Data Evaluation Report on the adsorption-desorption of RPA 203328, a transformation product of pyrasulfotole, in soil

PMRA Submission Number 2006-2445 EPA MRID Number 46801704

Data Requirement: PMRA Data Code: 8.2.4.2
EPA DP Barcode: D328639
OECD Data Point: IIA 7.4.2
EPA Guideline: 163-1

Test material:
Common name: RPA 203328.
Chemical name:
IUPAC name: 2-Mesyl-4-trifluoromethylbenzoic acid.
CAS name: Benzoic acid, 2-(methylsulfonyl)-4-(trifluoromethyl)-.
CAS No.: 142994-06-7.
Synonyms: AE B197555-benzoic acid; AE B197555; K-1198; K-1367.
Smiles string: O=C(c1ccc(cc1S(=O)(=O)C)C(F)(F)F)O (ISIS v2.3/Universal SMILES).
No EPI Suite, v3.12 SMILES String found as of 6/7/06.
CS(=O)(=O)c1cc(C(F)(F)F)ccc1C(=O)O.
CS(=O)(=O)c1cc(ccc1C(=O)O)C(F)(F)F.

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Essex, CM5 0GZ, United Kingdom; sponsored and submitted by Bayer CropScience AG, Monheim am Rhein, Germany. Battelle Laboratory Project ID/Report Number CX/03/061. Sponsor Reference MEISM001. Experimental start date October 6, 2003, and completion date January 31, 2004 (p. 5). Final report issued April 6, 2004.

EXECUTIVE SUMMARY

The adsorption/desorption characteristics of [U-^{14}C]ring-labeled 2-mesyl-4-trifluoromethylbenzoic acid (RPA 203328) were studied in four soils from the UK: a sandy loam [Little Shelford, pH 7.7, organic carbon 1.5%], a clay loam [Shelley Field, pH 7.6, organic carbon 1.9%], a sandy clay [Lockington, pH 6.6, organic carbon 3.3%], and a sandy loam [Manningtree, pH 7.1, organic carbon 1.0%]; and in a German silt loam soil [Goch, pH 6.5, organic carbon 1.6%], in a batch equilibrium experiment. The experiment was conducted in accordance with the USEPA Guidelines for Pesticides Registration, Subdivision N §163-1, and in compliance with OECD Good Laboratory Practices. The adsorption phase of the study was carried out by equilibrating air-dried soils with [^{14}C]RPA 203328 at nominal test concentrations of 0.01, 0.03, 0.1, 0.3, and 1.0 mg a.i./kg soil for all test soils. The samples were shaken in the dark at 20 ± 2°C for *ca.* 24 hours (Lockington sandy clay soil only) or for *ca.* 7 days. The equilibrating solution used was 0.01M $CaCl_2$ solution, with soil/solution ratios of 1:1 (w:v) for all test soils. The desorption phase of the study was carried out by replacing the adsorption solution with an equivalent amount volume of pesticide-free 0.01M $CaCl_2$ solution (*ca.* 10 mL for the Lockington soil) and equilibrating in the dark at 20 ± 2°C for *ca.* 24 hours. For all test soils, three desorption cycles were conducted for the desorption phase.

The supernatant after adsorption and each desorption cycle was separated by centrifugation and aliquots were analyzed for total radioactivity using LSC. Following the third desorption cycle, the soils were extracted with acetonitrile:water (50:50, v:v) and centrifuged, and aliquots of the extracts were analyzed using LSC. The remaining soils were air-dried, milled, and analyzed for total radioactivity using LSC following combustion. Aliquots of the adsorption supernatants, first desorption cycle supernatants, and soil extracts from the two highest treatment concentrations (0.3 and 1.0 mg a.i./kg soil) were analyzed for RPA 203328 using HPLC.

The incubation temperature during the study was maintained at 20 ± 2°C; no supporting information was provided. The pH of the supernatants solutions during the adsorption and desorption phases ranged from 6.28 to 7.15. Based on HPLC analysis, [^{14}C]RPA 203328 was stable in solution during the definitive study, comprising >98% of the radioactivity in the radio-chromatograms.

Mass balances at the end of the adsorption phase were not reported. Mean mass balances at the end of the desorption phase ranged from 100.5-103.5%, 101.3-124.2%, 100.2-102.7%, 98.6-101.9%, and 95.4-98.7% of the applied for the Little Shelford sandy loam, Shelley Field clay loam, Lockington sandy clay, Manningtree sandy loam, and Goch silt loam soils, respectively.

After 7 days of equilibration, 0.8-26.7%, 0.7-1.7%, and 1.6-13.6% of the applied [^{14}C]RPA 203328 was adsorbed to the Shelley Field clay loam, Manningtree sandy loam, and Goch silt loam soils, respectively (reviewer-calculated). Maximums of 1.0% and 3.2% of the applied [^{14}C]RPA 203328 were adsorbed to the Little Shelford sandy loam and Lockington sandy clay soils, respectively, after 7 days and 24 hours of equilibrium. Registrant-calculated adsorption K_d

and K_{oc} values were not reported. Registrant-calculated Freundlich adsorption K_F values were 0.0283, 0.0088, and 0.0183 for the Shelley Field clay loam, Manningtree sandy loam, and Goch silt loam soils, respectively; corresponding Freundlich adsorption K_{Foc} values were 1.49, 0.881, and 1.14. The study authors noted that for the Little Shelford sandy loam and Lockington sandy clay soils, there was insufficient correlation in the data for adsorption, $r^2 <0.6$, and therefore, did not consider the Freundlich constants to be valid. At the end of the desorption phase, 86.3-87.7%, 54.3-85.5%, 52.8-73.9%, 91.7-92.5%, and 73.2-91.4% of the applied [^{14}C]RPA 203328 desorbed from the Little Shelford sandy loam, Shelley Field clay loam, Lockington sandy clay, Manningtree sandy loam, and Goch silt loam soils, respectively (reviewer-calculated). Registrant-calculated desorption K_d and K_{oc} values were not reported. Registrant-calculated Freundlich desorption K_F values were 0.311, 0.620, and 0.135 for the Shelley Field clay loam, Manningtree sandy loam, and Goch silt loam soils, respectively; corresponding Freundlich desorption K_{Foc} values were 16.4, 62.0, and 8.46. The study authors did not consider the desorption results for the Little Shelford sandy loam and Lockington sandy clay desorption to be valid, due to the low correlation for the adsorption phase.

Adsorption coefficients were re-calculated by the secondary reviewer using slopes of adsorption isotherms rather than mean coefficients. $K_{d\text{-}ads}$ values were 0.0515, 0.00782 and 0.0205 for Shelley field clay loam, Manningtree sandy loam and Goch silt loam, respectively; corresponding $K_{OC\text{-}ads}$ values were 3, 1 and 2, respectively. Freundlich regressions gave $K_{F\text{-}ads}$ values of 0.03, 0.01 and 0.02 for Shelley field clay loam, Manningtree sandy loam and Goch silt loam, respectively; corresponding $K_{FOC\text{-}ads}$ values were 1, 1 and 2, respectively. Based on the $K_{FOC\text{-}ads}$ values and the mobility classification of McCall *et al.* (1981), RPA 203328 is expected to exhibit very high mobility in the range of soils studied.

Results Synopsis:

Soil type: **Little Shelford Sandy loam**

Amount adsorbed:	0.0-1.0% of the applied.
Freundlich adsorption K_F:	N/A
Freundlich adsorption K_{Foc}:	N/A
Amount desorbed:	86.3-87.7% of the adsorbed.
Freundlich desorption K_F:	N/A
Freundlich desorption K_{Foc}:	N/A

Soil type: **Shelley Field Clay loam**

Amount adsorbed:	0.8-26.7% of the applied.
Freundlich adsorption K_F:	0.0283
Freundlich adsorption K_{Foc}:	1.49
Amount desorbed:	54.3-85.5% of the adsorbed.
Freundlich desorption K_F:	0.311
Freundlich desorption K_{Foc}:	16.4

Soil type: **Lockington Sandy clay**
Amount adsorbed: 0.0-3.2% of the applied.
Freundlich adsorption K_F: N/A
Freundlich adsorption K_{Foc}: N/A
Amount desorbed: 52.8-73.9% of the adsorbed.
Freundlich desorption K_F: N/A
Freundlich desorption K_{Foc}: N/A
Soil type: **Manningtree Sandy loam**
Amount adsorbed: 0.7-1.7% of the applied.
Freundlich adsorption K_F: 0.00881
Freundlich adsorption K_{Foc}: 0.881
Amount desorbed: 91.7-92.5% of the adsorbed.
Freundlich desorption K_F: 0.620
Freundlich desorption K_{Foc}: 62.0

Soil type: **Goch Silt loam**
Amount adsorbed: 1.6-13.6% of the applied.
Freundlich adsorption K_F: 0.0183
Freundlich adsorption K_{Foc}: 1.14
Amount desorbed: 73.2-91.4% of the adsorbed.
Freundlich desorption K_F: 0.135
Freundlich desorption K_{Foc}: 8.46

PMRA Results Synopsis:

Soil type: **Shelley Field Clay loam**
Amount adsorbed: 0.8-26.7% of the applied.
Adsorption K_d: 0.0515
Adsorption K_{oc}: 3
Freundlich adsorption K_F: 0.03
Freundlich adsorption K_{Foc}: 1
Mobility classification: Very high

Soil type: **Manningtree Sandy loam**
Amount adsorbed: 0.7-1.7% of the applied.
Adsorption K_d: 0.00782
Adsorption K_{oc}: 1
Freundlich adsorption K_F: 0.01
Freundlich adsorption K_{Foc}: 1
Mobility classification: Very high

Soil type: **Goch Silt loam**
Amount adsorbed: 1.6-13.6% of the applied.

