(5-11-2004)

Data Evaluation Report on the adsorption-desorption of BSTCA, BST, and 5-OH-XDE-638, degradates of penoxsulam, in soil

PMRA Submission Number {.....} EPA MRID Number 45830802

Data Requirement: PMRA Data Code:
EPA DP Barcode: D288160
OECD Data Point:
EPA Guideline: 163-1

Test materials:

Common name: BSTCA (transformation product of penoxsulam).
Chemical name:
IUPAC: 3-[[[2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)phenyl]sulfonyl]amino]-1H-1,2,4-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: Not reported.
Synonyms: Not reported.
SMILES string:

Common name: BST (transformation product of penoxsulam).
Chemical name:
IUPAC: 2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazol-3-yl-6-(trifluoromethyl)-benzenesulfonamide.
CAS name: 2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazole-3-yl-6-(trifluoromethyl)benzenesulfonamide.
CAS No: Not reported.
Synonyms: Not reported.
SMILES string:

Common name: 5-OH-XDE-638 (transformation product of penoxsulam).
Chemical name:
IUPAC: 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).
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: Not reported.
Synonyms: Not reported.
SMILES string:

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PMRA Submission Number {.....} EPA MRID Number 45830802

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

CITATION: Yoder, R.N. 2002. Batch equilibrium adsorption of XDE-638 metabolites, 5-OH-XDE-638, BSTCA, and BST. Unpublished study performed, sponsored and submitted by Regulatory Laboratories- Indianapolis Lab, Dow AgroSciences LLC, Indianapolis, Indiana. Laboratory Study ID: 010092. Experiment initiation September 12, 2001, and completion November 2, 2001 (p.3). Final report issued February 12, 2002.

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Data Evaluation Report on the adsorption-desorption of BSTCA, BST, and 5-OH-XDE-638, degradates of penoxsulam, in soil

PMRA Submission Number {.....} EPA MRID Number 45830802

EXECUTIVE SUMMARY:

The adsorption/desorption characteristics of [triazolopyrimidine-2-^{14}C]-labeled 3-[[[2-(2,2-difluoroethoxy)-6-(trifluoromethyl)phenyl]sulfonyl]amino]-1H-1,2,4-triazole-5-carboxylic acid (BSTCA); [triazolopyrimidine-2-^{14}C]-labeled 2-(2,2-difluoroethoxy)-N-1H-1,2,4-triazol-3-yl-6-(trifluoromethyl)-benzenesulfonamide (BST); and [triazolopyrimidine-2-^{14}C]-labeled 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) were studied in four U.S soils: a sand soil from North Carolina [M538; pH 5.6, organic carbon 0.40%], a silt loam soil from Arkansas [M557; pH 5.8, organic carbon 0.97%], a clay loam soil from California [M562; pH 6.5, organic carbon 2.46%], and a loam soil from North Dakota [M563; pH 6.9, organic carbon 2.74%], and in four European soils: a silty clay loam [M570; pH 6.2, organic carbon 0.97%] and a sandy loam soil [M573; pH 6.3, organic carbon 0.86%] each from Italy; a silty clay loam soil from France [M571; pH 6.2, organic carbon 0.99%]; and a sandy clay loam soil from the UK [M572; pH 8.0, organic carbon 1.64%], in a batch equilibrium experiment. The experiment was conducted in accordance with the U.S. EPA Pesticide Assessment Guidelines, Subdivision N, Section 163-1, and in compliance with U.S. EPA, Title 40, Part 160. The adsorption phase of the study was carried out by equilibrating moist soil with [^{14}C]BSTCA/BST and [^{14}C]5-OH-XDE-638 at a nominal concentration of 0.4 mg a.i/kg soil at 20°C for 2 and 24 hours, respectively (lighting conditions not reported). The equilibrating solution used was 0.01M $CaCl_2$, with soil/solution ratios of 1:2 (w:v) for all soils. Desorption was not studied.

The supernatant solution after adsorption was separated by centrifugation, and aliquots of the supernatants were analyzed for total radioactivity using LSC. Following adsorption, samples were extracted three times by shaking with acetonitrile:0.1N HCl (90:10, v:v). The extracts were centrifuged, combined, and analyzed for total radioactivity using LSC. Portions of the extracts were concentrated, filtered, and analyzed using HPLC. [^{14}C]Residues remaining in the extracted soil were quantified by LSC following combustion.

Based on HPLC analyses of the supernatants and extracts, 5-OH-XDE-638 was stable in the test solutions for the Arkansas silt loam (M557) soil during the study, accounting for 100% of the total radioactivity. BSTCA was unstable in solution and continued to degrade to BST throughout the study. Mass balances at the end of the adsorption phase of the study were calculated by summing the radiocarbon recovered in the adsorption supernatants, soil extracts, and combusted soils. The overall mass balances at the end of adsorption for the **[^{14}C]BSTCA/BST-treated soils** were 97.4-99.8%, 96.8-97 9%, 93.0-94.8%, 92.7-96.1%, 90.5-92.6%, 98.2-100.2%, 89.7-94.2%, and 96.6-97.5% of the applied for the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively. The overall mass balances at the end of adsorption for the **[^{14}C]5-OH-XDE-638- treated soils** were 99.4-99.8%, 96.9-98.0%, 95.1-97.9%, 95.9-96.4%,

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97.1-97.9%, 97.6-97.9%, 94.6-95.1%, and 99.5-99.8% of the applied for the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively.

After 2 hours of equilibration, 8.2%, 24.6%, 9.2%, 45.5%, 14.0%, and 1.4% of the applied **[^{14}C]BSTCA** was adsorbed to the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), silty clay loam from Italy (M570), silty clay loam from France (M571), and sandy clay loam from the UK (M572) soils, respectively. Calculated simple adsorption K_d values were 0.185, 1.515, 0.605, 4.395, 0.720, and 0.085 for the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), silty clay loam from Italy (M570), silty clay loam from France (M571), and sandy clay loam from the UK (M572) soils, respectively. Corresponding K_{oc} values were 46, 156, 25, 444, 74, and 5.

After 2 hours of equilibration, 5.1%, 25.2%, 19.6%, 3.9%, 33.5%, 22.6%, 3.2%, and 4.9% of the applied **[^{14}C]BST** was adsorbed to the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively. Calculated adsorption K_d values were 0.135, 0.590, 0.420, 0.545, 0.840, 0.470, 0.075, and 0.610 for the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively. Corresponding K_{oc} values were 34, 61, 18, 21, 85, 48, 5, and 71.

After 24 hours of equilibration, 6.6%, 12.9%, 17.6%, 30.1%, 39.6%, 15.6%, 11.2%, and 13.1% of the applied **[^{14}C]5-OH-XDE-638** was adsorbed to the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), Sandy clay loam from the UK (M572), and Sandy loam from Italy (M573) soils, respectively. Calculated K_d values were 0.140, 0.325, 0.455, 1.030, 1.425, 0.400, 0.280, and 0.295 for the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively. Corresponding K_{oc} values were 34, 34, 18, 38, 144, 42, 18, and 34.

For **[^{14}C]BSTCA**, the calculated r^2 value for the relationship of Kd vs. % organic carbon is 0.1323, for Kd vs. pH is 0.0621, and for Kd vs. % clay is 0.6665. For **[^{14}C]BST**, the calculated r^2 value for the relationship of Kd vs. % organic carbon is 0.0875, for Kd vs. pH is 0.0151, and for Kd vs. % clay is 0.1558. For **[^{14}C]5-OH-XDE-638**, the calculated r^2 value for the relationship of Kd vs. % organic carbon is 0.1806, for Kd vs. pH is 0.0309, and for Kd vs. % clay is 0.3632.

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PMRA Submission Number {.....} EPA MRID Number 45830802

Results Synopsis: K_d values were calculated using the equation: $K_d = C_s \div C_{aq}$.

[^{14}C]BSTCA:
Soil type: North Carolina sand (M538)
Amount adsorbed: 8.2% of the applied
Adsorption K_d: 0.19
Adsorption K_{oc}: 46
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Arkansas silt loam (M557)
Amount adsorbed: 24.6% of the applied
Adsorption K_d: 1.5
Adsorption K_{oc}: 156
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: California clay loam (M562)
Amount adsorbed: 9.2% of the applied
Adsorption K_d: 0.61
Adsorption K_{oc}: 25
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Silty clay loam from Italy (M570)
Amount adsorbed: 45.5% of the applied
Adsorption K_d: 4.4
Adsorption K_{oc}: 444
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

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Soil type: Silty clay loam from France (M571)
Amount adsorbed: 14.0% of the applied
Adsorption K_d: 0.72
Adsorption K_{oc}: 74
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Sandy clay loam from the UK (M572)
Amount adsorbed: 1.4% of the applied
Adsorption K_d: 0.085
Adsorption K_{oc}: 5
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

[^{14}C]BST:
Soil type: North Carolina sand (M538)
Amount adsorbed: 5.1% of the applied
Adsorption K_d: 0.14
Adsorption K_{oc}: 34
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Arkansas silt loam (M557)
Amount adsorbed: 25.2% of the applied
Adsorption K_d: 0.59
Adsorption K_{oc}: 61
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: California clay loam (M562)
Amount adsorbed: 19.6% of the applied
Adsorption K_d: 0.42
Adsorption K_{oc}: 18
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

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Soil type: North Dakota loam (M563)
Amount adsorbed: 3.9% of the applied
Adsorption K_d: 0.55
Adsorption K_{oc}: 21
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Silty clay loam from Italy (M570)
Amount adsorbed: 33.5% of the applied
Adsorption K_d: 0.84
Adsorption K_{oc}: 85
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Silty clay loam from France (M571)
Amount adsorbed: 22.6% of the applied
Adsorption K_d: 0.47
Adsorption K_{oc}: 48
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Sandy clay loam from the UK (M572)
Amount adsorbed: 3.2% of the applied
Adsorption K_d: 0.075
Adsorption K_{oc}: 5
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Sandy loam from Italy (M573)
Amount adsorbed: 4.9% of the applied
Adsorption K_d: 0.61
Adsorption K_{oc}: 71
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

[^{14}C]5-OH-XDE-638:
Soil type: North Carolina sand (M538)
Amount adsorbed: 6.6% of the applied
Adsorption K_d: 0.14
Adsorption K_{oc}: 34
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Arkansas silt loam (M557)
Amount adsorbed: 12.9% of the applied
Adsorption K_d: 0.33
Adsorption K_{oc}: 34
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: California Clay loam (M562)
Amount adsorbed: 17.6% of the applied
Adsorption K_d: 0.46
Adsorption K_{oc}: 18
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: North Dakota loam (M563)
Amount adsorbed: 30.1% of the applied
Adsorption K_d: 1.0
Adsorption K_{oc}: 38
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Silty clay loam from Italy (M570)
Amount adsorbed: 39.6% of the applied
Adsorption K_d: 1.4
Adsorption K_{oc}: 144
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Silty clay loam from France (M571)
Amount adsorbed: 15.6% of the applied
Adsorption K_d: 0.40
Adsorption K_{oc}: 42
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Sandy clay loam from the UK (M572)
Amount adsorbed: 11.2% of the applied
Adsorption K_d: 0.28
Adsorption K_{oc}: 18
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Soil type: Sandy loam from Italy (M573)
Amount adsorbed: 13.1% of the applied
Adsorption K_d: 0.30
Adsorption K_{oc}: 34
Amount desorbed: Not performed
Desorption K_d: Not performed
Desorption K_{oc}: Not performed

Acceptability: This study is classified as **supplemental**. The study cannot be used toward the fulfilment of the mobility data requirement guideline, Subdivision N Guideline §163-1, because (i) the study was conducted using transformation products of penoxsulam rather than the parent compound, and (ii) desorption was not studied.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: The study was conducted according to the U.S. EPA Pesticide Assessment Guidelines, Subdivision N, Section 163-1; the Society of Environmental Toxicology and Chemistry (SETAC) Part 1, Section 4; the Organization for Economic Cooperation and Development (OECD) Method 106; and the U.S. EPA Fate, Transport, and Transformation Guidelines, OPPTS 835.1220 (p.9). Significant deviations from Subdivision N § 163-1 guidelines were:

The study was conducted using transformation products of penoxsulam, rather than the parent compound. This does not affect the validity of the study.

