TEXT SEARCHABLE DOCUMENT

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

PMRA Submission Number 2006-2445

EPA MRID Number 46801718

Data Requirement: PMRA Data Code: 8.3.2

EPA DP Barcode: D328639

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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

Concentration of a.i.: 4.32%

Formulation type: Suspo-emulsion

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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PMRA Submission Number 2006-2445

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PMRA Reviewer

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5/16/07

Final Reviewer: Olga Braga

DEH Reviewer

Signature:

Date:

Company Code: BCZ Active Code: PSA

Use Site Category: 13. 14 EPA PC Code: 000692

CITATION: Lenz, M. 2006. Terrestrial field dissipation of AE 0317309 in Washington soil, 2004. Unpublished study performed by Bayer CropScience, Stilwell, KS; AGVISE Laboratories, Northwood, ND; and Qualls Agricultural Laboratory, Inc., Ephrata, WA; and submitted by Bayer CropScience, Research Triangle Park, NC. Study No: MEAIY009. Experiment initiation June 8, 2004 and completion January 6, 2006 (p. 13). Final report issued March 10, 2006.

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 sandy loam soil in Washington. 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 45.7 x 36.6 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 7.6-12.7 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 53.83 inches or 478% of the 30-year average precipitation. A control plot was located approximately 46 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 was equivalent to an application rate of 62.8 g a.i./ha or a reviewer-calculated 114% of the 55 g a.i./ha target. Mean recovery of pyrasulfotole plus the transformation product AE B197555 from the pans was equivalent to an application rate of 47.8 g a.i./ha for the bare plot and 48.2 g a.i./ha for the cropped plot, which corresponds to 87.0% and 87.7% 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, 3, 7, 14, 28, 58, 120, 175, 269, 363, 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 μ g/kg and 0.5 μ g/kg, respectively, for both analytes. Soil samples were stored frozen for up to 577 days prior to analysis.

In the <u>bare test plot</u>, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 27.18 ppb or 109% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 25 μ g/kg). Pyrasulfotole decreased to 17.51-18.59 ppb by 1-3 days, 12.35 ppb by 7 days, was last detected above the LOQ at 1.10 ppb at 28 days, and was not detected following 175 days posttreatment. Pyrasulfotole moved into deeper soil layers over time, reaching the 45-60 cm layer at 28 days, the 75-90 cm layer at 58 days, and the 105-120 cm layer by 175 days. Pyrasulfotole was detected in the 15-30, 30-45, 45-60, 60-75, and 75-90 cm soil layers at maximum concentrations of 3.26 ppb (28 days), 1.84 ppb (28 days), 1.99 ppb (175 days), 1.24 ppb (58 days), and 0.57 ppb (58 days), respectively; residues were detected below the LOQ in the 90-105 and 105-120 cm soil layers. The major transformation

product AE B197555 was detected in the 0-15 cm soil depth at a maximum of 3.86 ppb at 7 days (which is equivalent to 5.21 ppb parent equivalents or 20.8% of the theoretical applied pyrasulfotole based on the target application rate), then decreased to below the LOQ by 28-58 days, and was not detected by 120 days posttreatment. AE B197555 was detected in the 15-30 cm soil depth at a maximum concentration of 0.94 ppb at 14 days, in the 30-45 cm soil depth at a maximum of 1.59 ppb at 28 days, and in the 45-60 cm soil depth at a maximum of 0.57 ppb at 28 days. AE B197555 was not detected above the LOQ in soil below the 45-60 cm depth; however, residues were detected below the LOQ to 120 cm, the maximum depth analyzed.

In the <u>cropped test plot</u>, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 24.05 ppb or 92.5% of the theoretical, based on the target application rate (reviewercalculated based on a theoretical day-0 recovery of 26 µg/kg). Pyrasulfotole decreased to 14.04-14.84 ppb by 3-7 days, 11.56 ppb by 14 days, was last detected above the LOQ at 0.58 ppb at 58 days, and was generally detected below the LOO from 120 to 526 days posttreatment. Pyrasulfotole moved into deeper soil layers over time, reaching the 30-45 cm layer at 28 days and the 105-120 cm layer by 58 days. Pyrasulfotole was detected in the 15-30, 30-45, 45-60, 60-75, 75-90, 90-105, and 105-120 cm soil layers at maximum concentrations of 8.54 ppb (28 days). 3.23 ppb (58 days), 2.48 ppb (58 days), 1.67 ppb (58 days), 0.68 ppb (120 days), 0.61 ppb (269 days), and 0.92 ppb (363 days), respectively. The major transformation product AE B197555 was detected in the 0-15 cm soil depth at a maximum of 2.85 ppb at 7 days (which is equivalent to 3.85 ppb parent equivalents or 14.8% of the theoretical applied pyrasulfotole based on the target application rate), then decreased to below the LOO by 28-58 days, and was not detected by 120 days posttreatment. AE B197555 was detected in the 15-30 cm soil depth at a maximum concentration of 1.27 ppb at 14 days and in the 30-45 cm soil depth at a maximum concentration of 0.90 ppb at 28 days. AE B197555 was not detected above the LOQ in soil below the 30-45 cm depth; however, residues were detected below the LOO to 120 cm, the maximum depth analyzed. The study author-calculated half-life value for AE B197555 was 18 days.

