

US EPA ARCHIVE DOCUMENT

3-16-04

Data Evaluation Report on the phototransformation of penoxsulam in natural water

PMRA Submission Number {.....}

EPA MRID Number 45830722

Data Requirement: PMRA Data Code:
EPA DP Barcode: D288160
OECD Data Point:
EPA Guideline: 161-2

Test material:

Common name: Penoxsulam.
Chemical names:

IUPAC: 6-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy-s-triazolo[1,5-c]pyrimidin-2-yl)- α,α,α -trifluoro-o-toluenesulfonamide
3-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)- α,α,α -trifluorotoluene-2-sulfonamide
CAS : 2-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide.
CAS No: 219714-96-2

Synonyms: XDE-638

SMILES string: n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F

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Company Code:
Active Code:
Use Site Category:
EPA PC Code: 119031

CITATION: Byrne, S.L., S.K. Embrey, R.N. Yoder and D.O. Duebelbeis. 1999. Natural water photolysis and outdoor aerobic aquatic metabolism and photolysis of the experimental rice herbicide XDE-638. Unpublished study performed by Global Environmental Chemistry Laboratory, Dow AgroSciences LLC, Indianapolis, IN; sponsored and submitted by Dow AgroSciences, LLC, Indianapolis, IN. Study ID: GH-C 4932. Study experimental start date May 1998, and experimental end date November 1998 (p.3). Final report issued on July 7, 1999.

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EXECUTIVE SUMMARY

The aqueous phototransformation of [triazolopyrimidine-¹⁴C]6-(2,2-difluoroethoxy)-N-(5,8-dimethoxy-s-triazolo[1,5-c]pyrimidin-2-yl)- α,α,α -trifluoro-o-toluenesulfonamide (penoxsulam, XDE-683) was studied at 23°C outdoors under natural light in both nonsterile pond water at a nominal concentration of 0.1 mg a.i./L for 28 days and in flooded silt loam soil [pH 5.8, organic carbon 0.72%] at 0.1 mg a.i./kg soil for 59 days. The pond water was obtained from an unspecified location in Arkansas. The silt loam soil was obtained from a field in the rice-growing region of Arkansas. This experiment was submitted under USEPA Subdivision N Guideline §161-2, but the guidance used to design the study was not reported. The study was *not* conducted in compliance with USEPA GLP Standards (40 CFR, Part 160). The irradiated natural water test system consisted of tightly capped quartz glass vials (not further described), each containing 10 mL of treated aerated pond water, that were kept in a continuously circulating waterbath. The irradiated flooded soil system consisted of loosely capped quartz glass flasks (50 mL), each containing 10 g (dry weight) of treated soil flooded with 40 mL of aerated pond water, that were kept in a continuously circulating waterbath. The system remained aerobic throughout the study (redox potential of 61.5-248.7 mV). Dark controls for both systems were stored in darkness at 25°C. Volatiles were not collected in either system. Single vials of the irradiated and dark control pond water test solutions were collected after 0, 1, 4, 7, 14, 21, and 28 days. Duplicate flasks of the irradiated flooded soil and dark controls were collected after 0, 1, 4, 11, 25, and 59 days. The water and soil phases were separated by centrifugation with decanting. The water from both experiments was analyzed directly using HPLC, but apparently only the water from the flooded soil was analyzed using LSC. The soil was extracted three times with acetonitrile:water (90:10, v:v), and the soil extracts were pooled and analyzed using HPLC. The extracted soil was analyzed using LSC following combustion. Identification of penoxsulam was done by co-chromatography with an unlabeled reference standard. No reference standards were identified for potential transformation products. Compounds associated with discrete HPLC peaks were further analyzed using MS.

Natural Water: A LSC material balance was not reported for the pond water. Overall average HPLC recoveries were $96.4 \pm 1.4\%$ of the applied for the irradiated samples and $99.0 \pm 0.8\%$ for the dark controls.

In the irradiated natural water, [¹⁴C]penoxsulam decreased from 98% of the applied at time 0 to 49% at 4 days posttreatment, 24% at 7 days, and 4% at 14 days. [¹⁴C]Penoxsulam was not detected at 21 and 28 days. The two major transformation products were D1 (5-OH, 2-amino TP; 8-methoxy[1,2,4]triazolo-[1,5-c]pyrimidin-5-ol-2-amine) and D2 (2-amino TP; 5,8-dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidine-2-amine). D1 was a maximum of 32% of the applied at 14 days posttreatment and decreased to 19% at 28 days (study termination). D2 was a maximum of 17% at 7-14 days and decreased to 10% at 28 days. The three minor transformation products, each present at a maximum of 3-7% of the applied, were D3 (unidentified; MW 220, Rt 15 minutes), D4 [BST; 2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazol-3-yl-6-(trifluoromethyl) benzenesulphonamide], and D5 [BSTCA-methyl; methyl 5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]

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amino]- 1H-1,2,4-triazole-3-carboxylic acid]. An unidentified peak (Rt 7 minutes) believed to consist of multiple polar compounds was a maximum 64% of the applied at 28 days posttreatment.

In the corresponding dark controls, [¹⁴C]penoxsulam was stable, ranging from 98 to 100% of the applied with no pattern of decline during the study. No major or minor transformation products were isolated from the dark controls at quantifiable levels. Volatiles were not collected from either the irradiated samples or the dark controls.

Flooded soil: The overall material balance of the irradiated flooded soil averaged $94.7 \pm 3.5\%$ of the applied and of the dark controls averaged $98.3 \pm 0.7\%$.

In the irradiated flooded soil, [¹⁴C]penoxsulam decreased from 98.6% of the applied at time 0 to 56.8% at 4 days posttreatment, 40.6% at 11 days, and 1.3% at 59 days. The three major transformation products were D1, which was a maximum of 19.4% of the applied at 25 days posttreatment and decreased to 5.5% at 59 days (study termination). D4, which was a maximum of 11.4% at 11 days and decreased to 4.4% at 59 days. D5, which was a maximum of 12.2% at 25 days and decreased to 3.5% at 59 days. The only identified minor transformation product was D2, which was a maximum of 9.4% at 59 days. Two unidentified peaks (Rt 5 and 34 minutes) were maximums of 26.4% and 8.6% of the applied, respectively at 59 days posttreatment.

In the corresponding dark controls, [¹⁴C]penoxsulam decreased from 98.6% at time 0, to 70.8% at 25 days, and 22.0% at 28 days. The major transformation products were D4 and D5, which reached a maximum of 23.3% and 26.9% of the applied, respectively, at 59 days posttreatment. One unidentified peak (Rt 34 minutes) totaled was 1.7% of the applied at 59 days posttreatment. Unextracted [¹⁴C]residues totaled 30.1% of the applied in the irradiated system and 22.4% in the dark control at 59 days. Volatiles were not collected from either system.

Based on first-order linear regression analysis (Excel 2000), penoxsulam degraded in natural water with a calculated half-life of 3.1 days in the irradiated samples, and was stable in the dark controls. In flooded soil, penoxsulam dissipated with a calculated half-life (corrected for dark control) of 14.2 days in the irradiated samples, and 27.7 days in the dark controls.

The study author suggested that the longer half-life in the flooded soil was due to the turbidity of the samples. It was proposed that the suspended soil reduced the amount of light available for photodegradation. However, it is also plausible that the pH of the test system effected the photolytic half-life. At a pH at or above 7, $\geq 99\%$ penoxsulam exists in an ionized form, as calculated from a reported pK_a of 5.1 for penoxsulam. At a pH of 5.8, as reported fro the flooded soil system, only 83% of the penoxsulam exists in an ionized form. The remaining 17% exists as the associated species. It is possible that this change in speciation from the associated to the ionized form could have influenced photodegradation.

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A transformation pathway was proposed by the study author. Penoxsulam is expected to degrade to 5-OH penoxsulam [2-(2,2-difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide; not identified in the current experiment]. Penoxsulam and 5-OH penoxsulam is expected to degrade to D2 (2-amino TP) via cleavage of the sulfonamide bridge. 5-OH Penoxsulam is expected to degrade to D5 (BSTCA-methyl) via degradation of the pyrimidine ring, which in turn is expected to degrade to BSTCA (3-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino]-1H-1,2,3-triazole-5-carboxylic acid; not identified in the current experiment). BSTCA in turn degrades to BST. Although not stated by the study author, significant quantities of polar compounds are formed.

Results Synopsis:

Test medium: Arkansas Pond Water.

Source of irradiation: Natural light.