The study was conducted using a single test concentration. Subdivision N guidelines specify that at least four test concentrations be used. This does not affect the validity of the study.

It was not stated whether the study was conducted in the dark. This does not affect the validity of the study since the test substance was stable in the test solutions during the study.

The test substances were not completely characterized. Complete physico-chemical properties were not reported. This does not affect the validity of the study.

COMPLIANCE: The study was conducted in compliance with the U.S. EPA, Title 40, Part 160 GLP (1989) and the OECD ISBN 92-64-12367-9 GLP (1982; p.3). Signed and dated No Data Confidentiality, GLP, and Quality Assurance statements were provided (pp.2-4). A Certificate of Authenticity was not provided.

A. MATERIALS:

1. Test Material

[Triazolopyrimidine-2-^{14}C]labeled [[[2-(2,2-Difluoroethoxy)-6-(trifluoromethyl)phenyl]sulfonyl]amino]-1H-1,2,4-triazole-5-carboxylic acid (BSTCA),

[Triazolopyrimidine-2-^{14}C]-labeled 2-(2,2-Difluoroethoxy)-N-1H-1,2,4-triazol-3-yl-6-(trifluoromethyl)-benzenesulfonamide (BST),

[Triazolopyrimidine-2-^{14}C] 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; pp.10-12; Figure 1, p.32).

Chemical Structures: See DER Attachment 1.

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Description:	[^{14}C]BSTCA was prepared as the Et_3N salt (p.11). Descriptions of BST and 5-OH-XDE-638 were not provided.
Purity:	
Radiolabelled:	
[^{14}C]BSTCA	Analytical purity: Not reported. Radiochemical purity: 52.7% (Figure 1, p.32). Inventory No. INV1618. Reference No. DE3-E1212-19A. Specific activity: 22.8 mCi/mmole. Locations of the label: 2-C in triazolopyrimidine ring.
[^{14}C]BST	Analytical purity: Not reported. Radiochemical purity: 46.9% (Figure 1, p.32). Inventory No. INV1618. Reference No. DE3-E1212-19A. Specific activity: 22.7 mCi/mmole. Locations of the label: 2-C in triazolopyrimidine ring.
[^{14}C]5-OH-XDE-638	Analytical purity: Not reported. Radiochemical purity: 99.9% (Figure 1, p.32). Inventory No. INV1627. Reference No. F0903-7c. Specific activity: 29.0 mCi/mmole. Locations of the label: 2-C in triazolopyrimidine ring.
Non-radiolabelled:	
BSTCA	Analytical purity: 98% (p.12). TSN No. TSN101979. Lot No. F0398-54A.
BST	Analytical purity: 99% (p.12). TSN No. TSN101806. Lot No. F0512-178A.
5-OH-XDE-638	Analytical purity: 99% (p.12). TSN No. TSN101756. Lot No. F0512-129A.
Storage conditions of test chemicals:	The radiolabeled test materials were stored frozen (Figure 1, p.32). Unlabeled BSTCA was stored frozen (p.12). Unlabeled BST and 5-OH-XDE-638 were stored under ambient conditions.

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Physico-chemical properties of BSTCA, BST, and 5-OH-XDE-638:

Parameter	Values	Comments
Water solubility	Not reported	
Vapour pressure	Not reported	
UV absorption	Not reported	
Molecular Formula	Not reported	
Molecular Weight	416 g/mole (BSTCA); 372 g/mole (BST); 469 g/mole (5-OH-XDE-638).	
Melting point	Not reported	
Bulk density	Not reported	
pK_a	Not reported	
K_{ow}	Not reported	
Stability of Compound at room temperature	Not reported	

Data were obtained from Figure 1, p.32 of the study report.

2. Soil Characteristics

Table 1: Description of soil collection and storage.

Description	M538	M557	M562	M563	M570	M571	M572	M573
Geographic location	North Carolina	Arkansas	California	North Dakota	Italy	France	UK	Italy
Pesticide use history at the collection site	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported
Collection procedures	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported
Sampling depth (cm)	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported
Storage conditions	Stored at 4°C; then at room temperature 2 months prior to treatment.	Stored at 4°C; then at room temperature 2 months prior to treatment.	Stored at 4°C; then at room temperature 2 months prior to treatment.	Stored at 4°C; then at room temperature 2 months prior to treatment.	Stored at 4°C; then at room temperature 2 months prior to treatment.	Stored at 4°C; then at room temperature 2 months prior to treatment.	Stored at 4°C; then at room temperature 2 months prior to treatment.	Stored at 4°C; then room temperature 2 months prior to treatment.
Storage length	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported
Soil preparation	Sieved, 2 mm	Sieved, 2 mm	Sieved, 2 mm	Sieved, 2 mm	Sieved, 2 mm	Sieved, 2 mm	Sieved, 2 mm	Sieved, 2 mm

Data were obtained from pp.14 and Table 3, p.26 of the study report.

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Table 2: Properties of the soils.

Property	M538	M557	M562	M563	M570	M571	M572	M573
Soil Texture	Sand	Silt loam	Clay loam	Loam	Silty clay loam	Silty clay loam	Sandy clay loam	Sandy loam
% sand	88.4	8.8	32.8	40.8	13.2	15.2	57.2	69.2
% silt	7.6	67.2	33.2	35.2	54.0	56.0	16.0	22.0
% clay	4.0	24.0	34.0	24.0	32.8	28.8	26.8	8.8
pH	5.6	5.8	6.5	6.9	6.2	6.2	8.0	6.3
Organic carbon (%)	0.40	0.97	2.46	2.74	0.99	0.97	1.64	0.86
Organic matter (%)[1]	0.69	1.67	4.23	4.71	1.70	1.67	2.82	1.48
CEC (meq/100 g)	1.16	16.54	21.67	21.99	10.73	13.08	16.45	3.80
Moisture at 1/3 atm (%)	3.59	24.82	29.84	28.53	27.25	24.59	19.44	11.48
Bulk density (g/cm^3)	1.68	1.11	1.18	1.02	1.23	1.20	1.21	1.29
Biomass (mg microbial C/100 g or CFU or other)	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported

Property	M538	M557	M562	M563	M570	M571	M572	M573
Soil taxonomic classification[2]	Loamy, Kaolinitic, thermic Arenic Kandiudults and Loamy, Kaolinitic, thermic Grossarenic Kandiudults.	Fine-silty, mixed, active, thermic Typic Endo-aqualfs.	Fine, smectitic, thermic, Aquic Haploxererts.	Coarse-silty, mixed superactive, frigid Aeric Calciaquolls and Coarse-loamy, mixed, superactive, frigid Typic Endoaquolls.	Greggio	Charentilly	Marcham	Ottobaiano
Soil mapping unit (for EPA)	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported

Data were obtained from Table 3, p.26 of the study report.

[1] Percent organic matter was calculated by the reviewer as follows: % organic carbon × 1.72.

[2] Soils M538, M557, M562, and M563 were classified according to the USDA Soil Classification for US Soils. The classification systems used for the remaining soils were not reported.

C. STUDY DESIGN:

1. Preliminary study: Preliminary studies were not conducted.

2. Definitive study experimental conditions:

Table 3a: Study design for the adsorption phase.

Parameters		M538 Sand	M557 Silt loam	M562 Clay loam	M563 Loam	M570 Silty clay loam	M571 Silty clay loam	M572 Sandy clay loam	M573 Sandy loam
Condition of soil (air dried/fresh)		Moist	Moist	Moist	Moist	Moist	Moist	Moist	Moist
Have these soils been used for other laboratory studies ? (specify which)		Yes, MRID 45830801	Yes, MRID 45830801	Yes, MRID 45830801	Yes, MRID 45830801	Yes, MRID 45830801	Yes, MRID 45830801	Yes, MRID 45830801	Yes, MRID 45830801
Soil (g/replicate)		5	5	5	5	5	5	5	5
Equilibrium solution used (name and concentration; eg: 0.01N $CaCl_2$)		0.01M $CaCl_2$	0.01M $CaCl_2$	0.01M $CaCl_2$	0.01M $CaCl_2$	0.01M $CaCl_2$	0.01M $CaCl_2$	0.01M $CaCl_2$	0.01M $CaCl_2$
Control used (with salt solution only) (Yes/No)		No	No	No	No	No	No	No	No
[^{14}C]BSTCA concentrations[1]	Nominal application rates (mg a.i./kg soil)	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4
	Analytically measured concentrations (mg a.i./kg soil)	0.4	0.24	0.2	Not analyzed*	0.3	0.24	0.18	Not analyzed*

Parameters		M538 Sand	M557 Silt loam	M562 Clay loam	M563 Loam	M570 Silty clay loam	M571 Silty clay loam	M572 Sandy clay loam	M573 Sandy loam
[^{14}C]BST concentrations[1]	Nominal application rates (mg a.i./kg soil)	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4
	Analytically measured concentrations (mg a.i./kg soil)	0.32	0.44	0.46	0.08	0.46	0.48	0.38	0.08
[^{14}C]5-OH-XDE-638 concentrations[1]	Nominal application rates (mg a.i./kg soil)	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4
	Analytically measured concentrations (mg a.i./kg soil)	0.4	0.38	0.4	0.36	0.38	0.38	0.38	0.4
Identity and concentration of co-solvent for [^{14}C]BSTCA/BST, if any[2]		Acetonitrile or acetone, concentrations not reported.	Acetonitrile or acetone, concentrations not reported.	Acetonitrile or acetone, concentrations not reported.	Acetonitrile or acetone, concentrations not reported.	Acetonitrile or acetone, concentrations not reported.	Acetonitrile or acetone, concentrations not reported.	Acetonitrile or acetone, concentrations not reported.	Acetonitrile or acetone, concentrations not reported.

