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### Data Evaluation Report on the aquatic field dissipation of penoxsulam

PMRA Submission Number {.....}

EPA MRID Number 46703502

Data Requirement: PMRA Data Code:

EPA DP Barcode: D325783

**OECD Data Point:** EPA Guideline: 164-2

Test material: Penoxsulam

Concentration of a.i.: 21.4% End Use Product name: GF-443 SC SF

Formulation type: Aqueous suspension concentrate

**Test material:** 

Penoxsulam. Common name:

Chemical name:

3-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-

2-vl)- $\alpha$ , $\alpha$ , $\alpha$ -trifluorotoluene-sulfonamide.

2-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-**IUPAC** name:

2-yl)-6-(trifluoromethyl)benzenesulfonamide.

6-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy-s-triazolo[1,5-c]pyrimidin-2-

yl)- $\alpha$ , $\alpha$ , $\alpha$ -trifluoro-o-toluenesulfonamide.

2-(2.2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-CAS name:

2-yl)-6-(trifluoromethyl)benzenesulfonamide.

219714-96-2. CAS No.:

XDE-638; DE-638; TSN101649; SP1019 (SePRO). Synonyms:

FC(c1cccc(c1S(=O)(=O)N(c1nn2c(n1)ccnc2))OCC(F)F)(F)F

(ISIS v2.3/Universal SMILES).

Smiles string: No EPI Suite, v3.12 SMILES String found as of 6/27/06.

n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F.

Primary Reviewer: Dan Hunt Signature: **Cambridge Environmental Date:** 6/30/06

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Final Reviewer: Lucy Shanaman

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Date: 08/15/06 **EPA Reviewer** 

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

**CITATION:** Newcombe, A.C., J.A. Knuteson and D.G. Petty. 2005. Penoxsulam aquatic dissipation in Florida after whole-pond treatment. Unpublished study performed by LFR Levine-Fricke, Tallahassee, FL; Pyxant Laboratories, Inc., Colorado Springs, CO; Enviro-Test Laboratories, Inc., Alberta, Canada; and Agvise Laboratories, Inc., Northwood, ND; and submitted by SePRO Corporation, Carmel, IN (p.16). Laboratory Study ID: PD-2004-01. Experiment initiation April 4, 2004 and completion April 27, 2005 (p.3). Final report issued November 14, 2005.

### **EXECUTIVE SUMMARY**

Penoxsulam (3-(2,2-difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)α.α.α-trifluorotoluene-2-sulfonamide; GF-443 SC SF, 21.4% a.i.) was applied once by subsurface injection to an approximately 0.9-ha pond in Florida to achieve a whole-pond water concentration of 150 ug penoxsulam/L to an approximately 0.3-ha application zone. The maximum proposed single use rate was reported as 150 µg penoxsulam/L. Water and sediment samples were collected for analysis of penoxsulam and the transformation products 5-OH (6- $(2,2-difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo-\underline{s}-triazolo[1,5-\underline{c}]pyrimidin-2-yl)-\alpha,\alpha,\alpha$ trifluoro-o-toluene sulfonamide); BSTCA (3-[6-(2,2-difluoroethoxy)- α,α,α-trifluoro-otoluenesulfonamidol-s-triazole-5-carboxylic acid); BSA (2-(2,2-difluoroethoxy)-6-(trifluoromethyl)benzenesulfonic acid); sulfonamide (2-(2,2-difluoroethoxy)-6-(trifluoromethyl)benzenesulfonamide); and 2-amino-TP (5,8-dimethoxy[1,2,4]triazole[1,5-c]pyrimidin-2-amine). Water samples were also analyzed for the transformation products TPSA (5,8dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)sulfamic acid) and 5-OH-2-amino-TP (2-amino-8-methoxy[1,2,4]triazolo[1,5-c]pyrimidin-5-ol). Water samples were collected at multiple depths from three sampling locations at 1, 3, 7, 14, 21, 28, 43, 57, 85, 114, 141, 169, 195, 223, 253, and 296 days posttreatment. Sediment samples were collected at the same sampling intervals for water. All samples were analyzed within 380 days of collection.

Penoxsulam dissipated in the water with a calculated half-life of 24.8 days ( $r^2 = 0.7313$ ). The half-life was calculated using linear regression analysis performed on a plot of ln-transformed penoxsulam concentrations vs. time and the equation  $t_{1/2} = -\ln 2 / k$ , where k is the rate constant.

The mean measured penoxsulam concentration in water was initially 167.05 ng/mL or 111% of the target concentration at 1 day, decreased to 130.29-134.04 ng/mL by 7-14 days, 74.22 ng/mL by 43 days, 16.40 ng/mL at 85 days, and was last detected at 3.73 ng/mL at 114 days posttreatment. Vertical mixing was accomplished by 3 days posttreatment at the two shallow-depth sampling stations, and at approximately 4 weeks posttreatment at the sampling station located in the deepest area of the pond. The study authors attributed the slow vertical mixing at the deep sampling station to the temperature gradient, adding that vertical mixing of penoxsulam was not complete until a significant rainfall event of 5.15 cm at 3.5 weeks posttreatment.

The transformation products 5-OH, BSTCA, and TPSA were detected in the pond water at the highest concentrations. **5-OH** was initially detected in the pond water at a mean concentration of 0.23 ng/mL at 3 days, increased to a maximum of 6.83 ng/mL by 57 days, and was last detected at 1.46 ng/mL at 114 days. **BSTCA** was initially detected in the pond water at a mean concentration of 0.13 ng/mL at 3 days, increased to a maximum of 13.57 ng/mL by 57 days, then decreased to 2.04 ng/mL by 141 days, and was last detected at 0.03 ng/mL at 223 days. **TPSA** was initially detected in the pond water at a mean concentration of 0.31 ng/mL at 14 days, increased to a maximum of 2.12 ng/mL by 57 days, and was last detected at 0.06 ng/mL at 114 days. The transformation products BSA, 2-amino-TP, sulfonamide, and 5-OH-2-amino-TP were detected in the pond water at maximum concentrations of 0.26 ng/mL (14 days), 0.63 ng/mL (43 days), 0.71 ng/mL (43 days), and 0.05 ng/mL (253 days), respectively.

Average penoxsulam and transformation product concentrations in pond water, expressed as ng/mL.

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Days	Average concentration (ng/mL)							
post-	Penoxsulam	5-OH	BSTCA	BSA	2-Amino-	Sulfona-	TPSA	5-OH-2-amino-
treatment					TP	mide		TP
1	167.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	160.83	0.23	0.13	0.04	0.00	0.00	0.00	0.00
7	130.29	0.91	0.10	0.00	0.00	0.00	0.00	0.00
14	134.04	2.00	2.16	0.26	0.13	0.00	0.31	0.00
21	121.00	3.22	3.17	0.00	0.00	0.00	1.12	0.00
28	94.13	3.73	4.61	0.00	0.10	0.00	1.12	0.00
43	74.22	5.71	10.35	0.00	0.63	0.71	2.04	0.00
57	59.41	6.83	13.57	0.00	0.54	0.00	2.12	0.00
85	16.40	3.98	13.52	0.00	0.26	0.00	0.89	0.00
114	3.73	1.46	4.78	0.00	0.00	0.00	0.06	0.00
141	0.00	0.00	2.04	0.00	0.00	0.00	0.00	0.00
169	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
195	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
223	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00
253	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05
296	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Values in bold are above the LOQ (3.0 ng/mL).