Under field conditions in the <u>bare test plot</u>, pyrasulfotole had a reviewer-calculated half-life value of 41.5 days in soil ($r^2 = 0.5835$; based on all available replicate data, using linear regression and the equation $t_2 = \ln 2 / k$, 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 from the top 15 cm soil layer was 8.2 days ($r^2 = 0.9462$). The reviewer calculated DT50 and DT90 values for pyrasulfotole in the whole soil column were 6 and 213 days, respectively (two compartment non-linear regression model; $r^2 = 0.94$). The reviewer calculated half-life value for AE B197555 residues in the whole soil column was 42.0 days (first order regression; $r^2 = 0.94$). Carryover of pyrasulfotole residues in the soil column was 8.8 and 3.1% of the applied pyrasulfotole at the beginning of the following growing season (i.e. Day 269) and at the end of the study period (i.e. Day 526), respectively, based on observed Day 0 concentrations.

Under field conditions in the <u>cropped test plot</u>, pyrasulfotole had a reviewer-calculated half-life value of 77.0 days in soil ($r^2 = 0.5914$; based on all available replicate data, 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 was 10.1 days ($r^2 = 0.8834$). The registrant-calculated DT90 value was 246 days for pyrasulfotole (DFOP model). Carryover of pyrasulfotole residues in the soil column was 11.0 and 11.3% of the applied pyrasulfotole at the beginning of the following growing season (i.e. Day 269) and at the end of the study period (i.e. Day 526), respectively, based on observed Day 0 concentrations.

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

RESULTS SYNOPSIS

Bare plot

Location/soil type: Grant County, WA/Sandy loam (0-30 cm) over loamy sand (30-90 cm). Half-life: 41.5 days ($r^2 = 0.5835$; based on all replicate detections in the top 15 cm soil layer; reviewer-calculated).

8.2 days ($r^2 = 0.9462$; based on 0-58 day data in the top 15 cm soil layer; reviewer-calculated).

DT₅₀: 6 days (reviewer calculated for whole soil column; $r^2 = 0.94$).

DT₉₀: 213 days (reviewer calculated for whole soil column; $r^2 = 0.94$).

Major transformation products detected: AE B197555:

Half-life: 42.0 days (reviewer calculated for whole soil column; $r^2 = 0.94$)

Dissipation routes: Transformation.

Carryover to following growing season: 8.8%

Cropped plot

Location/soil type: Grant County, WA/Sandy loam (0-15 cm) over loamy sand (15-60 cm) over sand (60-122 cm).

Half-life: 77.0 days ($r^2 = 0.5914$; based on all replicate detections in the top 15 cm soil layer; reviewer-calculated).

10.1 days ($r^2 = 0.8834$; based on 0-58 day data in the top 15 cm soil layer; reviewer-calculated).

DT90: 246 days (registrant-calculated).

Major transformation products detected: AE B197555.

Dissipation routes: Transformation.

Carryover to following growing season: 11.0%

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

I. MATERIALS AND METHODS

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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. 13). Signed and dated Data

Confidentiality, GLP compliance, Quality Assurance, 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 (12.3-25.5°C; p. 14).

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

Paramater	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	At 20°C
Vapor Pressure/Volatility	pH 9: 49.0 g/L 2.7x10 ⁻⁷ Pa	At 20°C
	6.8x10 ⁻⁷ Pa 4.8x10 ⁻⁵ Pa	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. 27 and 38 of the study report.

2. Test site: The test site was located in Ephrata, Grant County, Washington on a sandy loam soil (0-15 cm; Tables 1 and 5, pp. 26 and 30). The site was located in the market region for the product (p. 14). No hardpan or confining layer was found in the top 6 feet of the test site (p. 15). 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	Washington
Geographic	Latitude	47° 9' 0''
coordinates	Longitude	119° 33' 0"
	Province/State	Washington
	Country	USA
	Ecoregion	10.1/6.2
Slope Gradient		0-1%
Depth to ground	water (m)	>3 m
Distance from w	veather station used for ements	0.2 miles from on-site station; 16 miles from NOAA station
conditions before study were with	r the meteorological re starting or during the in 30 year normal	Total water input (rainfall plus irrigation) during the 526-day study period was 53.83 inches or 478% of the 30-year average precipitation.
levels (Yes/No).	If no, provide details.	

Data were obtained from pp. 14-15; Table 3, p. 28; and Appendix 4, Table 1, p. 105 of the study report.

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

Use	Year	Washington
Crops grown	Previous year	Wheat
	2 years previous	Alfalfa
	3 years previous	Wheat
Pesticides used	Previous year	Roundup Ultra and Weedar 64
	2 years previous	Gramoxone extra and Roundup ultra
	3 years previous	Gramoxone extra, Ally 60 WDC and Novaluron
Fertilizers used	Previous year	Not reported
	2 years previous	Not reported
	3 years previous	Not reported
Cultivation methods, if	Previous year	Not reported
provided (eg., Tillage)	2 years previous	Not reported
	3 years previous	Not reported

Data were obtained from Table 4, p. 29 of the study report.

^{*}The test plots were cultivated 7.5-10 cm using a 11-ft Northwest rototiller prior to the test application (p. 15).