Half-life/irradiated: 3.1 days (0-21 day data; $r^2 = 0.997$).

Half-life/dark: Stable.

Major and minor transformation products/dark:

None.

Major transformation products/irradiated:

D1 (5-OH, 2-amino TP; 8-methoxy[1,2,4]triazolo-[1,5-c]pyrimidin-5-ol-2-amine).

D2 (2-amino TP; 5,8-dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidine-2-amine).

Minor transformation products/irradiated:

D3 (Unidentified).

D4 [BST; 2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazol-3-yl-6-(trifluoromethyl)benzenesulphonamide].

D5 [BSTCA-methyl; methyl 5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-3-carboxylic acid].

Test medium: Flooded silt loam soil.

Source of irradiation: Natural light.

Half-life/irradiated (corrected for dark control): 14.2 days (0-59 day data; $r^2 = 0.95$).

Half-life/dark: 27.7 days (0-59 days data; $r^2 = 0.9534$).

Major transformation products/dark:

D4 [BST; 2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazol-3-yl-6-(trifluoromethyl)benzenesulphonamide].

D5 [BSTCA-methyl; methyl 5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-3-carboxylic acid].

Minor transformation products/dark:

None

Major transformation products/irradiated:

D1 (5-OH, 2-amino TP; 8-methoxy[1,2,4]triazolo-[1,5-c]pyrimidin-5-ol-2-amine).

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D4 [BST; 2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazol-3-yl-6-(trifluoromethyl) benzenesulphonamide].

D5 [BSTCA-methyl; methyl 5-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony] amino], 1H-1,2,4-triazole-3-carboxylic acid].

Minor transformation products/irradiated:

D2 (2-amino TP; 5,8-dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidine-2-amine).

Study Acceptability: This study is classified as supplemental. The study is scientifically valid, but cannot be used to satisfy the requirement for a photodegradation in water because the study was conducted using either nonsterile unbuffered pond water or flooded soil (4:1 water:soil ratio). In addition, environmental conditions during outdoor incubation were not adequately described (i.e., cloud cover, hours of sunlight) and it was not certain that all transformation products present $\geq 10\%$ were identified.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: The guidance used to design the study was not reported. Significant deviations from the Subdivision N guidelines were:

The study was conducted using either nonsterile unbuffered pond water or flooded soil. This does not affect the validity of the study.

It is not certain that all transformation products present at $>10\%$ were identified. HPLC peaks at 5 and 7 minutes that totaled up to 26 and 64% of the applied, respectively, were assumed to consist of polar compounds and were not analyzed further. This does not affect the validity of the study.

Characteristics of the natural sunlight, such as cloud cover and hours of daylight, were not described. This does not affect the validity of the study.

COMPLIANCE: The study was not conducted in compliance with USEPA GLP Standards (40 CFR, Part 160; p.3). Signed and dated GLP, Quality Assurance, Data Confidentiality and statements were provided (pp.2-4). A Certificate of Authenticity was not provided.

A. MATERIALS

1. Test Material

[¹⁴C]Penoxsulam (p.11).

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Chemical Structure: See DER Attachment 2.

Description: Not provided.

Purity: Radiochemical purity: 98.3% (p.11).
 Lot No.: 1352
 Analytical purity: Not provided.
 Specific activity: 25.65 mCi/mMol (117,800 dpm/μg).
 Location of the radiolabel: Labeled on the triazolopyrimidine moiety.

Storage conditions of test chemicals: Not reported.

Physico-chemical properties of penoxsulam.

Parameter	Values	Comments
Water solubility	42 ppm. 13,000 ppm	At pH 5.3; At pH 7.7.
Molecular formula	C ₁₆ H ₁₄ F ₅ N ₅ O ₅ S	
Molecular weight	483.38	
Vapor pressure	Not reported.	
UV absorption	254 nm	
pK _a	Not reported.	
K _{ow} /log K _{ow}	Not reported.	
Melting point	Not reported.	
Log K _{oc} :	Not reported.	
Stability of compound at room temperature	Not reported.	

Data obtained from pp.11, 16 in the study report.

2. Buffer Solution:

Table 1a: Description of buffer solution.

pH	Type and final molarity of buffer	Composition
Natural pond water was used. Information about the pond water, such as collection procedures and physical and chemical properties, were not provided.		

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Table 1b: Properties of the soil.

Property	Details
Soil texture:	Silt loam (from Arkansas).
% sand:	8.8
% silt:	68.0
% clay:	23.2
pH:	5.8
Organic carbon (%):	0.72
CEC (meq/100 g soil):	6.97
Moisture	13.94
Bulk density, disturbed (g/cm ³):	1.11
Soil Taxonomic classification:	Not reported.
Soil Mapping Unit:	Not reported.

Data obtained from p.13 of the study report.

3. Details of light source:

Table 2: Artificial light source.

Property	Details
Type of lamp used:	Not applicable.*
Emission wavelength spectrum:	Not applicable.*
Light intensity:	Not applicable.*
Filters used:	Not applicable.*
Relationship to natural sunlight:	Not applicable.*

* The pond water and flooded soil samples were incubated outdoors and exposed to natural sunlight. The study authors did not describe the cloud cover or report the hours of sunlight per day. The intensity of the light reaching the samples was measured using an actinometer.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: A preliminary study was conducted to determine if penoxsulam should be applied to the water or soil phases (p.13). Four soil and two water samples used for flooding were spiked with penoxsulam. Two soils were flooded immediately and two were flooded

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four days later. Samples were maintained in the dark at 25°C (p.14). After 11 days, the spiked soil samples had 73.4% of the applied in the water phase (Table I, p.32). In the spiked water samples, 89.3% remained in the water phase after 7 days. Penoxsulam primarily partitioned to the water phase regardless of the application site or the time to flooding (p.22).

2. Experimental conditions:

Table 3: Experimental design.

Parameter		Details
Duration of the test: Natural water: Flooded soil:		28 days 59 days
Application rate: Nominal Measured Natural water Flooded soil		0.10 ppm 0.132 mg a.i./L 0.124 mg a.i./kg
Dark controls used (Yes/No):		Yes.
Replications	Dark controls: Natural water Flooded soil	None. Only one sample was collected at each sampling interval. Duplicate.
	Irradiated: Natural water Flooded soil	None. Only one sample was collected at each sampling interval. Duplicate.
Preparation of the test medium:	Volume used/treatment: Natural water Flooded soil	300 mL of pond water were treated, and 10 mL aliquots were transferred to individual vials. 1.5 L of pond water were treated, and 40 mL aliquots were used to flood individual 10 g soil samples.
	Method of sterilization:	The samples were not sterile
	Co-solvent, if any:	Acetonitrile, <1% by volume.
Test apparatus (Type/material/volume):	Dark controls:	Dark controls were incubated in the dark at 25°C.
	Irradiated: Natural water Flooded soil	Quartz vial were tightly capped and incubated outdoors in a waterbath at ca. 23°C. Quartz jars were loosely capped and incubated outdoors in a waterbath at 23°C

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Parameter		Details
Details of traps for CO ₂ and organic volatiles, if any:		Volatiles were not trapped.
If no traps were used, is the system closed/open?		Closed.
Any indication of the test material adsorbing to the walls of the test apparatus?		None.
Experimental conditions.	Temperature (°C):	ca. 23°C.
	Duration of light/darkness:	The samples were irradiated under natural sunlight. The hours of sunlight/day were not reported.
Other details, if any:		None.

Data obtained from pp.12-14 in the study report.

3. Supplementary experiments: In an attempt to generate sufficient material to identify transformation products, a flask of HPLC grade water (50 mL) was treated with 0.5 mL of penoxsulam in acetonitrile and incubated under a xenon lamp (p.16). After 7 days, the sample was moved outdoors for 2 additional days. Then the sample was neutralized with 0.1N NaOH to increase the solubility of penoxsulam and incubated outdoors for an additional 3 days (p.17). Finally, the sample was partitioned with MTBE. The aqueous phase was neutralized to pH 12 with 2N NaOH, partitioned with MTBE, acidified to pH 2 with 2N HCl and partitioned with MTBE. Aliquots of the MTBE extracts were analyzed by LSC and HPLC. The initial MTBE extract was subjected to fractionation using HPLC. The fractions were analyzed using LC/MS.

