5-14-04

Data Evaluation Report on the aquatic field dissipation of penoxsulam

PMRA Submission Number {......} EPA MRID Number 45830805

Data Requirement: PMRA Data Code:
EPA DP Barcode: D288160
OECD Data Point:
EPA Guideline: 164-2

Test material: XDE-638

End Use Product name: XDE-638 GF-520 **Concentration of a.i.:** 0.11% (w/w)

Formulation type: Granule

Active ingredient
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.

Primary Reviewer: Dan Hunt **Signature:**
Dynamac Corporation **Date:**

QC Reviewer: Joan Harlin **Signature:**
Dynamac Corporation **Date:**

Secondary Reviewer: Lucy Shanaman **Signature:** Lucy Shanaman
EPA **Date:** May 14, 2004

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

CITATION: Roberts, D.W., S.C. Dolder and G.E. Schelle. 2002. Field dissipation of XDE-638 granule in California rice agriculture. Unpublished study performed by Dow AgroSciences LLC, Indianapolis, IN, AGVISE Laboratories, Inc., Northwood, ND and Agricultural Advisors, Inc., Live Oak, CA, and submitted by Dow AgroSciences LLC, Indianapolis, IN. Laboratory Study ID: 010072. Experiment initiation June 12, 2001, and completion August 14, 2002 (p.3). Final report issued September 6, 2002.

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ABSTRACT

Field Dissipation - Aquatic

Penoxsulam (6-(2,2-difluoroethoxy)-N-(5,8-dimethoxy-s-triazolo[1,5-c]pyrimidin-2-yl)-α,α,α-trifluoro-o-toluenesulfonamide; XDE-638; formulated as a granule containing a nominal 0.11% penoxsulam), was applied once at an application rate of 55.7 g a.i./ha (target application rate of 40 g a.i./ha) onto a flooded plot of Oswald clay soil planted with rice. Following application, water samples were collected for analysis of penoxsulam and seven transformation products: 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 (5-OH-XDE-638), 2-amino-8-methoxy[1,2,4]triazolo[1,5-c]pyrimidin-5-ol (2-amino-TP), 3-{[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulfonyl]amino]-1H-1,2,4-triazole-5-carboxylic acid (BSTCA), 2-(2,2-difluoroethoxy)-6-(trifluoromethyl)benzenesulfonic acid (BSA), 5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-ylsulfamic acid (XDE-638 TPSA), 2-(2,2-difluoroethoxy)-6-(trifluoromethyl)-benzenesulfonamide (sulfonamide), and 2-amino-8-methoxy[1,2,4]triazolo[1,5-c]pyrimidin-5-ol (5-OH-2-amino-TP) through 92 days after application (when the plots were drained). Soil samples were collected for analysis of penoxsulam and the transformation products 5-OH-XDE-638, 2-amino-TP, BSTCA, BSA, and sulfonamide through 306 days posttreatment.

Penoxsulam dissipated in the paddy water with a first-order calculated half-life value of 4.2 days ($r^2 = 0.91$). Penoxsulam was detected in the **paddy water** at 0.033 μg/mL at day 0, was 0.027-0.028 μg/mL from 4 hours to 2 days, decreased to 0.010 μg/mL by 7 days, and was detected below the LOQ at 14 and 21 days posttreatment. Transformation products of penoxsulam were not detected in the paddy water at any sampling interval except for a single trace detection of **BSTCA** at 21 days posttreatment at the LOD (0.001 μg/mL).

Penoxsulam was initially detected in the 0- to 3-inch depth of the **soil** at 0.0041 μg/g at day 0, was a maximum of 0.0046 μg/g at 2 days, decreased to 0.0033 μg/g by 14 days, and was detected below the LOQ at 21, 30 and 61 days posttreatment. The only two transformation products detected in the soil at a mean concentration above the LOD were 5-OH XDE-638 and BSTCA. **5-OH XDE-638** was detected in the 0- to 3-inch soil depth at a maximum of 0.0012 μg/g at 14 days, and was not detected in soil following 30 days posttreatment. **BSTCA** was detected in the 0- to 3-inch soil depth at a maximum of 0.0029 μg/g at 14 days, and decreased to 0.0020 μg/g by 306 days (the last sampling interval). No analytes were detected below the 0- to 3-inch soil depth except for BSTCA, which was detected once in the 3- to 6-inch depth, at 0.0012 μg/g at 306 days posttreatment. The data did not allow for the calculation of a half-life value for penoxsulam in soil.

Study Acceptability: This study is classified **acceptable** and partially satisfies the US EPA Subdivision N Guideline §164-2 for an aquatic field dissipation study.

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MATERIALS AND METHODS

The aquatic field dissipation of penoxsulam (6-(2,2-difluoroethoxy)-N-(5,8-dimethoxy-s-triazolo[1,5-c]pyrimidin-2-yl)-α,α,α-trifluoro-o-toluenesulfonamide; XDE-638), formulated as GF-520 (a granule containing a nominal 0.11% penoxsulam), was conducted on a flooded plot (17 x 145 ft; slope ≤1%; Figure 2, p.41) planted to rice in Sutter County, California (pp.11-13). The soil at the test site was an Oswald clay (0- to 12-inch depth: 37-39% sand, 27-29% silt, 32-36% clay, pH 6.5-6.6, 3.1-3.8% organic matter, CEC 23.2-24.5 meq/100 g, bulk density 1.31 g/cm^3; Table 1, p.30; Appendix D, p.58). The treated plot consisted of three replicate plots which were each divided into five equal-sized subplots (Figure 2, p.41). Each subplot consisted of 14 sub-subplots which comprised the sampling locations for water and soil samples. A control plot (13 x 46 ft) was also established at the test site and planted with rice. The control plot was located an unspecified distance from the treated plot. A three-year plot history indicated that Roundup was applied in 1998 (fallow), and that 2,4-D and Ordram were applied in 1999 and 2000 to rice (p.14). Approximately one month prior to treatment, both plots (treated and control) were disked and/or rolled to provide a weed-free bareground condition, and were planted with rice (M-202 variety) approximately two weeks later on May 30, 2001, 14 days prior to the test application.

