103-127% from 0 to 10 months. The study author did not state how long the stability study would be conducted.

III. STUDY DEFICIENCIES

No deficiencies were noted.

IV. REVIEWER'S COMMENTS

1. The storage stability study was on-going, and preliminary data could not confirm the stability of the parent and AE B197555 for the maximum duration that the test samples were stored. Test samples were stored frozen for up to 561 days prior to analysis, while preliminary storage stability data were available only for 10 months of storage (Appendix 10, p. 189). The study author stated that the results would be reported in a separate study report when finished.
2. The study author calculated half-lives using ModelMaker Version 4.0, using both a single first order model and a bi-exponential kinetic model or double first order in parallel (DFOP) model (p. 19). Simple first-order half-lives were 8 days for the bare plot and 13 days for the cropped plot (p. 21). Using the DFOP model, the study author reported a DT50 value for pyrasulfotole of 8 days and a DT90 of 75 days for the bare plot; corresponding DT50 and DT90 values for the cropped plot were 11 days and 94 days. The study author-calculated half-life values for AE B197555 were 6 days for the bare plot and 5 days for the cropped plot (p. 23).
3. The reviewer converted the concentration of AE B197555 in soil to parent equivalents by dividing by the molecular weight conversion factor 0.74. The molecular weight conversion factor was calculated by dividing the molecular weight of AE B197555 (268.2 g/mol) by the molecular weight of the parent (362.3 g/mol). AE B197555 concentrations were converted to parent equivalents by dividing the AE B197555 concentration by the molecular weight conversion factor.
4. The percent of AE B197555 in terms of percent of the applied pyrasulfotole was calculated by dividing the concentration of AE B197555 in parent equivalents (see above comment on how to convert to parent equivalents) by the theoretical day-0 concentration of pyrasulfotole in the 0-15 cm soil depth, based on the target application rate (see footnote to DER Table 4).
5. The study author stated that based on aerobic soil metabolism studies, biodegradation of pyrasulfotole to AE B197555 and subsequent biodegradation to non-extractable residues and mineralization to CO₂ are the major dissipation pathways for pyrasulfotole (p. 20). The author further stated that aerobic soil metabolism studies have shown that non-extractable residue can account for up to 50% of the total applied radioactivity after 100 days, and that mineralization to CO₂ can account for up to 40.5% of the applied after 358 days.
6. Mean method validation recoveries from soil samples fortified with pyrasulfotole at 0.5 ng/g (LOQ) and 2.5 ng/g (5x LOQ) were $87 \pm 7\%$ and $98 \pm 4\%$, respectively; corresponding recoveries for AE B197555 were $93 \pm 6\%$ and $96 \pm 3\%$, respectively (Appendix 3, p. 79).

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7. Mean recoveries of pyrasulfotole and AE B197555 from fortified control soil samples prepared with each sample set were $80 \pm 13\%$ for pyrasulfotole and $89 \pm 11\%$ for AE B197555 (Table 8, p. 36). The fortification level was not reported for parent or transformation product.
8. Kansas is located in EcoRegion 9.4, which is outside representative Canadian EcoRegions. Therefore, this study will not be used by the PMRA to assess pyrasulfotole's persistence in Canadian use regions.
9. The PMRA secondary reviewer re-calculated % carryover at Day 269 posttreatment (i.e., start of following growing season) and at the end of the study period (Day 526) as a function of the observed amount of parent found in the soil column on Day 0. This was done to determine the total amount of pyrasulfotole residue present in the soil prior to application in the following growing season.
10. The PMRA re-calculated expected DT50 and DT90 values for bare soil plots using a 2 compartment, 4 parameter model from Sigma Plot. This model appears to provide the optimal fit to the observed dissipation data. The PMRA assumed non-detects were equal to $\frac{1}{2}$ LOD, rather than 0 ug/kg as done by the study authors. Given the similar field dissipation characteristics of pyrasulfotole under bare and cropped plots, the PMRA will model field dissipation based on data from bare plots only to avoid potential confounding factors with vegetation on interpreting chemical dissipation.

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 164-1, Terrestrial Field Dissipation Studies. Office of Pesticide and Toxic Substances, Kansas, DC. EPA 540/9-82-021.
2. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Kansas, DC. EPA 738-R-93-010.
3. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Kansas, DC. EPA 540/09-90-078.

Attachment 1: Structures of Parent Compound and Transformation Products

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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].

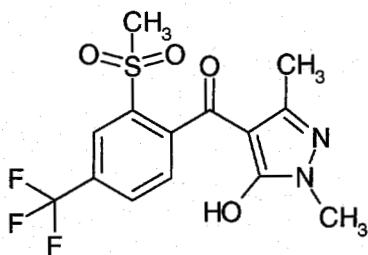
CAS Number: 365400-11-9.

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(ccc1)C(F)(F)F)C(=O)c1c(n(nc1C)C)O.



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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)-.