In order to determine the amount of light energy received by the definitive study samples, a dosing solution was prepared containing $1 \times 10^{-3}M$ *p*-nitroacetophenone (PNAP) and $1 \times 10^{-2}M$ pyridine (p.17). To simulate the flooded soil study, aliquots (40 mL) of the dosing solution were added to quartz flasks (50 mL) and placed in a shallow plastic container (p.18). To simulate the natural pond water study, aliquots (10 mL) of the dosing solution were added to quartz tubes (10 mL) and placed outdoors in a waterbath at 23°C. Samples were collected at approximately weekly intervals. Following collection, samples were wrapped in foil and refrigerated until analysis.



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4. Sampling:

Table 4: Sampling details.

Parameters	Details
Sampling intervals: Natural water Flooded soil	0, 1, 4, 7, 14, 21, 28 days. 0, 1, 4, 11, 25, 59 days.
Sampling method:	Entire vials/flasks were collected at each sampling interval.
Method of collection of volatile compounds, if any:	Volatiles were not collected.
Sampling intervals/times for: Sterility check: pH measurement:	Not applicable. Not reported.
Sample storage before analysis:	Not reported.
Other observations, if any:	None

Data obtained from Table III, p.34, Table IV, p.35, and Table VI, p.37 of the study report.

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods, if used: The flooded soils were swirled, then the water and soil phases were separated by centrifuging and decanting. Natural pond water samples and the aqueous portion of the flooded silt loam soils were analyzed by LSC and HPLC as collected, without manipulation or modification (pp.15, 16).

The soil was extracted three times with acetone:water (90:10, v:v) by shaking (33 mL/extraction; p.15). After each extraction, the samples were centrifuged and the supernatant removed. The extracts were combined and brought to 100 mL volume. Aliquots of the combined extract were analyzed for total radioactivity by LSC. The extract was then concentrated to dryness using rotary evaporation under vacuum, reconstituted in acetonitrile, brought to volume with water, and analyzed LSC and HPLC.

Volatile residue determination: Volatiles were not collected.

Total ^{14}C measurement: In the flooded soil, total ^{14}C was determined by summing the concentration of residues in the water, extracts, and extracted soil (Table III, p.34). In the natural pond water, total ^{14}C was the concentration in the water.

Nonextractable residue determination: The extracted flooded soil was analyzed for total radioactivity by LSC following combustion (p.19).

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

Identification and quantification of the parent: The samples were analyzed for penoxsulam using HPLC under the following conditions (pp.19-20): YMC ODS-AQ column (4.6 x 250 mm; 5 μ); **System 1:** gradient mobile phase consisting of (A) water with 1% acetic acid and (B) acetonitrile with 1% acetic acid [percent A:B (v:v) 0 minutes, 75:25, linear gradient to 30 minutes 25:75, 40 minutes re-equilibration, 50 minutes end]; **System 2:** [percent A:B (v:v) 0 minutes, 95:5, linear gradient to 30 minutes 0:100, 40 minutes re-equilibration, 50 minutes end]; flow rate 1.0 mL/minute, and UV detection. Penoxsulam was identified by comparison to the retention time of a penoxsulam reference standard that was cochromatographed with the samples.

Identification and quantification of transformation products: Transformation products were isolated and quantified using HPLC as described for the parent (p.19). No reference standards were reported.

Detection limits (LOD, LOQ) for the parent: The limits of detection were not reported. The LSC limit of quantification in the flooded soil study was 0.65% of the total recovered. The HPLC limit of quantification was 38 dpm (Tables III-V, pp.34-36).

Detection limits (LOD, LOQ) for the transformation products: The limits of detection and quantitation were not reported.

II. RESULTS AND DISCUSSION:

A. TEST CONDITIONS: The incubation temperatures were reported to be approximately 23°C during both studies. No supporting data were provided (pp.14, 15).

The pH for the natural pond water was not reported.

In the flooded soil, the pH of the solutions was ranged from 6.6-7.7 in the irradiated samples and 5.9-7.5 in the dark controls (Table II, p.33). The redox potentials ranged from 61.5-199.5 in the irradiated samples and 139.2-248.7 in the dark controls. Dissolved oxygen levels ranged from 2.2-8.1 mg/L in the irradiated and 1.7-7.2 mg/L in the dark controls.

B. MATERIAL BALANCE: An LSC material balance was not reported for the natural water. The calculated recoveries from the HPLC data averaged $96.4 \pm 1.4\%$ of the applied in the irradiated samples. Dark controls averaged $99.0 \pm 0.8\%$ (calculated from Table VI, p.37). The material balance of the irradiated flooded soil [^{14}C]penoxsulam was $94.7 \pm 3.5\%$ of the applied. The material balance of the dark controls averaged $98.3 \pm 0.7\%$ (calculated from Table III, p.34, Table IV, p.35).



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Table 5a: Phototransformation of [¹⁴C]penoxsulam in natural water expressed as percentage of applied radioactivity.

Compound		Sampling times (days)						
		0	1	4	7	14	21	28
Penoxsulam (XDE-638)	Irradiated	98	90	49	24	4	ND	ND
	Dark	98	99	100	99	99	98	100
7 minute (retention time)	Irradiated	ND	ND	5	10	30	48	64
	Dark	ND	ND	ND	ND	ND	ND	ND
D1 (5-OH, 2-amino TP)	Irradiated	ND	6	19	31	32	26	19
	Dark	ND	ND	ND	ND	ND	ND	ND
D2 (2-amino TP)	Irradiated	ND	1	12	17	17	14	10
	Dark	ND	ND	ND	ND	ND	ND	ND
D3 (MW 220) (No structure)	Irradiated	ND	ND	2	6	7	6	4
	Dark	ND	ND	ND	ND	ND	ND	ND
D4 (BST)	Irradiated	<LOQ	<LOQ	6	6	5	3	<LOQ
	Dark	ND	ND	ND	ND	<LOQ	<LOQ	<LOQ
D5 (BSTCA-methyl)	Irradiated	ND	<LOQ	1	3	<LOQ	ND	<LOQ
	Dark	ND	ND	ND	ND	<LOQ	ND	ND
Volatiles	Irradiated	Volatiles were not collected.						
	Dark	Volatiles were not collected						
Total Recovery*	Irradiated	98	97	94	97	95	97	97
	Dark	98	99	100	99	99	98	100

Data were obtained from Table VI, p.37 in the study report. Only a single value was reported for each sampling interval.

* Total recovery was calculated by adding the HPLC data points.

LOQ = 38 dpm, 0.65% TRR.

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Table 5b: Phototransformation of [¹⁴C]penoxsulam in flooded soil expressed as percentage of applied radioactivity (mean ± s.d., n = 1-2).

Compound		Sampling times (days)					
		0	1	4	11	25	59*
Penoxsulam (XDE-638)	Irradiated	98.6	76.3	56.8	40.6	6.0	1.3
	Dark	98.6	94.8	94.4	87.8	70.8	22.0
5 minute (retention time)	Irradiated	ND	12.1	19.8	6.9	23.1	26.4
	Dark	ND	<LOQ	ND	ND	ND	ND
D1 (5-OH, 2-amino TP)	Irradiated	ND	<LOQ	3.4	14.9	19.4	5.5
	Dark	<LOQ	ND	ND	ND	ND	ND
D2 (2-amino TP & unknown MW 220)	Irradiated	ND	<LOQ	0.8	5.4	7.9	9.4
	Dark	ND	ND	<LOQ	ND	<LOQ	ND
D4 (BST)	Irradiated	ND	1.8	2.0	11.4	0.3	4.4
	Dark	ND	<LOQ	<LOQ	<LOQ	8.2	23.3
D5 (BSTCA-methyl)	Irradiated	ND	0.3	0.2	4.6	12.2	3.5
	Dark	ND	0.8	2.2	7.4	14.2	26.9
Total dissolved (Water layer)	Irradiated	98.6 ± 0.6	89.3 ± 0.3	72.6 ± 0.7	78.4 ± 0.9	69.6 ± 0.4	62.7 ± 3.9
	Dark	98.6 ± 0.6	91.8 ± 0.3	95.3 ± 0.0	93.8 ± 0.3	88.9 ± 0.2	76.2 ± 1.3
Soil extract	Irradiated	0.3 ± 0.0	4.6 ± 0.7	9.5 ± 0.6	5.9 ± 0.1	2.3 ± 0.1	0.9 ± 0.8
	Dark	0.3 ± 0.0	4.8 ± 0.0	1.3 ± 0.3	1.3 ± 0.3	1.5 ± 1.7	0.3 ± 0.0
Unextracted	Irradiated	0.4 ± 0.1	2.2 ± 0.2	6.7 ± 0.4	12.3 ± 0.8	23.0 ± 0.2	30.1 ± 6.0
	Dark	0.4 ± 0.1	0.5 ± 0.0	1.6 ± 0.1	3.5 ± 0.4	8.7 ± 1.1	22.4 ± 1.6
Volatiles	Volatiles were not collected.						
Total Recovery	Irradiated	99.0 ± 0.5	96.1 ± 0.6	88.8 ± 0.3	96.5 ± 0.2	94.8 ± 0.2	93.4 ± 3.3
	Dark	99.0 ± 0.5	97.0 ± 0.3	98.2 ± 0.2	98.6 ± 0.1	98.9 ± 0.6	98.4 ± 0.0

Data were obtained from Tables III-V, pp.34-36 in the study report. Only a single value was reported for [¹⁴C]residue identification at each sampling interval. Means and sd for total dissolved, soil extract, unextracted residues and total recovery were calculated by the reviewer.