Following planting, the plots were flooded with water that was delivered by a nearby diversion canal (p.14). Characteristics of the water was as follows: pH 7.0, hardness 47 ppm, conductivity 0.17 mmhos/cm, total dissolved solids 178 ppm, turbidity 55 NTU, and alkalinity 64 mg (Table 1, p.30). Water was diverted as necessary in order to maintain an average 3-4 inch water level throughout the growing season. The flood water was drained from the test plot between September 13 and 19, 2001 (92-98 days posttreatment) just prior to rice crop harvest (p.14). The rice was harvested on September 30, 2001 and allowed to dry. One month later (October 29, 2001), the dried crop residue was burned within the test plot.

Meteorological and paddy water conditions were collected from an on-site weather station (p.15). The weather station recorded water level and temperature (approximately 2 inches from paddy bottom), soil temperatures (at 1- and 4-inch depth), relative humidity, wind speed and direction, air temperature, total solar radiation, and precipitation. In addition, a portable water quality station was placed inside the test plot to measure temperature, pH, dissolved oxygen, reduction/oxidation potential, specific conductivity, and total dissolved solids.

Penoxsulam was broadcast once, on June 13, 2001, at a target application rate of 40 g a.i./ha onto the flooded plot (p.16; Appendix E, p.60). The theoretical application rate was 55.7 g a.i./ha, based on calibration and pass-time data (Appendix E, p.60). The application was made using a hand-held granular drop-spreader, and was performed manually by the field investigator by turning the hand-crank of the drop spreader while walking on the levee along each 145-ft side of the plot at a timed pace. Meteorological conditions during application were as follows: wind speed and direction 5 mph, NW, air temperature 88°F, and relative humidity 29% (Appendix E, p.60). The rice was at the 3-4 leaf growth stage at the time of application. The test plots were fertilized once during the test period, with 15-15-15 fertilizer at a rate of 100 lb/acre in July 2001, and did not receive any other chemicals during the test duration (p.14).

To verify the application rate, three disposable aluminum pans (9 x 12.5 inches) were placed along each 145-ft side of the treated plot (6 pans total) prior to application (p.17). Following application, the pans were collected and the weight of the granules recovered was used to estimate the application efficiency. The weight of the granules recovered from the pans indicated that 122% of the target rate was achieved and 88% of the theoretical rate was achieved (Table 4, p.33).

Water samples were collected from the treated plot one day prior to the application and at 0, 4 and 8 hours and 1, 2, 7, 14, 21, 30, 61, and 92 days following the application (p.17; Table 2, p.31). Water samples (approximately 25 mL) were collected from the middle of the water column with disposable serological glass pipettes (p.18). Samples were capped and placed directly on dry ice immediately after sampling. Samples were frozen a few minutes after collection and were maintained in frozen condition during transport to the sponsor's facility. At the sponsor's facility, water samples were combined to produce three composite samples (one for each replicate plot) per sampling event (p.20). Water samples were stored frozen for up to 171 days prior to analysis (Appendix L, Table 1, p.115).

Soil samples were collected from the treated plot one day prior to the application and at 1, 2, 7, 14, 21, 30, 61, 92, 188, and 306 days following the application (p.17; Table 2, p.31). Soil samples were manually collected to a depth of 9 inches using a sampling tube fitted with an acetate liner (2.0- to 2.5-cm diameter; pp.18-19). Soil cores were placed on dry ice immediately after collection and placed in frozen storage at the field facility before being shipped frozen to the sponsor's facility. At the sponsor's facility, cores were sectioned into 3-inch segments and combined to produce three composite samples (one for each replicate plot) per segment and sampling event (p.19). Composite samples were then homogenized by grinding with dry ice, then were split into analytical and long-term samples and placed back into frozen storage (approximately -20°C) until analysis. Soil samples were stored frozen for up to 238 days prior to analysis (Appendix L, Table 1, p.115).

For each sampling event, one sub-subplot row (1-14) was randomly selected in each of the three replicate plots as the sampling location for that event (p.13; Figure 2, p.41). One sample was then collected from each of the five subplots corresponding to that row to produce a total of 15 samples per event (five from each replicate plot). When soil and water samples were to be collected from the same sampling area, water samples were collected first to prevent disturbance of the water column.

Water and soil samples were analyzed for penoxsulam and the transformation products 5-OH-XDE-638, 5,8-dimethoxy XDE-638 metabolite (2-amino-TP), triethylammonium of XDE-638 metabolite (BSTCA), XDE-638 sulfonic acid metabolite (BSA), and sulfonamide. Water samples were also analyzed for the additional transformation products XDE-638 TPSA and 2-amino-8-methoxy (5-OH-2-amino-TP; Appendix L, pp.102-103). Soil samples were not analyzed for TPSA and 5-OH-2-amino-TP because these transformation products were found only in the laboratory aqueous photolysis studies of penoxsulam (Appendix C, p.54).

Complete chemical names for penoxsulam and its transformation products.