Penoxsulam dissipated in the sediment with a calculated half-life of 34.5 days ( $r^2 = 0.5307$ ), based on detections following the maximum concentration at 21 days. The half-life was calculated using linear regression analysis performed on a plot of ln-transformed penoxsulam concentrations vs. time and the equation  $t_{1/2} = -ln \ 2 / k$ , where k is the rate constant.

The mean measured penoxsulam concentration in sediment was initially 2.63 ng/g at 1 day, increased to a maximum of 18.08 ng/g by 21 days, then decreased to 13.25 ng/g by 43 days and 4.41-4.59 ng/g by 57-85 days, and was last detected at 0.50 ng/g at 141 days (excluding a single replicate detection at 2.87 ng/g at 253 days).

The transformation products 5-OH and BSTCA were detected in the sediment at levels above the LOQ, 2-amino-TP was detected twice at levels below the LOQ, and BSA and sulfonamide were not detected in any sediment samples. **5-OH** was initially detected in the sediment at 14.08 ng/g at 1 day, increased to a maximum of 26.62 ng/g by 7 days, ranged from 15.39-20.20 ng/g from 14 to 28 days, decreased to 7.17 ng/g by 43 days, 1.01 ng/g by 141 days, and was last detected at 0.72 ng/g at 253 days. **BSTCA** was initially detected in the sediment at 0.98 ng/g at 7 days, increased to a maximum of 18.33 ng/g by 85 days, decreased to 7.17 ng/g by 141 days, and ranged from 4.10 to 7.13 ng/g from 169-296 days. The registrant-calculated half-lives of 5-OH and BSTCA in sediment were 28.6 days and 84.9 days, respectively.

Average penoxsulam and transformation product concentrations in pond sediment, expressed as

ng/g.						
Days			Average cor	ncentration (ng/	(g)	
posttreatment	Penoxsulam	5-OH	BSTCA	BSA	2-Amino-TP	Sulfonamide
1	2.63	14.08	0.00	0.00	0.00	0.00
3	9.68	10.75	0.00	0.00	0.00	0.00
7	5.22	26.62	0.98	0.00	0.00	0.00
14	17.37	15.39	3.08	0.00	0.00	0.00
21	18.08	18.04	8.32	0.00	1.56	0.00
28	13.83	20.20	2.85	0.00	1.47	0.00
43	13.25	7.17	9.82	0.00	0.00	0.00
57	4.41	4.98	12.56	0.00	0.00	0.00
85	4.59	3.39	18.33	0.00	0.00	0.00
114	1.34	1.65	10.22	0.00	0.00	0.00
141	0.50	1.01	7.17	0.00	0.00	0.00
169	0.00	0.00	7.00	0.00	0.00	0.00
195	0.00	0.00	5.58	0.00	0.00	0.00
223	0.00	0.00	4.62	0.00	0.00	0.00
253	2.87	0.72	4.10	0.00	0.00	0.00
296	0.00	0.00	7.13	0.00	0.00	0.00

Values in bold are above the LOQ (3.0 ng/g).

Total rainfall during the 9.5-month study period was 132.79 cm or 124% of the pro-rated annual historical rainfall total. The study authors stated that water quality parameters (pH range of approximately 5.2-7; dissolved oxygen range of 0.1-8.3 mg/L; conductivity range of 0.03 to 0.09 mS/cm) were typical for small water bodies in Florida, and that visibility readings indicated that the pond moved from a hypereutrophic state to a eutrophic state during the course of the study. The study authors stated that the test substance application had no obvious influence on water quality.

**Study Acceptability:** This study is classified as acceptable for fulfilling the data requirements for aquatic field dissipation of penoxsulam. No significant deviations from good scientific practices or Subdivision N Guidelines were noted.

### **MATERIALS AND METHODS**

The aquatic field dissipation of penoxsulam (GF-443 SC SF, 21.4% a.i.; water solubility = 0.408 g/L in pH 7 buffer at 19°C; vapor pressure = 2.49 x 10<sup>-14</sup> Pa at 20°C; p.24; Table 1, p.77) was conducted on an approximately 0.9-ha pond located in Madison County, Florida, approximately 2 kilometers southwest of the town of Madison (30.453433 N latitude, 83.430233 W longitude; pp.24-26; Table 4, p.80; Figure 2, p.152). The pond had one inflow channel (east end) and one outflow channel (west end), and both channels contained culvert type structures to control water flow. The maximum water depth of the pond was approximately 2.6 m (p.46). The greatest bank slope existed on the northern shoreline with an elevation increase of approximately 3 ft over 20 ft from the shoreline, and the smallest elevation increase was on the southern shoreline (Figure 5,

p.155). A bathymetric survey and a shoreline elevation survey were conducted as part of the site characterization (pp.26-27; Figure 4, p.154). Results indicated a mean water column depth of 3.76 ft (p.46). Three water and sediment samples were collected for characterization on the days prior to the test application (pp.27-28). Mean results for pond water were: pH 6.8, hardness 13 mg CaCO<sub>3</sub>/L, conductivity 0.06 mmhos/cm, total dissolved solids 15 ppm, turbidity 3.99 NTU, alkalinity 0.4 mg CaCO<sub>3</sub>/L (Table 13, p.89). The sediment was predominantly a clay loam (37.8% sand, 37.0% silt, 25.2% clay, pH 4.6, 16.0% organic carbon, CEC 62.6 meq/100 g, bulk density 0.69 g/cm<sup>3</sup>; Table 14, p.90). A three-year plot history was not provided for the test site. However, there was no documented history of penoxsulam use in the pond or on the adjacent land (p.25). An on-site meteorological station was installed on the north side of the pond to measure rainfall, air temperature, relative humidity, wind speed and direction, and solar radiation (p.29). Additionally, a thermocouple stack was installed in the deepest portion of the pond to measure the water temperature profile and surface sediment temperature, and a water quality meter was installed at approximately mid-depth in the water column at sampling stations A and C (Figure 1, p.151) to record dissolved oxygen, temperature, pH and electrical conductivity (p.30). Other instrumentation installed at sampling station A included a water depth gauge to measure fluctuations in the water depth. Also, visible light penetration and UV-B light penetration were measured at each sampling event (p.32). Visible light penetration was measured using a standard 20-cm diameter Secchi disk. UV-B light penetration was measured using a Skye Instruments UV-B light sensor and a portable hand-held SpectroSense meter. Light penetration measurements were conducted approximately 25 m east of sampling station B on the eastern side of the pond.

Prior to test application, three water and sediment sampling stations were positioned within the pond (p.33; Figure 1, p.151). Sampling stations B and C were positioned where the water column depth was 120 cm (4 ft). Sampling station A was positioned in the deepest section of the pond where the water column depth was 275 cm (9 ft). Station A was located just north of the center of the pond within the application zone. Station B was located on the east end of the pond just outside of the application zone. Station C was located on the southwest end of the pond just inside the application zone.