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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	Sandy loam	Sandy loam	Loamy sand	Loamy sand	Loamy sand	Loamy sand	Sand	Sand				
%sand	68	76	78	84	87	87	90	92				
%silt	22	16	18	12	9	9	6	14				
%clay	10	8	4	4	4	4	4	4				
pH (1:1 soil:water)	7.5	7.8	8.0	8.0	8.3	8.4	8.5	8.6				
Organic matter (%)	1.3	0.4	0.3	0.3	0.1	0.0	0.1	0.0				
Total organic carbon (%)	0.8	0.2	0.2	0.2	0.06	0.0	0.06	0.0				
CEC (meq/100 g)	14.5	13.9	15.3	13.3	13.0	13.7	12.6	12.3				
Bulk density (g/cm3)	1.45	1.51	1.61	1.65	1.69	1.67	1.63	1.61				
Moisture at 1/3 atm (%)	14.6	11.0	11.1	7.9	6.0	6.4	5.9	5.3				
Taxonomic classification (e.g., ferro-humic podzol)	Soil Orde Great Gro	Soil Series: Timmerman Soil Order: Aridisols Great Group: Haplcambids Mineralogy: Mixed										
Soil mapping unit	Timmerm	Timmerman sandy loam – grassland, Ap – 0 to 5 inches, Bw – 5 to 19 inches, Bk1 – 19 to 28 inches, Bk2 – 28 to 60 inches										

Data were obtained from Table 5, p. 30 of the study report. Organic carbon was calculated by the reviewer from percent organic matter (% o.c. = % o.m. \times 0.58). The particle distribution of the soil is presented graphically in Appendix 5, p. 124 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	Sandy loam	Loamy sand	Loamy sand	Loamy sand	Sand	Sand	Sand	Sand		
%sand	73	78	82	82	87	92	90	93		
%silt	21	17	14	15	11	6	7	5		
%clay	6	5	4	3	2	2	3	2		
pH (1:1 soil:water)	7.9	7.5	7.6	7.8	8.2	8.4	8.4	8.5		
Organic matter (%)	0.7	0.4	0.4	0.3	0.0	0.7	0.1	0.1		
Total organic carbon (%)	0.4	0.2	0.2	0.2	0.0	0.4	0.06	0.06		
CEC (meq/100 g)	12.8	13.4	13.6	13.1	12.2	12.2	13.1	13.0		
Bulk density (g/cm3)	1.43	1.53	1.62	1.62	1.69	1.69	1.68	1.64		
Moisture at 1/3 atm (%)	11.4	10.0	9.0	7.4	5.8	5.2	5.5	5.1		
Taxonomic classification (e.g., ferro-humic podzol)	Soil Orde Great Gro	Soil Series: Timmerman Soil Order: Aridisols Great Group: Haplcambids Mineralogy: Mixed								
Soil mapping unit		Timmerman sandy loam – grassland, Ap – 0 to 5 inches, Bw – 5 to 19 inches, Bk1 – 19 to 28 inches, Bk2 – 28 to 60 inches								

Data obtained from Table 5, p. 30 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. 124 of the study report.

B. EXPERIMENTAL DESIGN:

1. Experimental design:

Table 4: Experimental design.

Details		Bare plot	Cropped plot
Duration of stu	ıdy	526 days	526 days
Uncropped (bare) or cropped Control used (Yes/No)		Bare	Cropped
		Yes	No
No. of Controls replications Treatments		One	N/A
		Three	Three
Plot size	Controls	6 x 36.6 m	N/A
(L x W m)	Treatments	45.7 x 36.6 m	45.7 x 36.6 m
Distance betwee	een control plot and treated	45.7 m	N/A
Distance between	een treated plots	0 m	0 m
Application rat	te(s) used (g a.i/ha)	55 g a.i./ha	55 g a.i./ha
in study? (Yes/		110% of the proposed label rate	110% of the proposed label rate
Number of app	olications	One	One
Application Date(s) (dd mm yyyy)		08/06/2004	08/06/2004
	oplications, application rate t each application time (mg	0.025 mg a.i./kg soil ¹	0.026 mg a.i./kg soil ¹
	ethod (eg., spraying,	Liquid broadcast spray	Liquid broadcast spray
Type of spray of	equipment, if used	Boom sprayer equipped with flat fan nozzles spaced 20 inches apart and set at 19 inches above the ground	Boom sprayer equipped with flat fan nozzles spaced 20 inches apart and set at 19 inches above the ground
Total volume of applied/plot Of broadcasted/plot		228.5 L/ha	228.9 L/ha
	and volume of carrier (e.g.,	Water	Water
adjuvants and/o	centration of co-solvents, or surfactants, if used	None	None
Indicate whethereports were su	er the following monthly ibmitted:		
Precipitation:		Yes	Yes
temperature:	num and maximum air	Yes	Yes
temperature:	num and maximum soil	No (average at 3 and 6 inches)	No (average at 3 and 6 inches)
Average annua	I frost-free periods:	No	No