Applicant's Code Name	Chemical Name	Molecular Weight	Media Analyzed
XDE-638 (penoxsulam)	2-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)-benzenesulfonamide	483	Water Soil
5-OH XDE-638; 5-OH XDE-638; 5-OH	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	469	Water Soil
BSTCA	3-[[[2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)phenyl]sulfonyl]amino]-1H-1,2,4-triazole-5-carboxylic acid	416	Water Soil
BSA	2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)benzenesulfonic acid	306	Water Soil
XDE-638 TPSA; TPSA	5,8-Dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-ylsulfamic acid	275	Water
2-Amino-TP	2-Amino-8-methoxy{1,2,4]triazolo[1,5-c]pyrimidin-5-ol	195	Water Soil
5-OH-2-amino-TP; 5-OH-2-amino-TP; 5-OH-2-ATP	2-Amino-8-methoxy[1,2,4]triazolo[1,5-c]pyrimidin-5-ol	181	Water
Sulfonamide	2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)-benzenesulfonamide	305	Water Soil

Chemical names and molecular weights were obtained from Appendix A, pp.47-48 of the study report. A discussion of the rationale for the selection of transformation products analyzed for in water and soil samples can be found in Appendix C, pp.53-56 of the study report.

Water samples were analyzed according to the method GRM 01.30 (Appendix L, p.102). Sample aliquots were analyzed by HPLC with tandem mass spectrometry detection. Analysis was performed using a YMC ODS AM column and a PE/Sciex API 2000 tandem mass selective detector. The limits of detection and quantitation were 0.001 μg/mL and 0.003 μg/mL, respectively, for all analytes in water (Appendix L, p.104).

Soil samples were analyzed according to the method GRM 01.31 (Appendix L, p.102). Samples aliquots (5 g) were extracted twice by shaking with acetonitrile:1.0N HCl (90:10, v:v). The soil was centrifuged following each extraction step and the extracts were combined. An aliquot of the extract was evaporated and reconstituted in 0.1N HCl, and then purified using a hydrophilic-lipophilic balanced solid phase extraction plate using a Tecan Genesis Workstation 150. After evaporating to dryness, the eluate was reconstituted and analysed by HPLC with tandem mass spectrometry detection. Analysis was performed using a YMC ODS AM column and a PE/Sciex API 3000 tandem mass selective detector (p.102).

The limits of detection and quantitation were 0.001 µg/g and 0.003 µg/g, respectively, for all analytes in soil (Appendix L, p.104).

To determine the efficiency of the analytical methods, samples of water were fortified with penoxsulam and the transformation products 5-OH-XDE-638, 2-amino-TP, BSTCA, BSA, XDE-638 TPSA, sulfonamide, and 5-OH-2-amino-TP over the range of 0.003-0.09 µg/mL, and samples of soil were fortified with penoxsulam and the transformation products 5-OH-XDE-638; 2-amino-TP, BSTCA, BSA, and sulfonamide over the range of 0.003-0.20 µg/g (Appendix L, pp.103-104).

Mean (± SD) concurrent recoveries of penoxsulam and its transformation products from water and soil.

Analyte	Percent Recovery	
	Water	Soil
XDE-638 (penoxsulam)	100 ± 5	83 ± 10
5-OH XDE-638	94 ± 3	80 ± 5
BSTCA	93 ± 6	76 ± 5
BSA	115 ± 13	85 ± 6
XDE-638 TPSA	112 ± 11	NA
2-Amino-TP	93 ± 4	86 ± 9
5-OH-2-amino-TP	63 ± 13	NA
Sulfonamide	99 ± 6	75 ± 4

Means were obtained from Appendix L, p.104 and Tables 2-15, pp.116-122 of the study report.

RESULTS/DISCUSSION

Penoxsulam (6-(2,2-difluoroethoxy)-N-(5,8-dimethoxy-s-triazolo[1,5-c]pyrimidin-2-yl)-α,α,α-trifluoro-o-toluenesulfonamide [XDE-638] formulated as a granule containing a nominal 0.11% penoxsulam), applied once at a target application rate of 40 g a.i./ha (actual application rate of 55.7 g a.i./ha) onto a flooded plot of Oswald clay soil planted with rice, dissipated in the paddy water with a first-order calculated half-life value of 4.2 days (r^2 = 0.91). The data did not allow for the calculation of a half-life value for penoxsulam in soil.

Penoxsulam was detected in the **paddy water** at 0.033 µg/mL at day 0, was 0.027-0.028 µg/mL from 4 hours to 2 days, decreased to 0.010 µg/mL by 7 days, and was detected below the LOQ at 14 and 21 days posttreatment (Table 5, p.34; Appendix I, pp.79-80). Transformation products of penoxsulam were not detected in the paddy water at any sampling interval except for a single trace detection of **BSTCA** at 21 days posttreatment at the LOD (0.001 µg/mL; Table 6, p.35; Appendix I, pp.79-80).

Penoxsulam was initially detected in the 0- to 3-inch depth of the **soil** at 0.0041 µg/g at day 0, was a maximum of 0.0046 µg/g at 2 days, decreased to 0.0033 µg/g by 14 days, and was detected below the LOQ at 21 days (all three replicates), 30 days (2 of 3 replicates), and 61 days (1 of 3 replicates; Table 7, p.36; Appendix J, pp.82-87). Penoxsulam was not detected below the 0- to 3-inch soil depth at any sampling interval. The only two transformation products detected in the soil at a mean concentration above the LOD were 5-OH XDE-638 and BSTCA. **5-OH XDE-638** was detected in the 0- to 3-inch soil depth at a maximum of 0.0012 µg/g (mean of 3 replicates, with residues in 2 replicates detected above the LOD) at 14 days, and was not detected in soil following 30 days posttreatment. 5-OH XDE-638 was not detected below the 0- to 3-inch soil depth. **BSTCA** was detected in the 0- to 3-inch soil depth at a maximum of 0.0029 µg/g (mean of 3 replicates, with residues in 2 replicates detected above the LOD) at 14 days, and decreased to 0.0020 µg/g (mean of 3 replicates, with residues in 2 replicates detected above the LOD) by 306 days posttreatment (the last sampling interval). BSTCA was detected once in the 3- to 6-inch depth, at 0.0012 µg/g (mean of 3 replicates, with residues in 2 replicates detected above the LOD) at 306 days posttreatment, and was not detected below that depth.