* It was reported that on day 59, an additional peak was detected at 34 minutes and was 8.6% of the applied in the irradiated samples and 1.7% in the dark controls.

LOQ = 38 dpm; 0.65% TRR.

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Data Evaluation Report on the phototransformation of penoxsulam in natural water

PMRA Submission Number {.....}

EPA MRID Number 45830722

C. TRANSFORMATION OF PARENT COMPOUND: In the natural water dark controls, [¹⁴C]penoxsulam remained stable at 98% of the applied at time 0 and was 100% at 28 days posttreatment (Table VI, p.37). In the irradiated natural water, [¹⁴C]penoxsulam was 98% of the applied at time 0, 49% at 4 days posttreatment, 24% at 7 days, and was last detected at 4% at 14 days.

In the flooded soil dark controls, [¹⁴C]penoxsulam decreased from 98.6% of the applied at time 0 to 22.0% at 28 days posttreatment (Table V, p.36). In the irradiated flooded soil, [¹⁴C]penoxsulam decreased from 98.6% of the applied at time 0, to 56.8% at 4 days posttreatment, 40.6% at 11 days, and was 1.3% at 59 days.

HALF-LIVES: Based on first-order linear regression analysis (Excel 2000), penoxsulam dissipated in natural water with a calculated half-life of 3.1 days in the irradiated samples. Dark controls were stable. In flooded soil, penoxsulam dissipated with a calculated half-life of 14.2 days in the irradiated samples (corrected for dark controls) and 27.7 days in the dark controls.

The irradiated half-life in natural water calculated by the reviewer differed slightly from that calculated by the study author (3.8 and 2.9 days, respectively; DER attachment 1 and Figure 7, p.46). The study author stated that, based on the results from the actinometer, the natural water samples received only half the expected light energy, so the results were adjusted to approximate the intensity of light at 40°N latitude (pp.22, 23). The half-lives in flooded soil calculated by the study author were similar to the reviewer's values.

Half-lives*

Test system	First order linear			DT50	DT90
	Half-life (days)	Regression equation	r ²		
Irradiated					
Natural water	0-28 day data: 3.07 days	$y = -0.226x + 4.6841$	0.997	ND	ND
Flooded soil (dark corrected)	0-59 day data: 14.17 days	$y = -0.0739x + 4.3527$	0.95	ND	ND
Dark					
Natural water	Stable				
Flooded soil	0-59 day data: 27.73 days	$y = -0.025 + 4.6694$	0.9534	ND	ND

*Half-lives for irradiated samples calculated using data obtained from Table V, p.36, Table VI, p.37 of the study report.

ND = Not Determined.

TRANSFORMATION PRODUCTS:

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Natural water: In the irradiated system, two major transformation products were detected (pp.27-28, Table VI, p.37). D1 was a maximum of 32% of the applied at 14 days posttreatment and decreased to 19% at 28 days (study termination), and D2 was a maximum of 17% at 7-14 days and decreased to 10% at 28 days. Three minor transformation products were isolated: D3 (MW 220, Rt 15 minutes), D4 (MW 372), and D5 (MW 430). D3 was a maximum of 7% at 14 days and decreased to 4% at 28 days. D4 was a maximum of 6% at 1-4 days and was below the limit of quantification at 28 days. D5 was a maximum of 3% at 7 days and was below the limit of quantification thereafter. An unidentified peak (Rt 7 minutes), which was believed to consist of multiple polar compounds, was a maximum 64% of the applied at 28 days posttreatment.

Flooded soil: In the irradiated system, three major transformation products were detected (Table V, p.36). D1 was a maximum of 19.4% of the applied at 25 days posttreatment and decreased to 5.5% at 59 days (study termination). D4 was a maximum of 11.4% at 11 days and decreased to 4.4% at 59 days. D5 was a maximum of 12.2% at 25 days and decreased to 3.5% at 59 days. The only minor transformation product, D2, was a maximum of 9.4% of the applied at 59 days posttreatment. Two unidentified peaks (Rt 5 and 34 minutes) were a maximum 26.4% and 8.6% of the applied, respectively at 59 days posttreatment.

In the corresponding dark controls, D4 and D5 were a maximum of 23.3% and 26.9% of the applied, respectively at 59 days posttreatment. One unidentified peak (Rt 34 minutes), was 1.7% at 59 days.

Table 6: Chemical names for the transformation products of penoxsulam.

Applicant's Code Name	CAS Number	Chemical Names	Chemical formula	Molecular weight (g/mol)	Smiles string
D1; 5-OH, 2-amino TP		8-Dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidin-5-ol-2-amine		181	
D2; 2-amine TP		5,8-Dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidine-2-amine		195	
D3		No structure was provided.		220	
D4; BST		2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazol-3-yl-6-(trifluoromethyl) benzenesulphonamide		372	
D5; BSTCA-methyl		Methyl 3-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphony]amino], 1H-1,2,4-triazole-5-carboxylic acid		430	

Only structures and molecular weights were provided by the study author. Chemical names were determined by comparing the provided structures and mw with those presented in MRIDs 45830724 and 45830722.

VOLATILIZATION: Volatiles were not measured.

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TRANSFORMATION PATHWAY: A theoretical transformation pathway was provided by the study author (Figure 12, p.51). Penoxsulam is proposed to degrade into 5-OH penoxsulam (2-(2,2-difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl) benzenesulfonamide; not identified in the current experiment). Penoxsulam degraded to D2 (2-amino TP) via cleavage of the sulfonamide bridge. D2 and 5-OH penoxsulam degrades to D1. 5-OH Penoxsulam is proposed to degrade into D5 (BSTCA-methyl) via degradation of the pyrimidine ring, which in turn degrades to BSTCA (3-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulphonylamino]-1H-1,2,3-triazole-5-carboxylic acid; also not identified in the current experiment). BSTCA in turn degrades to BST. Although not stated by the study author, significant quantities of polar compounds are formed.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: In the degradate isolation study, four transformation products were tentatively identified. D1 (Rt 11-12 minutes) was the only transformation product in the aqueous phase following partitioning. It's molecular weight is 181 (p.26). The transformation products D2, D4 and D5 had a molecular weights of 195, 372 and 430, respectively (pp.27-28). Structures but not chemical names were provided for these compounds. The transformation product D3 had a Rt of 15 minutes and a molecular weight of 220. However, a tentative structure was not assigned.

The theoretical half-life for the actinometer was 7 days. The actual half-life for the flooded soil was 7.5 days (p.22). The half-life for the natural water was 14 days. The study author suggested that the reduction in light could be due to filtration by the water bath, the shape of the sample container, or the positioning of the samples.

III. STUDY DEFICIENCIES:

1. The experiments were conducted using either nonsterile unbuffered pond water or flooded soil (4:1 soil:water ratio). Subdivision N guidelines specify that sterile buffered water should be used in a photodegradation in water study. Also, photodegradation on soil studies are typically done using unflooded soil, and metabolism studies must be conducted in darkness.
2. It is not certain that all transformation products present at >10% were identified. HPLC peaks with retention times of 5 and 7 minutes totaled up to 26 and 64% of the applied, respectively. These were assumed to consist of multiple polar compounds and were not further analyzed. The study author should have determined whether these peaks were, in fact, comprised of multiple compounds and whether any of the compounds was present at >10% of the applied.
3. The study authors did not demonstrate that the degradates formed and identified by MS in the supplementary experiment were equivalent to the degradates formed in the definitive study. The conditions of the study were very different from the conditions of the definitive study.

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The authors stated that the degradate isolation study used HPLC grade water (without soil) rather than natural pond water to reduce the number of clean-up steps required. However, the natural water samples were analyzed directly by LSC and HPLC, so it is not clear what clean-up steps the study authors were referring to (p.16).