Adsorption K_d:	0.0205
Adsorption K_{oc}:	2
Freundlich adsorption K_F:	0.02
Freundlich adsorption K_{Foc}:	2
Mobility classification:	Very high

Study Acceptability: This study is classified as **supplemental**. No significant deviations from good scientific practices were noted. The study was conducted using a transformation product of pyrasulfotole, rather than the parent compound. Also, it could not be determined if the foreign soils used in the study were typical of the pesticide use area in the U.S.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with the USEPA Guidelines for Pesticides Registration, Subdivision N §163-1; the EU Commission Directive 95/36/EC; and the OECD Guideline for Testing of Chemicals No. 106 "Adsorption/-Desorption" (2000; p. 17). Significant deviations from the objectives of Subdivision N guidelines were:

> The study was conducted using a transformation product of pyrasulfotole, rather than the parent compound.
>
> It could not be determined if the foreign soils used in the study were typical of the pesticide use area in the U.S.

COMPLIANCE: This study was conducted in compliance with OECD Good Laboratory Practices (p. 3; Appendix 8, p. 105). 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 [^{14}C]RPA 203328 (p. 17).

Chemical Structure: See DER Attachment 1.

Description: Technical grade, white solid (p. 18).

Purity:

Radiolabeled: Radiochemical purity: 99.8% (p. 18).
Lot/Batch No.: SEL/1289.
Specific activity: 2.86 MBq/mg (769.3 MBq/mmol).
Location of the label: Uniformly ring labeled.

Unlabeled: Analytical purity: 99.6% (p. 18).
Lot/Batch No.: IGB 947.

Storage conditions of test chemicals: The radiolabeled test material was stored at <-15°C (p. 18).

Physico-chemical properties of RPA 203328:

Parameter	Value	Comment
Molecular weight	268.22 g/mole	
Molecular formula	$C_9H_7F_3O_4S$	
Water Solubility	8.5 g/L	
Vapor Pressure/Volatility	Not reported.	
UV Absorption	Not reported.	
Pka	Not reported.	
K_{ow}/log K_{ow}	Not reported.	
Stability of compound at room temperature, if provided	Not reported.	

Data were obtained from p. 17 of the study report.

2. Soil Characteristics

Table 1: Description of soil collection and storage.

Description	Little Shelford Sandy loam	Shelley Field Clay loam	Lockington Sandy clay	Manningtree Sandy loam	Goch Silt loam
Geographic location	Little Shelford, Field Station, Whittlesford Rd, Cambridgeshire, UK, CB5 5EU	Boarded Barns Farm, Fyfield Road, Ongar, Essex, UK, CM5 OHW	Lockington Grounds Farm, Lockington, Leicestershire, UK	Aldhams Farm, Dead lane, Lawford, Manningtree, Essex, UK, CO11 2NF	75 Berliner Str., Goch-Nierswald, D-47574, Germany
Pesticide use history at the collection site	Not reported.				
Collection procedures	Not reported.				
Sampling depth	Not reported.				
Storage conditions	Not reported.				
Storage length [1]	*ca.* 3 months.			*ca.* 1 month.	Collected after experimental initiation.
Soil preparation	Partially air-dried, sieved (2 mm).				

Data were obtained from pp. 18-19 and Table 1, p. 32 of the study report.

1 Storage length was determined by the reviewer as the interval between the field sampling date (July 2003 for the Little Shelford sandy loam, Shelley Field clay loam, and Lockington sandy clay soils, September 2003 for the Manningtree sandy loam soil, and December 2003 for the Goch silt loam soil) and the experimental study initiation (October 2003).

Table 2: Properties of the soils.

Property	Little Shelford	Shelley Field	Lockington	Manningtree	Goch
Soil texture (USDA)	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
% Sand	72.38	43.19	49.89	68.31	28.68
% Silt	10.98	23.48	14.14	25.31	61.06
% Clay	16.64	33.32	35.97	6.38	10.26
pH Deionized water 0.01M $CaCl_2$ 1M Potassium chloride	 7.7 7.6 7.2	 7.6 7.3 7.1	 6.6 5.9 6.3	 7.1 6.3 6.3	 6.5 5.6 5.6
Organic carbon (%)	1.5	1.9	3.3	1.0	1.6
Organic matter (%)	2.6	3.3	5.7	1.7	2.8
CEC (meq/100g)	39.4	17.2	17.8	8.3	9.6
Moisture at 1/3 bar (%)	20.7	30.6	44.0	17.6	28.5
Bulk density (g/cm^2)	Not reported.				
Biomass (mg microbial C/100 g or CFU or other)	Not reported.				
Soil taxonomic classification	Not reported.				
Soil mapping unit (for EPA)	Not reported.				

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

C. STUDY DESIGN:

1. Preliminary study: Preliminary experiments were conducted to determine the adsorption of the test material to the test vessels, and to determine the appropriate soil:solution ratio and equilibrium time to be used in the definitive study (pp. 20-21).

Prior to study initiation, stock solutions were prepared for the preliminary studies by dissolving the test substance in 0.01M $CaCl_2$ solution (p. 19). Triplicate aliquots of each stock solution were analyzed for total radioactivity suing LSC.

To determine the adsorption of the test material to the test containers, an aliquot (1 × *ca.* 75 mL) of [^{14}C]RPA 203328 stock solution was added to each of two borosilicate glass centrifuge tubes (pp. 19-20). The samples were capped and shaken in the dark at 20 ± 2EC for *ca.* 24 hours. Aliquots were analyzed for total radioactivity using LSC. No significant adsorption of the test material to the glass test containers was observed; [^{14}C]RPA 203328 averaged 100.7% of the applied radioactivity (duplicate samples; p. 28; Table 3, p. 33).

To determine background radioactivity, aliquots (2 × *ca.* 15 g) of each test soil were added to borosilicate glass centrifuge tubes, each containing *ca.* 75 mL 0.01M $CaCl_2$ solution (pp. 19-20).

The samples were shaken in the dark at 20 ± 2EC for *ca.* 24 hours, then centrifuged. Aliquots were analyzed for total radioactivity using LSC. The level of background radioactivity detected was negligible; therefore, no corrections were deemed necessary (p. 28; Table 4, p. 33).

To determine the soil:solution ratio, aliquots (1 × 20-, 26.7-, and 40-g) of each test soil were placed into borosilicate glass centrifuge tubes and mixed with 0.01M $CaCl_2$ solution to establish respective soil:solution ratios of *ca.* 1:2, 1:1.5, and 1:1 (w:v; pp. 19, 21). The samples were pre-equilibrated by shaking in the dark at 20 ± 2EC for at least 1 hour. Following pre-equilibration, the samples were treated with a *ca.* 1.0-mL aliquot of [^{14}C]RPA 203328 stock solution at a nominal test concentration of 1.0 mg/L. The sample tubes were capped, and the samples were shaken for 24 hours, then centrifuged. Aliquots of the supernatants were analyzed for total radioactivity using LSC. It was determined that 1.5%, 1.1% and 1.2% of the applied radioactivity was recovered in the supernatants for the Goch silt loam soil treated at soil:solution ratios of 1:2, 1:1.5, and 1:1 (w:v), respectively (p. 29; Table 5, p. 34). No radioactivity was recovered in the remaining test soils. Based on HPLC analysis, [^{14}C]RPA 203328 was stable when using a soil:solution ratio of 1:1 (w:v).

To determine the adsorption equilibration time, aliquots (6 × *ca.* 40 g) of each test soil were placed into borosilicate glass centrifuge tubes and mixed with *ca.* 40 mL of 0.01M $CaCl_2$ solution (pp. 19, 21). The samples were pre-equilibrated by shaking in the dark at 20 ± 2EC for at least 1 hour. Following pre-equilibration, the samples were treated with a *ca.* 1.0-mL aliquot of [^{14}C]RPA 203328 stock solution at a nominal test concentration of 0.03 mg/L. The samples were shaken in the dark at 20 ± 2EC for 2, 6, 24, 48, and 72 hours and 6 days. The samples were centrifuged, and aliquots of the resulting supernatants were analyzed for total radioactivity using LSC. All samples were then extracted by shaking in the dark at 20 ± 2EC for 24 hours with acetonitrile:water (50:50, v:v, *ca.* 40 mL). Following extraction, the samples were centrifuged and aliquots were analyzed using LSC. Selected adsorption supernatants and soil extracts were analyzed using HPLC. The results showed that equilibrium was reached after 24 hours for the Lockington sandy clay soil and after 6 days for the Little Shelford sandy loam, Shelley Field clay loam, Manningtree sandy loam, and Goch silt loam soils (p. 29; Figure 4, p. 44). Based on HPLC analysis of the adsorption supernatants and soil extracts, [^{14}C]RPA 203328 comprised >98% of the applied radioactivity, confirming the stability of the test material in soil following 6 days of incubation (Table 6, p. 34).