Penoxsulam was applied by subsurface injection to an approximate 0.3-ha application zone (75 x 42 m rectangular zone; p.36) located in the center of the pond on April 6, 2004 (pp.33-34). The test application was made to achieve a whole-pond water concentration of 150 µg penoxsulam/L. The application was made from a 4.3-m long fiberglass hulled Carolina skiff boat using three 1.8-m length rubber hoses equipped with a single Disc #12 spray nozzle and connected to a 1.8-m manifold boom. The hose arrangement provided an effective application-path width of 2.74 m. The test application required the preparation of two tank mixes (p.35). Only water obtained from the test site was used to prepare the tank mixes. A spray volume of 50 gal was prepared for the first tank mix, and a spray volume of 18 gal was prepared for the second tank mix (pp.35-36; Table 8, p.84). No tank mix adjuvants or antifoam agents were used. A total of 15 application passes were needed for the application (Figure 3, p.153). Application pass times and sprayer output following each pass were reported in Table 9 (p.85), and indicate the uniform output of spray solution and close adherence to the target output (p.36). Verification of the application rate

was not possible due to the subsurface application method. Following application, the spray tanks were rinsed with 5 gal of clean water followed by 10 gal of clean water, and the rinses applied to the pond in the center of the application zone and around the perimeter of the pond (pp.36-37). The spray tank was drained on the northern shore of the pond.

Tank mix samples were collected in duplicate just prior to application and just before the spray volume was exhausted for both tank mixes (p.38). Tank mix samples were mixed with approximately 75 mL of tetrahydrofuran (THF), and extracted by shaking by hand (pp.43-44). Samples were analyzed for penoxsulam by LC with UV detection (operating conditions reported in Appendix E, Figure 64, p.833). Samples were analyzed within 8 days of collection (p.44). The calculated recovery of penoxsulam in the tank mix was 93.8% of the theoretical value (Table 19, p.95; based on the registrant-calculated theoretical value reported on p.56).

Meteorological conditions during the application were as follows: air temperature 20.68-24.20°C, relative humidity 33.02-42.14%, wind speed: 0.78-4.38 m/s, cloud cover 5-10% (Table 6, p.82).

Water samples were collected prior to treatment and at 1, 3, 7, 14, 21, 28, 43, 57, 85, 114, 141, 169, 195, 223, 253, and 296 days posttreatment (Tables 10, p.86). At each sampling interval, duplicate samples (20 mL) were collected at approximately 25, 75, and 100 cm from the pond bottom from sampling stations B and C, and at approximately 25, 75, 100, 175, and 225 cm from pond bottom from sampling station A using a custom-made grab sampler (p.39; Figure 1, p.151). Samples were placed into an on-site freezer. Samples were analyzed within 380 days of collection (p.44).

Sediment samples were collected at the same sampling intervals for water (Table 10, p.86). Sediment samples were collected within a 3-m radius of sampling stations A, B, and C using a sediment dredge sampler (p.39; Figure 1, p.151). Following collection, the sediment was cleaned of any plant detritus and a 100-g aliquot was transferred to a metal sample container (p.40). The remainder was discarded back into the pond outside of the 3-m radius collection area. Samples were placed into an on-site freezer. Samples were analyzed within 369 days of collection (p.44).

Water and sediment samples were analyzed for penoxsulam and the transformation products 5-OH (6-(2,2-difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo-s-triazolo[1,5-c]pyrimidin-2-yl)- $\alpha$ , $\alpha$ , $\alpha$ -trifluoro-o-toluene sulfonamide); BSTCA (3-[6-(2,2-difluoroethoxy)- $\alpha$ , $\alpha$ , $\alpha$ -trifluoro-o-toluenesulfonamido]-s-triazole-5-carboxylic acid); BSA (2-(2,2-difluoroethoxy)-6-(trifluoromethyl)benzenesulfonic acid); sulfonamide (2-(2,2-difluoroethoxy)-6-(trifluoromethyl)-benzenesulfonamide); and 2-amino-TP (5,8-dimethoxy[1,2,4]triazole[1,5-c]pyrimidin-2-amine); water samples were also analyzed for the additional transformation products TPSA (5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-ylsulfamic acid) and 5-OH-2-amino-TP (2-amino-8-methoxy[1,2,4]triazolo[1,5-c]pyrimidin-5-ol; pp.41-43; Appendix F, pp.1042-1044).

Water samples were analyzed by DAS method GRM 02.15 with minor modifications, and select samples were analyzed for penoxsulam only (to improve the analytical sensitivity) by DAS method GRM 01.30 with minor modifications (pp.41-42; Appendix E, pp.586-588). For DAS Method 02.15, samples were thawed in the dark and a 1-mL aliquot was analyzed for penoxsulam and 2-amino-TP by HPLC (Varian Metasil AQ C18 column, 5 µm, 50 x 2 mm; mobile phase A: 1 mM ammonium acetate in water; mobile phase B: 1 mM ammonium acetate in methanol; A:B: 90:10 to 30:70 to 90:10, v:v; Appendix E, Figure 62, p.831) with tandem mass spectrometry (positive ion mode). The retention times of penoxsulam and 2-amino-TP were 1.47 and 0.80 min, respectively. Samples were analyzed for 5-OH, BSTCA, 5-OH-2-amino-TP, TPSA, BSA, and sulfonamide as described above but with the mobile phase gradient A:B 55:45 to 10:90 to 55:45, v:v, and with negative ion operating conditions. The retention times of 5-OH, BSTCA, 5-OH-2-amino-TP, TPSA, BSA, and sulfonamide were 4.70, 4.20, 1.20, 1.30, 4.20, and 4.70 min, respectively. The LOQ was 3.0 ng/mL and the LOD was 0.05 ng/mL. For DAS Method 01.30, samples were thawed in the dark and a 10-mL aliquot was purified by solid phase extraction (Waters Oasis® MAX 3 cartridge). The eluate was evaporated to dryness, reconstituted in 1 mL of acetonitrile:methanol:water:acetic acid (15:15:70:0.1; v:v:v:v), and analyzed for penoxsulam by LC-MS-MS (Zorbax SB C8 column, 3.5 m, 4.6 x 75 mm; mobile phase of A: water with 0.1% acetic acid and B; methanol; acetonitrile (1:1; v:v) with 0.1% acetic acid, A:B, 70:30 to 5:95 to 70:30, v:v; Appendix E, Figure 63, p.832). The retention time of penoxsulam was 5.30 min. The LOQ was 0.05 ng/mL and the LOD was 0.01 ng/mL.

Sediment samples were analyzed by DAS method GRM 01.31 with minor modifications (pp.42-43; Appendix F, pp.850-853). After thawing overnight, the samples were mixed with a spatula and approximately 5-g aliquots were extracted by shaking with 25 mL of acetonitrile: 0.1N hydrochloric acid (90:10, v:v) for 60 minutes. After the supernatant was decanted, the pellet was resuspended in 15 mL of the extraction solution and the extraction was repeated. The combined extracts were brought to volume with the extraction solution. Aliquots (4 mL) were then evaporated to near dryness, reconstituted in 4 mL of 0.1N hydrochloric acid, and 1.5-mL aliquots were purified by solid phase extraction (Waters Oasis® HLB cartridge). Analytes were eluted using 2.0 mL of acetonitrile:methanol with 0.1% acetic acid (80:20, v:v) The eluate was concentrated to near dryness, re-dissolved in methanol:acetonitrile (50:50, v:v), adjusted to 1 mL with 0.1% acetic acid in water, and analyzed for penoxsulam and 2-amino-TP by LC-MS-MS (YMC ODS-AM column, 3 x 150 mm, 5.0 μm; mobile phase gradient of A: 0.1% acetic acid in water; B: 0.1% acetic acid in 50:50 acetonitrile:methanol; A:B: 95:5 to 5:95 to 95:5, v:v; positive ion mode; Appendix F, Table 5, p.864). Samples were analyzed for 5-OH, BSTCA, BSA, and sulfonamide as described above but with the mobile phase gradient A: 1 mM ammonium acetate in water; B: 1 mM ammonium acetate in methanol; A:B: 95:5 to 5:95 to 95:5, v:v, and with negative ion operating conditions (Appendix F, Table 6, p.865). The LOO was 3.0 ng/g and the LOD was 1.0 ng/g (p.62).