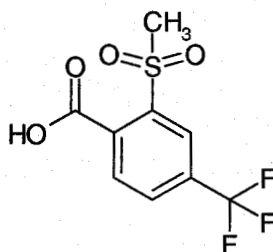
CAS Number: 142994-06-7.

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.



Chemical name Pyrasulfotole
 PC code 000692
 MRID 46801716
 Guideline No. 164-1

Bare plot
 0-15 cm depth

Half-life (days) = 87.7
 *Calculated using all available data
 Half-life (days) = 14.9
 *Calculated using 0-58 day data

Days posttreatment	Replicate plot	Pyrasulfotole (ppb)	Ln (pyrasulfotole)	Whole soil column		Day 0	Day 257	Day 526
				Pyrasulfotole (ppb)*	AE B197555 (ppb)**			
0	1	18.63	2.92	18.63	0.61			
0	2	19.18	2.95	19.18	0.53			
0	3	21.58	3.07	21.58	0.55			
1	1	15.19	2.72	15.19	2.60			
1	2	19.04	2.95	19.04	3.36			
1	3	16.60	2.81	16.6	2.53			
4	1	13.31	2.59	13.31	7.57			
4	2	14.35	2.66	14.35	7.14			
4	3	17.34	2.85	17.34	3.75			
7	1	9.02	2.20	9.02	6.44			
7	2	10.50	2.35	10.5	6.60			
7	3	14.07	2.64	14.07	5.33			
14	1	8.09	2.09	8.31	4.64			
14	2	6.48	1.87	6.53	4.59			
14	3	5.06	1.62	5.56	0.52			
27	1	3.69	1.31	3.69	2.72			
27	2	2.85	1.05	3.1	1.28			
27	3	2.90	1.06	3.12	2.19			
58	1	1.57	0.45	1.94	0.14			
58	2	1.26	0.23	1.53	0.17			
58	3	1.26	0.23	1.86	0.14			
127	1	1.29	0.25	1.49	0.15			
127	2	0.73	-0.31	0.93	0.13			
127	3	1.21	0.19	1.53	0.20			
166	1	1.00	0.00	1.1	0.12			
166	2	0.76	-0.27	0.76	0.10			
166	3	0.42	-0.87	0.59	0.05			
257	1	0.59	-0.53	0.78	0.05			
257	2	0.70	-0.36	0.86	0.05			
257	3	0.79	-0.24	1.06	0.05			
348	1	0.13	-2.04	0.29	0.05			
348	2	0.38	-0.97	0.52	0.05			
348	3	0.60	-0.51	0.8	0.05			
526	1	0.24	-1.43	0.24	0.05			
526	2	0.14	-1.97	0.14	0.05			
526	3	ND		0.13	0.05			

Sum of mean parent equivalents at

Day 0 Day 257 Day 526
 20.6 1.0 0.2

% carryover (vs. Day 0 observed)

Day 257 Day 526
 4.7 1.2

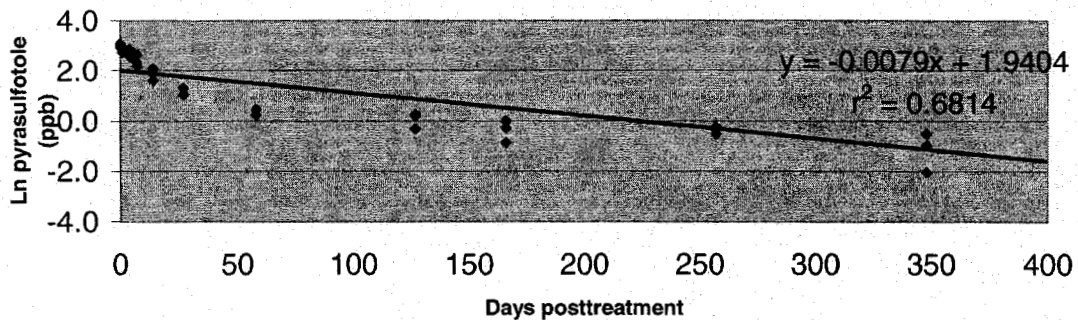
* Data obtained from Appendix 8, Table 1, p. 162 of the study report.

** Data obtained from Appendix 8, Table 2, p. 163 of the study report.

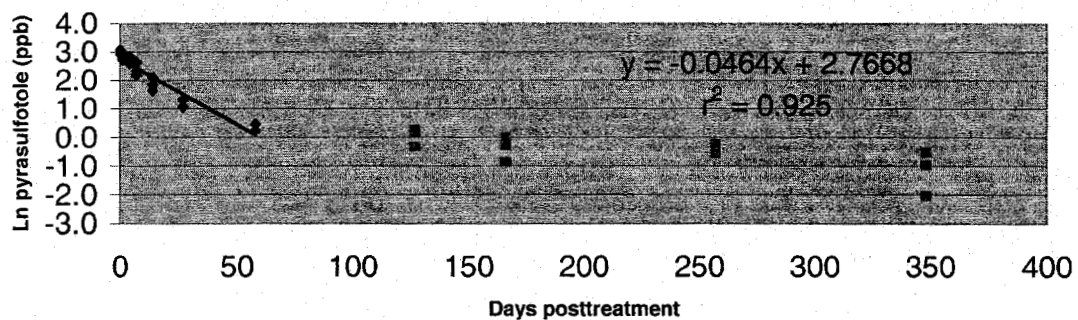
Shaded values were non-detects, set by peer reviewer to be 1/2 LOD (0.1 ug/kg soil)