Based on the results of these preliminary experiments, equilibration times of 24 hours for the Lockington sandy clay soil and 7 days for the Little Shelford sandy loam, Shelley Field clay loam, Manningtree sandy loam, and Goch silt loam soils, and a soil:solution ratio of 1:1 (w:v) for all test soils were selected for use in the definitive study (p. 29).

2. Definitive study experimental conditions:

Table 3: Study design for the adsorption phase.

Parameters		Little Shelford Sandy loam	Shelley Field Clay loam	Lockington Sandy clay	Manningtree Sandy loam	Goch Silt loam
Condition of soil (air dried/fresh) [1]		Air-dried.				
Have these soils been used for other laboratory studies? (specify which)		No.				
Soil (g/replicate)		*ca.* 40				
Equilibrium solution used (eg: 0.01N $CaCl_2$)		0.01M $CaCl_2$ solution.				
Control used (with salt solution only) (Yes/No)		Yes.				
Test material concentrations [2]	Nominal application rates (mg a.i./kg soil)	0.01, 0.03, 0.1, 0.3, 1.0				
	Analytically measured concentrations (mg a.i./kg soil)	0.00954-0.00963, 0.0286-0.0292, 0.0957-0.0965, 0.286-0.293, 0.962-0.984				
Identity and concentration of co-solvent, if any		0.01M $CaCl_2$ solution.				
Soil:solution ratio (w:v)		1:1				
Initial pH of the equilibration solution, if provided		Not reported.				
No. of replications	Controls	None.				
	Treatments	Duplicate.				
Equilibration	Time	*ca.* 7 days.		*ca.* 24 hours.	*ca.* 7 days.	
	Temperature (°C)	20 ± 2				
	Darkness (Yes/No)	Yes				
	Shaking method	End-over-end shaker.				
	Shaking time (hours)	*ca.* 7 days.		*ca.* 24 hours.	*ca.* 7 days.	
Method of separation of supernatant (eg., centrifugation)		Centrifugation				
Centrifugation	Speed (rpm)	2000				
	Duration (min)	10				
	Method of separation of soil and solution	Decanted.				

Data were obtained from pp. 19, 21-22 and Table 7, p. 35 of the study report.

1 Prior to use, aliquots of each test soil were pre-equilibrated by shaking for *ca.* 12 hours with *ca.* 40 mL of 0.01M $CaCl_2$ solution.

2 Test material concentrations were calculated by the reviewer by converting mg/L to mg a.i./kg using the following equation: [test concentration (mg/L) × total volume of test material (mL)] ÷ amount of soil (g); eg [0.01 mg/L × 40 mL] ÷ 40.0 g = 0.01 mg a.i./kg soil.

Table 4: Study design for the desorption phase.

Parameters		**Little Shelford Sandy loam**	**Shelley Field Clay loam**	**Lockington Sandy clay**	**Manningtree Sandy loam**	**Goch Silt loam**
Were the soil residues from the adsorption phase used? If not, describe the method for adsorption using a separate adsorption Table		Yes.				
Amount of test material present in the adsorbed state/adsorbed amount (mg a.i./kg soil)	0.01	0.00010	0.00267	0.00032	0.00016	0.00136
	0.03	-0.00004	0.00518	0.00023	0.00037	0.00287
	0.1	0.00000	0.00777	-0.00118	0.00172	0.00468
	0.3	-0.00082	0.01383	-0.00482	0.00336	0.00484
	1.0	-0.01471	0.00768	-0.04074	0.00729	0.01732
No. of desorption cycles		3				
Equilibration solution and quantity used per treatment for desorption (eg., 0.01M $CaCl_2$)		0.01M $CaCl_2$ solution; *ca.* 40 mL.		0.01M $CaCl_2$ solution; *ca.* 10 mL.	0.01M $CaCl_2$ solution; *ca.* 40 mL.	
Soil:solution ratio		1:1				
Replications	Controls	None.				
	Treatments	Duplicate.				
Desorption equilibration	Time (hours)	*ca.* 24				
	Temperature (°C)	20 ± 2				
	Darkness	Yes				
	Shaking method	End-over-end shaker.				
	Shaking time (hours)	*ca.* 24				
Centrifugation	Speed (G)	6000				
	Duration (min)	10				
	Method of separation of soil and solution	Decanted.				
Second desorption cycle		Followed same procedure as first desorption cycle; used ca. 40 mL 0.01M $CaCl_2$ solution per cycle.				
Third desorption cycle		Followed same procedure as first desorption cycle; used ca. 40 mL 0.01M $CaCl_2$ solution per cycle.				

Data were obtained from pp. 19, 21-22; Appendix 3, Table A3.2, p. 75; Table A3.4, p. 79; Table A3.6, p. 83; Table A3.8, p. 87; and Table A3.10, p. 91 of the study report.

3. Description of analytical procedures:

Extraction/clean up/concentration methods: Following the third desorption cycle, the soils were extracted by shaking for *ca.* 24 hours with acetonitrile:water (50:50, v:v, *ca.* 40 mL; p. 22). The extracted samples were centrifuged and the supernatants were removed for analysis.

Total ^{14}C measurement: Following adsorption, each desorption cycle, and extraction, aliquots of the supernatants were analyzed for total radioactivity using LSC (pp. 22-23). Mass balances were determined by summing the radioactivity recovered in the adsorption solutions, three desorption solutions, soil residues, and unextracted radiocarbon.

Non-extractable residues, if any: Following extraction, the soils were air-dried, milled to a fine powder, and analyzed for total radioactivity using LSC following combustion (p. 23). Combustion efficiency was not reported.

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

Identification and quantification of parent compound: Aliquots of the adsorption supernatants, first desorption cycle supernatants, and soil extracts from the two highest treatment concentrations (0.3 and 1.0 mg a.i./kg soil) were analyzed for RPA 203328 using HPLC under the following conditions (pp. 22, 23-24): Kromasil KR100 5C8 column (4.6 × 250 mm; particle size not reported), mobile phase combining (Solvent System A) water:acetonitrile:trifluoroacetic acid (70:30:0.5, v:v:v) and (Solvent System B) acetonitrile:trifluoroacetic acid (100:0.5, v:v) [percent A:B (v:v) at 0-5 min., 100:0; 22-27 min., 0:100, 30-35 min., 100:0], flow rate of 1 mL/minute, with UV (275 nm) detection. [^{14}C]RPA 203328 was identified by comparison to the retention time of an unlabeled reference standard (purity 99.6%, Rt = *ca.* 14.4 minutes; p. 18; Figure 1, p. 41; Figure 2, p. 42). HPLC column recoveries averaged 102.1% (range 100.7-105.8%; Appendix 7, pp. 100-104).

Identification and quantification of transformation products, if appropriate: Samples were not analyzed for transformation products of RPA 203328.

Detection limits (LOD, LOQ) for the parent compound: The Limit of Quantification (LOQ) for LSC analysis was 60 dpm and ranged from 0.03% to 0.9% of the applied for all test concentrations; the Limit of Detection (LOD) was not reported (p. 27). The LOQ for HPLC analysis was 255 dpm; the LOD was 77 dpm (p. 28).

Detection limits (LOD, LOQ) for the transformation products, if appropriate: Samples were not analyzed for transformation products of RPA 203328.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The incubation temperature during the study was maintained at 20 ± 2°C; no supporting information was provided (pp. 19, 28). The pH of the supernatants solutions during the adsorption and desorption phases ranged from 6.28 to 7.15 (p. 28; Table 2, p. 33). Based on HPLC analysis, [^{14}C]RPA 203328 was stable in solution during the definitive study, comprising >98% of the radioactivity in the radio-chromatograms (p. 29; Table 8, p. 36; Figures 5-19, pp. 45-59).

B. MASS BALANCE: Mass balances at the end of the adsorption phase were not reported. Mean mass balances at the end of the desorption phase ranged from 100.5-103.5%, 101.3-124.2%, 100.2-102.7%, 98.6-101.9%, and 95.4-98.7% of the applied for the Little Shelford sandy loam, Shelley Field clay loam, Lockington sandy clay, Manningtree sandy loam, and Goch silt loam soils, respectively (p. 29; Tables 9-13, pp. 37-39).

Table 5: Recovery of [^{14}C]RPA 203328, expressed as percentage of applied radioactivity, in high-dose soil after adsorption/desorption (mean ± s.d.; n = 2).