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	Details	Bare plot	Cropped plot
were submitted	the Pan evaporation data	Yes (Penman evapotranspiration)	Yes (Penman evapotranspiration)
Meteorological	Cloud cover	100%	100%
conditions during	Temperature (EC)	14.4	14.4
application	Humidity	70%	70%
	Sunlight (hr)	Not reported	Not reported
Pesticides used du	uring study:		
Name of product/ Amount applied:	a.i concentration:	Touchdown/glyphosate at 1.0 lb a.i./A; Gramoxone extra/paraquat at 0.75 lb a.i./A; Sencor/metribuzin at 0.5 lb a.i./A; Weedar 64/2,4-D at 0.95 lb a.i./A; Roundup ultra/glyphosate at 1.0 lb a.i./A; and Rozol/chlorophacinone-liphadone at 0.0005 lb a.i./A ²	Touchdown/glyphosate at 1.0 lb a.i./A; Gramoxone extra/paraquat at 0.75 lb a.i./A; Sencor/metribuzin at 0.5 lb a.i./A; Weedar 64/2,4-D at 0.95 lb a.i./A; Roundup ultra/glyphosate at 1.0 lb a.i./A; and Rozol/chlorophacinone-liphadone at 0.0005 lb a.i./A ²
Application method		Broadcast	Broadcast
Supplemental irri	gation used (Yes/No)	Yes	Yes
If yes, provide the	e following details:		
No. of irrigation:		59	59
Interval between i	rrigation:	1 day-6.5 months	1 day-6.5 months
Amount of water		0.09-1.26 inches	0.09-1.26 inches
Method of irrigati		Overhead sprinkler	Overhead sprinkler
rainfall + irrigatio average rainfall (Y		Yes	Yes
Were the applicat verified?	ion concentrations	Yes	Yes
Were field spikes	used?	No	No
Good agricultural or No)	practices followed (Yes	Yes	Yes
	normal climatic events	None	None
	ne study (eg., drought,		
heavy rainfall, flo		No. 10 No	
following details:	re used, provide the	N/A	
Plant - Common n	ame/variety:		Sunstar wheat
Details of planting			Planted May 4, 2004 using a 4-row
			planter Jr at a rate of 70 pounds
			seed per acre at 1 inch depth with
			12-ft John Deere Grain Drill and
			May 4, 2005 at a rate of 100
			pounds of seed per acre at 1 inch
			depth with John Deere 8300 Grain

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Details	Bare plot	Cropped plot				
Crop maintenance:		Drill No fertilizers were used				
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. 32-33; Appendix 4, Tables 1-2, pp. 105-106; and Appendix 5, Table 2, pp. 111-123 of the study report.

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 pans used to hold the pads were rinsed with extraction solvent and added to the pad extract. The combined 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 containing a layer of sieved, air-dried control soil was placed into each of the three replicate plots of the bare and cropped test plot 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. 17). 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.
- **5. Leaching:** Fifteen cores were taken from the bare and cropped plots at -7, 0, 1, 3, 7, 14, 28, 58, 120, 175, 269, 363, 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. 34).
- 6. Run off: Run off was not studied.

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 1.45 g/cm³ for the bare plot and one application at 0.049 lb a.i./A and a site-specific bulk density of 1.43 g/cm³ for the cropped plot.

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. 16; Appendix 10, p. 193). Soil samples were fortified with pyrasulfotole and AE B197555 at 0.005 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, 3, 7, 14, 28, 58, 120, 175, 269, 363, and 526 days	-7, 0, 1, 3, 7, 14, 28, 58, 120, 175, 269, 363, 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 Storage conditions	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 fixed inner paddles. Frozen	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 fixed inner paddles. Frozen
Storage length (days)	577 days	577 days

Data were obtained from p. 16 and Table 7, p. 34 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 pressure (p. 17; Appendix 3, pp. 62-65 and 102). 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 in water:acetonitrile (90:10, v:v).

Identification and quantification of parent compound: Extracts were fortified with an isotopic internal standard containing pyrasulfotole- d_3 , and analyzed for pyrasulfotole by LC/MS/MS (Phenomenex Prodigy 5μ C8 50 x 2.00 mm column; pp. 17-18; Appendix 3, p. 65

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and Table 1, p. 69). 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. 74). 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- 13 C₆, and analyzed for AE B197555 by LC/MS/MS (Phenomenex Prodigy 5μ C8 50 x 2.00 mm column; pp. 17-18; Appendix 3, p. 65 and Table 1, p. 69). 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 $0.1 \mu g/kg$ and $0.5 \mu g/kg$, respectively (p. 18).

II. RESULTS AND DISCUSSION

APPLICATION MONITORS: Mean recovery of pyrasulfotole from the solvent saturation pads (including the rinse from the aluminum pans) was equivalent to an application rate of 62.8 g a.i./ha or a reviewer-calculated 114% of the 55 g a.i./ha target (Appendix 7, Table 1, p. 157); results were not reported separately for the bare and cropped plots. Mean recovery of pyrasulfotole plus the transformation product AE B197555 from the pans was equivalent to an application rate of 47.8 g a.i./ha for the bare plot and 48.2 g a.i./ha for the cropped plot, which corresponds to 87.0% and 87.7% of the target rate, respectively (Appendix 7, Table 2, p. 158); AE B197555 accounted for only 1.3-1.7% of the parent equivalent recovery.