ND = Not detected

Dissipation of pyrasulfotole from soil
in the bare plot (0-15 cm depth)



Dissipation of pyrasulfotole from soil
in the bare plot (0-15 cm depth)



Chemical name Pyrasulfotole
 PC code 000692
 MRID 46801716
 Guideline No. 164-1

Cropped plot
 0-15 cm depth

Half-life (days) = 86.6
 *Calculated using all available data
 Half-life (days) = 15.4
 *Calculated using 0-58 day data

Days posttreatment	Replicate plot	Pyrasulfotole (ppb)	Ln (pyrasulfotole)	Whole soil column		Day 0	Day 257	Day 526
				Pyrasulfotole (ppb)*	AE B197555 (ppb)**			
0	1	17.77	2.88	17.77	0.60			
						Sum of mean parent equivalents at		
0	2	24.59	3.20	24.59	0.73	21.7	1.8	1.1
0	3	20.19	3.01	20.19	0.61			
1	1	19.16	2.95	19.16	3.11	Day 257	Day 526	
						% carryover (vs. Day 0 observed)		
1	2	25.25	3.23	25.25	4.52	8.1	5.1	
1	3	23.83	3.17	24.68	2.80			
4	1	14.64	2.68	14.64	5.55			
4	2	23.91	3.17	24.1	6.58			
4	3	16.56	2.81	16.56	5.40			
7	1	14.59	2.68	14.59	6.27			
7	2	17.79	2.88	17.79	5.08			
7	3	14.53	2.68	14.53	6.74			
14	1	7.65	2.03	7.65	1.43			
14	2	11.07	2.40	11.41	1.85			
14	3	12.20	2.50	13.13	2.31			
27	1	6.10	1.81	6.1	1.27			
27	2	5.93	1.78	5.93	1.40			
27	3	4.84	1.58	4.84	1.72			
58	1	1.51	0.41	2.3	0.37			
58	2	1.47	0.39	2.05	0.28			
58	3	2.03	0.71	3.3	0.24			
127	1	1.10	-0.10	2.55	0.23			
127	2	1.05	0.05	2.11	0.19			
127	3	0.87	-0.14	1.18	0.16			
166	1	0.77	-0.26	1.29	0.95			
166	2	0.77	-0.26	1.83	0.18			
166	3	0.57	-0.56	1	0.14			
257	1	0.65	-0.43	1.47	0.22			
257	2	0.71	-0.34	1.8	0.19			
257	3	0.68	-0.39	1.26	0.16			
348	1	0.61	-0.49	1.39	0.16			
348	2	0.53	-0.63	1.14	0.15			
348	3	0.71	-0.34	1.03	0.17			
526	1	0.38	-0.97	1.1	0.05			
526	2	0.38	-0.97	1.1	0.05			
526	3	0.30	-1.20	0.89	0.05			

* Data obtained from Appendix 8, Table 2, p. 164 of the study report.

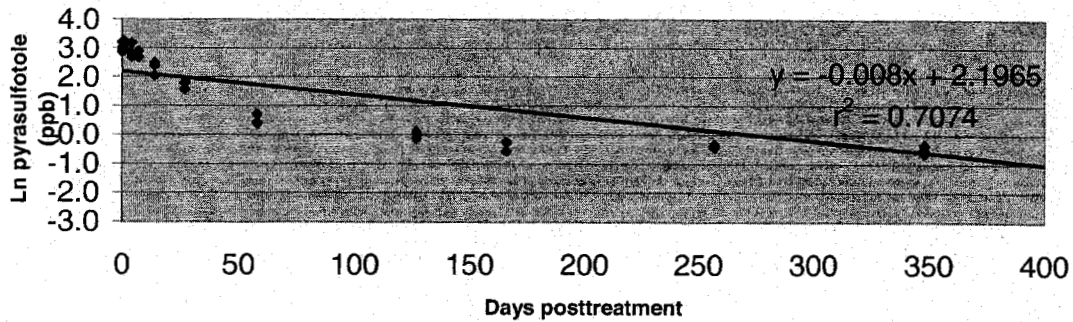
** Data obtained from Appendix 8, Table 2, p. 165 of the study report.

Shaded values were non-detects, set by peer reviewer to be 1/2 LOD (0.1 ug/kg soil)

ND = Not detected

US EPA ARCHIVE DOCUMENT

Dissipation of pyrasulfotole from soil
in the cropped plot (0-15 cm depth)



Dissipation of pyrasulfotole from soil
in the cropped plot (0-15 cm depth)