Matrices	**Little Shelford Sandy loam**	**Shelley Field Clay loam**	**Lockington Sandy clay**	**Manningtree Sandy loam**	**Goch Silt loam**
At the end of the adsorption phase					
Supernatant solution	35.9 ± 0.4	36.8 ± 1.7	25.2 ± 1.2	52.6 ± 1.0	44.1 ± 3.0
Solid phase (extracted)	Not determined.				
Non-extractable residues in soil, if measured	Not determined.				
Total recovery	Not determined.				
At the end of the desorption phase					
Supernatant solution (Desorption 1)	35.0 ± 0.7	30.7 ± 2.2	18.1 ± 1.0	30.8 ± 0.4	29.1 ± 1.8
Supernatant solution (Desorption 2)	16.2 ± 0.4	13.7 ± 1.5	20.4 ± 2.3	10.0 ± 0.2	11.0 ± 0.5
Supernatant solution (Desorption 3)	6.7 ± 0.1	5.9 ± 0.5	10.1 ± 2.4	3.3 ± 0.1	4.2 ± 0.1
Solid phase (extracted) [1]	2.8 ± 0.2	3.9 ± 1.4	9.9 ± 2.0	1.3 ± 0.1	3.0 ± 0.8
Non-extractable residues in soil, if measured	5.7 ± 0.7	16.8 ± 10.8	17.7 ± 4.8	2.5 ± 0.3	5.5 ± 3.4
Total recovery [5]	102.3 ± 0.9	107.8 ± 7.0	101.2 ± 0.8	100.6 ± 0.9	97.0 ± 1.1

Data were obtained from Tables 9-13, pp. 37-39 and Appendix 3, Tables A3.1-A3.10, pp. 73-92 of the study report. Means and standard deviations were determined by the reviewer using Excel.
1 All soils were extracted prior to combustion.

Table 6: Concentration of [^{14}C]RPA 203328 in the solid and liquid phases at the end of adsorption equilibration period (mean ± s.d.; n = 2).

Concentration (mg a.i./kg soil)	Little Shelford Sandy loam			Shelley Field Clay loam			Lockington Sandy clay		
	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]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.01	0.00010 ± 0.0	0.01007 ± 0.0	1.0 ± 1.6	0.00267 ± 0.0	0.00853 ± 0.0	26.7 ± 11.7	0.00032 ± 0.0	0.00940 ± 0.0	3.2 ± 5.6
0.03	-0.00004 ± 0.0	0.03058 ± 0.0	-0.1 ± 0.5	0.00518 ± 0.0	0.02735 ± 0.0	17.3 ± 6.5	0.00023 ± 0.0	0.02882 ± 0.0	0.8 ± 0.7
0.1	0.00000 ± 0.0	0.10109 ± 0.0	0.0 ± 0.6	0.00777 ± 0.0	0.09428 ± 0.0	7.8 ± 2.5	-0.00118 ± 0.0	0.09724 ± 0.0	-1.2 ± 1.9
0.3	-0.00082 ± 0.0	0.30623 ± 0.0	-0.3 ± 0.0	0.01383 ± 0.0	0.29219 ± 0.0	4.6 ± 0.9	-0.00482 ± 0.0	0.29596 ± 0.0	-1.6 ± 2.5
1.0	-0.01471 ± 0.0	1.02694 ± 0.0	-1.5 ± 0.1	0.00768 ± 0.0	0.98795 ± 0.0	0.8 ± 0.7	-0.04074 ± 0.0	1.01707 ± 0.0	-4.1 ± 0.3

Concentration (mg a.i./kg soil)	Manningtree Sandy loam			Goch Silt loam		
	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]
0.01	0.00016 ± 0.0	0.00976 ± 0.0	1.6 ± 0.1	0.00136 ± 0.0	0.00777 ± 0.0	13.6 ± 2.0
0.03	0.00037 ± 0.0	0.02917 ± 0.0	1.2 ± 0.1	0.00287 ± 0.0	0.02489 ± 0.0	9.6 ± 0.5
0.1	0.00172 ± 0.0	0.09555 ± 0.0	1.7 ± 0.0	0.00468 ± 0.0	0.08760 ± 0.0	4.7 ± 0.7
0.3	0.00336 ± 0.0	0.29190 ± 0.0	1.1 ± 0.1	0.00484 ± 0.0	0.27833 ± 0.0	1.6 ± 2.4
1.0	0.00729 ± 0.0	0.98440 ± 0.0	0.7 ± 0.2	0.01732 ± 0.0	0.92529 ± 0.0	1.7 ± 0.5

Data were obtained from Appendix 3, Table A3.2, p. 75, Table A3.4, p. 79, Table A3.6, p. 83, Table A3.8, p. 87, and Table A3.10, p. 91 of the study report. Means and standard deviations were determined by the reviewer using Excel.

1 Percent adsorbed was calculated by the reviewer using the following equation: [concentration on soil (mg a.i./kg) ÷ nominal test concentration (mg a.i./kg)] × 100; e.g. for the Little Shelford sandy loam soil at 0.01 mg a.i./kg, [0.00021 mg a.i./kg ÷ 0.01 mg a.i./kg soil] × 100 = 2.10%.

Table 7: Concentration of [^{14}C]RPA 203328 in the solid and liquid phases at the end of the third desorption cycle (mean ± s.d.; n = 2).

Concentration (mg a.i./kg soil)	Little Shelford Sandy loam			Shelley Field Clay loam			Lockington Sandy clay		
	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]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed[1]
0.01	0.00042 ± 0.0	0.00065 ± 0.0	86.3 ± 1.1	0.00328 ± 0.0	0.00053 ± 0.0	54.3 ± 8.5	0.00244 ± 0.0	0.00110 ± 0.0	52.8 ± 4.2
0.03	0.00098 ± 0.0	0.00197 ± 0.0	87.4 ± 0.8	0.00684 ± 0.0	0.00152 ± 0.0	64.2 ± 5.7	0.00549 ± 0.0	0.00366 ± 0.0	58.4 ± 0.7
0.1	0.00304 ± 0.0	0.00637 ± 0.0	87.7 ± 0.3	0.01192 ± 0.0	0.00555 ± 0.0	75.7 ± 1.5	0.01103 ± 0.0	0.01424 ± 0.0	65.8 ± 1.0
0.3	0.00953 ± 0.0	0.01972 ± 0.0	87.4 ± 0.9	0.02392 ± 0.0	0.01853 ± 0.0	80.7 ± 1.3	0.02076 ± 0.0	0.04813 ± 0.0	68.6 ± 0.5
1.0	0.02851 ± 0.0	0.06558 ± 0.0	87.7 ± 0.1	0.04405 ± 0.0	0.06283 ± 0.0	85.5 ± 0.1	0.03460 ± 0.0	0.15374 ± 0.0	73.9 ± 3.6

Concentration (mg a.i./kg soil)	Manningtree Sandy loam			Goch Silt loam		
	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]
0.01	0.00021 ± 0.0	0.00034 ± 0.0	92.0 ± 0.7	0.00121 ± 0.0	0.00043 ± 0.0	73.2 ± 4.5
0.03	0.00064 ± 0.0	0.00101 ± 0.0	91.8 ± 1.6	0.00235 ± 0.0	0.00127 ± 0.0	80.3 ± 0.4
0.1	0.00236 ± 0.0	0.00316 ± 0.0	91.7 ± 0.6	0.00472 ± 0.0	0.00409 ± 0.0	85.9 ± 0.5
0.3	0.00610 ± 0.0	0.00942 ± 0.0	92.3 ± 0.3	0.00847 ± 0.0	0.01254 ± 0.0	89.7 ± 0.0
1.0	0.01855 ± 0.0	0.03188 ± 0.0	92.5 ± 0.1	0.02014 ± 0.0	0.04079 ± 0.0	91.4 ± 0.4

Data were obtained from Appendix 3, Table A3.2, p. 76, Table A3.4, p. 80, Table A3.6, p. 84, Table A3.8, p. 88, and Table A3.10, p. 92 of the study report. Means and standard deviations were determined by the reviewer using Excel.

1 Percent desorbed as percent of the adsorbed was calculated by the reviewer using data obtained from Tables 9-13, pp. 37-39 and the following equation: [% Desorbed (Desorption cycles 1 + 2 + 3)÷ (% Total Recovery - % Adsorbed)] × 100; e.g. for the Little Shelford sandy loam soil at 0.01 mg a.i./kg soil [(35.66% + 16.01% + 6.67%) ÷ (103.5% - 35.26%] × 100 = 85.49%.