Initially the HPLC grade water was incubated indoors using a xenon lamp, however, degradation was proceeding too slowly, therefore, the samples were moved outdoors in an attempt to speed the process up. The authors did not report the temperature (indoors or outdoors) or the xenon/sunlight duration or intensity.

Also, the pH was neutralized from 4 to approximately 7.7 due to low solubility of penoxsulam. The pH of the natural water systems was not reported and could not be compared.

The authors noted that not all of the penoxsulam was available for photolysis. No further explanation was provided.

4. Structures were provided for D1, D2, D4, and D5, but chemical names were not provided. Chemical names were determined by comparing the structures of these degradates to structures of reference compounds used in other studies in this data package. The structure for D3 was not provided.

IV. REVIEWER'S COMMENTS:

1. The contribution from the dark control system was removed from the empirical photolytic half-life from the flooded soil system using the method outlined in Part C of the EPA OPP draft document, *Guidance for Chemistry and Management Practice Input Parameters For Use in Modeling the Environmental Fate and Transport of Pesticides* for calculating aqueous photolysis half-lives in the presence of a significant contribution from hydrolysis ($k_{\text{total hv}} - k_{\text{dark}} = k_{\text{hv}}$). The resulting adjusted, photolytic half-life was calculated to be 14.2 days ($\text{time}_{1/2} = \ln 2 / k_{\text{hv}} = \ln 2 / 0.0489$)
2. In MRID 45830721, the hydrolysis of [triazolopyrimidine-¹⁴C]- and [phenyl-¹⁴C]- labeled penoxsulam were studied at 25°C for 30 days in sterile aqueous buffer solutions at pH 5 (acetate), pH 7 (piperazineethanesulfonic acid), pH 9 (borate), and in natural water (pH 8.0; from White River, Indiana) at a nominal application rate of 1 mg/L. Penoxsulam was stable in all buffer solutions and in the natural water.
3. The study author stated that, based on the results from the actinometer, the natural water samples received only half the expected light energy, so the results should be adjusted to approximate the intensity of light at 40°N latitude (pp.22, 23). Subdivision N guidelines do not

Data Evaluation Report on the phototransformation of penoxsulam in natural water

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EPA MRID Number 45830722

specify that studies conducted under natural light conditions should be adjusted so as to be equivalent to 40°N latitude, but only that climatological conditions be defined. However, the temperature, humidity, cloud conditions, and hours of sunlight per day were not reported as required by Subdivision N Guideline §161-2. Characteristics of the natural sunlight, such as cloud cover and hours of daylight, were not described.

4. For the natural pond water, the study author only reported the HPLC data. It appeared that the material balance was never determined by LSC.
5. For the flooded soils, the study author noted that noted peak D2, which appeared as a single peak in HPLC system 1, separated into two components (MW 195 and 220) using HPLC system 2 (Table V, p.36). However, only the data for the combined D2 were reported. In the natural water study, the data from HPLC method 2 are reported and the two components (D2 and D3) are reported as separate compounds (Table VI, p.37). The study author does not state why the two systems are handled differently. This reviewer suspects that the difference is due to the fact that in the flooded soil, the combined D2 has a maximum concentration of <10% of the applied, while in the natural water, the combined D2 (actually D2 plus D3) has a maximum concentration of 24% of the applied. The structure of D3 was not determined and identification is not required. However, it would have been useful if the individual concentrations of D2 and D3 in the flooded soil had been provided.
6. Although not stated, it appeared that only one sample was collected at each sampling interval in the natural water portion of the study. At least two samples should be collected at each sampling interval, in part to allow the reviewer to assess the variation between replicates. In the flooded soil portion of the study, the study author specifically states that duplicate samples were prepared, and provides two data points for each sampling interval in Table IV (p.35). However, in the flooded soil portion of the study, only a single value is provided for [¹⁴C]residue identification. It could not be determined if this represented a mean of the two samples or if only one extract was analyzed by HPLC at each sampling interval.
7. The incubation temperature was reported to be approximately 23°C. More detailed information was not provided. It is preferred that the minimum, maximum, and average temperatures be reported, and any significant deviations from the average and their duration should be noted.
8. Dark controls were maintained at 25°C. Subdivision N guidelines specify that the irradiated and dark controls samples should be held at the same temperature.
9. In MRID 45834801, the aqueous phototransformation of [triazolopyrimidine-3-¹⁴C]- and [phenyl-U-¹⁴C]- labeled penoxsulam were studied at 25°C in lake water from England for 28 days at a nominal concentration of 0.15 µg a.i./mL under continuous irradiation using a UV-filtered xenon arc lamp. The half-life of penoxsulam (combined labels) was 0.36 days in natural water, based on the continuous irradiation used in the study. No degradation occurred in the

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EPA MRID Number 45830722

dark control. The predicted environmental phototransformation half-life in both the buffer solution and natural water is slightly less than 1.5 day. Major transformation products were TPSA, which was a maximum 56.0% of the applied, 5-OH, 2-amino TP, which was a maximum 23.4% at 14 days), 2-amino TP (which was a maximum 17.8% at 3 days), and BSA (which was a maximum 33.5% of the applied at 1.5 days). Minor identified transformation products were BSTCA, BSTCA-methyl, and di-FESA. Polar compounds comprised >70% of the applied by 28 days.

10. The day 0 soil samples were initially extracted with acetone:0.1N HCl. However, penoxsulam was found to be unstable at low pH and higher temperatures (p.15). The authors recommended that penoxsulam not be extracted with an acid, or if extracted with an organic acidic solvent, then removal of the acid prior to concentration is recommended (p.29).
11. The Limits of Detection were not reported. Limits of Detection and Quantification should be reported to allow the reviewer to evaluate the adequacy of the test method.
12. The study authors state that the flooded soil was sampled on day 60. However, the data tables indicate that the samples were collected at 59 days.
13. No transformation product reference standards were reported.
14. The soil remained aerobic during the course of the study. However, the study authors noted that the dark controls separated into two layers with the bottom layer appearing less aerobic (gray) using the Munsell color chart (p.23).
15. An aqueous storage stability study (MRID 45830803) indicated that penoxsulam did not significantly degrade after 130 days of refrigerated storage (average recovery 100.7% of applied) or 221 days of frozen storage (average recovery 96.0%), while recoveries of 5-OH-XDE-638 and BSTCA after 284 days of refrigerated storage averaged 99.7% and 90.7%, respectively (Tables 2-3, pp.28-35 in MRID 45830803). BSTCA-methyl and 5,8-diOH were not tested.

V. REFERENCES:

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 161-2. Photolysis studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.
2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.

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

20

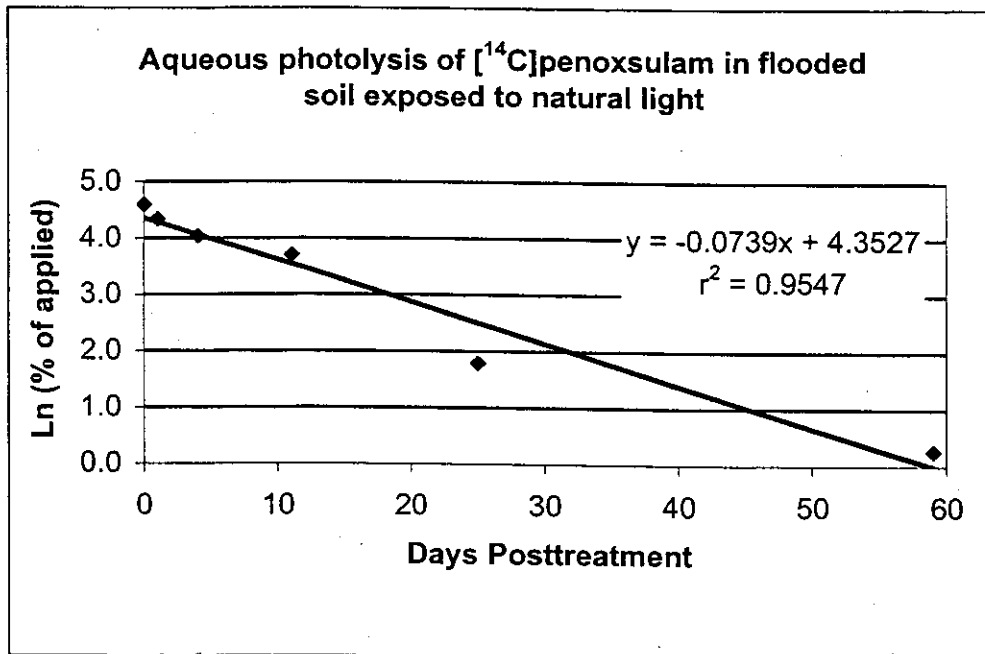
Attachment 1
Excel Spreadsheets

Chemical: Penoxsulam
MRID: 45830722
PC: 119031
Guideline No.: 161-2

Irradiated Flooded soil
Half-life (days) = 9.38

Interval (days)	Penoxsulam (% of applied)	Ln (% of applied)
0	98.6	4.5911
1	76.3	4.3347
4	56.8	4.0395
11	40.6	3.7038
25	6.0	1.7918
59	1.3	0.2624

Data obtained from Table V, p. 36 in the study report.