Method validation recoveries of penoxsulam and its transformation products from sediment samples fortified over the range of 3.0-100 ng/g were  $88 \pm 14\%$  for penoxsulam,  $85 \pm 13\%$  for 2-amino-TP,  $88 \pm 9.0\%$  for sulfonamide,  $86 \pm 12.2\%$  for 5-OH,  $101 \pm 9.5\%$  for BSA, and  $87 \pm 9.8\%$  for BSTCA (Appendix F, Tables 3-4, pp.862-863).

The efficiency of the analytical methods was determined by fortifying control water and sediment samples collected from the pond pretreatment with penoxsulam and its transformation products at the LOQ and five times the LOQ (p.38; Appendix E, p.598 and Appendix F, p.853). Mean recovery of penoxsulam from pond water was 92.8  $\pm$  11.0% for DAS method GRM 02.15 and 100  $\pm$  9.0% for DAS method GRM 01.30 (Appendix E, Tables 4-5, pp.628-632). Mean recoveries of the transformation products from pond water were 99.5  $\pm$  9.4% for 5-OH, 103  $\pm$  10.0% for BSTCA, 101  $\pm$  15.0% for BSA, 94.9  $\pm$  14.1% for 2-amino-TP, 96.2  $\pm$  12.1% for sulfonamide, 96.3  $\pm$  9.8% for TPSA, and 96.5  $\pm$  9.4% for 5-OH-2-amino-TP (p.55; Appendix E, Tables 6-12, pp.633-660). Mean recoveries from sediment were 107  $\pm$  19% for penoxsulam, 95  $\pm$  13% for 2-amino-TP, 93  $\pm$  13% for sulfonamide, 94  $\pm$  14% for 5-OH, 113  $\pm$  10.2% for BSA, and 97  $\pm$  14% for BSTCA (Appendix F, Table 7, pp.866-867). Recoveries from sediment were generally higher for the lower level fortifications.

Separate storage stability studies were conducted for penoxsulam and the transformation products 5-OH, sulfonamide, BSTCA, BSA, 2-amino-TP, TPSA, and 5-OH-2-amino-TP in water (MRID 46433901), and for penoxsulam and the transformation products 5-OH, BSTCA, BSA, XDE-638 sulfonamide, and 2-amino-TP in soil (MRID 46433902). In brief, in MRID 46433901, 25-ml aliquots of water samples acquired from a California study site were fortified with penoxsulam and its transformation products separately at 0.03 mg/L and stored refrigerated for up to 433 days (penoxsulam) or 270-284 days (transformation products), and separate samples were stored frozen for up to 320 days (penoxsulam). In MRID 46433902, 5-g aliquots of soil samples (from California) were fortified with penoxsulam and its transformation products separately at  $0.03 \mu g/g$  and stored frozen for up to 781 days.

### **RESULTS AND DISCUSSION**

Penoxsulam (GF-443 SC SF, 21.4% a.i.) was applied once by subsurface injection to achieve a whole-pond water concentration of 150 µg penoxsulam/L to an approximately 0.3-ha application zone of an approximately 0.9-ha pond in Florida.

Penoxsulam dissipated in the water with a calculated half-life of 24.8 days ( $r^2 = 0.7313$ ), calculated using linear regression analysis performed on a plot of ln-transformed penoxsulam concentrations vs. time and the equation  $t_{1/2} = -ln \ 2 / k$ , where k is the rate constant.

The mean measured penoxsulam concentration in water was initially 167.05 ng/mL or 111% of the target concentration at 1 day, decreased to 130.29-134.04 ng/mL by 7-14 days and 74.22 ng/mL by 43 days, was 16.40 ng/mL at 85 days, and was last detected at 3.73 ng/mL at 114 days posttreatment (Table 28, p.144). The study authors attributed the elevated concentration of penoxsulam at 24 hours to sampling variability and incomplete mixing in the water column, and to a band of emergent vegetation around the periphery of the test system that could have reduced the potential for convective mixing (p.60). Vertical mixing was accomplished by 3 days posttreatment at sampling stations B and C and at approximately 4 weeks posttreatment at sampling station A (located in the deepest area of the pond; p.57; Table 20, pp.96-101). The

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study authors attributed the slow vertical mixing at sampling station A to the temperature gradient, adding that vertical mixing of penoxsulam was not complete until a significant rainfall event of 5.15 cm on April 30, 2004.

The transformation products 5-OH (6-(2,2-difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo-striazolo[1,5-c]pyrimidin-2-yl)-α,α,α-trifluoro-o-toluene sulfonamide), BSTCA (3-[6-(2,2difluoroethoxy)-  $\alpha,\alpha,\alpha$ -trifluoro-o-toluenesulfonamido]-s-triazole-5-carboxylic acid), and TPSA (5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-ylsulfamic acid) were detected in the pond water at the highest concentrations (Table 28, p.144; Figure 20, p.165). 5-OH was initially detected in the pond water at a mean concentration of 0.23 ng/mL at 3 days, increased to a maximum of 6.83 ng/mL by 57 days, and was last detected at 1.46 ng/mL at 114 days. **BSTCA** was initially detected at a mean concentration of 0.13 ng/mL at 3 days, increased to a maximum of 13.57 ng/mL by 57 days, decreased to 2.04 ng/mL by 141 days, and was last detected at 0.03 ng/mL at 223 days. TPSA was initially detected at a mean concentration of 0.31 ng/mL at 14 days, increased to a maximum of 2.12 ng/mL by 57 days, and was last detected at 0.06 ng/mL at 114 days. The transformation products BSA (2-(2,2-difluoroethoxy)-6-(trifluoromethyl)benzenesulfonic acid); 2-amino-TP (5,8-dimethoxy-dimethoxy[1,2,4]triazole[1,5-c]pyrimidin-2amine); sulfonamide (2-(2,2-difluoroethoxy)-6-(trifluoromethyl)-benzenesulfonamide); and 5-OH-2-amino-TP (2-amino-8-methoxy[1,2,4]triazolo[1,5-c]pyrimidin-5-ol) were detected at maximum concentrations below 1 ng/mL. **BSA** was detected at 0.04-0.26 ng/mL at 3 and 14 days; 2-amino-TP was detected at a maximum of 0.63 ng/mL at 43 days, and was last detected at 0.26 ng/ml at 85 days; sulfonamide was detected once at 0.71 ng/mL at 43 days; and 5-OH-2**amino-TP** was detected once at 0.05 ng/mL at 253 days.

Average penoxsulam and transformation product concentrations in pond water, expressed as ng/mL.