Parameters		M538 Sand	M557 Silt loam	M562 Clay loam	M563 Loam	M570 Silty clay loam	M571 Silty clay loam	M572 Sandy clay loam	M573 Sandy loam
Identity and concentration of co-solvent for [^{14}C]5-OH-XDE-638, if any		Acetonitrile, concen-tration not reported.	Acetonitrile, concen-tration not reported.	Acetonitrile, concen-tration not reported.	Acetonitrile, concen-tration not reported.	Acetonitrile, concen-tration not reported.	Acetonitrile, concen-tration not reported.	Acetonitrile, concen-tration not reported.	Acetonitrile, concen-tration not reported.
Soil:solution ratio[3]		1:2	1:2	1:2	1:2	1:2	1:2	1:2	1:2
Initial pH of the equilibration solution, if provided		Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported
No. of replications	Controls	0	0	0	0	0	0	0	0
	Treatments	2	2	2	2	2	2	2	2
Equilibration	[^{14}C]BSTCA/ BST Time (hours)	2	2	2	2	2	2	2	2
	[^{14}C]5-OH-XDE-638 Time (hours)	24	24	24	24	24	24	24	24
	Temperature (°C)	20	20	20	20	20	20	20	20
	Darkness	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported	Not reported
	Shaking method	Horizontal shaker	Horizontal shaker	Horizontal shaker	Horizontal shaker	Horizontal shaker	Horizontal shaker	Horizontal shaker	Horizontal shaker

Parameters		M538 Sand	M557 Silt loam	M562 Clay loam	M563 Loam	M570 Silty clay loam	M571 Silty clay loam	M572 Sandy clay loam	M573 Sandy loam
	[^{14}C]BSTCA/ BST Shaking time (hours)	2	2	2	2	2	2	2	2
	[^{14}C]5-OH-XDE-638 Shaking time (hours)	24	24	24	24	24	24	24	24
Method of separation of supernatant (eg., centrifugation)		Centri-fugation	Centri-fugation	Centri-fugation	Centri-fugation	Centri-fugation	Centri-fugation	Centri-fugation	Centri-fugation
Centrifugation	Speed (rpm)	2,000-2,500	2,000-2,500	2,000-2,500	2,000-2,500	2,000-2,500	2,000-2,500	2000-2500	2000-2500
	Duration (min)	5	5	5	5	5	5	5	5
	Method of separation of soil and solution	Decanted	Decanted	Decanted	Decanted	Decanted	Decanted	Decanted	Decanted

Data were obtained from pp.12-15 and Table 2, p.25 of the study report.

[1] Test material concentrations were calculated as follows: [test concentration (ppm) x total volume of test material solution (mL)] ÷ amount of soil (g); eg. [0.2 µg/mL x 10.0 mL) ÷ 5.0 g = 0.4 mg a.i./kg soil.

[2] Two separate batches of the BSTCA/BST test solution (80:20) were prepared due to the instability of BSTCA (p.12). One was dissolved in acetone (1 mL) and the other was dissolved in acetonitrile (1 mL).

[3] The actual soil:solution ratios and application rates are presented in Table 2 of the study report (p.25). For both the 5-OH and BSTCA/BST treatments, the actual soil:solution ratios ranged from 1:2.0 to 1:2.3 (w:v).

Table 4: Study design for the desorption phase.[1]

Parameters		M538 Sand	M557 Silt loam	M562 Clay loam	M563 Loam	M570 Silty clay loam	M571 Silty clay loam	M572 Sandy clay loam	M573 Sandy loam
Were the soil residues from the adsorption phase used? If not, describe the method for adsorption using a separate adsorption Table									
Amount of test material present in the adsorbed state/adsorbed amount (mg a.i./kg soil)									
No. of desorption cycles									
Equilibration solution and quantity used per treatment for desorption (eg., 0.01M $CaCl_2$)									
Soil:solution ratio									
Replications	Controls								
	Treatments								
Desorption equilibrium	Time (hours)								
	Temperature (°C)								
	Darkness								
	Shaking method								
	Shaking time (hours)								
Centrifugation	Speed (rpm)								
	Duration (min)								
	Method of separation of soil and								

[1] Desorption was not studied.

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3. Description of analytical procedures:

Extraction/clean up/concentration methods: Following adsorption, the soils were extracted a total of three times by vortexing briefly to break up the soil pellets, and shaking on a horizontal shaker for one half hour with 7 mL of acetonitrile:0.1N HCl (90:10, v:v; p.15). The samples were centrifuged and the supernatants were pipetted into a 25-mL volumetric flask. The extracts were combined and brought to volume (25 mL) with additional acetonitrile:0.1N HCl. A 10-mL aliquot of each organic extract was concentrated for about one hour on a Turbovap, then concentrated under nitrogen in a water bath at 30°C. The resulting concentrates were filtered through a 0.2-µm PTFE filter.

An aliquot (10 mL) of each extract was then concentrated to approximately 2 mL by placing the samples in a waterbath at 30°C under nitrogen for approximately 1 hour. The concentrated extracts were filtered (0.2 µm) and analyzed using HPLC. The organic extracts were refrigerated when not undergoing analysis.

Total ^{14}C measurement: Aliquots of the adsorption and extraction supernatants were analyzed for total radioactivity using LSC (p.15). Following extraction, triplicate samples of soil residues were air-dried for at least one week, and analyzed for total radioactivity using LSC following combustion. Oxidizer efficiency was not reported. The data were corrected for combustion efficiency.

Non-extractable residues, if any: Not applicable.

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

Identification and quantification of BSTCA, BST, and 5-OH-XDE-638: Aliquots of the BSTCA/BST samples were analyzed immediately using HPLC (p.15). The 5-OH-XDE-638 samples were refrigerated and representative samples were analyzed using HPLC within one week of sampling. Aqueous samples were filtered through a 0.2 µm PTFE filter prior to HPLC analysis. The pore water remaining in the soil after the aqueous phase was decanted was measured by weight. The aqueous samples were then refrigerated. Organic extracts for the BSTCA/BST samples were analyzed on the day of extraction, and the 5-OH-XDE-638 samples were analyzed within one week of extraction.

Aliquots of the adsorption and extraction supernatants were analyzed for [^{14}C]BSTCA and [^{14}C]BST by HPLC using the following operating conditions: YMC-ODS AQ SN160212005 (Column A; dimensions and particle size not reported) and YMC-ODS AQ SN042513608 (Column B; dimensions and column size not reported), combining (A) water + 1% acetic acid and (B) acetonitrile + 1% acetic acid [%A:B at 0 minutes 95:5, 20 minutes 50:50, and 20.1-30 minutes

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95:5], flow rate 1 mL/min (p.13, 15; Table 1, p.24). [^{14}C]5-OH-XDE-638 was analyzed by HPLC using the following operating conditions: YMC-ODS AQ SN042513608 (Column B; dimensions and column size not reported)), combining (A) water + 1% acetic acid and (B) acetonitrile + 1% acetic acid [%A:B at 0 minutes 95:5, 15-20 minutes 5:95, and 20.1-30 minutes 95:5], flow rate 1 mL/min. Unlabeled reference standards of each test compound were analyzed using a UV-VIS detector (254 nm). It was not stated whether the reference compounds were cochromatographed with the supernatant and extract samples, or whether they were chromatographed separately. Retention times for BSTCA were 14.0 and 16.5 minutes using HPLC Column A and B, respectively. Retention times for BST were 15.5 and 17.5 minutes using HPLC Column A and B, respectively. Retention times for 5-OH-XDE-638 were 14-15 minutes using HPLC Column B.

Identification and quantification of transformation products, if appropriate: Samples were not analyzed for transformation products of BSTCA, BST, and 5-OH-XDE-638.

Detection limits (LOD, LOQ) for BSTCA, BST, and 5-OH-XDE-638: The LOD and LOQ for LSC and HPLC analyses of BSTCA, BST, and 5-OH-XDE-638 were 10 and 40 dpm, respectively (pp.17-18).

Detection limits (LOD, LOQ) for the transformation products: Samples were not analyzed for transformation products of BSTCA, BST, and 5-OH-XDE-638.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: Based on HPLC analyses of the supernatants and extracts, 5-OH-XDE-638 was stable during the study, accounting for 100% of the total radioactivity in the test solutions for the Arkansas silt loam (M557) soil (p.19; Figures 5-6, pp.36-37). BSTCA was unstable in solution and continued to degrade to BST throughout the study (p.20; Figures 7-9, pp.38-40). The temperature during the study was reported to be 20°C. However, temperature records were not provided. The pH of the test solutions during the study were not reported.

B. MASS BALANCE: Mass balances at the end of the adsorption phase of the study were calculated by summing the radiocarbon recovered in the adsorption supernatants, soil extracts, and combusted soils (p.19).

[^{14}C]BSTCA/BST treatment: Material balances at the end of the adsorption phase were 97.4-99.8%, 96.8-97.9%, 93.0-94.8%, 92.7-96.1%, 90.5-92.6%, 98.2-100.2%, 89.7-94.2%, and 96.6-97.5% of the applied for the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively (Table 8, p.31).

[^{14}C]5-OH-XDE-638 treatment: Material balances at the end of the adsorption phase were 99.4-99.8%, 96.9-98.0%, 95.1-97.9%, 95.9-96.4%, 97.1-97.9%, 97.6-97.9%, 94.6-95.1%, and 99.5-99.8% of the applied for the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively (Table 6, p.29).

Table 5a: Recovery of [^{14}C]BSTCA/BST, expressed as percentage of applied radioactivity, in soil after adsorption/desorption (mean ± s.d.).

Matrices	M538 Sand	M557 Silt loam	M562 Clay loam	M563 Loam	M570 Silty clay loam	M571 Silty clay loam	M572 Sandy clay loam	M573 Sandy loam
At the end of the adsorption phase								
Supernatant solution	91.3 ± 1.3	69.8 ± 0.5	75.8 ± 0.5	73.0 ± 0.9	53.8 ± 0.6	76.8 ± 0.9	87.0 ± 5.3	74.3 ± 0.8
Solid phase (extracted)[1]	7.3 ± 0.4	26.3 ± 0.4	16.8 ± 0.8	17.5 ± 0.8	37.4 ± 0.8	19.3 ± 0.4	3.2 ± 1.8	22.3 ± 0.4
Non-extractable residues in soil, if measured	0.1 ± 0.1	1.2 ± 0.1	1.2 ± 0.0	3.9 ± 0.6	0.4 ± 0.1	3.1 ± 0.1	1.8 ± 0.4	0.4 ± 0.3
Total recovery	98.6 ± 1.7	97.4 ± 0.8	93.9 ± 1.3	94:4 ± 2.4	91.6 ± 1.5	99.2 ± 1.4	92.0 ± 3.2	97.1 ± 0.6
At the end of the desorption phase[2]								
Supernatant solution	Not measured							
Solid phase (extracted)	Not measured							
Non-extractable residues in soil, if measured	Not measured							
Total recovery	Not measured							

Data were obtained from Table 8, p.31 of the study report. Means and standard deviations were calculated using Excel.

[1] All soils were extracted prior to combustion.

[2] Desorption was not studied.

Table 5b: Recovery of [^{14}C]5-OH-XDE-638, expressed as percentage of applied radioactivity, in

soil after adsorption/desorption (mean ± s.d.).

