

**Data Evaluation Report on the adsorption-desorption of the transformation product
JAU6476-S-methyl in soil**

PMRA Submission Number 2004-0843

EPA MRID Number 46246501



Data Requirement: PMRA DATA CODE: 8.2.4.2
EPA DP Barcode: DP 303488
OECD Data Point: IIA 7.4.2
EPA Guideline: 163-1

Test material: JAU6476-S-methyl

Common name
chemical name:

IUPAC: (alpha-1(1-chlorocyclopropyl)-alpha-[(2-chlorophenyl)methyl]-3-(methylthio)-1H-1,2,4-triazole-1-ethanol)

CAS name: (alpha-1(1-chlorocyclopropyl)-alpha-[(2-chlorophenyl)methyl]-3-(methylthio)-1H-1,2,4-triazole-1-ethanol)

CAS No: 178928-71-7

synonyms: WAK 7861

SMILES string: ClC1(C(Cc2ccccc2Cl)(CN2N=CNC2SC)O)CC1.

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EPA/OPP/EFED/ERB4

Dirk Young
Date: Aug. 22, 2005

Company Code BCZ

Active Code PRB

Use Site Category 7, 13, 14 (Industrial Oil Seed Crops and Fibre Crops, Terrestrial Feed Crops, Terrestrial Food Crops)

EPA PC Code 113961

CITATION Hein, W. 1999. Adsorption/Desorption of S-methyl-JAU6476 on Four Different Soils. Performing Laboratory: Staatliche Lehr- und Forschungsanstalt für Landwirtschaft, Weinbau und Gartenbau (SLFA). Bayer CropScience, North Carolina. Unpublished. Report No. FM774. December 21, 1999.

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EXECUTIVE SUMMARY:

The adsorption/desorption characteristics of [phenyl-UL-¹⁴C]JAU6476-S-methyl (purity >98%), a transformation product of prothioconazole (JAU6476), was studied two German and two American soils in a batch equilibrium experiment: a sandy loam (Laacher Hof AXXa), a silt (Höfchen am Hohenseh 4a), a silty clay loam (Stanley) and a loamy sand (Byromville). The soil characteristics were the following: *sandy loam*: pH 7.2, 2.02% organic carbon, 72.4% sand, 22.6% silt, 5% clay; *silt*: pH 7.1, 2.14% organic carbon, 8.5% sand, 81.3% silt, 10.2% clay; *silty clay loam*: pH 5.9, 1.66% organic carbon, 12.4% sand, 48% silt, 39.6% clay; *loamy sand*: pH 6.8, 0.79% organic carbon, 86.8% sand, 7.6% silt, 5.6% clay. The experiment was conducted in accordance with the USEPA Pesticide Assessment Guidelines, Subdivision N, Section §163-1, OECD Guideline 106 and EC, Commission Directive 95/36/EC Amending Council Directive 91/41/EEC (Annexes I + II, Fate and Behaviour in the Environment), July 14, 1995 and in compliance with German and OECD Good Laboratory Practice Standards. The adsorption phase of the study was carried out by equilibrating air-dried soil with [phenyl-UL-¹⁴C]JAU6476-S-methyl at 0.6, 1.2, 4.2 and 13.4 mg/kg soil in the dark at 20°C for 27 hours (51 hours for the loamy sand). The equilibrating solution used was 0.01M CaCl₂, with a soil/solution ratio of 1:20. The desorption phase of the study was carried out by replacing the adsorption solution with an equivalent volume (20 mL) of pesticide-free 0.01M CaCl₂ solution and equilibrating in the dark for 27 hours (51 hours for the loamy sand) at 20 ± 1°C. The desorption step was conducted once for all soils.

The supernatant solution after adsorption and desorption was separated by centrifugation, decanted and analysed by Liquid Scintillation Counting (LSC) without extraction. Following desorption, the soil was mixed with 0.4 g cellulose/g soil, air-dried, homogenised and combusted prior to LSC analysis. To improve mass balance, the soil samples of Stanley silty clay loam were extracted three times with 20 mL acetonitrile for 30 minutes. High dose [phenyl-UL-¹⁴C]JAU6476-S-methyl residues in all soils were analysed by radio-High Performance Liquid Chromatography (HPLC).