22

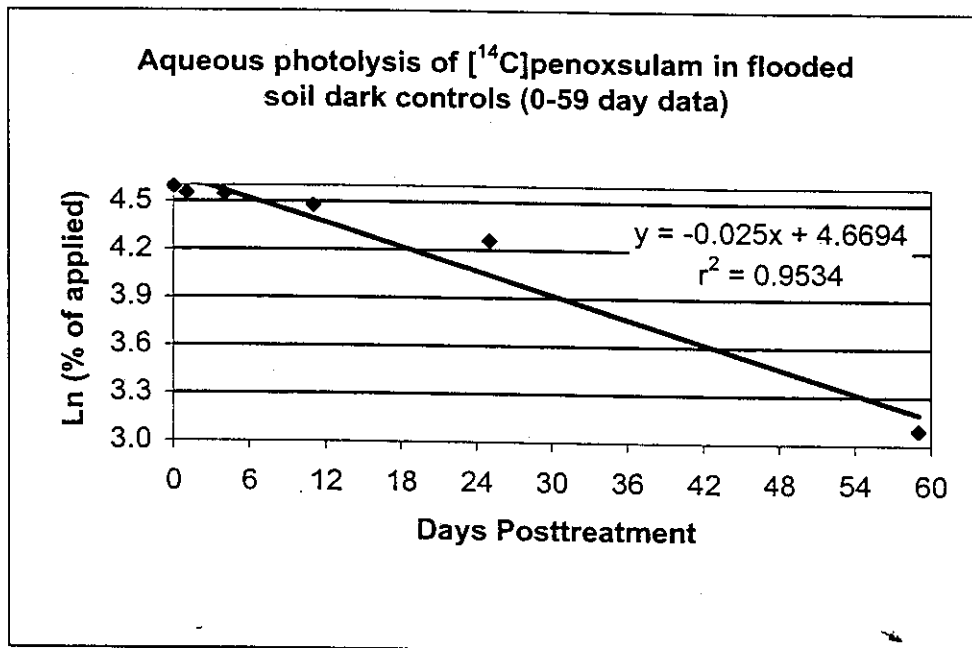
Chemical: Penoxsulam
MRID: 45830722
PC: 119031
Guideline No.: 161-2

Dark Flooded soil

Half-life (days) = 27.73

Interval (days)	Penoxsulam (% of applied)	Ln (% of applied)
0	98.6	4.5911
1	94.8	4.5518
4	94.4	4.5475
11	87.8	4.4751
25	70.8	4.2599
59	22.0	3.0910

Data obtained from Table V, p. 36 in the study report.



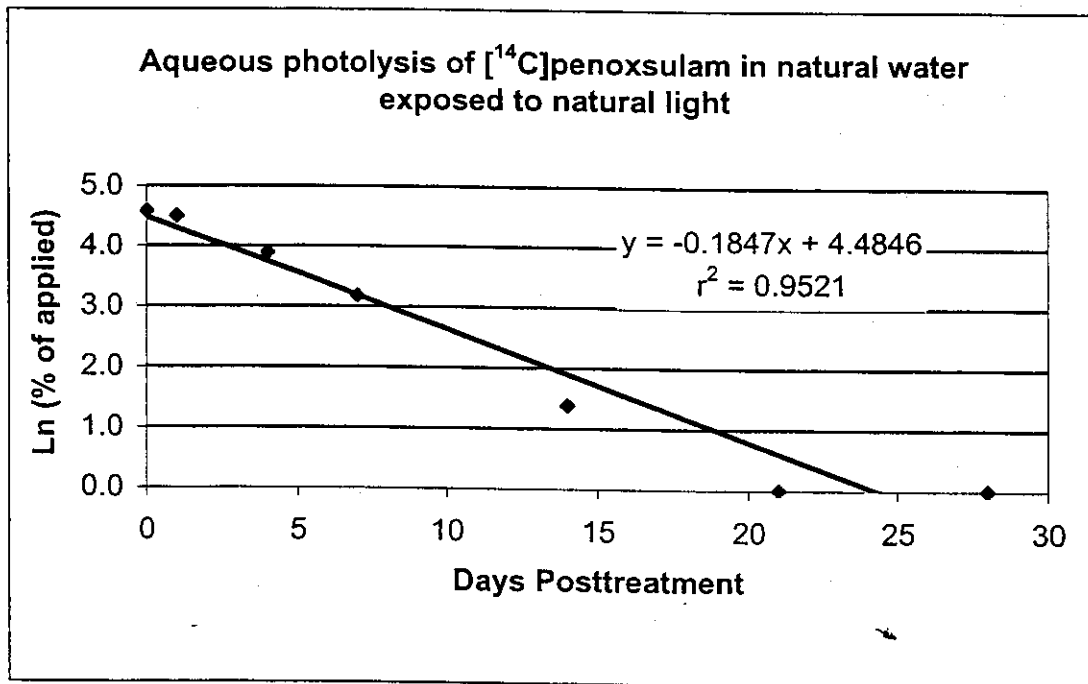
23

Chemical: Penoxsulam
MRID: 45830722
PC: 119031
Guideline No.: 161-2

Natural Water
Half-life (days) = 3.75

Interval (days)	Penoxsulam (% of applied)	Ln (% of applied)
0	98.0	4.5850
1	90.0	4.4998
4	49.0	3.8918
7	24.0	3.1781
14	4.0	1.3863
21	0.0	#NUM!
28	0.0	#NUM!

Data obtained from Table VI, p. 37 in the study report.



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Chemical: Penoxsulam
 MRID: 45830722
 PC: 119031

**Flooded soil
 Irradiated**

Days	Water		Soil		Total
	layer	extract	extract	soil	
0	98.2	0.3	0.3	0.4	98.6
0	99.0	0.3	0.3	0.3	99.3
average	98.6	0.3	0.3	0.4	99.0
sd	0.6	0.0	0.0	0.1	0.5
1	89.1	5.1	2.3	2.3	96.5
1	89.5	4.1	2.0	2.0	95.6
average	89.3	4.6	2.2	2.2	96.1
sd	0.3	0.7	0.2	0.2	0.6
4	73.1	9.1	6.4	6.4	88.6
4	72.1	9.9	7.0	7.0	89.0
average	72.6	9.5	6.7	6.7	88.8
sd	0.7	0.6	0.4	0.4	0.3
11	77.7	5.8	12.8	12.8	96.3
11	79.0	6.0	11.7	11.7	96.6
average	78.4	5.9	12.3	12.3	96.5
sd	0.9	0.1	0.8	0.8	0.2
25	69.3	2.2	23.1	23.1	94.6
25	69.8	2.3	22.8	22.8	94.9
average	69.6	2.3	23.0	23.0	94.8
sd	0.4	0.1	0.2	0.2	0.2
59	65.4	0.3	25.8	25.8	91.0
59	59.9	1.5	34.3	34.3	95.7
average	62.7	0.9	30.1	30.1	93.4
sd	3.9	0.8	6.0	6.0	3.3

Dark

Days	Water		Soil		Total
	layer	extract	extract	soil	
0	98.2	0.3	0.3	0.4	98.6
0	99.0	0.3	0.3	0.3	99.3
average	98.6	0.3	0.3	0.4	99.0
sd	0.6	0.0	0.0	0.1	0.5
1	92.0	4.8	4.8	0.5	97.2
1	91.6	4.8	4.8	0.5	96.8
average	91.8	4.8	4.8	0.5	97.0
sd	0.3	0.0	0.0	0.0	0.3
4	95.3	1.1	1.1	1.6	98.0
4	95.3	1.5	1.5	1.5	98.3
average	95.3	1.3	1.3	1.6	98.2
sd	0.0	0.3	0.3	0.1	0.2
11	93.6	1.3	1.3	3.8	98.7
11	94.0	1.2	1.2	3.2	98.5
average	93.8	1.3	1.3	3.5	98.6
sd	0.3	0.1	0.1	0.4	0.1
25	89.0	0.3	0.3	9.5	98.5
25	88.7	2.7	2.7	7.9	99.3
average	88.9	1.5	1.5	8.7	98.9
sd	0.2	1.7	1.7	1.1	0.6
59	77.1	0.3	0.3	21.3	98.4
59	75.2	0.3	0.3	23.5	98.4
average	76.2	0.3	0.3	22.4	98.4
sd	1.3	0.0	0.0	1.6	0.0

Data obtained from Table III, p. 34, and Table IV, p. 35.
 Values reported as <LOQ were averaged as 0.3%, which was approximately half of the reported LOQ of 0.65% TRR.