Matrices	M538 Sand	M557 Silt loam	M562 Clay loam	M563 Loam	M570 Silty clay loam	M571 Silty clay loam	M572 Sandy clay loam	M573 Sandy loam
At the end of the adsorption phase								
Supernatant solution	93.1 ± 0.8	83.6 ± 0.1	77.9 ± 3.1	64.6 ± 0.5	58.0 ± 0.8	81.0 ± 0.1	82.5 ± 0.1	86.6 ± 0.8
Solid phase (extracted)[1]	6.3 ± 0.6	12.3 ± 0.8	17.1 ± 1.2	29.1 ± 0.6	38.2 ± 0.0	15.2 ± 0.1	10.8 ± 0.4	12.6 ± 0.6
Non-extractable residues in soil, if measured	0.3 ± 0.0	1.5 ± 0.0	1.5 ± 0.1	2.5 ± 0.3	1.4 ± 0.1	1.6 ± 0.1	1.5 ± 0.6	0.4 ± 0.1
Total recovery	99.6 ± 0.3	97.4 ± 0.8	96.5 ± 2.0	96.2 ± 0.4	97.5 ± 0.6	97.8 ± 0.2	94.8 ± 0.4	99.6 ± 0.2
At the end of the desorption phase[2]								
Supernatant solution	Not measured							
Solid phase (extracted)	Not measured							
Non-extractable residues in soil, if measured	Not measured							
Total recovery	Not measured							

Data were obtained from Table 6, p.29 of the study report. Means and standard deviations were calculated using Excel.

[1] All soils were extracted prior to combustion.

[2] Desorption was not studied.

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Table 6a: Concentration of [^{14}C]BSTCA in the solid and liquid phases at the end of adsorption equilibration period (mean ± s.d.).

Concentration (mg a.i./kg soil)	North Carolina sand (M538)			Arkansas silt loam (M557)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.0330 ± 0.0	0.1800 ± 0.0	8.2 ± 0.7	0.0985 ± 0.0	0.0650 ± 0.0	24.6 ± 5.8

Concentration (mg a.i./kg soil)	California clay loam (M562)			North Dakota loam (M563)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.0370 ± 0.0	0.0600 ± 0.0	9.2 ± 0.7	Not analyzed		

Concentration (mg a.i./kg soil)	Silty clay loam from Italy (M570)			Silty clay loam from France (M571)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.1820 ± 0.0	0.0400 ± 0.0	45.5 ± 7.1	0.0560 ± 0.0	0.0800 ± 0.0	14.0 ± 0.0

Concentration (mg a.i./kg soil)	Sandy clay loam from the UK (M572)			Sandy loam from Italy (M573)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.0055 ± 0.0	0.0650 ± 0.0	1.4 ± 0.9	Not analyzed		

Data were obtained from Appendix A, pp.46-49 of the study report. Means and standard deviations were calculated using Excel.

[1] % Adsorbed as the % of the applied was calculated by dividing the amount in soil after adsorption by the applied; e.g. [(0.035 µg/g ÷ 0.4 mg a.i./kg] × 100 = 8.8%.

Table 6b: Concentration of [^{14}C]BST in the solid and liquid phases at the end of adsorption equilibration period (mean ± s.d.).

Concentration (mg a.i./kg soil)	North Carolina sand (M538)			Arkansas silt loam (M557)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.0205 ± 0.0	0.1450 ± 0.0	5.1 ± 0.2	0.1010 ± 0.0	0.1700 ± 0.0	25.2 ± 6.0

Concentration (mg a.i./kg soil)	California clay loam (M562)			North Dakota loam (M563)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.0785 ± 0.0	0.1850 ± 0.0	19.6 ± 0.9	0.0155 ± 0.0	0.0300 ± 0.0	3.9 ± 0.2

Concentration (mg a.i./kg soil)	Silty clay loam from Italy (M570)			Silty clay loam from France (M571)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.1340 ± 0.0	0.1600 ± 0.0	33.5 ± 8.1	0.0905 ± 0.0	0.1950 ± 0.0	22.6 ± 0.5

Concentration (mg a.i./kg soil)	Sandy clay loam from the UK (M572)			Sandy loam from Italy (M573)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.0130 ± 0.0	0.1700 ± 0.0	3.2 ± 1.8	0.0195 ± 0.0	0.0300 ± 0.0	4.9 ± 0.2

Data were obtained from Appendix A, pp.46-49 of the study report. Means and standard deviations were calculated by the reviewer using Excel.

[1] % Adsorbed as the % of the applied was calculated by dividing the amount in soil after adsorption by the applied; e.g. [(0.02 µg/g ÷ 0.4 mg a.i./kg] × 100 = 5%.

Table 6c: Concentration of [^{14}C]5-OH-XDE-638 in the solid and liquid phases at the end of

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adsorption equilibration period (mean ± s.d.).

Concentration (mg a.i./kg soil)	North Carolina sand (M538)			Arkansas silt loam (M557)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.0265 ± 0.0	0.1900 ± 0.0	6.6 ± 0.5	0.0515 ± 0.0	0.1600 ± 0.0	12.9 ± 0.9

Concentration (mg a.i./kg soil)	California clay loam (M562)			North Dakota loam (M563)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.0705 ± 0.0	0.1550 ± 0.0	17.6 ± 1.2	0.1205 ± 0.0	0.1200 ± 0.0	30.1 ± 0.5

Concentration (mg a.i./kg soil)	Silty clay loam from Italy (M570)			Silty clay loam from France (M571)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.4	0.1585 ± 0.0	0.1100 ± 0.0	39.6 ± 0.2	0.0625 ± 0.0	0.1600 ± 0.0	15.6 ± 0.2

Concentration (mg a.i./kg soil)	Sandy clay loam from the UK (M572)			Sandy loam from Italy (M573)		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution(µg a.i./mL)	% adsorbed[1]
0.4	0.0450 ± 0.0	0.1600 ± 0.0	11.2 ± 0.4	0.0525 ± 0.0	0.1800 ± 0.0	13.1 ± 0.5

Data were obtained from Appendix A, pp.43-44 of the study report. Means and standard deviations were calculated using Excel.

[1] % Adsorbed as the % of the applied was calculated by dividing the amount in soil after adsorption by the applied; e.g. [(0.025 µg/g ÷ 0.4 mg a.i./kg] × 100 = 6.25%.

Table 7: Concentration of [^{14}C]BSTCA, [^{14}C]BST, and [^{14}C]5-OH-XDE-638 in the solid and liquid

phases at the end of desorption (n=0).[1]

Concentration (mg a.i./kg soil)						
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed[1]

[1] Desorption was not studied.

Table 8a: Adsorption and desorption constants of [^{14}C]BSTCA in the soils.

Soil	Adsorption				Desorption[1]			
	K_d	1/N	R^2	K_{oc}	K_d	1/N	R^2	K_{oc}
North Carolina sand (M538)	0.185	NA	NA	46				
Arkansas silt loam (M557)	1.515	NA	NA	156				
California clay loam (M562)	0.605	NA	NA	25				
North Dakota loam (M563)	Not analyzed							
Silty clay loam from Italy (M570)	4.395	NA	NA	444				
Silty clay loam from France (M571)	0.720	NA	NA	74				
Sandy clay loam from the UK (M572)	0.085	NA	NA	5				
Sandy loam from Italy (M573)	Not analyzed							

Data were obtained from Table 7, p.30 of the study report. Means and standard deviations were calculated by the reviewer using Excel.
NA - not applicable
K_d -Adsorption and desorption coefficients; K - Freundlich adsorption and desorption coefficients; 1/N -Slope of Freundlich adsorption/desorption isotherms.
K_{oc} - Coefficient adsorption per organic carbon (K_d or K x 100/% organic carbon).
R^2 - Regression coefficient of Freundlich equation.
K_d values were calculated using the following equation (p.16):

$$K_d = C_s \div C_{aq}$$

where
Kd = partitioning coefficient;
Cs = concentration of test substance adsorbed to the soil; and
Caq = concentration of test substance in solution at equilibrium.
[1] Desorption was not studied.

Table 8b: Adsorption and desorption constants of [^{14}C]BST in the soils.

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Soil	Adsorption				Desorption[1]			
	K_d	1/N	R^2	K_{oc}	K_d	1/N	R^2	K_{oc}
North Carolina sand (M538)	0.135	NA	NA	34				
Arkansas silt loam (M557)	0.590	NA	NA	61				
California clay loam (M562)	0.420	NA	NA	18				
North Dakota loam (M563)	0.545	NA	NA	21				
Silty clay loam from Italy (M570)	0.840	NA	NA	85				
Silty clay loam from France (M571)	0.470	NA	NA	48				
Sandy clay loam from the UK (M572)	0.075	NA	NA	5				
Sandy loam from Italy (M573)	0.610	Not reported	Not reported	71				

Data were obtained from Table 7, p.30 of the study report. Means and standard deviations were calculated using Excel.

K_d -Adsorption and desorption coefficients; K - Freundlich adsorption and desorption coefficients; 1/N - Slope of Freundlich adsorption/desorption isotherms.

K_{oc} - Coefficient adsorption per organic carbon (K_d or K x 100/% organic carbon).

R^2 - Regression coefficient of Freundlich equation.

K_d values were calculated by the study author using the following equation (p.16):

$$K_d = C_s \div C_{aq}$$

where

K_d = partitioning coefficient;

Cs = concentration of test substance adsorbed to the soil; and

Caq = concentration of test substance in solution at equilibrium.

[1] Desorption was not studied.

Table 8c: Adsorption and desorption constants of [^{14}C]5-OH-XDE-638 in the soils.

Soil	Adsorption				Desorption[1]			
	K_d	1/N	R^2	K_{oc}	K_d	1/N	R^2	K_{oc}
North Carolina sand (M538)	0.140	NA	NA	34				
Arkansas silt loam (M557)	0.325	NA	NA	34				
California clay loam (M562)	0.455	NA	NA	18				
North Dakota loam (M563)	1.030	NA	NA	38				
Silty clay loam from Italy (M570)	1.425	NA	NA	144				
Silty clay loam from France (M571)	0.400	NA	NA	42				
Sandy clay loam from the UK (M572)	0.280	NA	NA	18				
Sandy loam from Italy (M573)	0.295	NA	NA d	34				

Data were obtained from Table 5, p.28 of the study report. Means and standard deviations were calculated using Excel.

K_d -Adsorption and desorption coefficients; K - Freundlich adsorption and desorption coefficients; 1/N -Slope of Freundlich adsorption/desorption isotherms.

K_{oc} - Coefficient adsorption per organic carbon (K_d or K x 100/% organic carbon).

R^2 - Regression coefficient of Freundlich equation.

K_d values were calculated by the study author using the following equation (p.16):

$K_d = C_s \div C_{aq}$

where

K_d = partitioning coefficient;

Cs = concentration of test substance adsorbed to the soil; and

Caq = concentration of test substance in solution at equilibrium.

[2] Desorption was not studied.

C. ADSORPTION:

[^{14}C]BSTCA: After 2 hours of equilibration, 8.2%, 24.6%, 9.2%, 45.5%, 14.0%, and 1.4% of the applied [^{14}C]BSTCA was adsorbed to the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), silty clay loam from Italy (M570), silty clay loam from France (M571), and sandy clay loam from the UK (M572) soils, respectively (Appendix A, pp.46-49). Calculated simple K_d values were 0.185, 1.515, 0.605, 4.395, 0.720, and 0.085 for the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), silty clay loam from Italy (M570), silty clay loam from France (M571), and sandy clay loam from the UK (M572) soils, respectively. Corresponding K_{oc} values were 46, 156, 25, 444, 74, and 5 (Table 7, p.30).