[Phenyl-UL-¹⁴C]JAU6476-S-methyl accounted for 91% of the radioactivity recovered in the high-dose adsorption supernatants. The mass balance at the end of the adsorption phase was not reported. The mean mass balance at the end of desorption phase ranged from 94.1-102.5% in all soils.

A summary of results following the 24 hours equilibration period is given in Table 1. Desorption results are summarized in Table 2. Note that desorption was carried out for only one desorption step, which is somewhat different than guideline studies normally submitted in which several desorption steps are performed. The desorption portion of the study is not acceptable to the PMRA. These results indicate that JAU6476-S-methyl has slight mobility in the sandy loam, the silt and the silty clay loam and low mobility in the the loamy sand tested, according to the classification scheme of McCall *et al.* (1981).

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Table 1. Summary of Adsorption Results

Registrant's Name of soil	Classification	% uptake	Freundlich Coefficient (mg/Kg) ^N /(mg/L)	Freundlich Exponent	Approximated * K _{oc} (mL/g)
Laacher Hof	Sandy loam	79-85	56	0.87	2772
Höfchen am Hohenseh	Silt	81-86	64.1	0.88	2995
Stanley	Silty clay loam	70-76	41.2	0.91	2484
Byromville	Loamy sand	48-56	15.6	0.85	1973

* Based on the Freundlich Coefficient values.

Table 2. Summary of Desorption Results (Note that the desorption portion of this study is not acceptable to the PMRA)

Registrant's Name of soil	Freundlich Coefficient (mg/Kg) ^N /(mg/L)	Freundlich Exponent	Approximated* K _{oc} (mL/g)
Laacher Hof	63.1	0.86	3124
Höfchen am Hohenseh	71.9	0.88	3358
Stanley	48.6	0.91	2926
Byromville	20.0	0.85	2532

* Based on the Freundlich Coefficient values.

Study Acceptability: This study is classified acceptable. It fulfills the Subdivision N Guideline §163-1 data requirements for a mobility study using unaged soil for a major transformation product of prothioconazole, JAU6476-S-methyl. However, the desorption portion of this study was conducted with only one desorption cycle. Three to five cycles are required (Guideline 106, OECD; T-1-255, Agriculture Canada). A new study will not be required.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED:

The study was conducted according to the following guidelines: EC, Commission Directive 95/36/EC Amending Council Directive 91/41/EEC (Annexes I + II, Fate and Behaviour in the Environment), July 14, 1995; OECD Guideline 106; EPA Pesticide Assessment Guidelines, Subdivision N, Chemistry: 163-1 and the Addendum on Data Reporting, September 30, 1988

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A deviation was noted by the study author:
The total amount of soil (1 g) was oxidized.
Therefore the described homogenisation and aliquot analysis was not conducted. The mass balances obtained indicate that this procedure is acceptable. This deviation is not expected to alter the results of the study.

A significant deviation under Guideline 106, OECD; T-1-255, Agriculture Canada was:

The study was conducted using only one desorption cycle rather than the three to five cycles required.

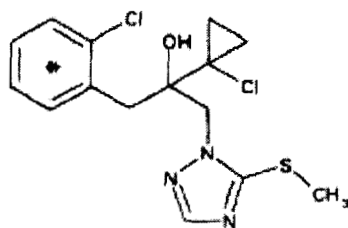
COMPLIANCE: The study was conducted in compliance with Chemikaliengesetz, Appendix 1 of July 25, 1994 and OECD (1981) GLP standards. Signed and dated GLP, Quality Assurance and Data Confidentiality statements were provided.