Table 8: Adsorption and desorption constants of [^{14}C]RPA 203328 in the soils. [1]

Soil	Adsorption						Third Desorption					
	K_d	K_F	1/N	R^2	K_{oc}	K_{Foc}	K_d	K_F	1/N	R^2	K_{oc}	K_{Foc}
Little Shelford Sandy loam[1]	NR	0.000494	0.298	NR	NR	0.0329	NR	0.158	0.793	NR	NR	10.5
Shelley Field Clay loam	NR	0.0283	0.569	NR	NR	1.49	NR	0.311	0.634	NR	NR	16.4
Lockington Sandy clay[1]	NR	0.000779	0.4991	NR	NR	0.02361	NR	0.1177	0.543	NR	NR	3.57
Manningtree Sandy loam	NR	0.00881	0.853	NR	NR	0.881	NR	0.620	0.995	NR	NR	62.0
Goch Silt loam	NR	0.0183	0.527	NR	NR	1.14	NR	0.135	0.610	NR	NR	8.46

Data were obtained from p. 30, Table 14 p. 39, Table 15, p. 40, Figures 20-29, pp. 60-64, and Appendix 4, Table A4.1-A4.5, pp. 93-97 of the study report.
1 The study authors noted that for the Little Shelford sandy loam and Lockington sandy clay soils, there was insufficient correlation in the data for adsorption, r^2 <0.6, and therefore, concluded that valid Freundlich constants could not be obtained. As a result of the low correlation for the adsorption phase, the authors concluded that the desorption results were not valid.
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.
1 Freundlich K_F values were calculated by the study author using the following equation (p. 25):

$C_s = K_F C_w^{(1/n)}$, where

C_s = soil concentration after adsorption or desorption (Φg/g);
C_w = concentration of supernatant after adsorption or desorption (Φg/g);
1/n = Freundlich exponent; and
K_F = Freundlich coefficient.

NR = Not reported.

Table 8b: Adsorption and desorption constants of [^{14}C]RPA 203328 in the soils, as determined by the PMRA. [1]

	Adsorption							Consecutive desorption (after two cycles)						
Soil	K_d	R^2	K_{oc}	K_F	1/N	R^2	K_{Foc}	K_d	R^2	K_{oc}	K_F	1/N	R^2	K_{Foc}
Shelley Field Clay loam	0.0515	0.732	3	0.03	0.568	0.967	1	-0.0376	0.764	-2	0.01	-0.194	0.627	1
Manningtree Sandy loam	0.00782	0.873	1	0.01	0.856	0.973	1	-0.0121	0.888	-1	0.01	-0.260	0.636	1
Goch Silt loam	0.02047	0.736	2	0.02	0.527	0.979	2	-0.00506	0.288	-1	0.02	-0.0438	0.0869	2

Data were obtained from p. 30, Table 14 p. 39, Table 15, p. 40, Figures 20-29, pp. 60-64, and Appendix 4, Table A4.1-A4.5, pp. 93-97 of the study report.

1 The study authors noted that for the Little Shelford sandy loam and Lockington sandy clay soils, there was insufficient correlation in the data for adsorption, r^2 <0.6, and therefore, concluded that valid Freundlich constants could not be obtained. As a result of the low correlation for the adsorption phase, the authors concluded that the desorption results were not valid.

K_d - Adsorption and desorption coefficients; K_F - 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.

C. ADSORPTION: After 7 days of equilibration, 0.8-26.7%, 0.7-1.7%, and 1.6-13.6% of the applied [^{14}C]RPA 203328 was adsorbed to the Shelley Field clay loam, Manningtree sandy loam, and Goch silt loam soils, respectively (reviewer-calculated; Appendix 3, Table A3.2, p. 75, Table A3.4, p. 79, Table A3.6, p. 83, Table A3.8, p. 87, and Table A3.10, p. 91). Maximums of 1.0% and 3.2% of the applied [^{14}C]RPA 203328 were adsorbed to the Little Shelford sandy loam and Lockington sandy clay soils, respectively, after 7 days and 24 hours of equilibrium. Registrant-calculated adsorption K and K_{oc} values were not reported. Registrant-calculated Freundlich adsorption K values were 0.000494, 0.0283, 0.000779, 0.00881, and 0.0183 for the Little Shelford sandy loam, Shelley Field clay loam, Lockington sandy clay, Manningtree sandy loam, and Goch silt loam soils, respectively; corresponding Freundlich adsorption K_{oc} values were 0.0329, 1.49, 0.02361, 0.881, and 1.14. The study authors noted that for the Little Shelford sandy loam and Lockington sandy clay soils, there was insufficient correlation in the data for adsorption, r^2 <0.6, and therefore, did not consider the Freundlich constants to be valid.

Adsorption coefficients were re-calculated by the secondary reviewer using slopes of adsorption isotherms rather than mean coefficients (Table 8b). $K_{d\text{-}ads}$ values were 0.0515, 0.00782 and 0.0205 for Shelley field clay loam, Manningtree sandy loam and Goch silt loam, respectively; corresponding $K_{OC\text{-}ads}$ values were 3, 1 and 2, respectively. Freundlich regressions gave $K_{F\text{-}ads}$ values of 0.03, 0.01 and 0.02 for Shelley field clay loam, Manningtree sandy loam and Goch silt loam, respectively; corresponding $K_{FOC\text{-}ads}$ values were 1, 1 and 2, respectively. Given the low r^2 values for the adsorption isotherms (see Table 8b), $K_{FOC\text{-}ads}$ values were used to determine the mobility classification of RPA 203328. According to McCall *et al.* (1981), RPA 203328 is expected to exhibit very high mobility in the range of soils studied.

D. DESORPTION: At the end of the desorption phase, 86.3-87.7%, 54.3-85.5%, 52.8-73.9%, 91.7-92.5%, and 73.2-91.4% of the applied [^{14}C]RPA 203328 desorbed from the Little Shelford sandy loam, Shelley Field clay loam, Lockington sandy clay, Manningtree sandy loam, and Goch silt loam soils, respectively (reviewer-calculated; Tables 9-13, pp. 37-39). Registrant-calculated desorption K and K_{oc} values were not reported. Registrant-calculated Freundlich desorption K values were 0.158, 0.311, 0.1177, 0.620, and 0.135 for the Little Shelford sandy loam, Shelley Field clay loam, Lockington sandy clay, Manningtree sandy loam, and Goch silt loam soils, respectively; corresponding Freundlich desorption K_{oc} values were 10.5, 16.4, 3.57, 62.0, and 8.46. The study authors did not consider the desorption results for the Little Shelford sandy loam and Lockington sandy clay desorption to be valid, due to the low correlation for the adsorption phase.

III. STUDY DEFICIENCIES

1. The study was conducted using a transformation product of pyrasulfotole, rather than the parent compound.

2. It was not established that the foreign soils used in this study were comparable to soils that would be found at the intended use sites in the United States. The foreign test soils were from Germany and the United Kingdom, and the FAO classifications were not provided.

IV. REVIEWER'S COMMENTS

1. To confirm adsorption constant data reported in the study report, the reviewer calculated adsorption K_d values using the following EPA-approved equation:

   $K_d = [(C_0V_0 - C_{eq}V_0) \div m] \div C_{eq}$ where

   S = the sorbed phase concentration with units of mass of sorbate per solid sorbent mass;
   C_0 = the concentration in the water before sorption;
   V_0 = the total water volume in the batch system;
   C_{eq} = the aqueous-phase equilibrium concentration; and
   m = the dry mass of sorbent.

   Adsorption K_d values determined by the reviewer are tabulated below:

Table 9: Reviewer-calculated adsorption constants of [^{14}C]RPA 203328 in the soils.

Soil	K_d
Little Shelford Sandy loam	-0.02
Shelley Field Clay loam	0.07
Lockington Sandy clay	0.03
Manningtree Sandy loam	0.03
Goch Silt loam	0.16

K_d values were reviewer-calculated using data obtained from Appendix 3, Table A3.2, p. 75, Table A3.4, p. 79, Table A3.6, p. 83, Table A3.8, p. 87, and Table A3.10, p. 91 of the study report.

   The reviewer-calculated r^2 value for the relationship of K_d vs. % organic carbon is 0.0037, for K_d vs. pH is 0.3503, and for K_d vs. % clay is 0.03.

2. RPA 203328 is weakly adsorbed to soil, based on the low Freundlich adsorption K values obtained for the test soils (pp. 30, 31). According to the Briggs Classification System, RPA 203328 is potentially very mobile in soil, based on the low Freundlich adsorption K_{oc} values obtained for all test soils (p. 31; Appendix 5, p. 98).

3. None of the test soils had an organic matter content ≤1%, as recommended by Subdivision N guidelines.

4. The study authors reported the following information following the first and second desorption cycles:

Table 10: Desorption constants of [^{14}C]RPA 203328 in the soils.

Soil	First desorption			Second desorption		
	K_F	K_{Foc}	1/N	K_F	K_{Foc}	1/N
Little Shelford Sandy loam	0.0159	1.06	0.692	0.072	4.77	0.790
Shelley Field Clay loam	0.0840	4.42	0.613	0.153	8.05	0.600
Lockington Sandy clay	0.0759	2.30	0.747	0.0646	1.96	0.599
Manningtree Sandy loam	0.0523	5.23	0.944	0.173	17.3	0.956
Goch Silt loam	0.0460	2.87	0.594	0.0803	5.02	0.602

Data were obtained from Table 15, p. 40 of the study report.