The average air temperature for the study duration was near normal (pp.23-24; Table 3, p.32). After the plots were drained at 92-98 days posttreatment, rainfall totaled 15.19 inches through the end of the study, which was 87% of the 30-year normal precipitation for the same period. Precipitation was not supplemented with irrigation after the plots were drained. The average daily water level during the flooded period fluctuated from between approximately 2 to 5 inches (p.24; Figure 3, p.42). Daily environmental data (air and soil temperature, relative humidity, rainfall, wind speed, solar radiation, water level, and water temperature) were reported in Appendix G (pp.65-73), and water quality measurements were reported graphically in Appendix H (pp.75-77).

DEFICIENCIES/DEVIATIONS

1. The study authors stated that the field investigator observed granules bouncing out of the application verification pans during application and that therefore, the application rate verification data were not used to establish the theoretical application rate (p.25). Instead, the theoretical application rate used, 55.7 g a.i./ha (139% of the target application rate), was obtained from the calibration discharge rate of the spreader (13.37 g/sec) and the pass-time data (43.335 sec/145 ft; p.24; Appendix E, p.60). The day-0 concentration of penoxsulam in the paddy water was 0.033 µg/mL, which was 101% of the theoretical application rate (p.25). The maximum proposed seasonal application rate of penoxsulam for agricultural use was reported as 40 g a.i./ha (p.9).

2. The study authors stated that a frozen storage stability study of penoxsulam and transformation products in soil and water is currently in progress, and that preliminary results indicate that penoxsulam and its transformation products are stable in frozen soil for at least 327 days, and in frozen water for at least 221 days (p.20). The reviewer notes that these storage periods exceed the maximum length of storage for the test samples (238 days for soil

and 171 days for water; Appendix L, Table 1, p.115). The authors stated that the storage stability study is scheduled to continue for up to approximately 2 years (Appendix L, p.101).

3. The calculated DT_{50} and DT_{90} values for penoxsulam in rice paddy water were 3 days and 10 days ($r^2 = 0.9707$), respectively, calculated using non-linear regression (SigmaPlot software; p.22; Figure 5, p.44). The calculated DT_{50} and DT_{90} values for penoxsulam in the total system (water plus soil) were 4 days and 15 days ($r^2 = 0.9709$), respectively (Figure 6, p.45). Dissipation of penoxsulam from the total system was determined after converting concentrations in water (µg/mL) and soil (µg/g) to g a.i./ha (Table 10, p.39). Sample conversion calculations were provided in Appendix K (pp.89-90).

4. The study authors stated that the rapid half-life of penoxsulam in this study was consistent with the 4-6 day field half-life observed in a similar study conducted using a liquid formulation of penoxsulam in Arkansas and California (MRID 45830804), and is consistent with the 2-day aqueous photolysis half-life (p.28). Physical/chemical and environmental properties of penoxsulam are reported in Appendix B (pp.50-51).

5. The study authors stated that four additional transformation products were detected in laboratory studies at ≥10% of the applied penoxsulam, besides the seven transformation products analyzed for in this study, but that in a meeting with US EPA EFED on January 23, 2001, it was agreed upon to not include these transformation products in the analytical methods (Appendix C, pp.53-56). A complete discussion of the rationale for the selection of transformation products analyzed for in water and soil samples can be found in Appendix C of the study report.

6. The study authors stated that laboratory environmental fate and chemistry studies indicated that penoxsulam degrades through two separate pathways, the photolytic degradation pathway which is initiated by cleavage of the sulfonamide bridge portion of the parent molecule, and the biodegradation pathway which proceeds through degradation of the pyrimidine ring and its substituents (p.10).

7. Signed and dated Good Laboratory Practice, Quality Assurance and No Data Confidentiality statements were provided with the study (pp.2-4).

Attachment 1

Excel Spreadsheets

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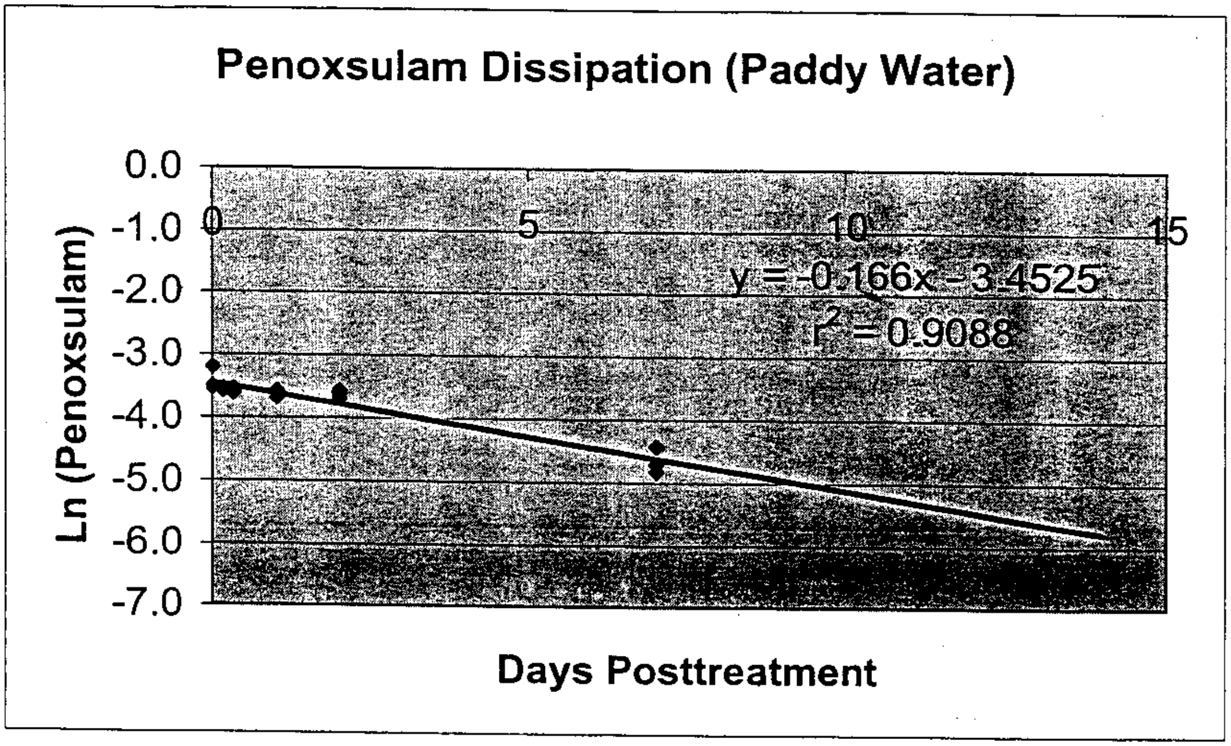
Chemical Name	Penoxsulam	**Water**
PC Code	119031	
MRID	45830805	
Guideline No.	164-2	