A. MATERIALS:

1. Test Material

S-methyl-JAU6476

Chemical Structure:



* denotes radiolabel position

Description: [phenyl-UL-¹⁴C]JAU6476-S-methyl: Technical, solid, white (p.9)
Non-radiolabelled JAU6476-S-methyl: Technical, yellowish powder (p.10)

Purity:

[phenyl-UL-¹⁴C]JAU6476-S-methyl:
Analytical purity: Not reported
Synthesis ID: THS 5083

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Radiochemical purity: >98.0%
Specific activity: 3.67 MBq/mg
Locations of the label: phenyl ring

Non-radiolabelled JAU6476-desthio:

Analytical purity: 99%
Reference Substance No.: M00892

**Storage conditions of
test chemicals:**

[phenyl-UL-¹⁴C]SXX0665: stored as cool as possible to
protect from autoradiolysis (data provided by sponsor);
stored ≤ -18 °C (at test facility)

Non-radiolabelled JAU6476-desthio: 0-10 °C (data
provided by sponsor); +1-10 °C (at test facility)

Table 3: Physico-chemical properties of JAU6476-S-methyl.

Parameter	Values	Comments
Water solubility	1.456 mg/L	Estimated by modeling. Extra information provided by the sponsor. (p. 9)
Vapour pressure	not reported	
UV absorption	not reported	
pKa	not reported	
Kow	not reported	
Stability of Compound at room temperature	not reported	Results of stability tests show that the test substance was stable under test conditions (>94% after 51 hours) (p.16)

2. Soil Characteristics

Table 4: Description of soil collection and storage.

Description	Laacher Hof AXXa sandy loam	Höfchen am Hohenseh 4a silt	Stanley silty clay loam	Byromville loamy sand
Geographic location	Germany	Germany	Stilwell, KS, USA	Byromville, GA, USA

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Pesticide use history at the collection site	not reported (Biotransformation in aerobic soil study reports (MR-549/99, MR-340/00 and MR-327/00) state no pesticide use since 1988)	not reported (Biotransformation of JAU6476-S-methyl and JAU6476-desthio in aerobic soil study reports (MR-340/00 and MR-327/00) state no pesticide use)	not reported (Biotransformation in aerobic soil study reports (MR-549/99, MR-340/00 and MR-327/00) state no pesticide use)	not reported (Soil phototransformation of prothioconazole on soil study report (MR-242/00) states no pesticide use)
Collection procedures	Not reported	Not reported	Not reported	Not reported
Sampling depth (cm)	0-30 cm	0-30 cm	0-15.24 cm	0-15.24 cm
Storage conditions	Soils were shipped moist and unsieved. They were air-dried and sieved just prior to study initiation. Sieved soils were stored in plastic containers at room temperature.	Soils were shipped moist and unsieved. They were air-dried and sieved just prior to study initiation. Sieved soils were stored in plastic containers at room temperature.	Soils were shipped moist and unsieved. They were air-dried and sieved just prior to study initiation. Sieved soils were stored in plastic containers at room temperature.	Soils were shipped moist and unsieved. They were air-dried and sieved just prior to study initiation. Sieved soils were stored in plastic containers at room temperature.
Storage length	Feb. 98 to January 5, 1999	Feb. 98 to January 5, 1999	December 5, 1995 to January 5, 1999	January 26, 1998 to January 5, 1999
Soil preparation	Air-dried; sieved, 2 mm.	Air-dried; sieved, 2 mm.	Air-dried; sieved, 2 mm.	Air-dried; sieved, 2 mm.

Data obtained from Appendix 4, p. 34; pp. 8, 12.

Table 5: Properties of the soils.

Property	Laacher Hof AXXa	Höfchen am Hohenseh 4a	Stanley	Byromville
Soil Texture	sandy loam	silt	silty clay loam	loamy sand
% sand	72.4	8.5	12.4	86.8
% silt	22.6	81.3	48	7.6
% clay	5	10.2	39.6	5.6
pH (in H ₂ O)	7.2	7.1	5.9	6.8
Organic carbon (%)	2.02	2.14	1.66	0.79
CEC (meq/100 g)	8	15	18.5	4.29

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Moisture at 1/3 atm (%)	Not reported	Not reported	Not reported	Not reported
Bulk density (g/cm ³)	Not reported	Not reported	Not reported	1.59
Biomass (mg microbial C/100 g or CFU or other)	Not reported	Not reported	Not reported	Not reported
Soil taxonomic classification	Not reported	Not reported	Not reported	Not reported
Soil mapping unit (for EPA)	Not reported	Not reported	Not reported	Not reported