[^{14}C]BST: After 2 hours of equilibration, 5.1%, 25.2%, 19.6%, 3.9%, 33.5%, 22.6%, 3.2%, and 4.9% of the applied [^{14}C]BST was adsorbed to the North Carolina sand (M538), Arkansas silt loam

(M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively (Appendix A, pp.46-49). Calculated simple adsorption K_d values were 0.135, 0.590, 0.420, 0.545, 0.840, 0.470, 0.075, and 0.610 for the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively. Corresponding K_{oc} values were 34, 61, 18, 21, 85, 48, 5, and 71 (Table 7, p.30).

[^{14}C]5-OH-XDE-638: After 24 hours of equilibration, 6.6%, 12.9%, 17.6%, 30.1%, 39.6%, 15.6%, 11.2%, and 13.1% of the applied **[^{14}C]5-OH-XDE-638** was adsorbed to the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively (Appendix A, pp.43-44). Calculated simple adsorption K_d values were 0.140, 0.325, 0.455, 1.030, 1.425, 0.400, 0.280, and 0.295 for the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils, respectively. Corresponding K_{oc} values were 34, 34, 18, 38, 144, 42, 18, and 34 (Table 5, p.28).

D. DESORPTION: Desorption was not studied.

III. STUDY DEFICIENCIES: This study is scientifically valid but cannot be used to fulfill the Subdivision N Guideline §163-1 data requirements for a mobility study using unaged soil because (i) the study was conducted using transformation products of penoxsulam rather than the parent compound, (ii) desorption was not studied, and (iii) the test substances were incompletely characterized. In addition, soil characterization data for three of the test soils (Silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils) were inconsistent throughout the study report. However, the information provided by this study does aid in understanding the overall environmental fate of penoxsulam in unaged soil.

IV. REVIEWER'S COMMENTS:

1. The study was conducted using only one test concentration. Subdivision N guidelines specify that a batch equilibrium study must be conducted using a minimum of four test concentrations of the parent and each of the transformation products. In addition, the low and high test

concentrations must differ by a factor of at least 10, to determine whether adsorption is concentration-dependent and to calculate an accurate Freundlich K value. If possible, one of the test concentrations should be approximately equivalent to the maximum proposed or registered field application rate of the parent compound.

2. Preliminary experiments were not conducted to determine the conditions to be used in the definitive study, such as the equilibration times soil:solution ratios to be used in the definitive study. Also, a preliminary experiment should be conducted to determine whether the test substances adsorbed to the test container walls.

3. It was not stated whether the definitive study was conducted in the dark. The equilibration should be conducted in the dark to minimize photodegradation. In this study, the test substances did not degrade during the course of the experiment. However, the lighting conditions used in the experimental design should be reported.

4. Four of the eight test soils were foreign in origin (Table 3, p.26). However, these soils were characterized using the USDA classification system and were comparable to U.S. soils.

5. The physico-chemical properties of the test substances were incomplete. Water solubility, vapour pressure, UV adsorption, molecular formula, melting point, bulk density, pk_a, K_{ow}, and the stability of the test substance were not reported. Descriptions of the test substances BST and 5-OH-XDE-638 were not provided. It was reported that [^{14}C]BSTCA was prepared as the Et_3N salt (p.11). The physical descriptions of the three test substances were not reported.

6. The soil biomass of the test soils was not reported.

7. A complete description of the test soil collection and storage was not provided. Pesticide use history at the collection site, collection procedures, sampling depth, and storage length were not reported.

8. The definitive study temperature was reported as 20°C. More detailed information was not provided. It is preferred that minimum, maximum, and average temperatures be reported. Any significant deviations from the average and their duration should be noted.

9. Soil characterization were inconsistent for three of the eight test soils. Specifically, the US Soil Texture Classifications presented in Table 3, p.26 of the study report for the silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils do not correspond with the US Soil Textural Classifications presented in Tables 4-8, pp.27-31 and Figure 9, p.40 of the study. Clarification by the registrant may be necessary.

10. BSTCA is unstable in solution and readily degrades to BST (pp.11-12, 18). Two separate

batches of [^{14}C]BSTCA/BST test solutions were prepared for use in the definitive study. Prior to adsorption, BSTCA completely degraded to BST in the dosing solutions for the North Dakota loam (M563) and sandy loam from Italy (M573) soils (p.20; Table 4, p.27). Therefore, sorption of [^{14}C]BSTCA was determined in six of the eight test soils. A short equilibration time of 2 hours was used in the definitive study for [^{14}C]BSTCA/BST to minimize degradation of BSTCA (p.15).

11. Controls were not used in the definitive study.

12. The study author stated that the aqueous solubility of penoxsulam is approximately 6 µg/mL, and that the transformation products 5-OH-XDE-638, BSTCA, and BST are likely to be more soluble than the parent compound (Figure 1, p.32).

13. Following adsorption, all samples were analyzed immediately for total radioactivity using LSC (pp.15, 17). Due to the instability of BSTCA in solution, all BSTCA/BST samples were immediately analyzed using HPLC following adsorption and extraction. All 5-OH-XDE-638 samples were refrigerated and analyzed using HPLC within one week following adsorption and extraction.

14. Only one replicate of each soil type treated with 5-OH-XDE-638 was analyzed using HPLC (p.13). It is preferred that at least two samples be analyzed in order to determine between-sample variability and identify outliers.

15. Complete details of the analytical methods were not reported. Oxidizer efficiency was not reported. For the HPLC method, the dimensions and particle size of the HPLC column were not reported, and it was not stated how [^{14}C]penoxsulam was identified in the samples.

16. The study author stated that only one radiolabel of each test substance was used in the definitive study, since the purpose of the study was to determine the sorptive behavior of penoxsulam, rather than to determine its transformation products (p.11).

17. Stock solutions were prepared by dissolving the test material in 1 mL of acetonitrile or 1 mL of acetone (p.12). However, the concentration of the co-solvents were not reported. Insufficient information was provided in the study report for the reviewer to determine the concentration of acetonitrile or acetone in the test solutions.

18. The study author concluded that [^{14}C]5-OH-XDE-638 and [^{14}C]BST are potentially mobile in the North Carolina sand (M538), Arkansas silt loam (M557), California clay loam (M562), North Dakota loam (M563), silty clay loam from Italy (M570), silty clay loam from France (M571), sandy clay loam from the UK (M572), and sandy loam from Italy (M573) soils (pp.19-20). [^{14}C]BSTCA was considered to be potentially mobile to moderately mobile in the test

3

soils.

19. The radiochemical purities of [^{14}C]5-OH-XDE-638 and both batches of [^{14}C]BSTCA/BST were confirmed using HPLC analysis (p.12; Figures 2-4, pp.33-35).

V. REFERENCES:

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 163-1. Mobility 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.

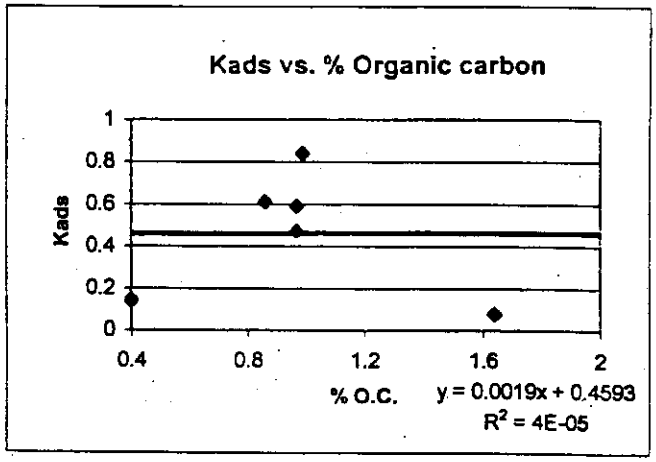
3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738.

4. U.S. Environmental Protection Agency. 2003. Guidance for Calculating Sorption Coefficients in Batch Equilibrium Studies.

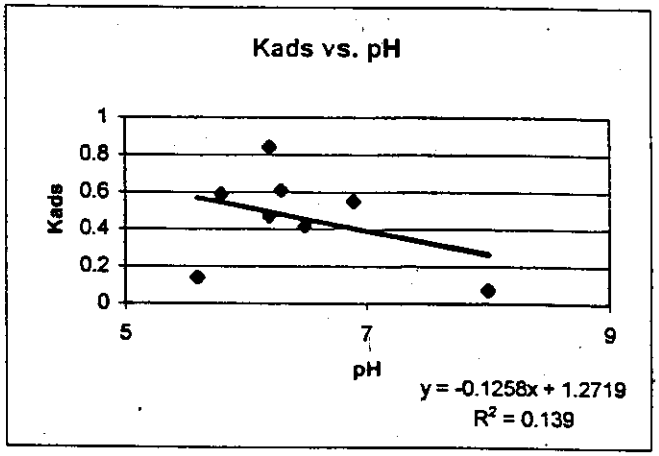
34

Chemical: BST
PC Code: 118205
MRID: 45830802
Guideline No: 163-1

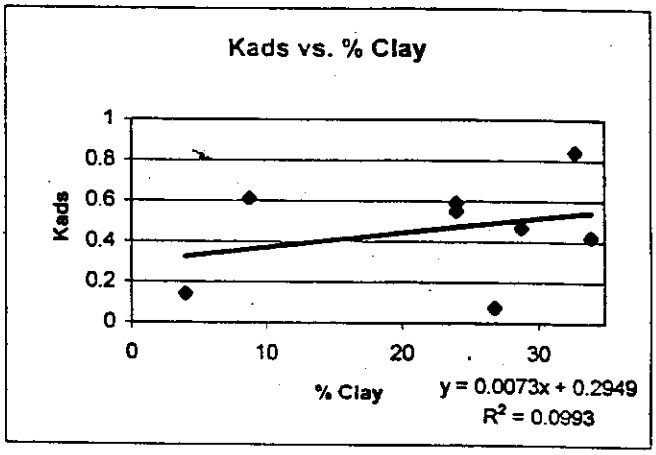
Soil	Kads	% organic carbon
Sand	0.14	0.4
Silt loam	0.59	0.97
Clay loam	0.42	2.46
Loam	0.55	2.74
Silty clay loam	0.84	0.99
Silty clay loam	0.47	0.97
Sandy clay loam	0.075	1.64
Sandy loam	0.61	0.86



Soil	Kads	pH
Sand	0.14	5.6
Silt loam	0.59	5.8
Clay loam	0.42	6.5
Loam	0.55	6.9
Silty clay loam	0.84	6.2
Silty clay loam	0.47	6.2
Sandy clay loam	0.075	8
Sandy loam	0.61	6.3