		F	Average concer	tration (ng/mL	.)		
Penoxsulam	5-OH	BSTCA	BSA	2-Amino-	Sulfona-	TPSA	5-OH-2-
				TP	mide		amino-TP
167.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
160.83	0.23	0.13	0.04	0.00	0.00	0.00	0.00
130.29	0.91	0.10	0.00	0.00	0.00	0.00	0.00
134.04	2.00	2.16	0.26	0.13	0.00	0.31	0.00
121.00	3.22	3.17	0.00	0.00	0.00	1.12	0.00
94.13	3.73	4.61	0.00	0.10	0.00	1.12	0.00
74.22	5.71	10.35	0.00	0.63	0.71	2.04	0.00
59.41	6.83	13.57	0.00	0.54	0.00	2.12	0.00
16.40	3.98	13.52	0.00	0.26	0.00	0.89	0.00
3.73	1.46	4.78	0.00	0.00	0.00	0.06	0.00
0.00	0.00	2.04	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	167.05 160.83 130.29 134.04 121.00 94.13 74.22 59.41 16.40 3.73 0.00 0.00 0.00 0.00	167.05         0.00           160.83         0.23           130.29         0.91           134.04         2.00           121.00         3.22           94.13         3.73           74.22         5.71           59.41         6.83           16.40         3.98           3.73         1.46           0.00         0.00           0.00         0.00           0.00         0.00           0.00         0.00           0.00         0.00           0.00         0.00           0.00         0.00           0.00         0.00           0.00         0.00	Penoxsulam         5-OH         BSTCA           167.05         0.00         0.00           160.83         0.23         0.13           130.29         0.91         0.10           134.04         2.00         2.16           121.00         3.22         3.17           94.13         3.73         4.61           74.22         5.71         10.35           59.41         6.83         13.57           16.40         3.98         13.52           3.73         1.46         4.78           0.00         0.00         2.04           0.00         0.00         0.00           0.00         0.00         0.00           0.00         0.00         0.00           0.00         0.00         0.00           0.00         0.00         0.00           0.00         0.00         0.00           0.00         0.00         0.00	Penoxsulam         5-OH         BSTCA         BSA           167.05         0.00         0.00         0.00           160.83         0.23         0.13         0.04           130.29         0.91         0.10         0.00           134.04         2.00         2.16         0.26           121.00         3.22         3.17         0.00           94.13         3.73         4.61         0.00           74.22         5.71         10.35         0.00           59.41         6.83         13.57         0.00           16.40         3.98         13.52         0.00           3.73         1.46         4.78         0.00           0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00	Penoxsulam         5-OH         BSTCA         BSA         2-Amino-TP           167.05         0.00         0.00         0.00         0.00           160.83         0.23         0.13         0.04         0.00           130.29         0.91         0.10         0.00         0.00           134.04         2.00         2.16         0.26         0.13           121.00         3.22         3.17         0.00         0.00           94.13         3.73         4.61         0.00         0.10           74.22         5.71         10.35         0.00         0.63           59.41         6.83         13.57         0.00         0.54           16.40         3.98         13.52         0.00         0.26           3.73         1.46         4.78         0.00         0.00           0.00         0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00         0.00           0.00         0.00         0.00	167.05         0.00         0.00         0.00         0.00         0.00           160.83         0.23         0.13         0.04         0.00         0.00           130.29         0.91         0.10         0.00         0.00         0.00           134.04         2.00         2.16         0.26         0.13         0.00           121.00         3.22         3.17         0.00         0.00         0.00           94.13         3.73         4.61         0.00         0.10         0.00           74.22         5.71         10.35         0.00         0.63         0.71           59.41         6.83         13.57         0.00         0.54         0.00           16.40         3.98         13.52         0.00         0.26         0.00           3.73         1.46         4.78         0.00         0.00         0.00           0.00         0.00         0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00         0.00         0.00           0.00         0.00         0.00         0.00         0.00         0.00           0.00         0.00 <th< td=""><td>Penoxsulam         5-OH         BSTCA         BSA         2-Amino-TP         Sulfonamide         TPSA           167.05         0.00         0.00         0.00         0.00         0.00         0.00         0.00           160.83         0.23         0.13         0.04         0.00         0.00         0.00         0.00           130.29         0.91         0.10         0.00         0.00         0.00         0.00         0.00           134.04         2.00         2.16         0.26         0.13         0.00         0.31           121.00         3.22         3.17         0.00         0.00         0.00         1.12           94.13         3.73         4.61         0.00         0.10         0.00         1.12           74.22         5.71         10.35         0.00         0.63         0.71         2.04           59.41         6.83         13.57         0.00         0.54         0.00         2.12           16.40         3.98         13.52         0.00         0.26         0.00         0.89           3.73         1.46         4.78         0.00         0.00         0.00         0.00           0.00</td></th<>	Penoxsulam         5-OH         BSTCA         BSA         2-Amino-TP         Sulfonamide         TPSA           167.05         0.00         0.00         0.00         0.00         0.00         0.00         0.00           160.83         0.23         0.13         0.04         0.00         0.00         0.00         0.00           130.29         0.91         0.10         0.00         0.00         0.00         0.00         0.00           134.04         2.00         2.16         0.26         0.13         0.00         0.31           121.00         3.22         3.17         0.00         0.00         0.00         1.12           94.13         3.73         4.61         0.00         0.10         0.00         1.12           74.22         5.71         10.35         0.00         0.63         0.71         2.04           59.41         6.83         13.57         0.00         0.54         0.00         2.12           16.40         3.98         13.52         0.00         0.26         0.00         0.89           3.73         1.46         4.78         0.00         0.00         0.00         0.00           0.00

Data were obtained from Table 28, p.144 of the study report. Individual sample concentrations of the parent and transformation products from each of the three sampling stations were reported in Tables 20-27, pp.96-143 of the study report. Concentrations are corrected for method recoveries. Values in bold are above the LOQ (3.0 ng/mL).

Penoxsulam dissipated in the sediment with a calculated half-life of 34.5 days ( $r^2 = 0.5307$ ), based on detections following the maximum concentration at 21 days. The half-life was calculated using linear regression analysis performed on a plot of ln-transformed penoxsulam concentrations vs. time and the equation  $t_{1/2} = -ln \ 2 / k$ , where k is the rate constant.

The mean measured penoxsulam concentration in sediment was initially 2.63 ng/g at 1 day, increased to a maximum of 18.08 ng/g by 21 days, then decreased to 13.25 ng/g by 43 days, 4.41-4.59 ng/g by 57-85 days, and was last detected at 0.50 ng/g at 141 days (excluding a single replicate detection at 2.87 ng/g at 253 days; Tables 29 and 31, pp.145-146 and 149, respectively).

The transformation products 5-OH and BSTCA were detected in the sediment at levels above the LOQ, 2-amino-TP was detected twice at levels below the LOQ, and BSA and sulfonamide were not detected in any sediment samples (Tables 29-31, pp.145-149). **5-OH** was initially detected in the sediment at 14.08 ng/g at 1 day, increased to a maximum of 26.62 ng/g by 7 days, ranged from 15.39-20.20 ng/g from 14 to 28 days, decreased to 7.17 ng/g by 43 days, 1.01 ng/g by 141 days, and was last detected at 0.72 ng/g at 253 days. **BSTCA** was initially detected in the sediment at 0.98 ng/g at 7 days, increased to a maximum of 18.33 ng/g by 85 days, decreased to 7.17 ng/g by 141 days, and ranged from 4.10 to 7.13 ng/g from 169-296 days. The registrant-calculated half-lives of 5-OH and BSTCA in sediment were 28.6 days and 84.9 days, respectively (Figure 23, p.168).

Average penoxsulam and transformation product concentrations in pond sediment, expressed as ng/g.