C. STUDY DESIGN:

1. Preliminary study: Preliminary tests were conducted to determine the appropriate soil:solution ratio and equilibration times to be used in the definitive study and to evaluate the stability of the test substance in aqueous solution (pp. 12-13). Prior to the initiation of the preliminary tests, two application solutions containing a mixture of [phenyl-UL-¹⁴C]JAU6476-S-methyl and non-radiolabelled JAU6476-S-methyl were prepared using three stock solutions. Stock Solution I was prepared by dissolving a 1.1 g aliquot of CaCl₂ in 1000 mL of distilled water (0.01 M CaCl₂; p. 10). Standard Stock Solution I was prepared by dissolving [phenyl-UL-¹⁴C]JAU6476-S-methyl in 5 mL of acetonitrile. The radioactivity of the solution was measured by LSC and the purity was determined by HPLC. The concentration of the test substance in Standard Stock Solution I was 0.73 µg/µL and the purity was >98.0%. Standard Stock Solution II was prepared by dissolving 21.06 mg of non-radiolabelled test substance in 100 mL of acetonitrile. The final concentration was 210.6 mg/L.

To make the application solution for the Preliminary Test I (PRE I) (determination of appropriate soil:solution ratio), aliquots of 0.10 mL radioactive and 0.47 mL non-radioactive solution from Standard Stock Solutions I and II (equivalent to 0.07 mg of labelled and 0.10 mg of non-labelled test substance) were added to a 250-mL volumetric flask. The organic solvent was evaporated and the volumetric flask was filled with Stock Solution I. The concentration of the [¹⁴C]labelled test substance in solution was measured by LSC and determined to be 0.24 mg/L, and the purity was determined to be greater than 98.0% by HPLC.

The application solution for the Preliminary Test II (PRE II) (determination of equilibration time and stability) was made by combining aliquots of 0.20 mL radioactive and 0.12 mL non-radioactive solution from Standard Stock Solutions I and II (equivalent to 0.14 mg of labelled and 0.03 mg of non-labelled test substance) in a 250-mL volumetric flask. The organic solvent was evaporated and the volumetric flask was filled with Stock Solution I. The concentration of the [¹⁴C]labelled test substance in solution was measured by LSC and determined to be 0.53 mg/L, and the purity was determined to be greater than 98.0% by HPLC.

Application Solution A (0.70 mg/L) for the definitive test was prepared by adding approximately 0.57 mL of Standard Stock Solution I (0.42 mg of [phenyl-UL-¹⁴C]JAU6476-desthio) to a

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500 mL volumetric flask. (About 20% of the test substance volatilized during the preparation of the application solutions PRE I and PRE II. Therefore, the amount of test substance was increased by 20%.) The organic solvent was evaporated and the flask was filled with Stock Solution I. Four aliquots were taken for HPLC analysis of radiopurity. Application Solutions B, C and D (0.25, 0.08 and 0.04 mg/L, respectively) were prepared by mixing 71.4, 22.9 and 11.4 mL of Solution A to 200 mL of Stock Solution I, respectively. Four 100 μ L aliquots of each solution were taken for LSC analysis (p. 11).

To determine the soil:solution ratio to be used in the definitive study, 6-, 3- and 1-g portions (dry weight equivalent) of all the test soils were added to 20-mL aliquots of PRE I Application Solution at a nominal concentration of 0.7 mg/L (p. 12). The samples were shaken in the dark at $20 \pm 1^\circ\text{C}$ for 24 hours. The samples were centrifuged and duplicate 100 μ L aliquots of the supernatants were analyzed for total radioactivity using LSC. The soils were combusted and aliquots were analyzed for total radioactivity using LSC. Based on the results of this preliminary test, a soil:solution ratio of 1:20 (corresponding to 1 g soil and 20 mL solution) was selected for all soils.