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Chemical: Penoxsulam
MRID: 45830722
PC: 119031

Natural water

Overall Recovery

Days	Irradiated	Dark
0	98	98
1	97	99
4	94	100
7	97	99
14	95	99
21	97	98
28	97	100
Average	96.4	99.0
SD	1.4	0.8

Recoveries for individual sampling intervals calculated by the reviewer by summing the HPLC data in Table VI, p. 37.

Flooded soil

Overall Recovery

Days	Irradiated	Dark
0	98.6	98.6
0	99.3	99.3
1	96.5	97.2
1	95.6	96.8
4	88.6	98.0
4	89.0	98.3
11	96.3	98.7
11	96.6	98.5
25	94.6	98.5
25	94.9	99.3
59	91.0	98.4
59	95.7	98.4
Average	94.7	98.3
SD	3.5	0.7

Data obtained from Table III, p. 34, and Table IV, p. 35.

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Attachment 2

Structures of Parent and Transformation Products

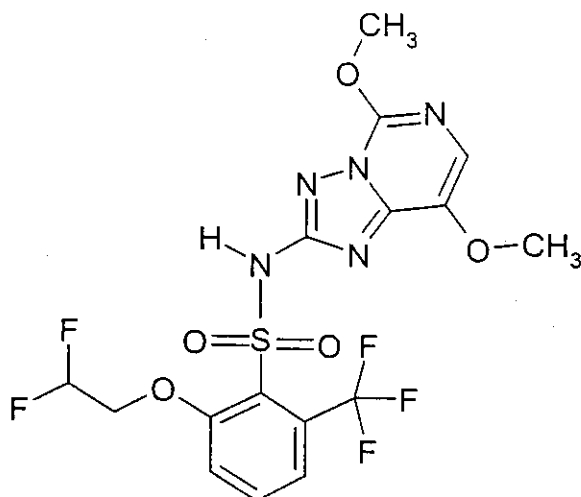
Penoxsulam

IUPAC name: 3-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)- α,α,α -trifluorotoluene-2-sulfonamide

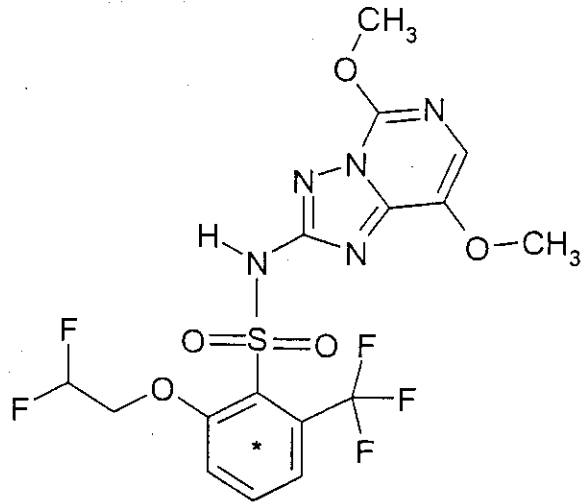
CAS name: 2-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide

CAS No: 219714-96-2

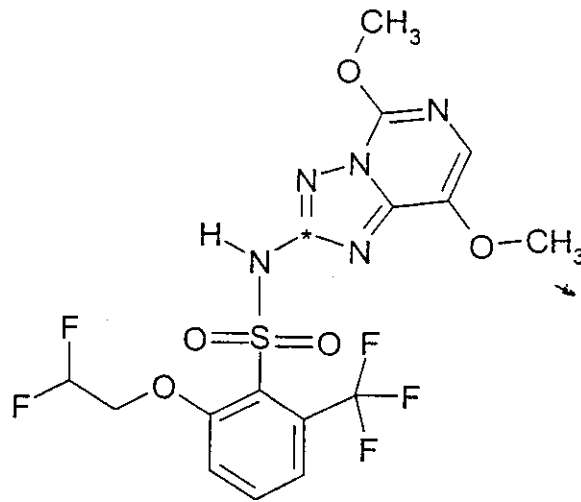
Unlabeled



[Phenyl-U-¹⁴C] label



[Triazolopyrimidine-2-¹⁴C] label



* Position of the radiolabel.

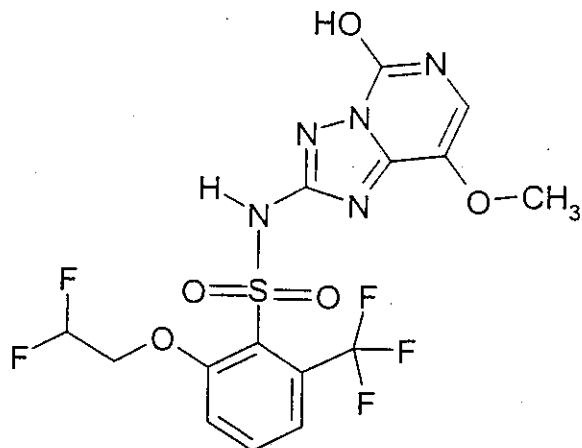
5-OH-XDE-638

IUPAC name: 6-(2,2-Difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo-s-triazolo[1,5-c]pyrimidin-2-yl)- α,α,α -trifluoro-o-toluenesulfonamide

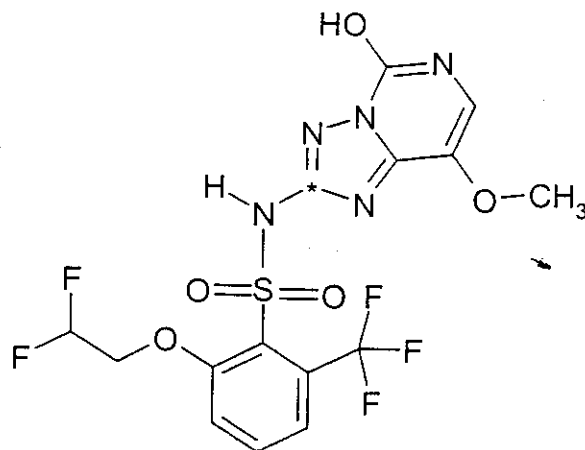
CAS name: 2-(2,2-Difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide

CAS No: NA

Unlabeled



[Triazolopyrimidine-2-¹⁴C] label



* Position of the radiolabel.

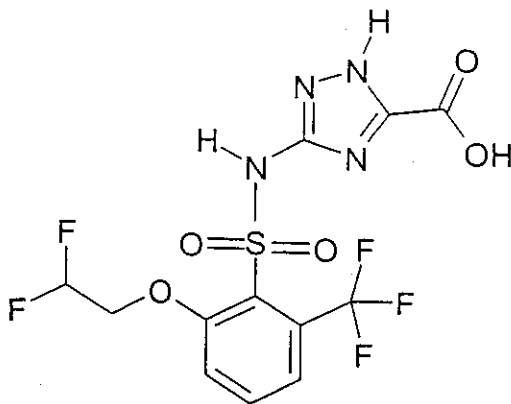
BSTCA

IUPAC name: 3-[6-(2,2-Difluoroethoxy)- α,α,α -(trifluoro-*o*-toluenesulfonyl)-*s*-
triazole-5-carboxylic acid

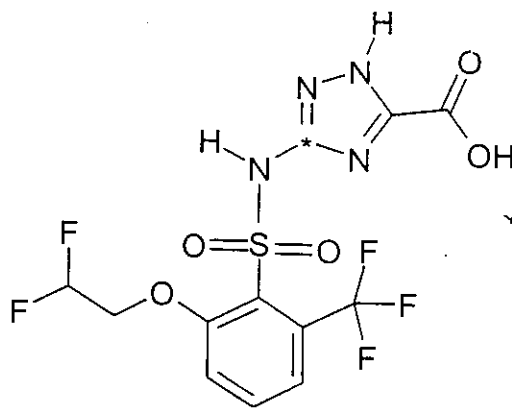
CAS name: 3-[[[2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)phenyl]-sulfonyl]amino]-
1H-1,2,4-triazole-5-carboxylic acid

CAS No: NA

Unlabeled



[Triazolopyrimidine-2-¹⁴C] label



* Position of the radiolabel.