Half-life (days) = **4.2** * Half-life based on all data points

Days Posttreatment	Penoxsulam (ug/mL)	Ln (Penoxsulam)
0	0.041	-3.1942
0	0.030	-3.5066
0	0.029	-3.5405
0.167	0.028	-3.5756
0.167	0.029	-3.5405
0.167	0.028	-3.5756
0.333	0.027	-3.6119
0.333	0.028	-3.5756
0.333	0.029	-3.5405
1	0.025	-3.6889
1	0.027	-3.6119
1	0.028	-3.5756
2	0.027	-3.6119
2	0.028	-3.5756
2	0.025	-3.6889
7	0.008	-4.8283
7	0.009	-4.7105
7	0.012	-4.4228
14	<LOQ	
14	<LOQ	

Data obtained from Appendix I, pp. 79-80 in the study report.

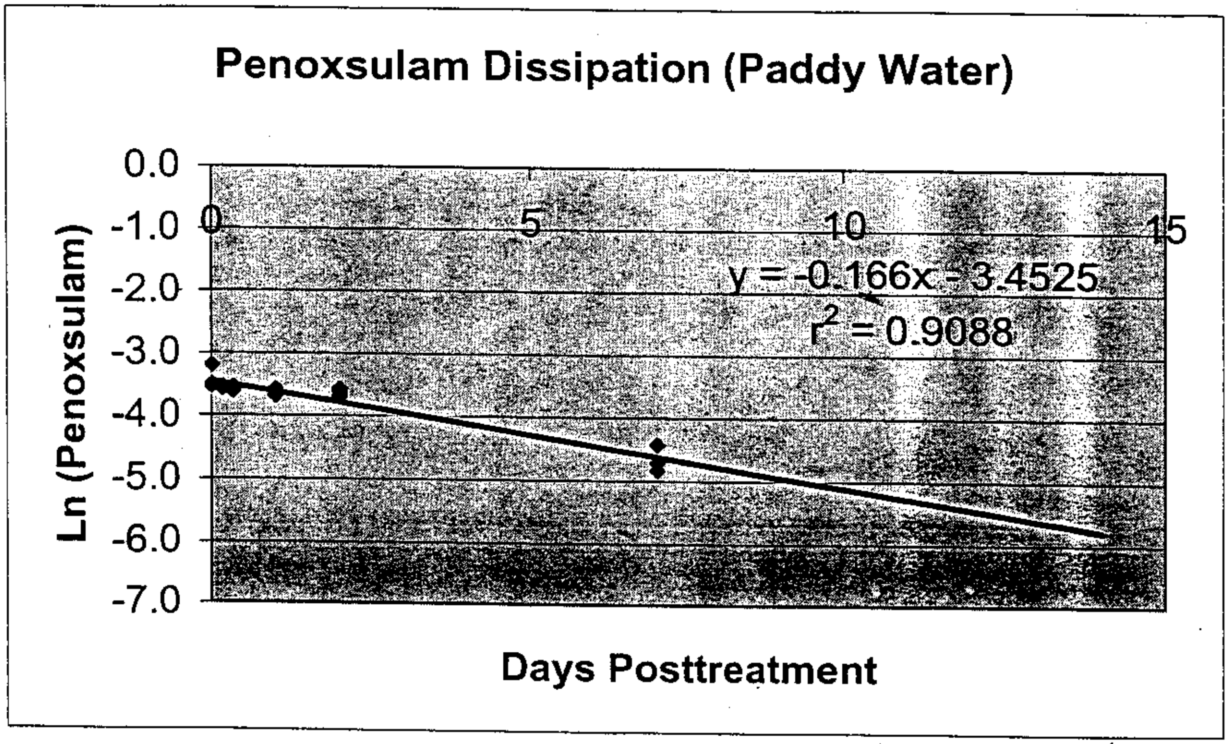


Chemical Name	Penoxsulam	**Water**
PC Code	119031	
MRID	45830805	
Guideline No.	164-2	

Half-life (days) = **4.2** * Half-life based on all data points.