To determine the equilibration time to be used in the definitive study and to evaluate the stability of the test substance in aqueous solution, the correct soil:solution ratio determined in PRE I was treated to 1g portions (dry weight equivalent) of each test soil were added to 20-mL aliquots of Application Solution A, at a nominal concentration of 0.7 mg/L (p. 13). The samples were shaken in the dark at $20 \pm 1^\circ\text{C}$ for 1, 3, 6, 27, 51, 75 and 99 hours (p. 13). The samples were centrifuged and 100- μ L aliquots of the supernatants were analyzed for total radioactivity using LSC. The 27-, 51-, 75- and 99-hour samples were also analyzed by HPLC to investigate the stability of the test substance. Duplicate soilless control samples were also prepared and were shaken for 99 hours to evaluate the adsorption of the test substance to the surface of the test vessels. It was determined that the concentration of the test solution remained consistent after 27 hours of shaking (51 hours for Byromville loamy sand) (pp. 14, 19-23; Figure 1, p.25). No adsorption of the test substance to the surface of the test vessels was observed (mean recovery was 97.4%; p. 17).

Based on the results of this preliminary test, a soil:solution ratio of 1:20 (corresponding to 1 g soil and 20 mL solution) was selected. and an equilibrium time of 27 hours (51 hours for Byromville loamy sand) were selected for use in the definitive study (p.16).

2. Definitive study experimental conditions:

Table 6: Study design for the adsorption phase.

Parameters	Laacher Hof AXXa sandy loam	Höfchen am Hohenseh 4a silt	Stanley silty clay loam	Byromville loamy sand
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Condition of soil (air dried/fresh)		air-dried	air-dried	air-dried	air-dried
Have these soils been used for other laboratory studies ?		Yes (Bayer Report Nos. MR-549/99, MR-340/00, MR-327/00, MR-098/99 - Aerobic soil biotransformation, leaching)	Yes (Bayer Report Nos. MR-104/01, MR-340/00, MR-327/00, MR-098/99 - Aerobic soil biotransformation, leaching)	Yes (Bayer Report Nos. MR-549/99, MR-340/00, MR-327/00, MR-098/99 - Aerobic soil biotransformation, leaching)	Yes (Bayer Report No. MR-104/01, MR-242/00, MR-098/99, MR-364/00- Aerobic soil biotransformation, phototransformation on soil, leaching, aged soil leaching)
Soil (g/replicate)		1	1	1	1
Equilibrium solution used (name and concentration; eg: 0.01N CaCl ₂)		0.01 M CaCl ₂	0.01 M CaCl ₂	0.01 M CaCl ₂	0.01 M CaCl ₂
Control used (with salt solution only) (Yes/No)		Yes	Yes	Yes	Yes
Test material concentrations ¹	Nominal application rates	0.04, 0.08, 0.25, 0.70 mg/L, equivalent to 0.8, 1.6, 5.0, 14.0 mg/kg soil	0.04, 0.08, 0.25, 0.70 mg/L, equivalent to 0.8, 1.6, 5, 14 mg/kg soil	0.04, 0.08, 0.25, 0.70 mg/L, equivalent to 0.8, 1.6, 5, 14 mg/kg soil	0.04, 0.08, 0.25, 0.70 mg/L, equivalent to 0.8, 1.6, 5, 14 mg/kg soil
	Analytically measured concentrations	0.03, 0.06, 0.21, 0.67 mg/L, equivalent to 0.6, 1.2, 4.2, 13.4 mg/kg soil	0.03, 0.06, 0.21, 0.67 mg/L, equivalent to 0.6, 1.2, 4.2, 13.4 mg/kg soil	0.03, 0.06, 0.21, 0.67 mg/L, equivalent to 0.6, 1.2, 4.2, 13.4 mg/kg soil	0.03, 0.06, 0.21, 0.67 mg/L, equivalent to 0.6, 1.2, 4.2, 13.4 mg/kg soil
Identity and concentration of co-solvent, if any		Acetonitrile (evaporated)	Acetonitrile (evaporated)	Acetonitrile (evaporated)	Acetonitrile (evaporated)
Soil:solution ratio		1:20	1:20	1:20	1:20
Initial pH of the equilibration solution, if provided		Not reported	Not reported	Not reported	Not reported
No. of replications	Controls	2	2	2	2
	Treatments	2	2	2	2
Equilibration	Time (hours)	27	27	27	51
	Temperature (°C)	20 ± 1	20 ± 1	20 ± 1	20 ± 1