- 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					Sampl	ing tin	ıes (da	ys)				
	depth (cm)	0	1	3	7	14	28	58	120	175	269	363	526
Pyrasulfotole (AE	0-15	27.18	17.51	18.59	12.35	8.93	1.10	0.17	0.11	0.19	ND	ND	ND
0317309)	15-30	NS	0.34	ND	ND	0.21	3.26	0.27	0.23	0.30	0.19	ND	ND
	30-45	NS	ND	ND	ND	ND	1.84	0.89	0.78	0.92	0.10	0.29	ND
	45-60	NS	ND		ND	ND	0.61	1.10	0.55	1.99	ND	0.41	0.16
	60-75	NS					ND	1.24	0.51	0.33	0.13	0.32	0.17
	75-90	NS	7.1				ND	0.57	0.46	0.26	0.24	0.25	0.18
	90-105	NS					-	ND	0.17	0.14	0.42	ND	0.19
	105-120	NS						ND		0.27	0.29		
	Total	27.18	17.85	18.59	12.35	9.14	6.81	4.24	2.81	4.40	1.37	1.27	0.70
AE B197555	0-15	0.21	2.07	3.24	3.86	2.87	0.40	0.11	ND	ND	ND	ND	ND
	15-30	NS	ND	ND	ND	0.94	0.70	ND	ND	ND	ND	ND	ND
	30-45	NS	ND	ND	ND	ND	1.59	ND	ND	ND	0.13	ND	ND
	45-60	NS	ND		ND	ND	0.57	0.23	ND	ND	ND	ND	ND
	60-75	NS					0.15	0.42	ND	ND	ND	ND	ND
	75-90	NS					ND	0.33	ND	ND	ND	ND	ND
	90-105	NS						0.25	0.13	0.16	ND	ND	ND
	105-120	NS						0.20		ND	0.14		
	Total	0.21	2.07	3.24	3.86	3.81	3.41	1.54	0.13	0.16	0.14	ND	ND

Residue data were obtained from Table 9, p. 36 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					Samp	ling tim	es (day	s)				
	depth (cm)	0	1	3	7	14	28	58	120	175	269	363	526
Pyrasulfotole	0-15	24.05	17.31	14.84	14.04	11.56	1.38	0.58	0.16	ND	0.14	0.12	0.18
(AE 0317309)	15-30	NS	ND	ND	ND	2.99	8.54	2.35	0.52	ND	0.17	0.17	0.14
	30-45	NS	ND	ND	ND	ND	1.37	3.23	1.28	ND	0.14	0.19	0.26
	45-60	NS		ND		ND	ND	2.48	0.67	0.27	0.26	0.25	0.40
	60-75	NS					ND	1.67	1.13	1.15	0.26	0.35	0.46
	75-90	NS						0.15	0.68	0.61	0.61	0.42	0.49
	90-105	NS						0.16	0.55	0.25	0.61	0.56	0.53
	105-120	NS						0.47	0.45	ND	0.69	0.92	0.36
	Total	24.05	17.31	14.84	14.04	14.55	11.29	11.09	5.44	2.28	2.88	2.98	2.82
AE B197555	0-15	0.23	1.74	2.63	2.85	1.74	0.22	0.16	ND	ND	ND	ND	ND
	15-30	NS	ND	ND	ND	1.27	1.11	0.27	ND	ND	ND	ND	ND
	30-45	NS	ND	ND	ND	ND	0.90	0.34	ND	ND	ND	ND	ND
	45-60	NS		ND		ND	0.18	0.36	ND	ND	ND	ND	ND
	60-75	NS					ND	0.35	ND	0.19	ND	ND	ND
	75-90	NS						0:17	ND	0.17	ND	ND	ND
	90-105	NS						ND	ND	0.11	ND	ND	ND
	105-120	NS		,				0.27	0.11	ND	ND	ND	ND
	Total	0.23	1.74	2.63	2.85	3.01	2.41	1.92	0.11	0.47	ND	ND	ND

Residue data were obtained from Table 10, 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.

4. PARENT COMPOUND: In the <u>bare test plot</u>, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 27.18 ppb or 109% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 25 μg/kg; Table 9, p. 36; see footnote to DER Table 4). Pyrasulfotole decreased to 17.51-18.59 ppb by 1-3 days, 12.35 ppb by 7 days, was last detected above the LOQ at 1.10 ppb at 28 days, and was not detected following 175 days posttreatment. Pyrasulfotole moved into deeper soil layers over time, reaching the 45-60 cm layer at 28 days, the 75-90 cm layer at 58 days, and the 105-120 cm layer by 175 days. Pyrasulfotole was detected in the 15-30, 30-45, 45-60, 60-75, and 75-90 cm soil layers at maximum concentrations of 3.26 ppb (28 days), 1.84 ppb (28 days), 1.99 ppb (175 days), 1.24 ppb (58 days), and 0.57 ppb (58 days), respectively; residues were detected below the LOQ in the 90-105 and 105-120 cm soil layers.

In the <u>cropped test plot</u>, the measured zero-time recovery of pyrasulfotole in the 0-15 cm soil layer was 24.05 ppb or 92.5% of the theoretical based on the target application rate (reviewer-calculated based on a theoretical day-0 recovery of 26 μg/kg; Table 10, p. 37; see footnote to DER Table 4). Pyrasulfotole decreased to 14.04-14.84 ppb by 3-7 days, 11.56 ppb by 14 days, was last detected above the LOQ at 0.58 ppb at 58 days, and was generally detected below the LOQ from 120 to 526 days posttreatment. Pyrasulfotole moved into deeper soil layers over time, reaching the 30-45 cm layer at 28 days and the 105-120 cm layer by 58 days. Pyrasulfotole was detected in the 15-30, 30-45, 45-60, 60-75, 75-90, 90-105, and 105-120 cm soil layers at maximum concentrations of 8.54 ppb (28 days), 3.23 ppb (58 days), 2.48 ppb (58 days), 1.67 ppb (58 days), 0.68 ppb (120 days), 0.61 ppb (269 days), and 0.92 ppb (363 days), respectively.