5. The mass balances for two of the Shelley Field clay loam soil samples were 115.2% and 124.2% of the applied, which are significantly outside the range of recommended material balances (90-110% of the applied) specified by Subdivision N guidelines (p. 29; Table 10, p. 37). The results for these two samples were rejected and not used by the registrant to calculate the Freundlich coefficients.

6. The radiopurity of the treatment solution was ≥99.5% of the recovered radioactivity, based on HPLC analysis (p. 28; Figure 2, p. 42; Appendix 6, p. 99). The identity of RPA 203328 was confirmed using LC/MS analysis.

7. The Freundlich 1/n values for the adsorption and each of the three desorption cycles for all test soils were below 0.9. Subdivision N guidelines specify that 1/n values should be in the range of 0.9 to 1.1.

8. Sample storage stability was investigated using an adsorption supernatant from the Little Shelford sand loam soil, which was reanalyzed after being stored with 0.5% trifluoroacetic acid in an HPLC vial at ambient temperature for 2 days (p. 29). It was reported that no qualitative differences (<1%) were observed between the initial and day 2 chromatograms.

9. The maximum field application rate for pyrasulfotole was not reported. Subdivision N guidelines specify that one test concentration should be roughly equivalent to the maximum proposed or registered field application rate of the parent compound.

10. The secondary reviewer (PMRA) re-calculated Kd and Kf coefficients based on current PMRA practices. The reviewer agrees with the study author that adsorption and desorption data from Little Shelford and Lockington soils were not valid. However, pyrasulfotole concentrations in the soil appear to **increase** through consecutive desorption cycles, resulting in negative K_{des} values (which is theoretically impossible). Therefore, the PMRA reviewer recommends not using desorption data for the remaining soils (Shelley Field clay loam, Manningtree sandy loam and Goch sandy silt). Although this study has severe data limitations, it does demonstrate the pyrasulfotole transformation product AE B197555 (i.e.

RPA 230328) does not readily adsorb to soils and is expected to be highly mobile in the terrestrial environment.

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.

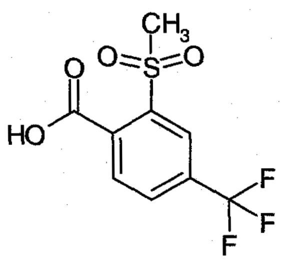
4. U.S. Environmental Protection Agency. 2003. Guidance for Calculating Sorption Coefficients in Batch Equilibrium Studies.

Attachment 1: Structures of Parent Compound and Transformation Products

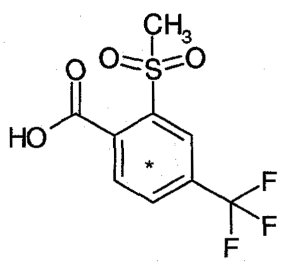
RPA 203328 [AE B197555-benzoic acid; AE B197555; K-1198; K-1367]

IUPAC Name: 2-Mesyl-4-trifluoromethylbenzoic acid.
CAS Name: Benzoic acid, 2-(methylsulfonyl)-4-(trifluoromethyl)-.
CAS Number: 142994-06-7.
SMILES String: O=C(c1ccc(cc1S(=O)(=O)C)C(F)(F)F)O (ISIS v2.3/Universal SMILES).
No EPI Suite, v3.12 SMILES String found as of 6/7/06.
CS(=O)(=O)c1cc(C(F)(F)F)ccc1C(=O)O.
CS(=O)(=O)c1cc(ccc1C(=O)O)C(F)(F)F.

Unlabeled



[^{14}C]RPA 203328

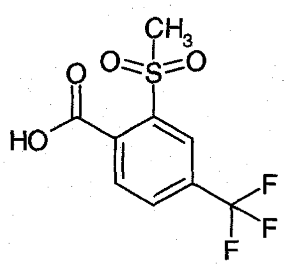


^{14}C = Position of radiolabel.

Identified Compounds

RPA 203328 [AE B197555-benzoic acid; AE B197555; K-1198; K-1367]

IUPAC Name:	2-Mesyl-4-trifluoromethylbenzoic acid.
CAS Name:	Benzoic acid, 2-(methylsulfonyl)-4-(trifluoromethyl)-.
CAS Number:	142994-06-7.
SMILES String:	O=C(c1ccc(cc1S(=O)(=O)C)C(F)(F)F)O (ISIS v2.3/Universal SMILES). No EPI Suite, v3.12 SMILES String found as of 6/7/06. CS(=O)(=O)c1cc(C(F)(F)F)ccc1C(=O)O. CS(=O)(=O)c1cc(ccc1C(=O)O)C(F)(F)F.



Chemical: RPA-203328
PC Code: 000692
MRID: 46801704
Guideline No: 163-1

Little Shelford Sandy loam- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
1	40	1.03175	40	40	-0.0317	-0.03	
1	40	1.02212	40	40	-0.0221	-0.02	
0.3	40	0.30759	40	40	-0.0076	-0.02	
0.3	40	0.30486	40	40	-0.0049	-0.02	
0.1	40	0.10062	40	40	-0.0006	-0.01	
0.1	40	0.10155	40	40	-0.0016	-0.02	
0.03	40	0.03049	40	40	-0.0005	-0.02	
0.03	40	0.03066	40	40	-0.0007	-0.02	
0.01	40	0.00997	40	40	0.0000	0.00	
0.01	40	0.01017	40	40	-0.0002	-0.02	
						-0.02	AVG

Shelley Field Clay loam- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
1	40	0.99253	40	40	0.0075	0.01	
1	40	0.98337	40	40	0.0166	0.02	
0.3	40	0.29340	40	40	0.0066	0.02	
0.3	40	0.29097	40	40	0.0090	0.03	
0.1	40	0.09322	40	40	0.0068	0.07	
0.1	40	0.09533	40	40	0.0047	0.05	
0.03	40	0.02755	40	40	0.0025	0.09	
0.03	40	0.02715	40	40	0.0029	0.10	
0.01	40	0.00845	40	40	0.0016	0.18	
0.01	40	0.00860	40	40	0.0014	0.16	
						0.07	AVG

Lockington Sandy clay- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
1	40	1.01642	40	40	-0.0164	-0.02	
1	40	1.01771	40	40	-0.0177	-0.02	
0.3	40	0.29203	40	40	0.0080	0.03	
0.3	40	0.29988	40	40	0.0001	0.00	
0.1	40	0.09857	40	40	0.0014	0.01	
0.1	40	0.09590	40	40	0.0041	0.04	
0.03	40	0.02903	40	40	0.0010	0.03	
0.03	40	0.02860	40	40	0.0014	0.05	
0.01	40	0.00910	40	40	0.0009	0.10	
0.01	40	0.00970	40	40	0.0003	0.03	
						0.03	AVG

Data were obtained from Appendix 3, Table A3.2, p. 75, Table A3.4, p. 79, Table A3.6, p. 83, Table A3.8, p. 87, and Table A3.10, p. 91 of the study report.

Chemical: RPA-203328
PC Code: 000692
MRID: 46801704
Guideline No: 163-1

Manningtree Sandy loam- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
1	40	0.98483	40	40	0.0152	0.02	
1	40	0.98396	40	40	0.0160	0.02	
0.3	40	0.29062	40	40	0.0094	0.03	
0.3	40	0.29317	40	40	0.0068	0.02	
0.1	40	0.09499	40	40	0.0050	0.05	
0.1	40	0.09610	40	40	0.0039	0.04	
0.03	40	0.02913	40	40	0.0009	0.03	
0.03	40	0.02920	40	40	0.0008	0.03	
0.01	40	0.00981	40	40	0.0002	0.02	
0.01	40	0.00971	40	40	0.0003	0.03	
						0.03	AVG

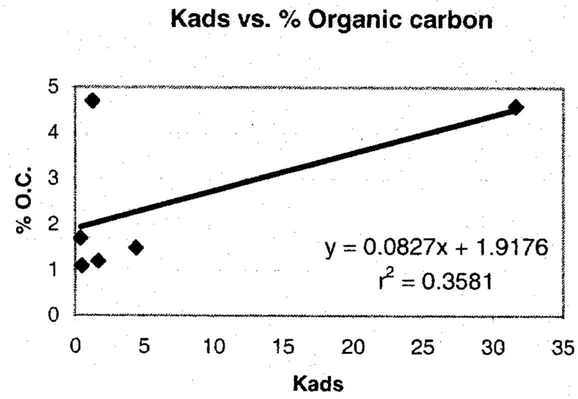
Goch Silt loam- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
1	40	0.92469	40	40	0.0753	0.08	
1	40	0.92589	40	40	0.0741	0.08	
0.3	40	0.28461	40	40	0.0154	0.05	
0.3	40	0.27205	40	40	0.0280	0.10	
0.1	40	0.08780	40	40	0.0122	0.14	
0.1	40	0.08739	40	40	0.0126	0.14	
0.03	40	0.02494	40	40	0.0051	0.20	
0.03	40	0.02483	40	40	0.0052	0.21	
0.01	40	0.00759	40	40	0.0024	0.32	
0.01	40	0.00794	40	40	0.0021	0.26	
						0.16	AVG

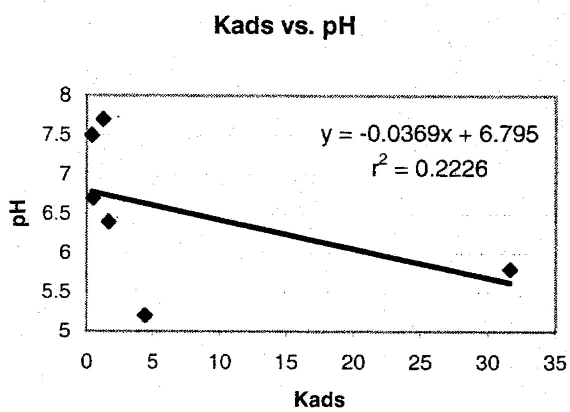
Data were obtained from Appendix 3, Table A3.2, p. 75, Table A3.4, p. 79, Table A3.6, p. 83, Table A3.8, p. 87, and Table A3.10, p. 91 of the study report.