Days			Average conce	entration (ng/g)		
posttreatment	Penoxsulam	5-OH	BSTCA	BSA	2-Amino-TP	Sulfonamide
1	2.63	14.08	0.00	0.00	0.00	0.00
3	9.68	10.75	0.00	0.00	0.00	0.00
7	5.22	26.62	0.98	0.00	0.00	0.00
				0.00	0.00	0.00
14	17.37	15.39	3.08			
21	18.08	18.04	8.32	0.00	1.561	0.00
28	13.83	20.20	2.85	0.00	1.471	0.00
43	13.25	7.17	9.82	0.00	$0.00^{2}$	0.00
57	4.41	4.98	12.56	0.00	0.00	0.00
85	4.59	3.39	18.33	0.00	0.00	0.00
114	1.34	1.65	10.22	0.00	0.00	0.00
141	0.50	1.01	7.17	0.00	0.00	0.00
169	0.00	0.00	7.00	0.00	0.00	0.00
195	0.00	0.00	5.58	0.00	0.00	0.00
223	0.00	0.00	4.62	0.00	0.00	0.00
253	2.871	0.72	4.10	0.00	0.00	0.00
296	$0.00^{2}$	0.00	7.13	0.00	0.00	0.00

Data were obtained from Table 31, p.149 of the study report. Individual sample concentrations of the parent and transformation products from each of the three sampling stations are reported in Tables 29-30, pp.145-147 of the study report. Values in bold are above the LOQ (3.0 ng/g).

Total rainfall during the 9.5-month study period was 132.79 cm or 124% of the pro-rated annual historical rainfall total (p.48). The unusually high rainfall total was the result of rainfall from three tropical storms that occurred in August and September of 2004. The lowest monthly rainfall total occurred in January 2005 (2.11 cm over 27 days) and the highest occurred in September 2004 (41.09 cm) and included 12.34 cm on September 6, 2004 (Appendix A, pp.172-181). Pond water levels ranged from a low of 244.7 cm on May 31, 2004 to a maximum of 296.3 cm on September 27, 2004 (p.53). Water temperatures monitored via a thermocouple stack ranged from a low of 6.29°C on December 27, 2004 (measured at 50 cm from the sediment) to a high of 34.55°C on August 6, 2004 (measured at 35 cm from the pond surface; p.50); the study authors stated that significant water-column temperature gradients were observed in July and August of 2004 and in early January 2005 due to periods of intense rainfall (p.49). Water temperatures as measured by the Datasonde showed similar results (p.51; Figure 7, p.157); temperatures followed a diurnal pattern, with temperatures highest in the late afternoon due to solar warming (Figure 8, p.157).

The pH of the pond ranged from approximately 5.2 to 7 during the study period (p.51; Figure 9, p.158). Dissolved oxygen (DO) levels ranged from approximately 0.1 mg/L to 8.3 mg/L (p.52; Figure 11, p.159); DO levels generally remained very low particularly in the deep part of the pond, rarely rising above 1 mg/L until late in the study. The authors stated that water

<sup>1</sup> Single replicate detection as reported in Table 29, pp.145-146; values reported in Table 31 are not consistent with values reported in Table 29 of the study report.

<sup>2</sup> Not detected as reported in Table 29, pp.145-146; values reported in Table 31 are not consistent with values reported in Table 29 of the study report.

conductivity was low, ranging from 0.03 to 0.09 mS/cm (p.52; Figure 13, p.160). The authors added that water quality parameters were typical of small water bodies in Florida (p.54). Light penetration measurements indicated that 54% of the UV-B light was extinguished in the top 2 cm of the water column, and 97% was extinguished in the top 10 cm (p.54; Table 17, p.93); Secchi readings showed visibility increasing from an average visibility limit of 79 cm through mid-October to 117 cm for the last two months of the study (p.55; Table 18, p.94; Figure 19, p.164). The authors stated that the readings indicated that the pond moved from a hypereutrophic state (extremely high level of biological productivity) to a eutrophic state (high level of biological productivity) during the course of the study (p.55). The study authors stated that the test substance application had no obvious influence on water quality (p.64).

The storage stability study MRID 46433901 indicated that penoxsulam declined slightly in stored water samples, but that penoxsulam was stable for at least 230 days in water, and that the transformation products 5-OH, sulfonamide, BSTCA, BSA, 2-amino-TP, TPSA, and 5-OH-2amino-TP were stable in water for the duration of the 270-284 day storage interval. Corrected recoveries of penoxsulam from refrigerated samples were 109% at day 0, and decreased to 101% by 230 days and 93% by 433 days. Corrected recoveries of penoxsulam from frozen samples were 109% at day 0, 96% at 221 days, and decreased to 61% by 320 days. Corrected recoveries of 5-OH, sulfonamide, BSTCA, BSA, 2-amino-TP, TPSA, and 5-OH-2-amino-TP ranged from 98-115%, 103-115%, 85-94%, 102-114%, 105-124%, 93-107%, and 105-116%, respectively, throughout the 284-day storage interval, with no pattern of decline. The storage stability study MRID 46433902 indicated that penoxsulam and the transformation products 5-OH, sulfonamide, and BSA were stable in soil for the duration of the storage interval, 781 days, and that the stability of BSTCA and 2-amino-TP was questionable. Corrected recoveries of penoxsulam, 5-OH, sulfonamide and BSA ranged from 80-97%, 70-84%, 90-102%, and 90-108%, respectively, throughout the storage interval. Corrected recoveries of 2-amino-TP were initially 53% at day 0, were 43-44% from 91-196 days, 52% at 327 days, and ranged from 40-43% form 594-781 days, which indicates that recoveries were consistent, although low. Corrected recoveries of BSTCA ranged from 80-89% from 0 to 182 days, then decreased to 64-68% from 196-781 days.

### STUDY DEFICIENCIES

1. The stability of penoxsulam in water and sediment could not be confirmed because the storage stability study was not conducted using control samples from the test site fortified at a known concentration and stored frozen for the maximum length of storage of the test samples. Rather, separate stability studies were conducted with penoxsulam and its transformation products in water samples (MRID 46433901) and soil samples (MRID 46433902) obtained from California. The stability studies could not confirm the stability of penoxsulam in water for greater than 221 days or the stability of its transformation products in water for greater than 270-284 days. These periods of storage are insufficient because the test water samples were stored for a maximum of 380 days. In addition, the stability of BSTCA and 2-amino-TP from soil samples was questionable. The authors also stated that field spikes were prepared for both water and sediment samples, but that

the experiment was rejected due to degradation of the analytical standard used to prepare the travel spikes (p.45).

### **REVIEWER'S COMMENTS**

- 1. It is interesting to note that average measured concentration (167  $\mu$ g/L) 24 hours after application was 11% higher than the targeted whole-lake concentrations of 150  $\mu$ g/L. Individual sample concentrations were in excess of the targeted concentration rate of 150  $\mu$ g/L as much as three weeks after application. Some individual samples were more than 70% higher than the targeted concentration. This observation suggests that, in actual usage, initial concentrations of penoxsulam may exceed the intended applied concentration, and therefore might, in some places, inadvertently exceed maximum labeled concentrations for short periods following application at maximum application rates.
- 2. There was no pesticide use history for the test site. A three-year use history is needed to determine if pesticides related to the test chemical were applied in recent years that could have affected the degradation rate of the test chemical.
- 3. Sediment samples were analyzed on a wet-weight basis (Appendix F, p.846). The reviewer notes that samples analyzed on a wet-weight basis can have a dilution or concentration effect due to differences in soil moisture levels between samples. It is recommend that samples be analyzed on a dry-weight basis to control for the effects of soil moisture on the analyte concentrations.
- 4. The authors stated that the outlet culvert to the pond was opened between September 4 and 7, 2004 due to the heavy rainfall associated with a tropical storm system, and to prevent flooding of the surrounding land (p.53). The authors added that the outlet culvert was an overflow for surface water only and therefore, no significant test system water volume was lost.
- 5. The study authors stated that data gaps due to equipment malfunction of the on-site automated weather station were supplemented with data from three other sources; a station installed approximately 6 kilometers from the test site for use in a companion study; a NOAA weather station (station id 085275) located approximately 1 kilometer from the test site; and a NOAA station (station id 084394) located approximately 38 kilometers from the test site (pp.29-30).
- 6. The study authors stated that instrumentation to measure the oxidation-reduction potential of the bottom sediment was installed at sampling station C, but that due to failure of the pH sensors and fouling of the reference electrode, the oxidation-reduction monitoring equipment was removed and the data were not reported (pp.31-32).