HALF-LIFE: Under field conditions in the <u>bare test plot</u>, pyrasulfotole had a reviewer-calculated half-life value of 41.5 days in soil ($r^2 = 0.5835$; based on all available replicate data, using linear regression and the equation $t_2 = \ln 2 / k$, 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 8.2 days ($r^2 = 0.9462$). The registrant-calculated DT50 and DT90 values were 7 and 208 days, respectively for pyrasulfotole (DFOP model, p. 21). The reviewer calculated DT50 and DT90 were 5.7 and 213 days, respectively (two-compartment, four parameter non-linear regression; $r^2 = 0.94$; using Sigma Plot equation solver for 0.5x and 0.1x mean Day 0 concentrations).

Under field conditions in the <u>cropped test plot</u>, pyrasulfotole had a reviewer-calculated half-life value of 77.0 days in soil ($r^2 = 0.5914$; 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 10.1 days ($r^2 = 0.8834$). The registrant-calculated DT90 value was 246 days for pyrasulfotole (DFOP model, p. 21).

5. TRANSFORMATION PRODUCTS: In the <u>bare test plot</u>, the major transformation product AE B197555 (2-(methylsulfonyl)-4-(trifluoromethyl) benzoic acid) was initially detected in the

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0-15 cm soil depth below the LOQ at day 0, increased to a maximum of 3.86 ppb by 7 days (which is equivalent to 5.21 ppb parent equivalents or 20.8% of the theoretical applied pyrasulfotole based on the target application rate), then decreased to below the LOQ by 28-58 days, and was not detected by 120 days posttreatment. AE B197555 was detected in the 15-30 cm soil depth at a maximum concentration of 0.94 ppb at 14 days, in the 30-45 cm soil depth at a maximum concentration of 1.59 ppb at 28 days, and in the 45-60 cm soil depth at a maximum concentration of 0.57 ppb at 28 days. AE B197555 was not detected above the LOQ in soil below the 45-60 cm depth; however, residues were detected below the LOQ to 120 cm, the maximum depth analyzed. The study author-calculated half-life value for AE B197555 was 21 days (p. 22). The reviewer calculated half-life value for AE B197555 residues in the whole soil column was 42.0 days (first order regression; y = 4.664*exp(-0.0165*x); r² = 0.94).

In the <u>cropped test plot</u>, the major transformation product AE B197555 was initially detected in the 0-15 cm soil depth below the LOQ at day 0, increased to a maximum of 2.85 ppb by 7 days (which is equivalent to 3.85 ppb parent equivalents or 14.8% of the theoretical applied pyrasulfotole based on the target application rate), then decreased to below the LOQ by 28-58 days, and was not detected by 120 days posttreatment. AE B197555 was detected in the 15-30 cm soil depth at a maximum concentration of 1.27 ppb at 14 days, and in the 30-45 cm soil depth at a maximum concentration of 0.90 ppb at 28 days. AE B197555 was not detected above the LOQ in soil below the 30-45 cm depth; however, residues were detected below the LOQ to 120 cm, the maximum depth analyzed. The study author-calculated half-life value for AE B197555 was 18 days (p. 22).

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
		2-(Methylsulfonyl)-4-			CS(=O)(=O)c1
AE B197555	142994-06-7	(trifluoromethyl) benzoic	C ₉ H ₇ F ₃ O ₄ S	268.2097	cc(ccc1C(=O)
		acid			O)C(F)(F)F

Data were obtained from Table 11, p. 38 and Figure 1, p. 40 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., 269 days post treatment).		8.8%	11.0%	
Accumulation (residues) in soil at study termination (i.e., 526 days post treatment)		3.1%	11.3%	
Transformation (% of transformation products) ¹		20.9% (day 7)	15.6% (day 14)	
Leaching, if measured (maximum depth detected)	Pyrasulfotole	105-120 cm*	105-120 cm*	
	AE B197555	105-120 cm*	105-120 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. 36-37 of the study report. Determined by reviewer as proportion of total amount of parent equivalents 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).

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

8. PLANT UPTAKE: N/A.

9. LEACHING: Pyrasulfotole and AE B197555 moved into deeper soil layers over time, with residues of both parent and transformation product reaching the lowest soil layer sampled, the 105-120 cm layer (Tables 9-10, pp. 36-37). In the <u>bare test plot</u>, pyrasulfotole reached the 45-60 cm layer by 28 days, the 75-90 cm layer by 58 days, and the 105-120 cm layer by 175 days; residues of pyrasulfotole were not detected above the LOQ in soil below the 75-90 cm layer. Residues of AE B197555 were detected above the LOQ at a maximum depth of 45-60 cm; however, residues were detected below the LOQ to 105-120 cm. In the <u>cropped test plot</u>, pyrasulfotole was detected at levels above the LOQ in the 60-75 cm layer by 58 days, the 90-105 cm layer by 120 days, and the 105-120 cm layer by 269 days. Residues of AE B197555 were detected above the LOQ at a maximum depth of 30-45 cm; however, residues were detected below the LOQ to 105-120 cm.

The high sand content of the soils (approximately 70-90%) and the high water input produced an environment conducive to leaching. Total water input was much greater than historic rainfall for the study site for the duration of the study (478% of the 30-year average). The first significant water input event was a rainfall of approximately 0.5 inches at 2 days posttreatment (Appendix 5, Table 2, p. 111). The test plots received 19.38 cm or 7.63 inches of water over the first 30 days

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

^{*} Maximum depth analyzed.

N/A = Not applicable.