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	Darkness (Yes/No)	Yes	Yes	Yes	Yes
	Shaking method	Rotary shaker	Rotary shaker	Rotary shaker	Rotary shaker
	Shaking time (hours)	27	27	27	51
Method of separation of supernatant		Centrifugation	Centrifugation	Centrifugation	Centrifugation
Centrifugation	Speed (rpm)	≈5000	≈5000	≈5000	≈5000
	Duration (min)	≈20	≈20	≈20	≈20
	Method of separation of soil and solution	Decanted	Decanted	Decanted	Decanted

Data were obtained from Table 2, p. 11; pp. 12, 14 of the study report.

¹ Test material concentrations were calculated by the reviewer by converting mg/L to mg/kg soil using the following equation: [test concentration (mg/L) x total volume of test material solution (L)] ÷ amount of soil (kg); eg. (0.04 mg/L x 0.02 L) ÷ 0.001 kg = 0.8 mg/kg soil.

Table 7: Study design for the desorption phase.

Parameters		Laacher Hof AXXa sandy loam	Höfchen am Hohenseh 4a silt	Stanley silty clay loam	Byromville loamy sand
Were the soil residues from the adsorption phase used? If not, describe the method for adsorption using a separate adsorption Table		Yes	Yes	Yes	Yes
Amount of test material present in the adsorbed state/adsorbed amount (mg a.i./kg soil)	0.6	0.58062	0.58932	0.51703	0.41357
	1.2	1.0581	1.0644	0.94017	0.71205
	4.2	3.3533	3.442	3.0205	2.2017
	13.4	10.618	10.862	9.4799	6.4412
No. of desorption cycles		1	1	1	1
Equilibration solution and quantity used per treatment for desorption (eg., 0.01M CaCl ₂)		0.01M CaCl ₂ 20 mL	0.01M CaCl ₂ 20 mL	0.01M CaCl ₂ 20 mL	0.01M CaCl ₂ 20 mL
Soil:solution ratio		0.0555556	0.0555556	0.0555556	0.0555556
Replications	Controls	0	0	0	0
	Treatments	2	2	2	2

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Desorption equilibration	Time (hours)	27	27	27	51
	Temperature (°C)	20 ± 1	20 ± 1	20 ± 1	20 ± 1
	Darkness	Yes	Yes	Yes	Yes
	Shaking method	Shaking method	Rotary shaker	Rotary shaker	Rotary shaker
	Shaking time	Shaking time (hours)	24	24	24
Centrifugation	Speed (rpm or g)	≈ 5000	≈ 5000	≈ 5000	≈ 5000
	Duration (min)	≈ 20	≈ 20	≈ 20	≈ 20
	Method of separation of soil and solution	Decanted	Decanted	Decanted	Decanted

Data were obtained from pp.11, 13, and Tables 11-14, pp. 20-23 of the study report.

3. Description of analytical procedures:

Extraction/clean up/concentration methods: To improve mass balance, the soil samples of Stanley sitly clay loam were extracted three times with 20 mL acetonitrile for 30 minutes. Extraction/clean up/concentration methods were not employed for the other three soils.

Total ¹⁴C measurement: Following adsorption and desorption, aliquots of the supernatants were analyzed for total radioactivity using LSC (p. 14). Following desorption, soil samples were mixed with approximately 0.4 g cellulose/g soil, air dried, homogenised and combusted in the Sample Oxidiser 307 (Canberra Packard Corp.) prior to LSC analysis. Combustion efficiency was not reported. Recovery of total radioactivity was determined by summing the [¹⁴C]residues measured in the supernatants after equilibrium (adsorption) and after desorption, and the [¹⁴C]residues remaining in the soil after desorption for each test soil.

Non-extractable residues, if any: Not applicable.