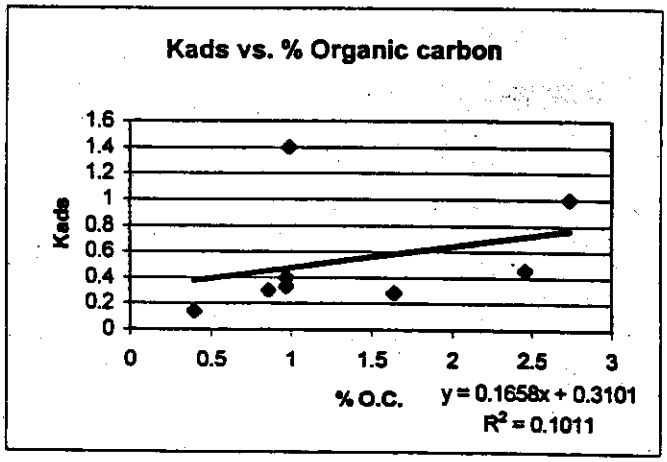
Soil	Kads	% clay
Sand	0.14	4
Silt loam	0.59	24
Clay loam	0.42	34
Loam	0.55	24
Silty clay loam	0.84	32.8
Silty clay loam	0.47	28.8
Sandy clay loam	0.075	26.8
Sandy loam	0.61	8.8



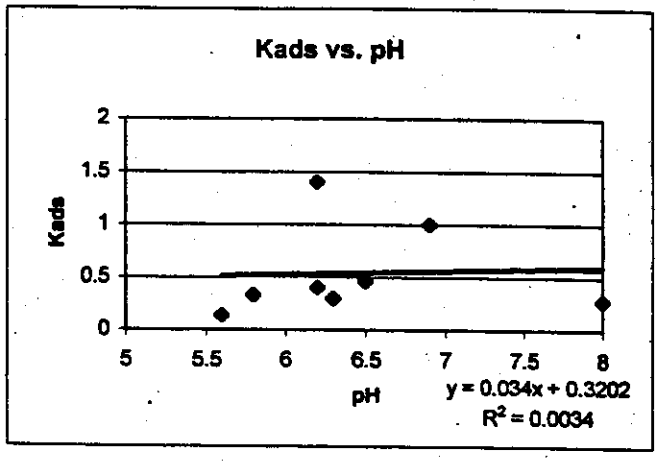
Data were obtained from Table 3, p. 26 and Appendix A, p. 48 of the study report.

Chemical: 5-OH-XDE-638
PC Code: 118205
MRID: 45830802
Guideline No: 163-1

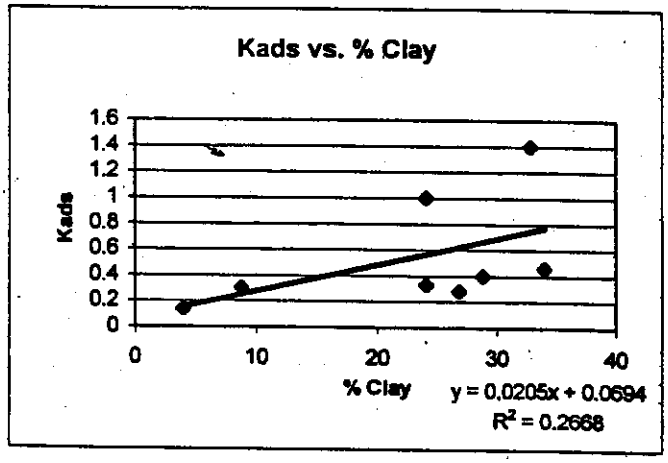
Soil	Kads	% organic carbon
Sand	0.14	0.4
Silt loam	0.33	0.97
Clay loam	0.46	2.46
Loam	1	2.74
Silty clay loam	1.4	0.99
Silty clay loam	0.4	0.97
Sandy clay loam	0.28	1.64
Sandy loam	0.3	0.86



Soil	Kads	pH
Sand	0.14	5.6
Silt loam	0.33	5.8
Clay loam	0.46	6.5
Loam	1	6.9
Silty clay loam	1.4	6.2
Silty clay loam	0.4	6.2
Sandy clay loam	0.28	8
Sandy loam	0.3	6.3



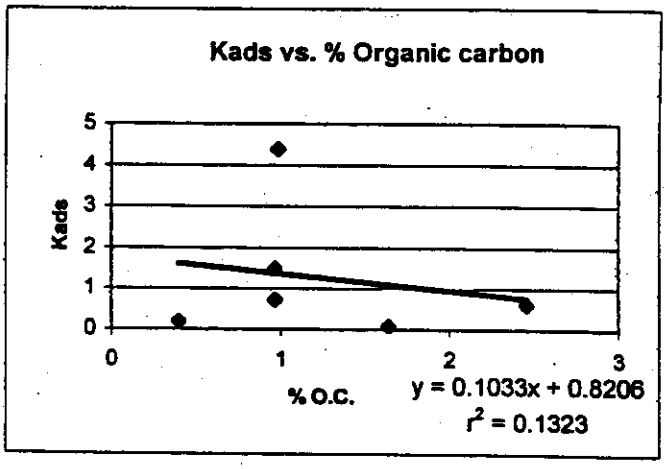
Soil	Kads	% clay
Sand	0.14	4
Silt loam	0.33	24
Clay loam	0.46	34
Loam	1	24
Silty clay loam	1.4	32.8
Silty clay loam	0.4	28.8
Sandy clay loam	0.28	26.8
Sandy loam	0.3	8.8



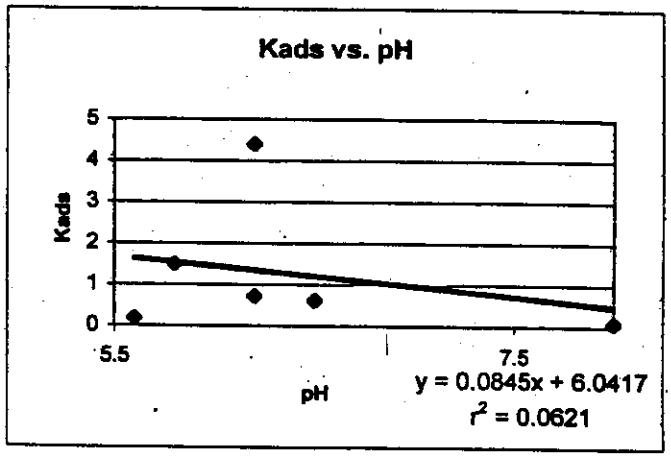
Data were obtained from Table 3, p. 26 and Appendix A, p. 43 of the study report.

Chemical: BSTCA
PC Code: 118205
MRID: 45830802
Guideline No: 163-1

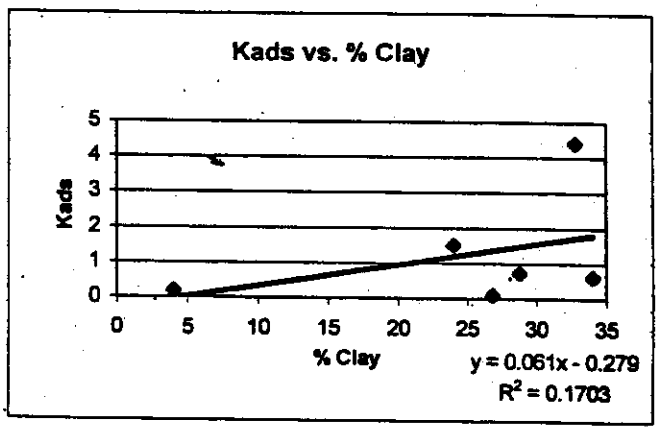
Soil	Kads	% organic carbon
Sand	0.19	0.4
Silt loam	1.5	0.97
Clay loam	0.61	2.46
Loam		
Silty clay loam	4.4	0.99
Silty clay loam	0.72	0.97
Sandy clay loam	0.085	1.64
Sandy loam		



Soil	Kads	pH
Sand	0.19	5.6
Silt loam	1.5	5.8
Clay loam	0.61	6.5
Loam		
Silty clay loam	4.4	6.2
Silty clay loam	0.72	6.2
Sandy clay loam	0.085	8
Sandy loam		



Soil	Kads	% clay
Sand	0.19	4
Silt loam	1.5	24
Clay loam	0.61	34
Loam		
Silty clay loam	4.4	32.8
Silty clay loam	0.72	28.8
Sandy clay loam	0.085	26.8
Sandy loam		



Data were obtained from Table 3, p. 26 and Appendix A, p. 48 of the study report.

Chemical: BSTCA
PC Code: 119031
MRID: 45830802
Guideline: 163-1

M538 Sand- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd
0.2	10	0.18	10	5	0.0400	0.2222
0.2	10	0.18	10	5	0.0400	0.2222
						0.2222 AVG

M557 Silt loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd
0.2	10	0.07	10	5	0.2600	3.7143
0.2	10	0.06	10	5	0.2800	4.6667
						4.1905 AVG

M562 Clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd
0.2	10	0.06	10	5	0.2800	4.6667
0.2	10	0.06	10	5	0.2800	4.6667
						4.6667 AVG

M570 Silty clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd
0.2	10	0.04	10	5	0.3200	8.0000
0.2	10	0.04	10	5	0.3200	8.0000

M571 Silty clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd
0.2	10	0.08	10	5	0.2400	3.0000
0.2	10	0.08	10	5	0.2400	3.0000
						3.0000 AVG

M572 Sandy clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd
0.2	10	0.06	10	5	0.2800	4.6667
0.2	10	0.07	10	5	0.2600	3.7143
						4.1905 AVG

Data were obtained from Appendix A, p. 48 of the study report.

Chemical: BST
PC Code: 119031
MRID: 45830802
Guideline: 163-1

M538 Sand- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.15	10	5	0.1000	0.6667	
0.2	10	0.14	10	5	0.1200	0.8571	
						0.7619	AVG

M557 Silt loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.17	10	5	0.0600	0.3529	
0.2	10	0.17	10	5	0.0600	0.3529	
						0.3529	AVG

M562 Clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.19	10	5	0.0200	0.1053	
0.2	10	0.18	10	5	0.0400	0.2222	
						0.1637	AVG

M563 Loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.03	10	5	0.3400	11.333	
0.2	10	0.03	10	5	0.3400	11.333	
						11.333	AVG

M570 Silty clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd
0.2	10	0.16	10	5	0.0800	0.5000
0.2	10	0.16	10	5	0.0800	0.5000

Data were obtained from Appendix A, p. 48 of the study report.

Chemical: BST
PC Code: 119031
MRID: 45830802
Guideline: 163-1

M571 Silty clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.2	10	5	0.0000	0.0000	
0.2	10	0.19	10	5	0.0200	0.1053	
						0.0526	AVG

M572 Sandy clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.16	10	5	0.0800	0.5000	
0.2	10	0.18	10	5	0.0400	0.2222	
						0.3611	AVG

M573 Sandy loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.03	10	5	0.3400	11.333	
0.2	10	0.03	10	5	0.3400	11.333	
						11.333	AVG

Data were obtained from Appendix A, p. 48 of the study report.

Chemical: 5-OH-XDE-638
PC Code: 119031
MRID: 45830802
Guideline: 163-1

M538 Sand- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.19	10	5	0.0200	0.1053	
0.2	10	0.19	10	5	0.0200	0.1053	
						0.1053	AVG

M557 Silt loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.16	10	5	0.0800	0.5000	
0.2	10	0.16	10	5	0.0800	0.5000	
						0.5000	AVG

M562 Clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.15	10	5	0.1000	0.6667	
0.2	10	0.16	10	5	0.0800	0.5000	
						0.5833	AVG

M563 Loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.12	10	5	0.1600	1.333	
0.2	10	0.12	10	5	0.1600	1.333	
						1.333	AVG

M570 Silty clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd
0.2	10	0.11	10	5	0.1800	1.6364
0.2	10	0.11	10	5	0.1800	1.6364

Data were obtained from Appendix A, p. 43 of the study report.