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. 127-128.

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 269 days post treatment), carryover of residues was 8.8% of the applied pyrasulfotole for the bare plot and 11.0% for the cropped plot. By the end of the study period (i.e., 526 days post treatment), 3.1 and 11.3% 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 indicated that pyrasulfotole and the transformation product AE B197555 were stable through 10 months of storage (Appendix 10, p. 193). Corrected recoveries of pyrasulfotole ranged from 110-114% from 0 to 5 months and were 128% at 10 months. Corrected recoveries of AE B197555 ranged from 100-115% 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. REVIEWERS' 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 577 days prior to analysis, while preliminary storage stability data was available only for 10 months of storage (Appendix 10, p. 193). 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 (pp. 18-19). Simple first-order half-lives were 12 days for the bare plot and 69 days for the cropped plot (pp. 20-21). Using the DFOP model, the study author reported a DT50 value for pyrasulfotole of 7 days and a DT90 of 208 days for the bare plot; corresponding DT50 and DT90 values for the cropped plot were 31 days and 246 days. The study author-calculated half-life values for AE B197555 were 21 days for the bare plot and 18 days for the cropped plot (p. 22).

- 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 to AE B197555 and subsequent biodegradation to non-extractable residues and mineralization to CO₂ are the major dissipation pathways for pyrasulfotole (pp. 19-20). 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 and were $93 \pm 6\%$ and $96 \pm 3\%$, respectively (Appendix 3, p. 77).
- 7. Mean recoveries of pyrasulfotole and AE B197555 from fortified control soil samples prepared with each sample set were $78 \pm 11\%$ for pyrasulfotole and $84 \pm 11\%$ for AE B197555 (Table 8, p. 35). The fortification level was not reported for parent or transformation product.
- 8. 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 + metabolite found in the soil column on Day 0. This was done to determine the total amount of residue present in the soil prior to application in the following growing season.
- 9. 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 ½ 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.

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V. REFERENCES

- 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, Washington, DC. EPA 540/9-82-021.
- 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.
- 3. 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.

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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(=0)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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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 000692

PC code

MRID Guideline No. 46801718 164-1

Bare plot 0-15 cm depth

Day 0

Day 269

27.4

11.1

Day 269 Day 526

0.9

3.0

3.3

Day 526

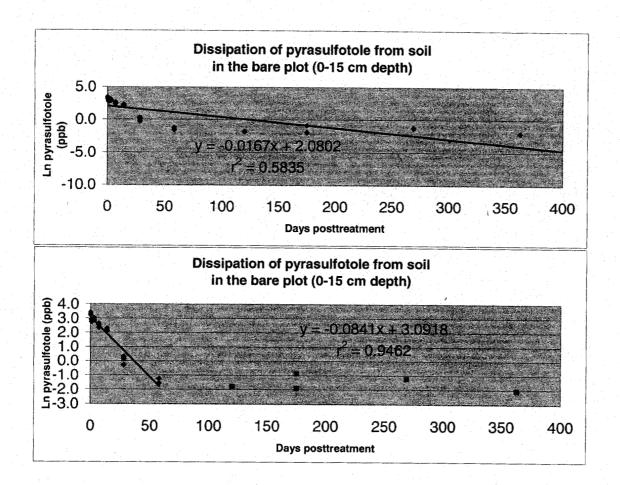
Half-life (days) = 41.5 *Calculated using all available data

Half-life (days) =

8.2

*Calculated using 0-58 day data

Days		Replicate	Pyrasulfotole	Ln Whole soil column		il column	
po	sttreatment	plot	(ppb)	(pyrasulfotole)	Pyrasulfotole (ppb)*	AE B197555 (ppb)**	
	0	1.	25.55	3.24	25.55	0.20	
							Sum of mean
	_				30.03		parent
	0	2	30.06	3.40		0.21	equivalents at
	0	3	25.92	3.26	25.92	0.21	•
	1	1	15.60	0.75	16.50		
	'		15.62	2.75		1.62	
					10.00		% carryover
	1	2 -	10.10	0.00	18.28		(vs. Day 0
	1	3	18.13	2.90		2.18	observed)
	3		18.78	2.93	18.78	2.43	
		1	17.90	2.88	17.90	2.59	
	3	2	20.36	3.01	20.36	3.43	
	3	3	17.51	2.86	17.51	3.70	
	7	S - 1 - 1	12.47	2.52	12.47	4.03	
	7	2	14.08	2.64	14.08	3.94	
	7	3	10.50	2.35	10.50	3.62	
	14	1	8.61	2.15	9.23		
	.14	2	8.38	2.13	8.38	3.82	
	14	3	9.80	2.28		3.32	
	28	1	0.76		9.80	4.29	
	28	2		-0.27	7.39	3.88	
			1.36	0.31	7.34	2.97	
	28	3	1.17	0.16	5.67	3.40	
	58	1	0.29	-1.24	3.99	2.10	
	58	2	ND		3.57	1.27	
	58	3	0.21	-1.56	5.35	1.11	
	120	1	0.16	-1.83	3.54	0.58	
	120	2	ND		2.53	0.69	
	120	3	0.17	-1.77	2.38	0.15	
- 1	175	1	0.42	-0.87	5.29		
	175	2	ND	0.07		0.50	
	175	3	0.15	-1.90	3.26	0.15	
	269	1	0.29	-1.24	4.14	0.14	
	269	2	ND	-1.24	4.56	0.95	
	269	3	ND		1.55	0.42	
	363	1		0.04		0.05	
			0.13	-2.04	2.76	0.13	
	363	2	ND		0.19	0.05	
	363	3	ND		1.30	0.05	
	526	1 .	ND		0.76	0:05	
	526	2	ND		0.14	0.05	
	526	3	ND		1 62	0.05	
Data	obtained fro	m Appendix 8	, Table 1, p. 160	of the study repo	ert.		
* Data	a obtained fro	om Appendix 8	3, Table 2, p. 16:	3 of the study rep	ort		
Shade	d values wer	e non-detects	. set by peer rev	iewer to he 1/2 I	OD (0.1 ug/kg soil)		
ID - 8	Not detected		, co. by poor lev	ionol to be 1/2 Lt	JD (U. I ug/kg son)		