Chemical: Pyrasulfotole
PC Code: 000692
MRID: 46801703
Guideline No: 163-1

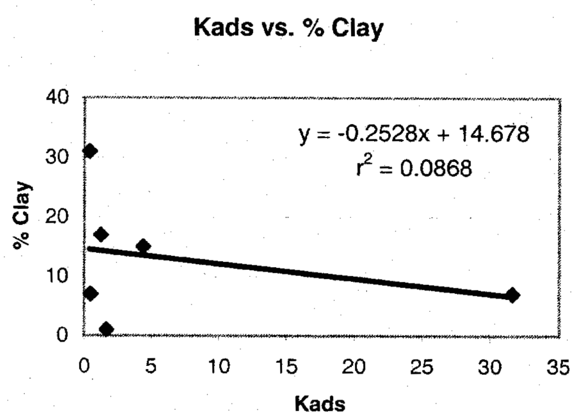
Soil	Kads	% organic carbon
Silt loam	1.24	4.7
Loamy sand	1.68	1.2
Clay loam	0.38	1.7
Sandy loam	0.48	1.1
Silt loam	4.41	1.5
Sandy loam	31.63	4.6



Soil	Kads	pH
Silt loam	1.24	7.7
Loamy sand	1.68	6.4
Clay loam	0.38	7.5
Sandy loam	0.48	6.7
Silt loam	4.41	5.2
Sandy loam	31.63	5.8



Soil	Kads	% clay
Silt loam	1.24	17
Loamy sand	1.68	1
Clay loam	0.38	31
Sandy loam	0.48	7
Silt loam	4.41	15
Sandy loam	31.63	7



Data were obtained from Table 2, p. 41. Kads values were reviewer-calculated using data obtained from Table 9, p. 50, Table 12, p. 53, Table 15, p. 56, Table 18, p. 59, Table 21, p. 62, and Table 24, p. 65 of the study report.

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PC Code: 000692
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Table 4/6 Adsorption on soil

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	-0.01553	0.00280	-0.04305	0.00881	0.01404
1	-0.01389	0.01256	-0.03843	0.00576	0.02060
AVG	-0.01471	0.00768	-0.04074	0.00729	0.01732
STDEV	0.00	0.01	0.00	0.00	0.00
0.3	-0.00090	0.01578	0.00056	0.00357	-0.00020
0.3	-0.00074	0.01188	-0.01019	0.00314	0.00988
AVG	-0.00082	0.01383	-0.00482	0.00336	0.00484
STDEV	0.00	0.00	0.01	0.00	0.01
0.1	0.00041	0.00951	-0.00250	0.00175	0.00421
0.1	-0.00041	0.00603	0.00014	0.00169	0.00515
AVG	0.00000	0.00777	-0.00118	0.00172	0.00468
STDEV	0.00	0.00	0.00	0.00	0.00
0.03	0.00006	0.00380	0.00008	0.00035	0.00296
0.03	-0.00014	0.00655	0.00038	0.00038	0.00277
AVG	-0.00004	0.00518	0.00023	0.00037	0.00287
STDEV	0.00	0.00	0.00	0.00	0.00
0.01	0.00021	0.00350	0.00071	0.00015	0.00150
0.01	-0.00001	0.00184	-0.00008	0.00016	0.00122
AVG	0.00010	0.00267	0.00032	0.00016	0.00136
STDEV	0.00	0.00	0.00	0.00	0.00

Data were obtained from Appendix 3, Table A3.2, p. 75, Table A3.4, p. 79, Table A3.6, p. 83, Table A3.8, p. 87, and Table A3.10, p. 91 of the study report.

Table 5 Adsorption solution

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	35.89	38.18	26.56	52.65	47.16
1	35.65	37.82	26.49	53.83	47.91
0.3	35.68	38.26	25.44	53.14	43.12
0.3	36.34	38.15	25.78	53.73	47.26
0.1	36.19	37.33	26.46	51.05	45.10
0.1	36.36	38.15	24.63	52.12	44.99
0.03	35.99	36.22	24.90	51.11	43.25
0.03	36.35	35.67	24.69	52.26	43.20
0.01	35.26	33.76	22.85	53.39	38.74
0.01	35.69	34.17	24.33	52.59	40.70
AVG	35.94	36.77	25.21	52.59	44.14
STDEV	0.4	1.7	1.2	1.0	3.0

Data were obtained from Tables 9-13, pp. 37-39 and Appendix 3, Tables A3.1-A3.10, pp. 73-92 of the study report.

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Table 5 Desorption 1 solution

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	34.44	33.12	19.07	30.94	30.56
1	34.50	32.82	18.72	30.45	31.02
0.3	34.05	31.88	18.76	30.48	30.89
0.3	34.89	31.92	19.10	30.83	30.66
0.1	35.66	31.38	18.27	30.18	29.02
0.1	36.12	31.60	18.61	30.67	29.05
0.03	34.53	30.37	17.47	30.83	28.71
0.03	34.52	29.69	17.31	31.37	27.86
0.01	35.66	26.82	15.93	30.99	25.30
0.01	35.65	27.27	17.42	31.38	27.39
AVG	35.00	30.69	18.07	30.81	29.05
STDEV	0.7	2.2	1.0	0.4	1.8

Table 5 Desorption 2 solution

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	15.84	15.10	22.76	10.05	11.38
1	15.96	15.40	22.86	9.76	11.27
0.3	16.56	15.07	21.67	9.94	11.91
0.3	16.03	14.80	21.61	9.94	11.31
0.1	15.93	14.27	20.83	9.98	11.10
0.1	15.76	14.07	21.79	9.80	11.18
0.03	16.58	12.91	20.32	10.33	10.76
0.03	16.91	12.77	18.33	10.28	10.65
0.01	16.01	11.27	16.38	10.10	10.12
0.01	16.32	11.77	16.90	10.04	10.75
AVG	16.19	13.74	20.35	10.02	11.04
STDEV	0.4	1.5	2.3	0.2	0.5

Table 5 Desorption 3 solution

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	6.87	6.12	14.75	3.32	4.11
1	6.49	6.11	12.20	3.29	4.15
0.3	6.83	6.61	11.82	3.29	4.29
0.3	6.67	6.47	11.15	3.12	4.19
0.1	6.65	5.91	9.89	3.23	4.13
0.1	6.53	5.70	8.84	3.24	4.18
0.03	6.68	5.20	7.44	3.44	4.26
0.03	6.75	5.35	8.73	3.33	4.32
0.01	6.67	5.60	7.45	3.31	4.26
0.01	6.85	5.52	8.25	3.56	4.41
AVG	6.70	5.86	10.05	3.31	4.23
STDEV	0.1	0.5	2.4	0.1	0.1

Data were obtained from Tables 9-13, pp. 37-39 and Appendix 3, Tables A3.1-A3.10, pp. 73-92 of the study report.

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Table 5 Extracted

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	2.80	2.58	7.80	1.22	2.21
1	2.94	2.40	7.28	1.13	2.11
0.3	2.32	2.76	9.46	1.27	2.48
0.3	2.61	2.96	8.21	1.18	2.33
0.1	2.77	3.34	9.35	1.24	2.70
0.1	2.79	3.51	9.19	1.26	2.80
0.03	2.92	4.67	11.01	1.43	3.55
0.03	2.97	4.52	10.75	1.33	3.52
0.01	2.81	6.10	13.34	1.37	4.48
0.01	2.95	6.25	12.75	1.49	4.11
AVG	2.79	3.91	9.91	1.29	3.03
STDEV	0.2	1.4	2.0	0.1	0.8

Table 5 Combusted

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	5.22	6.65	9.69	2.44	2.30
1	5.00	6.79	14.38	2.35	2.13
0.3	6.50	10.85	14.89	2.43	2.94
0.3	5.24	9.04	15.16	2.42	2.98
0.1	5.48	14.19	16.40	2.91	4.31
0.1	5.28	12.09	17.22	2.51	4.73
0.03	5.90	17.95	20.42	3.14	7.00
0.03	4.98	27.18	21.47	2.10	7.16
0.01	7.06	40.61	26.75	2.75	12.50
0.01	5.81	23.06	21.00	2.15	9.01
AVG	5.65	16.84	17.74	2.52	5.51
STDEV	0.7	10.8	4.8	0.3	3.4

Table 5 Recovery

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	101.1	101.8	100.6	100.6	97.7
1	100.5	101.3	101.9	100.8	98.6
0.3	101.9	105.4	102.0	100.6	95.6
0.3	101.8	103.3	101.0	101.2	98.7
0.1	102.7	106.4	100.2	98.6	96.4
0.1	102.8	105.1	100.3	99.6	96.9
0.03	102.6	107.3	101.6	100.3	97.5
0.03	102.5	115.2	101.3	100.7	96.7
0.01	103.5	124.2	102.7	101.9	95.4
0.01	103.3	108.0	100.7	101.2	96.4
AVG	102.3	107.8	101.2	100.6	97.0
STDEV	0.9	7.0	0.8	0.9	1.1

Data were obtained from Tables 9-13, pp. 37-39 and Appendix 3, Tables A3.1-A3.10, pp. 73-92 of the study report.