Days Posttreatment	Penoxsulam (ug/mL)	Ln (Penoxsulam)
0	0.041	-3.1942
0	0.030	-3.5066
0	0.029	-3.5405
0.167	0.028	-3.5756
0.167	0.029	-3.5405
0.167	0.028	-3.5756
0.333	0.027	-3.6119
0.333	0.028	-3.5756
0.333	0.029	-3.5405
1	0.025	-3.6889
1	0.027	-3.6119
1	0.028	-3.5756
2	0.027	-3.6119
2	0.028	-3.5756
2	0.025	-3.6889
7	0.008	-4.8283
7	0.009	-4.7105
7	0.012	-4.4228
14	<LOQ	
14	<LOQ	

Data obtained from Appendix I, pp. 79-80 of the study report.

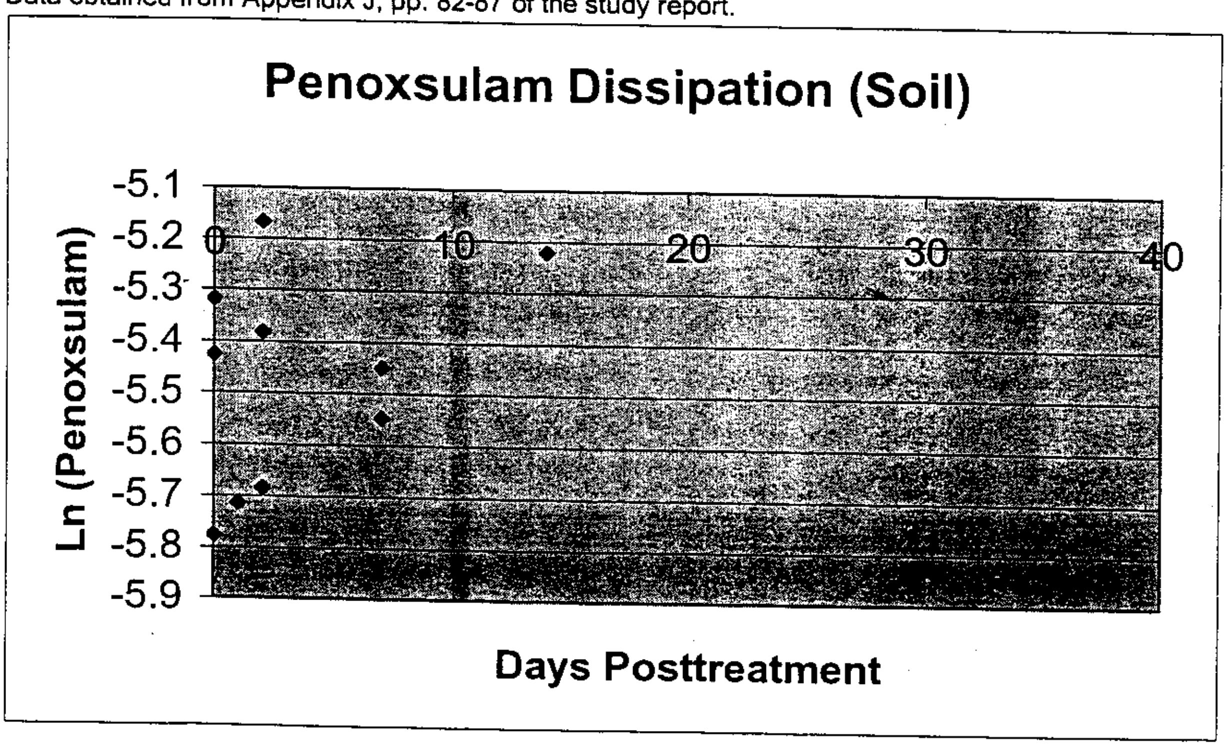


Chemical Name	Penoxsulam	**Soil (0- to 3-inch depth)**
PC Code	119031	
MRID	45830805	
Guideline No.	164-2	

Half-life (days) = **Not Calculated**

Days Posttreatment	Penoxsulam (ug/g)	Ln (Penoxsulam)
0	0.0031	-5.7764
0	0.0044	-5.4262
0	0.0049	-5.3185
1	<LOQ	
1	<LOQ	
1	0.0033	-5.7138
2	0.0046	-5.3817
2	0.0034	-5.6840
2	0.0057	-5.1673
7	0.0043	-5.4491
7	0.0039	-5.5468
7	ND	
14	<LOQ	
14	<LOQ	
14	0.0054	-5.2214
21	<LOQ	
21	<LOQ	
21	<LOQ	
30	ND	
30	<LOQ	
30	<LOQ	

Data obtained from Appendix J, pp. 82-87 of the study report.



Attachment 2

Structures of Parent and Transformation Products

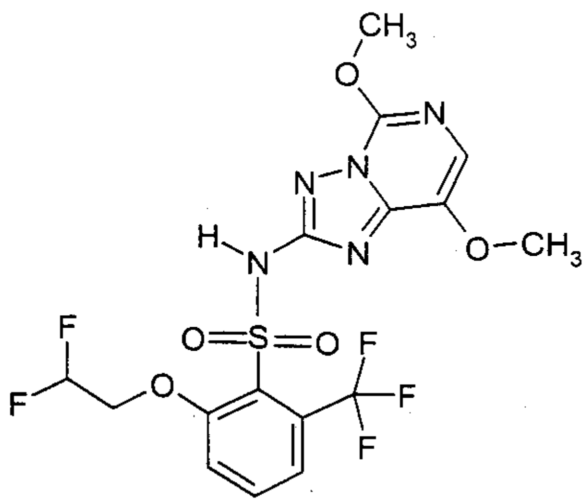
Penoxsulam

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

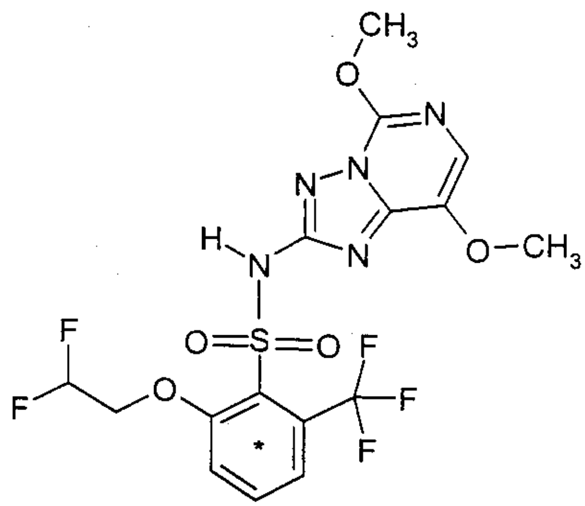
CAS name: 2-(2,2-Difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide

CAS No: 219714-96-2

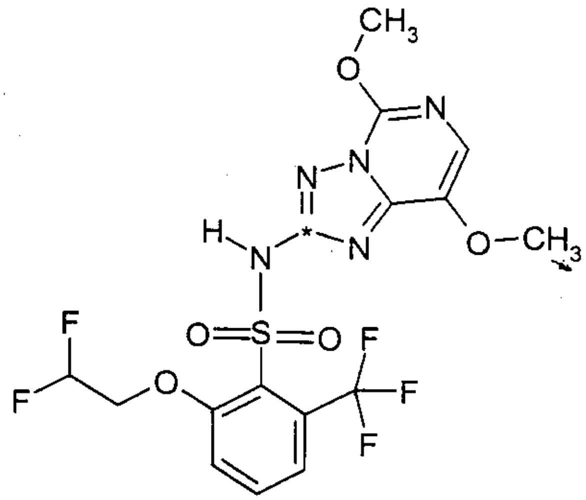
Unlabeled



[Phenyl-U-^{14}C] label



[Triazolopyrimidine-2-^{14}C] label

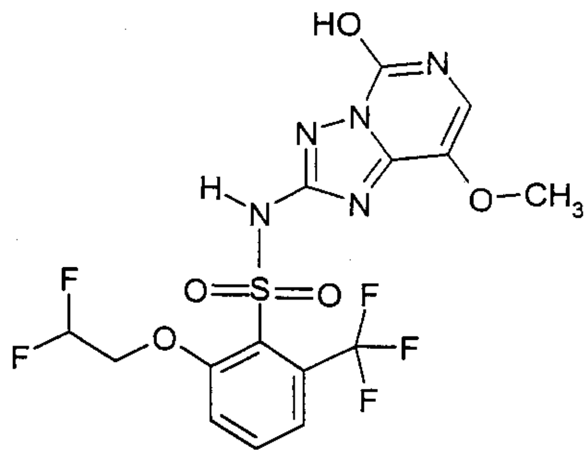


* Position of the radiolabel.

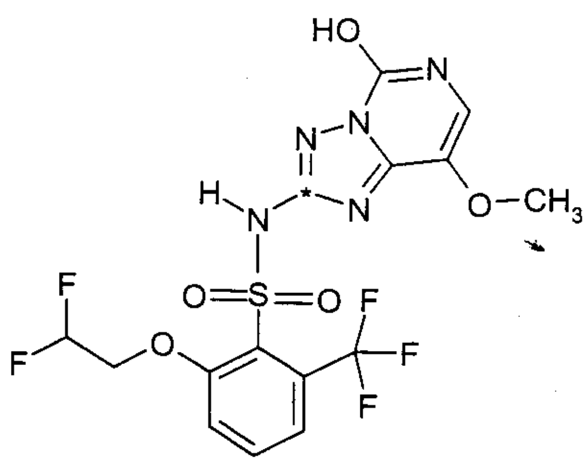
5-OH-XDE-638

IUPAC name: 6-(2,2-Difluoroethoxy)-N-(5,6-dihydro-8-methoxy-5-oxo-s-triazolo[1,5-c]pyrimidin-2-yl)-□,□,□-trifluoro-o-toluenesulfonamide
CAS name: (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-^{14}C] label



* Position of the radiolabel.

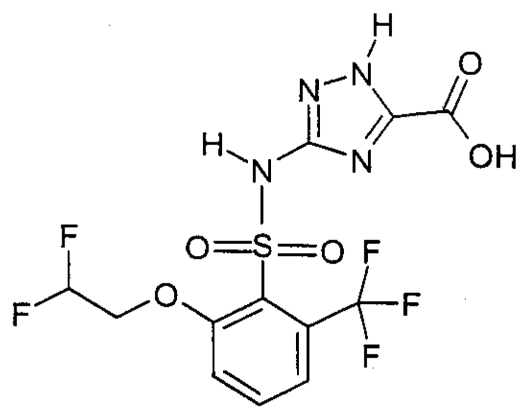
BSTCA

IUPAC name: 3-[6-(2,2-Difluoroethoxy)-□,□,□-(trifluoro-o-toluenesulfonamido]-s-triazole-5-carboxylic acid

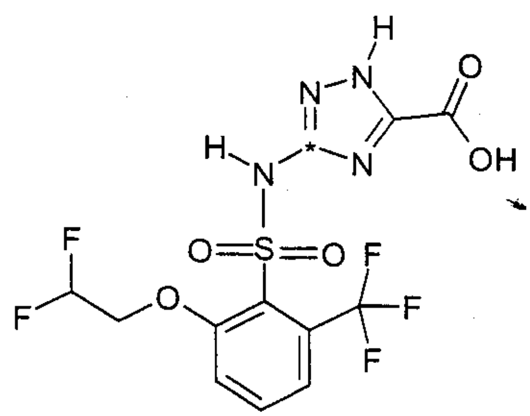
CAS name: 3-[[[2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)phenyl]-sulfonyl]amino]-1H-1,2,4-triazole-5-carboxylic acid

CAS No: NA

Unlabeled



[Triazolopyrimidine-2-^{14}C] label

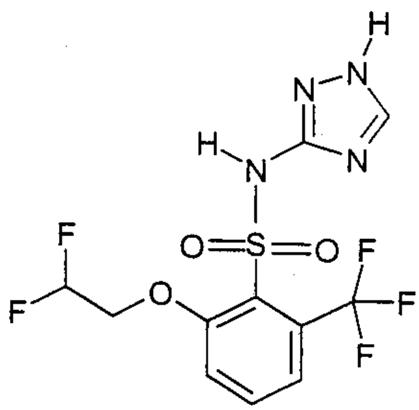


* Position of the radiolabel.