Chemical name Pyrasulfotole PC code Pyrasulfotole 000692 MRID 46801718 Guideline No. 164-1

Bare plot 0-15 cm depth

Day 269

#DIV/0!

Day 526

#DIV/0!

Day 526

#DIV/0!

Half-life (days) = 77.0

*Calculated using all available data
Half-life (days) = 10.1

*Calculated using 0-58 day data

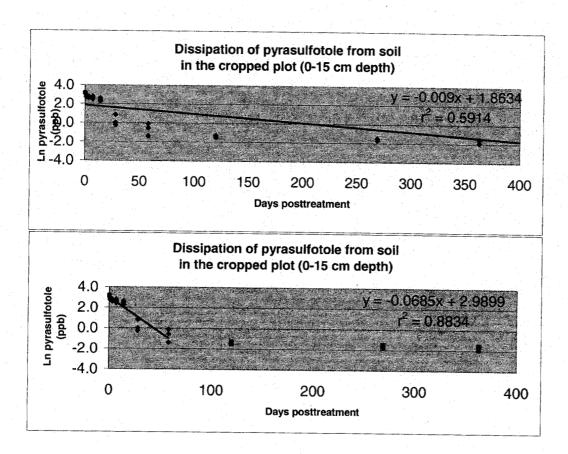
Days posttreatment	Replicate plot	Pyrasulfotole (ppb)	Ln (nyrasulfotole)	Whole so Pyrasulfotole (ppb)*	oil column AE B197555 (ppb)**		
0	1	25.55	3.24	25.55	Ac 6197353 (ppb)***		Day 0
							Day 0
				25.38		Sum of mean	
	_			20.00		parent	
0	2	25.38	3.23			equivalents at	#DIV/0!
. 0	3	21.21	3.05	21.21			
1	1	15.31	2.73	15.31			Day 269
						% carryover	
				18.18		(vs. Day 0	
1	2	18.03	2.89			observed)	#DIV/0!
1	3	18.60	2.92	18.60			
3	1	13.68	2.62	13.68			
3	2	14.70	2.69	14.70			
3	3	16.13	2.78	16.13			
7	1	11.80	2.47	11.80			
7	2	16.16	2.78	16.16			
7	3	14.18	2.65	14.18			
14	1	9.72	2.27	12.87			
14	2	13.50	2.60	13.75			
14	3	11.45	2.44	17.01			
28	1	1.01	0.01	12.14			
28	2	2.34	0.85	10.05			
28	3	0.78	-0.25	11.82			
58	1	0.91	-0.09	8.07			
58	2	0.25	-1.39	19.07			
58	3	0.58	-0.54	5.64			
120	. 1	0.27	-1.31	4.34			
120	2	ND		7.23			
120	3	0.22	-1.51	4.78			
175	1	ND .		3.67	, v		
175	2	ND		1.48			
175	3	ND		1.93			
269	1	ND		3.31			
269	2	0.18	-1.71	1.91			
269	3	0.23	-1.47	2.72	THE STATE OF THE STATE OF		
363	1	ND		1.99			
363	2	0.22	-1.51	2.54	A PARTY AND MAN		,
363	3	0.15	-1.90	2.57	to the company of the party of		
526	. 1	0.24	-1.43	3.32			
526	2	0.16	-1.83	2.85	The Land States		
526	3	0.13	-2.04	1.96			
* Data obtained fro	m Annondiy O	Toble 0 - 400			A CONTRACTOR OF THE PROPERTY OF THE PARTY OF		

^{*} Data obtained from Appendix 8, Table 3, p. 165 of the study report.

** Data obtained from Appendix 8, Table 4, p. 168 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



Days	Replicate	AE B197555
posttreatment	plot	(ppb)
. 0	1	0.24
0	2	0.24
0	3	0.20
1	1	1.99
1	2	1.61
1	3	1.61
3	1	2.09
3	2	2.86
3	3	2.95
7	. 1	2.55
7	2	2.91
7	3	3.11
14	1	2.55
14	2	3.35
14	3	3.43
28	1	2.33
28	2	1.90
28	3	3.02
58	1	0.82
58	2	3.08
58	3	1.84
120	1	0.36
120		0.79
120	3	nd .
175	1	0.37
175	2	0.91
175	3	0.12
269	1	0.12
269	2	nd
269	3	nd
363	1	0.17
363	2	0.13
363	3	nd ·
526	1	nd
526	2	0.11
526	3	nd
	Day 0	Day 269

Sum of mean parent equivalents at

24.4

0.4

vs. vs. Theoretical observed applied

% Carryover at Day 269

1.5

1.5