### Data Evaluation Report on the aquatic field dissipation of penoxsulam

### PMRA Submission Number {.....}

EPA MRID Number 46703502

- 7. Application equipment calibration data reported in Table 7 (p.83) of the study report show that the relative standard deviation determined during the nozzle output calibration was 0.59% (pp.34-35).
- 8. The study authors stated that the stability and uniformity of this test substance formulation was studied in a referenced laboratory study in which a penoxsulam SC formulation was evaluated when mixed with water and adjuvant (Agri-Dex crop-oil-concentrate; p.37). The results indicated that penoxsulam was uniformly distributed in the tank, and was chemically stable, for more than 12 hours in the tank mixture.

### **REFERENCES**

**US EPA ARCHIVE DOCUMENT** 

- 1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 164-1, Terrestrial Field Dissipation Studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.
- 2. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, 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.

**Attachment 1: Structures of Parent Compound and Transformation Products** 

### Penoxsulam [XDE-638; DE-638; TSN101649; SP1019 (SePRO)]

**IUPAC Name:** 3-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-

c]pyrimidin-2-yl)- $\alpha$ , $\alpha$ , $\alpha$ -trifluorotoluene-sulfonamide.

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

6-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy-s-triazolo[1,5-c]pyrimidin-

2-yl)-\alpha,\alpha,\alpha-trifluoro-o-toluenesulfonamide.

CAS Name: 2-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-

c|pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide.

**CAS Number:** 219714-96-2.

SMILES String: FC(c1cccc(c1S(=O)(=O)N(c1nn2c(n1)ccnc2))OCC(F)F)(F)F

(ISIS v2.3/Universal SMILES).

No EPI Suite, v3.12 SMILES String found as of 6/27/06.

n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F.

$$F \xrightarrow{F} CH_2$$

$$OMe$$

$$F \xrightarrow{O} S = O$$

$$N \xrightarrow{N} N$$

$$OMe$$

$$OMe$$

# **Identified Compounds**

# Penoxsulam [XDE-638; DE-638; TSN101649; SP1019 (SePRO)]

**IUPAC Name:** 3-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-

c]pyrimidin-2-yl)- $\alpha$ , $\alpha$ , $\alpha$ -trifluorotoluene-sulfonamide.

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

6-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy-s-triazolo[1,5-c]pyrimidin-

2-yl)- $\alpha$ , $\alpha$ , $\alpha$ -trifluoro-o-toluenesulfonamide.

CAS Name: 2-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-

c|pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide.

**CAS Number:** 219714-96-2.

**SMILES String:** FC(c1cccc(c1S(=O)(=O)N(c1nn2c(n1)ccnc2))OCC(F)F)(F)F

(ISIS v2.3/Universal SMILES).

No EPI Suite, v3.12 SMILES String found as of 6/27/06.

n1c(nc2n1c(ncc2OC)OC)NS(=O)(=O)c3c(cccc3C(F)(F)F)OCC(F)F.

# BSTCA [TSN103610; TSN101979]

**IUPAC Name:** 3-[6-(2,2-Difluoroethoxy)-α,α,α-trifluoro-o-toluenesulfonamido]-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 Number:** Not reported.

**SMILES String:** n1c(nc(n1)C(O)=O)NS(=O)(=O)c2c(ccc2C(F)(F)F)OCC(F)F.

## BSA [Penoxsulam sulfonic acid; TSN101980]

IUPAC Name: 6-(2,2-Difluoroethoxy)-α,α,α-trifluoro-o-toluenesulfonic acid.
 CAS Name: 2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)benzenesulfonic acid.

**CAS Number:** Not reported.

**SMILES String:** S(=O)(=O)(c1c(ccc1C(F)(F)F)OCC(F)F)O.

### 2-Amino-TP [TSN101824]

IUPAC Name: 2-Amino-5,8-dimethoxy-s-triazolo[1,5-c]pyrimidine. 5,8-Dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-amine.

**CAS Number:** Not reported.

SMILES String: n1c(nc2n1c(ncc2OC)OC)N.

### Sulfonamide [TSN102354]

IUPAC Name: 2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)-benzenesulfonamide. 2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)-benzenesulfonamide.

**CAS Number:** Not reported.

**SMILES String:** NS(=O)(=O)c1c(cccc1C(F)(F)F)OCC(F)F.

$$\begin{array}{c|c} & & & & F \\ & & & & & \\ & & & & & \\ \hline & & & & & \\ F & & & & & \\ \hline & & & & & \\ F & & & & & \\ \hline \end{array}$$

## 5-OH-2-Amino-TP [Analyte of XDE-638; TSN101837]

**IUPAC Name:** Not reported.

2-Amino-8-methoxy[1,2,4]triazolo[1,5-c]pyrimidin-5-ol. **CAS Name:** 

Not reported. **CAS Number:** 

**SMILES String:** n1c(nc2n1c(ncc2OC)O)N.

# TPSA [Analyte of XDE-638; TSN102025]

**IUPAC Name:** Not reported.

(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)sulfamic acid. **CAS Name:** 

**CAS Number:** Not reported.

**SMILES String:** nlc(nc2nlc(ncc2OC)OC)NS(=O)(=O)O.

# 5-OH-XDE-638 [5-Hydroxy-XDE-638; 5-OH-DE-638; TSN101756; 5-OH]

**IUPAC Name:** 6-(2,2-Difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo-s-

triazolo[1,5-c]pyrimidin-2-yl)- $\alpha$ , $\alpha$ , $\alpha$ -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 Number:** Not reported.

**SMILES String:** n1c(nc20C)O)NS(=O)(=O)c3c(ccc3C(F)(F)F)OCC(F)F.

# **Attachment 2: Excel Spreadsheets**

Chemical name Penoxsulam
PC code 119031

Water

MRID 46703502 Guideline No. 164-2

# Half-life (days) = 24.8

Days	Penoxsulam	Ln
posttreatment	(ng/mL)	(penoxsulam)
1	` 26.9 ´	" 3.29 ´
1	24.3	3.19
1	21.9	3.09
1	17.0	2.83
1	19.4	2.97
1	36.2	3.59
1	33.1	3.50
1	33.0	3.50
1	56.5	4.03
1	42.1	3.74
1	54.5	4.00
1	200	5.30
1	254	5.54
1	197	5.28
1	217	5.38
1	201	5.30
1	233	5.45
1	235	5.46
1	257	5.55
1	275	5.62
1	217	5.38
1	219	5.39
1	181	5.20
1	227	5.42
1	176	5.17
1	215	5.37
1	173	5.15
1	220	5.39
3	38.8	3.66
3	36.1	3.59
3	27.8	3.33
3	41.5	3.73
3	41.0	3.71
3	35.2	3.56
3	36.0	3.58
3	142	4.96
3	113	4.73
3	118	4.77
3	214	5.37
3 3 3 3 3 3 3	178	5.18
3	212	5.36
3	177	5.18
3	293	5.68