Chemical: 5-OH-XDE-638
PC Code: 119031
MRID: 45830802
Guideline: 163-1

M571 Silty clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.16	10	5	0.0800	0.5000	
0.2	10	0.16	10	5	0.0800	0.5000	
						0.5000	AVG

M572 Sandy clay loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.16	10	5	0.0800	0.5000	
0.2	10	0.16	10	5	0.0800	0.5000	
						0.5000	AVG

M573 Sandy loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.2	10	0.18	10	5	0.0400	0.222	
0.2	10	0.18	10	5	0.0400	0.222	
						0.222	AVG

Data were obtained from Appendix A, p. 43 of the study report.

Chemical: 5-OH-XDE-638
PC Code: 119031
MRID: 45830802
Guideline: 163-1

Table 4/6 Adsorption soil

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	0.025	0.049	0.074	0.122	0.158	0.062	0.044	0.054
0.4	0.028	0.054	0.067	0.119	0.159	0.063	0.046	0.051
AVG	0.0265	0.0515	0.0705	0.1205	0.1585	0.0625	0.0450	0.0525
STDEV	0.0021	0.0035	0.0049	0.0021	0.0007	0.0007	0.0014	0.0021

Data were obtained from Appendix A, p. 44 of the study report.

Table 5 Adsorption supernatant

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	93.6	83.7	75.7	64.2	58.5	81.1	82.6	86.1
0.4	92.5	83.6	80.1	64.9	57.4	80.9	82.4	87.2
AVG	93.05	83.65	77.90	64.55	57.95	81.00	82.50	86.65
STDEV	0.78	0.07	3.11	0.49	0.78	0.14	0.14	0.78

Table 5 Extracted

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	5.9	11.7	17.9	29.5	38.2	15.1	10.5	13
0.4	6.7	12.9	16.2	28.7	38.2	15.2	11.1	12.2
AVG	6.30	12.30	17.05	29.10	38.20	15.15	10.80	12.60
STDEV	0.57	0.85	1.20	0.57	0.00	0.07	0.42	0.57

Table 5 Combusted

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	0.3	1.5	1.4	2.7	1.3	1.7	1.9	0.3
0.4	0.3	1.5	1.6	2.3	1.5	1.6	1.1	0.5
AVG	0.30	1.50	1.50	2.50	1.40	1.65	1.50	0.40
STDEV	0.00	0.00	0.14	0.28	0.14	0.07	0.57	0.14

Data were obtained from Table 6, p. 29 of the study report.

Chemical: 5-OH-XDE-638
PC Code: 119031
MRID: 45830802
Guideline: 163-1

Table 5 Recovery

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	99.8	96.9	95.1	96.4	97.9	97.9	95.1	99.5
0.4	99.4	98	97.9	95.9	97.1	97.6	94.6	99.8
AVG	99.60	97.45	96.50	96.15	97.50	97.75	94.85	99.65
STDEV	0.28	0.78	1.98	0.35	0.57	0.21	0.35	0.21

Data were obtained from Table 6, p. 29 of the study report.

Table 6 Adsorption supernatant

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	0.19	0.16	0.15	0.12	0.11	0.16	0.16	0.18
0.4	0.19	0.16	0.16	0.12	0.11	0.16	0.16	0.18
AVG	0.1900	0.1600	0.1550	0.1200	0.1100	0.1600	0.1600	0.1800
STDEV	0.0000	0.0000	0.0071	0.0000	0.0000	0.0000	0.0000	0.0000

Table 6 % Adsorption

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	6.25	12.25	18.5	30.5	39.5	15.5	11	13.5
0.4	7	13.5	16.75	29.75	39.75	15.75	11.5	12.75
AVG	6.63	12.88	17.63	30.13	39.63	15.63	11.25	13.13
STDEV	0.53	0.88	1.24	0.53	0.18	0.18	0.35	0.53

Data were obtained from Appendix A, pp. 43-44 of the study report.

Table 8d K_d 5-OH-XDE-638

	M538	M557	M562	M563	M570	M571	M572	M573
	0.13	0.31	0.49	1.05	1.41	0.4	0.27	0.31
	0.15	0.34	0.42	1.01	1.44	0.4	0.29	0.28
AVG	0.14	0.325	0.455	1.03	1.425	0.4	0.28	0.295

Table 8d 5-OH-XDE-638

	M538	M557	M562	M563	M570	M571	M572	M573
	32	32	20	38	142	41	17	36
	37	35	17	37	145	42	18	33
AVG	34.5	33.5	18.5	37.5	143.5	41.5	17.5	34.5

Data were obtained from Table 5, p. 28 of the study report.

Chemical: BSTCA/BST
PC Code: 119031
MRID: 45830802
Guideline: 163-1

Table 4/6 Adsorption soil BSTCA

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	0.035	0.115	0.039	0	0.162	0.056	0.008	0
0.4	0.031	0.082	0.035	0	0.202	0.056	0.003	0
AVG	0.0330	0.0985	0.0370	0.0000	0.1820	0.0560	0.0055	0.0000
STDEV	0.0028	0.0233	0.0028	0.0000	0.0283	0.0000	0.0035	0.0000

Table 4/6 Adsorption soil BST

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	0.02	0.084	0.081	0.016	0.157	0.092	0.018	0.02
0.4	0.021	0.118	0.076	0.015	0.111	0.089	0.008	0.019
AVG	0.0205	0.1010	0.0785	0.0155	0.1340	0.0905	0.0130	0.0195
STDEV	0.0007	0.0240	0.0035	0.0007	0.0325	0.0021	0.0071	0.0007

Data were obtained from Appendix A, p. 49 of the study report.

Table 5 Adsorption supernatant

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	92.2	69.4	76.2	73.6	54.3	77.5	83.2	73.7
0.4	90.4	70.1	75.5	72.3	53.4	76.2	90.7	74.9
AVG	91.30	69.75	75.85	72.95	53.85	76.85	86.95	74.30
STDEV	1.27	0.49	0.49	0.92	0.64	0.92	5.30	0.85

Table 5 Extracted

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	7.6	26	17.4	18.1	37.9	19.5	4.4	22.6
0.4	7	26.6	16.3	16.9	36.8	19	1.9	22
AVG	7.30	26.30	16.85	17.50	37.35	19.25	3.15	22.30
STDEV	0.42	0.42	0.78	0.85	0.78	0.35	1.77	0.42

Table 5 Combusted

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	0.1	1.3	1.2	4.3	0.5	3.1	2.1	0.2
0.4	0	1.1	1.2	3.5	0.3	3	1.6	0.6
AVG	0.05	1.20	1.20	3.90	0.40	3.05	1.85	0.40
STDEV	0.07	0.14	0.00	0.57	0.14	0.07	0.35	0.28

Data were obtained from Table 8, p. 31 of the study report.

Chemical: BSTCA/BST
PC Code: 119031
MRID: 45830802
Guideline: 163-1

Table 5 Recovery

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	99.8	96.8	94.8	96.1	92.6	100.2	89.7	96.6
0.4	97.4	97.9	93	92.7	90.5	98.2	94.2	97.5
AVG	98.60	97.35	93.90	94.40	91.55	99.20	91.95	97.05
STDEV	1.70	0.78	1.27	2.40	1.48	1.41	3.18	0.64

Data were obtained from Table 8, p. 31 of the study report.

Table 6 Adsorption supernatant BSTCA

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	0.18	0.07	0.06	0	0.04	0.08	0.06	0
0.4	0.18	0.06	0.06	0	0.04	0.08	0.07	0
AVG	0.1800	0.0650	0.0600	0.0000	0.0400	0.0800	0.0650	0.0000
STDEV	0.0000	0.0071	0.0000	0.0000	0.0000	0.0000	0.0071	0.0000

Table 6 Adsorption supernatant BST

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	0.15	0.17	0.19	0.03	0.16	0.2	0.16	0.03
0.4	0.14	0.17	0.18	0.03	0.16	0.19	0.18	0.03
AVG	0.1450	0.1700	0.1850	0.0300	0.1600	0.1950	0.1700	0.0300
STDEV	0.0071	0.0000	0.0071	0.0000	0.0000	0.0071	0.0141	0.0000

Table 6 % Adsorption BSTCA

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	8.75	28.75	9.75	-	40.5	14	2	-
0.4	7.75	20.5	8.75	-	50.5	14	0.75	-
AVG	8.25	24.63	9.25	-	45.50	14.00	1.38	-
STDEV	0.71	5.83	0.71	-	7.07	0.00	0.88	-

Table 6 % Adsorption BST

	M538	M557	M562	M563	M570	M571	M572	M573
0.4	5	21	20.25	4	39.25	23	4.5	5
0.4	5.25	29.5	19	3.75	27.75	22.25	2	4.75
AVG	5.13	25.25	19.63	3.88	33.50	22.63	3.25	4.88
STDEV	0.18	6.01	0.88	0.18	8.13	0.53	1.77	0.18

Data were obtained from Appendix A, pp. 46-49 of the study report.

Chemical: BSTCA/BST
PC Code: 119031
MRID: 45830802
Guideline: 163-1

Table 8b K_d BSTCA

	M538	M557	M562	M563	M570	M571	M572	M573
	0.2	1.75	0.63	-	3.84	0.74	0.12	-
	0.17	1.28	0.58	-	4.95	0.7	0.05	-
AVG	0.185	1.515	0.605	-	4.395	0.72	0.085	-

Table 8b K_{oc} BSTCA

	M538	M557	M562	M563	M570	M571	M572	M573
	49	181	26	-	388	76	7	-
	43	132	24	-	500	72	3	-
AVG	46	156.5	25	-	444	74	5	-

Table 8c K_d BST

	M538	M557	M562	M563	M570	M571	M572	M573
	0.13	0.5	0.43	0.56	0.98	0.47	0.11	0.62
	0.14	0.68	0.41	0.53	0.7	0.47	0.04	0.6
AVG	0.135	0.59	0.42	0.545	0.84	0.47	0.075	0.61

Table 8c K_{oc} BST

	M538	M557	M562	M563	M570	M571	M572	M573
	33	51	18	21	99	48	7	72
	35	70	17	20	71	49	3	69
AVG	34	60.5	17.5	20.5	85	48.5	5	70.5

Data were obtained from Table 7, p. 30 of the study report.