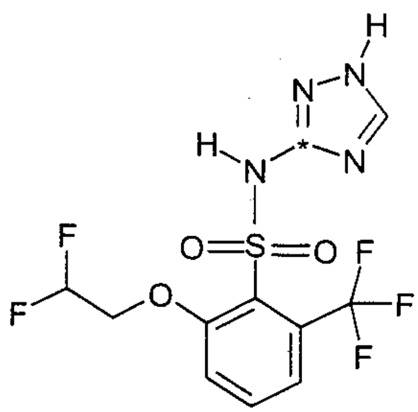
BST

IUPAC name: 6-(2,2-Difluoroethoxy)-□,□,□-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



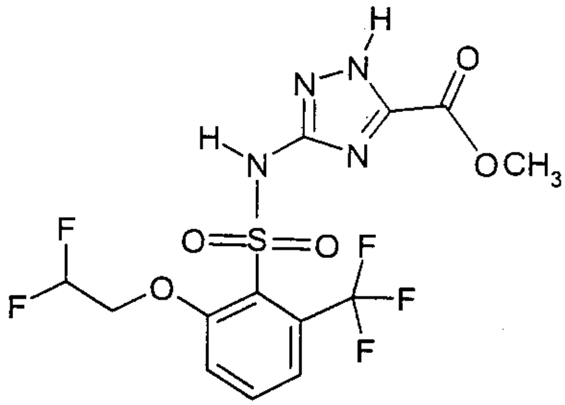
[Triazolopyrimidine-2-^{14}C] label



* Position of the radiolabel.

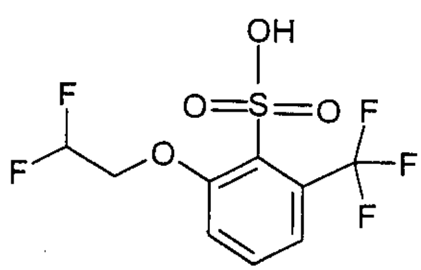
BSTCA-methyl

IUPAC name: Methyl 3-[6-(2,2-difluoroethoxy)-□,□,□-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



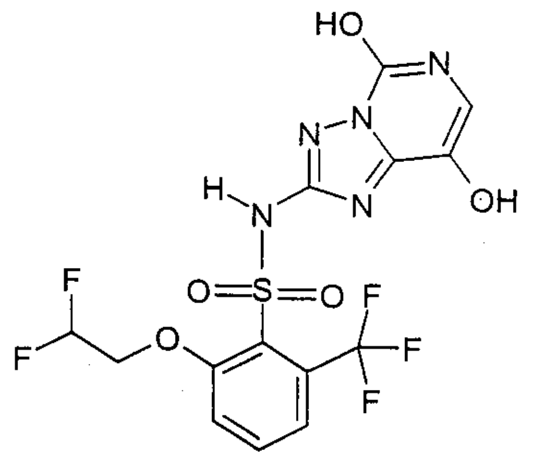
BSA

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



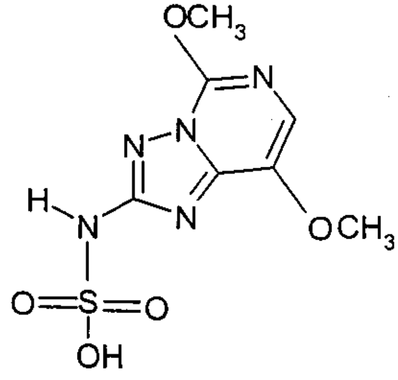
5,8-diOH

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



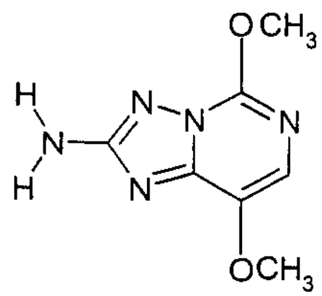
TPSA

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



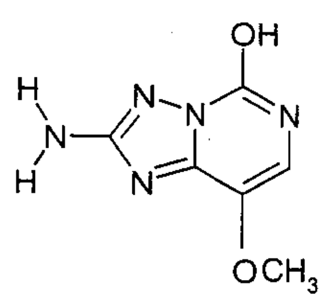
2-Amino TP

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



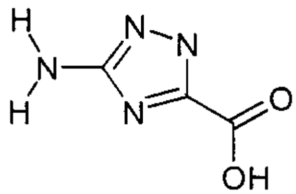
5-OH, 2-Amino TP

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



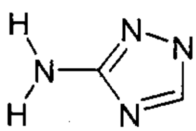
2-Amino TCA

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



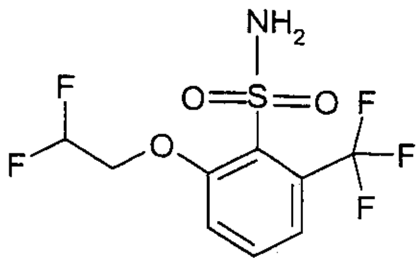
2-Amino-1,3,4-triazole

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