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Table 6 Adsorption solution

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	1.03175	0.99253	1.01642	0.98483	0.92469
1	1.02212	0.98337	1.01771	0.98396	0.92589
AVG	1.02694	0.98795	1.01707	0.98440	0.92529
STDEV	0.01	0.01	0.00	0.00	0.00
0.3	0.30759	0.29340	0.29203	0.29062	0.28461
0.3	0.30486	0.29097	0.29988	0.29317	0.27205
AVG	0.30623	0.29219	0.29596	0.29190	0.27833
STDEV	0.00	0.00	0.01	0.00	0.01
0.1	0.10062	0.09322	0.09857	0.09499	0.08780
0.1	0.10155	0.09533	0.09590	0.09610	0.08739
AVG	0.10109	0.09428	0.09724	0.09555	0.08760
STDEV	0.00	0.00	0.00	0.00	0.00
0.03	0.03049	0.02755	0.02903	0.02913	0.02494
0.03	0.03066	0.02715	0.02860	0.02920	0.02483
AVG	0.03058	0.02735	0.02882	0.02917	0.02489
STDEV	0.00	0.00	0.00	0.00	0.00
0.01	0.00997	0.00845	0.00910	0.00981	0.00759
0.01	0.01017	0.00860	0.00970	0.00971	0.00794
AVG	0.01007	0.00853	0.00940	0.00976	0.00777
STDEV	0.00	0.00	0.00	0.00	0.00

Data were obtained from Appendix 3, Table A3.2, p. 75, Table A3.4, p. 79, Table A3.6, p. 83, Table A3.8, p. 87, and Table A3.10, p. 91 of the study report.

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MRID: 46801704
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Table 6 % Adsorbed

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	-1.55	0.28	-4.31	0.88	1.40
1	-1.39	1.26	-3.84	0.58	2.06
AVG	-1.47	0.77	-4.07	0.73	1.73
STDEV	0.12	0.69	0.33	0.22	0.46
0.3	-0.30	5.26	0.19	1.19	-0.07
0.3	-0.25	3.96	-3.40	1.05	3.29
AVG	-0.27	4.61	-1.61	1.12	1.61
STDEV	0.04	0.92	2.53	0.10	2.38
0.1	0.41	9.51	-2.50	1.75	4.21
0.1	-0.41	6.03	0.14	1.69	5.15
AVG	0.00	7.77	-1.18	1.72	4.68
STDEV	0.58	2.46	1.87	0.04	0.66
0.03	0.20	12.67	0.27	1.17	9.87
0.03	-0.47	21.83	1.27	1.27	9.23
AVG	-0.13	17.25	0.77	1.22	9.55
STDEV	0.47	6.48	0.71	0.07	0.45
0.01	2.10	35.00	7.10	1.50	15.00
0.01	-0.10	18.40	-0.80	1.60	12.20
AVG	1.00	26.70	3.15	1.55	13.60
STDEV	1.56	11.74	5.59	0.07	1.98

Data were obtained from Appendix 3, Table A3.2, p. 75, Table A3.4, p. 79, Table A3.6, p. 83, Table A3.8, p. 87, and Table A3.10, p. 91 of the study report.

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PC Code: 000692
MRID: 46801704
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Table 7 Desorption 3 on soil

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	0.02913	0.04340	0.02225	0.02022	0.02109
1	0.02789	0.04469	0.04695	0.01687	0.01919
AVG	0.02851	0.04405	0.03460	0.01855	0.02014
STDEV	0.00	0.00	0.02	0.00	0.00
0.3	0.01087	0.02618	0.02220	0.00640	0.00832
0.3	0.00819	0.02165	0.01931	0.00580	0.00861
AVG	0.00953	0.02392	0.02076	0.00610	0.00847
STDEV	0.00	0.00	0.00	0.00	0.00
0.1	0.00293	0.01277	0.01013	0.00246	0.00446
0.1	0.00315	0.01107	0.01192	0.00225	0.00497
AVG	0.00304	0.01192	0.01103	0.00236	0.00472
STDEV	0.00	0.00	0.00	0.00	0.00
0.03	0.00110	0.00553	0.00549	0.00069	0.00235
0.03	0.00085	0.00815	0.00548	0.00059	0.00234
AVG	0.00098	0.00684	0.00549	0.00064	0.00235
STDEV	0.00	0.00	0.00	0.00	0.00
0.01	0.00047	0.00412	0.00277	0.00023	0.00140
0.01	0.00036	0.00244	0.00211	0.00018	0.00101
AVG	0.00042	0.00328	0.00244	0.00021	0.00121
STDEV	0.00	0.00	0.00	0.00	0.00

Data were obtained from Appendix 3, Table A3.2, p. 76, Table A3.4, p. 80, Table A3.6, p. 84, Table A3.8, p. 88, and Table A3.10, p. 92 of the study report.

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PC Code: 000692
MRID: 46801704
Guideline No: 163-1

Table 7 Desorption 3 in solution

	Sandy loam	Clay loam	Sandy clay	Sandy loam	Silt loam
1	0.06615	0.06350	0.14517	0.03222	0.04091
1	0.06501	0.06216	0.16230	0.03154	0.04066
AVG	0.06558	0.06283	0.15374	0.03188	0.04079
STDEV	0.00	0.00	0.01	0.00	0.00
0.3	0.01987	0.01868	0.04815	0.00957	0.01280
0.3	0.01956	0.01837	0.04811	0.00927	0.01227
AVG	0.01972	0.01853	0.04813	0.00942	0.01254
STDEV	0.00	0.00	0.00	0.00	0.00
0.1	0.00649	0.00564	0.01485	0.00314	0.00406
0.1	0.00625	0.00545	0.01362	0.00318	0.00412
AVG	0.00637	0.00555	0.01424	0.00316	0.00409
STDEV	0.00	0.00	0.00	0.00	0.00
0.03	0.00196	0.00150	0.00361	0.00103	0.00125
0.03	0.00197	0.00154	0.00371	0.00098	0.00128
AVG	0.00197	0.00152	0.00366	0.00101	0.00127
STDEV	0.00	0.00	0.00	0.00	0.00
0.01	0.00064	0.00053	0.00109	0.00033	0.00042
0.01	0.00065	0.00053	0.00111	0.00035	0.00043
AVG	0.00065	0.00053	0.00110	0.00034	0.00043
STDEV	0.00	0.00	0.00	0.00	0.00

Data were obtained from Appendix 3, Table A3.2, p. 76, Table A3.4, p. 80, Table A3.6, p. 84, Table A3.8, p. 88, and Table A3.10, p. 92 of the study report.

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Table 7 % Desorbed as % of the adsorbed

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam
1	87.64	85.41	76.42	92.41	91.12
1	87.82	85.59	71.32	92.61	91.62
AVG	87.73	85.50	73.87	92.51	91.37
STDEV	0.13	0.12	3.61	0.14	0.35

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam
0.3	86.74	79.77	68.25	92.10	89.73
0.3	87.98	81.64	68.94	92.46	89.74
AVG	87.36	80.71	68.60	92.28	89.73
STDEV	0.87	1.32	0.49	0.25	0.00

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam
0.1	87.57	74.65	66.44	91.25	86.26
0.1	87.91	76.73	65.07	92.06	85.55
AVG	87.74	75.69	65.75	91.66	85.90
STDEV	0.25	1.47	0.96	0.57	0.50

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam
0.03	86.76	68.20	58.97	90.67	80.61
0.03	87.95	60.12	57.92	92.86	80.06
AVG	87.36	64.16	58.44	91.76	80.33
STDEV	0.84	5.72	0.74	1.55	0.39

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam
0.01	85.49	48.31	49.79	91.53	70.03
0.01	87.00	60.35	55.74	92.53	76.39
AVG	86.25	54.33	52.77	92.03	73.21
STDEV	1.07	8.52	4.21	0.71	4.50

Data were obtained from Tables 9-13, pp. 37-39 of the study report.