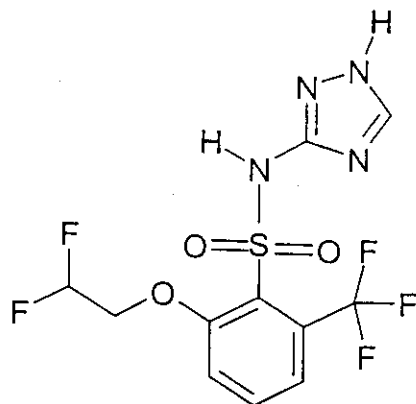
BST

IUPAC name: 6-(2,2-Difluoroethoxy)- α,α,α -trifluoro-N-s-triazol-3-yl-o-toluenesulfonamide

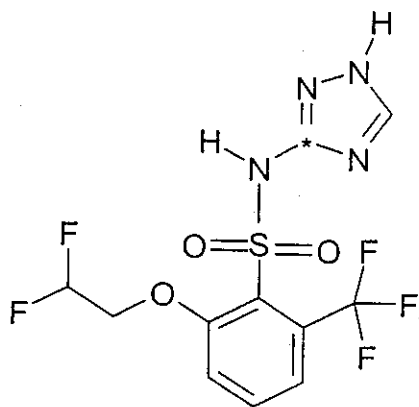
CAS name: 2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazole-3-yl-6-(trifluoromethyl)benzenesulfonamide

CAS No: NA

Unlabeled



[Triazolopyrimidine-2-¹⁴C] label

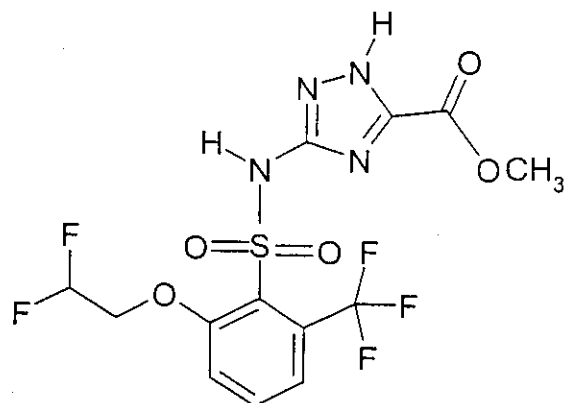


* Position of the radiolabel.

30

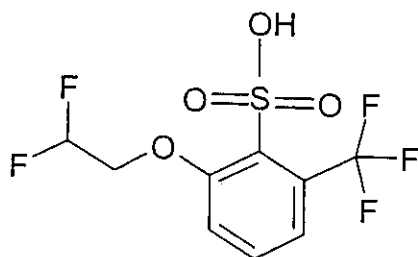
BSTCA-methyl

IUPAC name: Methyl 3-[6-(2,2-difluoroethoxy)- α,α,α -trifluoro-*o*-toluenesulfonamido]-s-triazole-5-carboxylate
CAS name: Methyl 3-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulfonyl]amino]-1H-1,2,4-triazole-5-carboxylate
CAS No: NA



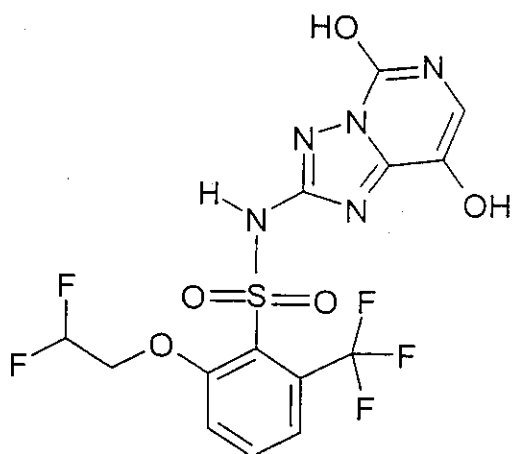
BSA

IUPAC name: 6-(2,2-Difluoroethoxy)- α,α,α -trifluoro-*o*-toluenesulfonic acid
CAS name: 2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)benzenesulfonic acid
CAS No: NA



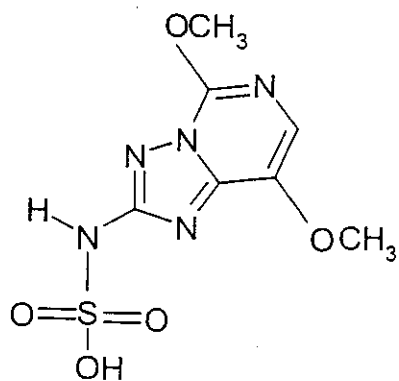
5,8-diOH

IUPAC name: NA
CAS name: 2-(2,2-Difluoroethoxy)-6-trifluoromethyl-N-(5,8-dihydroxy-
[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)benzenesulfonamide
CAS No: NA



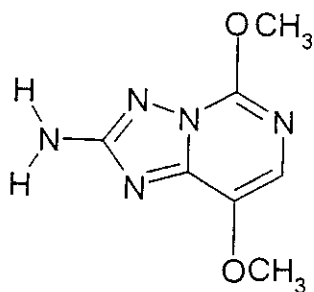
TPSA

IUPAC name: NA
CAS name: 5,8-Dimethoxy[1,2,4]triazolo-[1,5-c]pyrimidin-2-yl-sulfamic acid
CAS No: NA



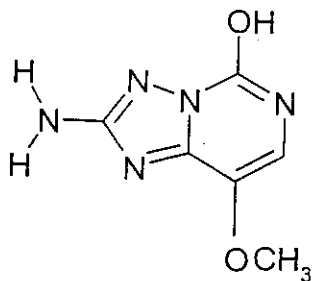
2-Amino TP

IUPAC name: 2-Amino-5,8-dimethoxy-s-triazolo[1,5-c]pyrimidine
CAS name: 5,8-Dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-amine
CAS No: NA



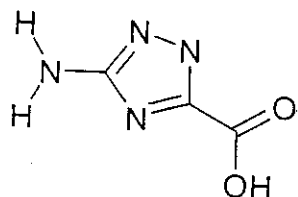
5-OH, 2-Amino TP

IUPAC name: NA
CAS name: 8-Methoxy[1,2,4]triazolo-[1,5-c]pyrimidin-5-ol-2-amine
CAS No: NA



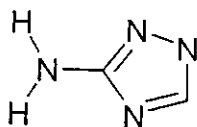
2-Amino TCA

IUPAC name: NA
CAS name: 2-Amino-1,3,4-triazole-5-carboxylic acid
CAS No: NA



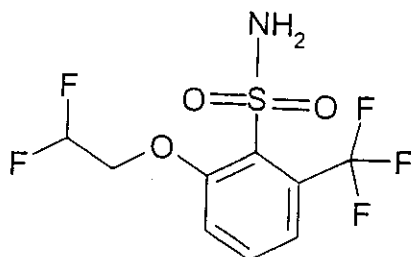
2-Amino-1,3,4-triazole

IUPAC name: NA
CAS name: 2-Amino-1,3,4-triazole
CAS No: NA



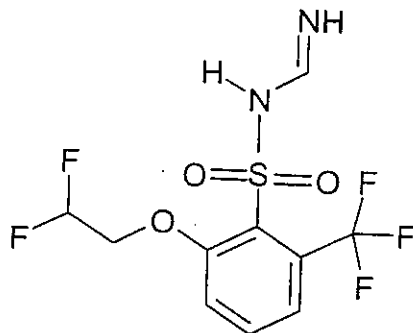
Sulfonamide

IUPAC name: 2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)-benzenesulfonamide
CAS name: 2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)-benzenesulfonamide
CAS No: NA



Sulfonylformamidine

IUPAC name: 2-(2,2-Difluoroethoxy)-N-[(E)iminomethyl]-6-(trifluoromethyl)benzenesulfonamide
CAS name: 2-(2,2-Difluoroethoxy)-N-(iminomethyl)-6-(trifluoromethyl)-benzenesulfonamide
CAS No: NA



Attachment 3

Transformation Pathway Presented by Registrant
Illustration of Test System

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DER CN Photoreproduction Of Neworsulard

Page is not included in this copy.

Pages 39 through 40 are not included.

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