3	190	5.25	
3	154	5.04	
3	210	5.35	
3	179	5.19	
3 3	213	5.36	
3	143	4.96	
3	176	5.17	
3	237	5.47	
3 3 3 3	165	5.11	
3	186	5.23	
3	228	5.43	
3	170	5.14	
3 3	220	5.39	
	184	5.21	
7	29.9	3.40	
7	24.3	3.19	
7	24.9	3.21	
7	56.1	4.03	
7 7	46.6 48.0	3.84 3.87	
7	48.0 112	3.67 4.72	
7	97.4	4.58	
7	111	4.71	
, 7	144	4.97	
7	150	5.01	
7	152	5.02	
7	116	4.75	
7	175	5.16	
7	167	5.12	
7	136	4.91	
7	158	5.06	
7	112	4.72	
7	137	4.92	
7	203	5.31	
7	172	5.15	
7	217	5.38	
7	160	5.08	
7 7	127	4.84	
7	182 151	5.20 5.02	
7	136	4.91	
7	138	4.93	
7	164	5.10	
7	179	5.19	
7	150	5.01	
7	160	5.08	
7	167	5.12	
7	168	5.12	
14	111	4.71	
14	118	4.77	
14	132	4.88	
14	135	4.91	

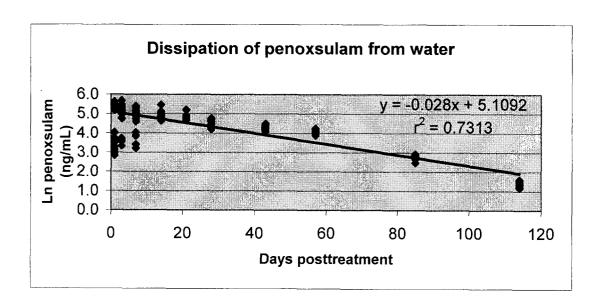
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14	126	4.84
14	133	4.89
14	132	4.88
14	233	5.45
14	157	5.06
14	132	4.88
14	165	5.11
14	145	4.98
14	141	4.95
	140	4.94
14		
14	129	4.86
14	131	4.88
14	117	4.76
14	137	4.92
14	149	5.00
14	130	4.87
14	137	4.92
14	130	4.87
14	135	4.91
14	131	4.88
14	101	4.62
14	124	4.82
14	129	4.86
14	130	4.87
14	152	5.02
14	133	4.89
14	126	4.84
14		
	126	4.84
14	120	4.79
14	121	4.80
21	105	4.65
21	107	4.67
21	107	4.67
21	117	4.76
21	111	4.71
21	183	5.21
21	176	5.17
21	107	4.67
21	111	4.71
21	137	4.92
21	119	4.78
21	127	4.84
21	123	4.81
21	128	4.85
21	113	4.73
21	119	4.78
28	112	4.72
28	104	4.64
28	111	4.71
28	87.1	4.47
28	98.1	4.59
28	70.4	4.25
20	10.7	7.20

28	110	4.70
28	80.2	4.38
28	113	4.73
28	78.2	4.36
28	98.2	4.59
28	82.2	4.41
28	95.7	4.56
28	82.5	4.41
28	102	4.62
28	84.5	4.44
28	117	4.76
28	84.3	4.43
28	109	4.69
28	82.8	4.42
28	113	4.73
28	72.5	4.28
28	65.6	4.18
43	88.6	4.48
43	84.8	4.44
43	58.8	4.07
43	67.4	4.21
43	71.5	4.27
43	71.4	4.27
43	64.1	4.16
43	76.5	4.34
43	73.7	4.30
43	72.9	4.29
43	74.0	4.30
43	85.8	4.45
43	66.9	4.20
43	81.9	4.41
43	70.7	4.26
43 43	86.1 72.5	4.46 4.28
43	65.6	4.20
43	75.9	4.33
43	68.4	4.23
43	67.3	4.21
43	87.9	4.48
57	49.2	3.90
57	47.9	3.87
57	69.0	4.23
57	56.1	4.03
57	70.0	4.25
57	61.4	4.12
57	68.5	4.23
57	48.9	3.89
57	61.5	4.12
57	69.6	4.24
57	58.4	4.07
57 57	49.8	3.91
57	66.9	4.20

57	58.2	4.06
57	69.9	4.25
57	59.4	4.08
57	68.5	4.23
57	51.9	3.95
57	67.5	4.21
57	51.1	3.93
85	17.6	2.87
85	11.7	2.46
85	17.1	2.84
85	17.2	2.84
85	16.5	2.80
85	17.4	2.86
85	18.1	2.90
85	16.3	2.79
85	16.5	2.80
85	17.7	2.87
85	15.4	2.73
85	18.4	2.91
85	16.1	2.78
85	16.7	2.82
85	14.1	2.65
85	16.3	2.79
85	16.5	2.80
85	16.8	2.82
85	14.3	2.66
114	3.41	1.23
114	4.00	1.39
114	3.84	1.35
114	4.94	1.60
114	4.77	1.56
114	4.75	1.56
114	3.88	1.36
114	4.66	1.54
114	4.36	1.47
114	3.25	1.18
114	3.30	1.19
114	3.66	1.30
114	3.47	1.24
114	3.36	1.24
114	4.05	1.40
114	4.05 4.42	1.40
114	4.42 3.25	
114	3.25 3.46	1.18 1.24
114	3.46 3.71	1.24
114	3.71 3.36	1.31
114		
114	3.20	1.16

114 3.20 1.16
Data obtained from Table 20, pp. 96-101 of the study report.



Chemical name Penoxsulam Sediment

PC code 119031 MRID 46703502 Guideline No. 164-2

### Half-life (days) = 34.5

### \*Calculated using 21-141 day data

Days	Penoxsulam	Ln (nanayaylam)	Moon (ng/g)
posttreatment 1	(ng/g) 0	(penoxsulam)	Mean (ng/g)
1	3.62	1.29	
1	4.27	1.45	2.63
3	5.58	1.72	
3	3.86	1.35	
3	19.6	2.98	9.68
7	2.09	0.74	
7	4.85	1.58	
7	8.73	2.17	5.22
14	21.7	3.08	
14 14	14.5 15.0	2.67	17.37
21	15.9 27.3	2.77 3.31	17.37
21	18.9	2.94	
21	8.03	2.08	18.08
28	3.49	1.25	
28	5.41	1.69	
28	32.6	3.48	13.83
43	18.2	2.90	
43	7.36	2.00	
43	14.2	2.65	13.25
57	6.97	1.94	
57	2.14	0.76	
57	4.12	1.42	4.41
85	1.45	0.37	
85 85	6.77	1.91	4.50
85 114	5.56 1.18	1.72 0.17	4.59
114	0	0.17	
114	2.83	1.04	1.34
141	0	1.04	1.04
141	0		
141	1.5	0.41	0.50
169	0		
169	0		
169	0		0.00
195	0		
195	0		
195	0		0.00
223	0		
223	0 0		0.00
223	U		0.00

253	0		
253	0		
253	2.87	1.05	0.96
296	0		
296	0		
296	0		0.00

Data obtained from Table 29, pp. 145-146, and Table 31, p. 149 of the study report.