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

Identification and quantification of parent compound: For each test soil, aliquots of the high-dose (13.4 mg/kg soil) adsorption and desorption supernatants were analyzed for [phenyl-UL-¹⁴C]JAU6476-S-methyl by radio-HPLC under the following conditions: Pharmacia LKB Low Pressure Mixer, LKB LC Gradient Pump, Pharmacia LKB Autosampler, Lichrospher 60, RP select (5 µm, 4 mm x 125 mm incl.), Pre-column (4 mm x 4 mm, same material), gradient mobile phase (A) 0.2% (w/w) H₃PO₄ in water or (B) acetonitrile [percent A:B at 0 min. 100:0 (v:v), 5

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min.100:0, 35 min. 0:100, 40 min. 0:100, 45 min 100:0], flow rate 1.50 mL/minute, Radio-HPLC-Detector A-525 AX (p.15).

Identification and quantification of transformation products, if appropriate: Samples were not analyzed for transformation products of JAU6476-S-methyl.

Detection limits (LOD, LOQ) for the parent compound: In a company response to a clarifax received by the PMRA on September 7, 2004, the LOD is approximately 50 dpm (0.83 Bq) per Liquid Scintillation (LS) sample. This is equivalent to less than 0.036% of the applied radioactivity. The LOQ is in the range of 100 dpm per LS sample. This is the equivalent to less than 0.072% of the applied radioactivity.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The incubation temperature was reported to be $20 \pm 1^\circ\text{C}$ during the study; temperature records were not provided (p. 12). The pH of the adsorption equilibrium solutions and in the supernatant of the highest concentration samples after the desorption ranged from 6.3 to 7.5 for all test soils (Table 17, p. 24). Based on HPLC analysis, [phenyl-UL- ^{14}C]JAU6476-S-methyl accounted for more than 91% of the radioactivity recovered in the high-dose adsorption supernatants (p. 17; Figure 2, p. 26).

B. MASS BALANCE: The mass balance at the end of adsorption phase was not determined as the soils were used in the desorption phase. The mass balance at the end of desorption phase ranged from 97.4-101.4%, 97.3-101.0%, 99.1-102.5 and 94.1-100.9% of the applied radioactivity in Laacher Hof AXXa sandy loam, Höfchen am Hohenseh 4a silt, Stanley silty clay loam Byromville loamy sand, respectively (Tables 11-14, pp. 20-23).

Table 8: Recovery of [phenyl-UL- ^{14}C]JAU6476-S-methyl, expressed as percentage of applied radioactivity, in soil after adsorption/desorption (mean \pm s.d.) (n=2).

Matrices		Laacher Hof AXXa sandy loam	Höfchen am Hohenseh 4a silt	Stanley silty clay loam	Byromville loamy sand
At the end of the adsorption phase					
Supernatant solution	0.03 mg/L	14.9 \pm 0.2	13.6 \pm 0.4	24.2 \pm 0.1	39.4 \pm 0.6
	0.06 mg/L	16.1 \pm 0.2	15.6 \pm 0.2	25.4 \pm 0.9	43.5 \pm 1.2
	0.21 mg/L	19.5 \pm 0.2	17.3 \pm 0.0	27.5 \pm 1.1	47.1 \pm 1.9
	0.67 mg/L	21.2 \pm 0.4	19.4 \pm 0.4	29.7 \pm 1.0	52.2 \pm 1.0
Solid phase (total ^{14}C)		Not analyzed			