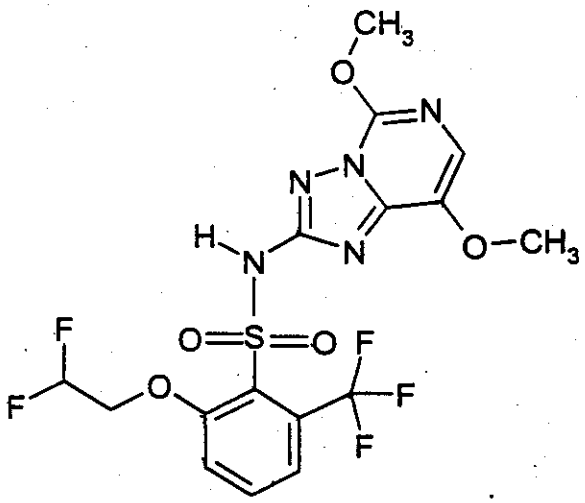
Attachment 2

Structures of Parent and Transformation Products

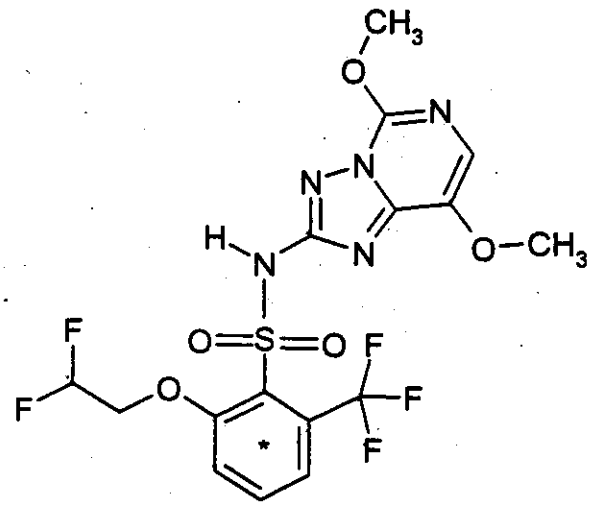
Penoxsulam

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

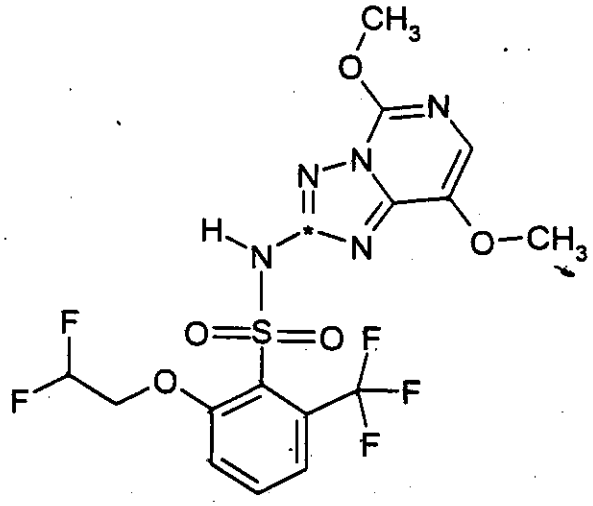
Unlabeled



[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

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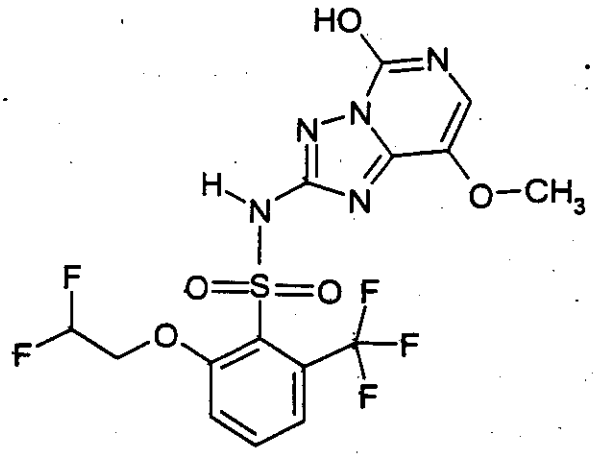
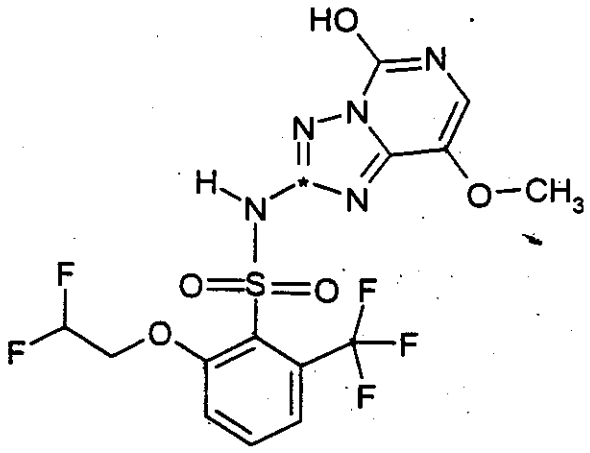


[Triazolopyrimidine-2-^{14}C] label



* 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

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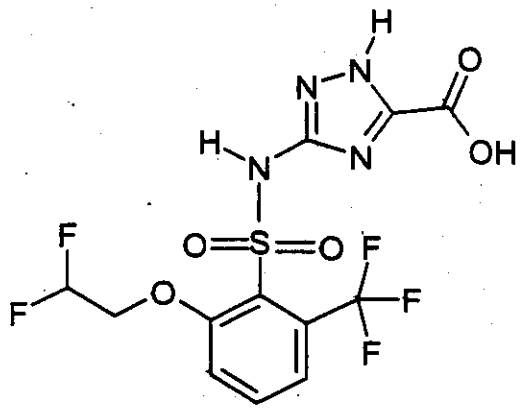
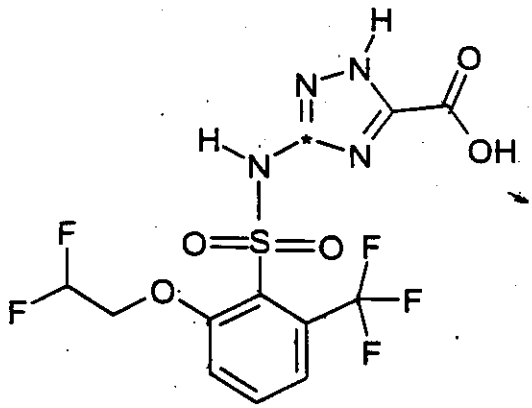


[Triazolopyrimidine-2-^{14}C] label



* 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

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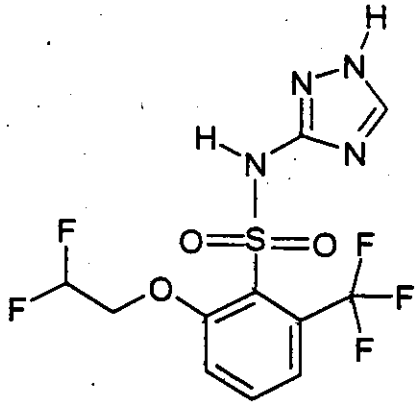
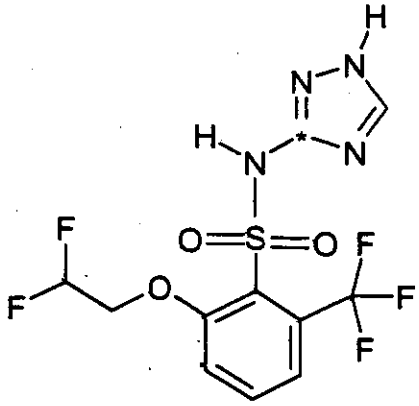


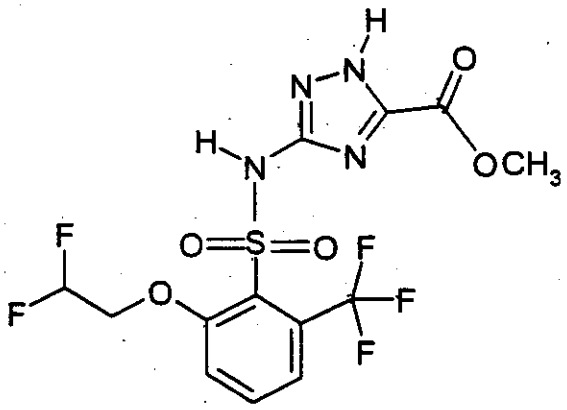
[Triazolopyrimidine-2-^{14}C] label



* Position of the radiolabel.

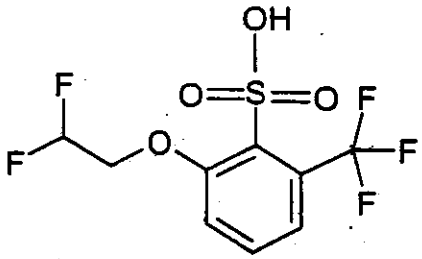
BSTCA-methyl

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



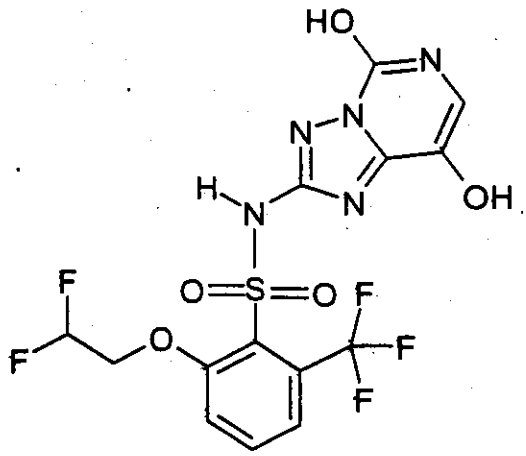
BSA

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



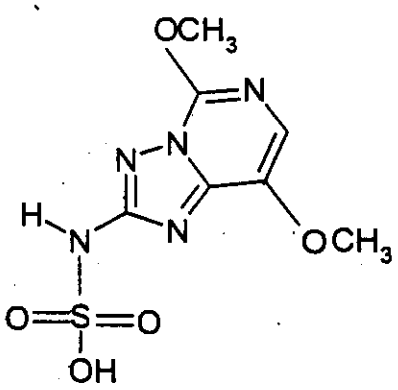
5,8-diOH

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



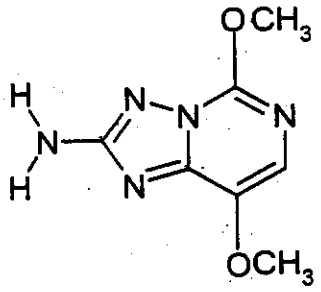
TPSA

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



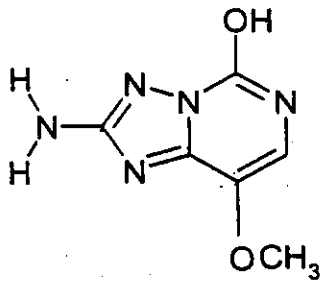
2-Amino TP

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



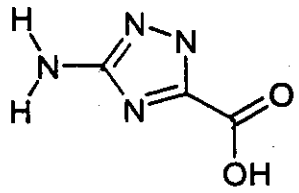
5-OH, 2-Amino TP

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



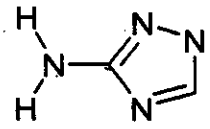
2-Amino TCA

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



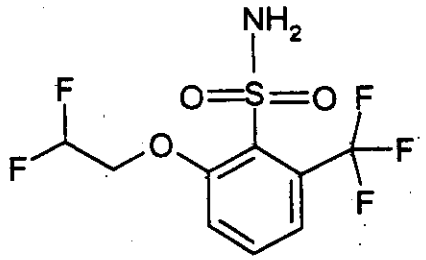
2-Amino-1,3,4-triazole

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