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Non-extractable residues in soil, if measured		Not measured			
Total recovery		Not determined			
At the end of the desorption phase					
Supernatant solution	0.03 mg/L	10.3 ± 0.0	10.3 ± 0.3	15.3 ± 0.0	17.5 ± 0.4
	0.06 mg/L	11.7 ± 0.1	11.3 ± 0.1	15.8 ± 0.5	19.4 ± 0.1
	0.21 mg/L	13.1 ± 0.3	12.5 ± 0.1	17.1 ± 0.7	19.7 ± 0.2
	0.67 mg/L	14.4 ± 0.4	13.4 ± 0.7	18.2 ± 0.0	19.6 ± 0.4
Solid phase (total ¹⁴ C) ¹	0.03 mg/L	72.2 ± 0.2	73.5 ± 0.7	59.6 ± 2.4	37.2 ± 3.4
	0.06 mg/L	73.2 ± 0.3	74.1 ± 0.9	61.3 ± 0.3	38.0 ± 1.1
	0.21 mg/L	68.8 ± 0.0	70.2 ± 0.1	54.8 ± 1.3	33.7 ± 1.5
	0.67 mg/L	62.9 ± 0.3	64.5 ± 0.9	54.3 ± 1.4	25.7 ± 0.4
Non-extractable residues in soil, if measured		Not measured			
Total recovery	0.03 mg/L	97.4 ± 0.4	97.4 ± 0.1	99.1 ± 2.5	94.1 ± 2.4
	0.06 mg/L	101.0 ± 0.4	101.0 ± 0.5	102.5 ± 1.7	100.9 ± 0.3
	0.21 mg/L	101.4 ± 0.6	100.0 ± 0.1	99.4 ± 0.4	100.5 ± 0.3
	0.67 mg/L	98.5 ± 0.4	97.3 ± 0.0	102.2 ± 0.1	97.5 ± 0.2

Data were obtained from Tables 11-14, pp. 20-23 of the study report.

¹ All soils were combusted following desorption.

Table 9: Concentration of [phenyl-UL-¹⁴C]JAU6476-S-methyl in the solid and liquid phases at the end of adsorption equilibration period (mean ± s.d.) (n=2).

Concentration (mg a.i./kg soil)	Laacher Hof AXXa sandy loam			Höfchen am Hohenseh 4a silt		
	on soil (mg a.i./kg)	in solution (µg a.i./mL) ¹	% adsorbed	on soil (mg a.i./kg)	in solution (µg a.i./mL) ¹	% adsorbed
0.6	0.581 ± 0.001	0.005 ± 0.000	85.1 ± 1.4	0.589 ± 0.003	0.005 ± 0.000	86.4 ± 3.1
1.2	1.058 ± 0.002	0.010 ± 0.000	83.9 ± 1.1	1.064 ± 0.003	0.010 ± 0.000	84.4 ± 1.3
4.2	3.353 ± 0.009	0.040 ± 0.000	80.5 ± 1.1	3.442 ± 0.001	0.036 ± 0.000	82.7 ± 0.2
13.4	10.618 ± 0.051	0.143 ± 0.002	78.8 ± 1.8	10.862 ± 0.028	0.131 ± 0.001	80.6 ± 1.1

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Concentration (mg a.i./kg soil)	Stanley silty clay loam			Byromville loamy sand		
	on soil (mg a.i./kg)	in solution ($\mu\text{g a.i./mL}$) ¹	% adsorbed	on soil (mg a.i./kg)	in solution ($\mu\text{g a.i./mL}$) ¹	% adsorbed
0.6	0.517 \pm 0.001	0.008 \pm 0.000	75.8 \pm 0.4	0.414 \pm 0.004	0.013 \pm 0.000	60.6 \pm 1.6
1.2	0.940 \pm 0.011	0.016 \pm 0.000	74.6 \pm 3.4	0.712 \pm 0.015	0.027 \pm 0.001	56.5 \pm 2.7
4.2	3.020 \pm 0.047	0.057 \pm 0.002	72.5 \pm 4.1	2.202 \pm 0.079	0.098 \pm 0.004	52.9 \pm 4.0
13.4	9.480 \pm 0.129	0.200 \pm 0.006	70.3 \pm 3.2	6.441 \pm 0.141	0.352 \pm 0.007	47.8 \pm 2.0

Data were obtained from Tables 11-14, pp. 20-23 of the study report.

¹Amount in solution was calculated by the reviewer by dividing the amount in solution at equilibration by the amount of initial solution; e.g. 0.10978 $\mu\text{g} \div 20 \text{ mL} = 0.00549 \mu\text{g/mL}$.

Table 10: Concentration of [phenyl-UL-¹⁴C]JAU6476-S-methyl in the solid and liquid phases at the end of desorption (n = 1). The desorption phase of the study is NOT acceptable to the PRMA, as only one desorption cycle was conducted instead of three to five cycles.

Concentration (mg a.i./kg soil)	Laacher Hof AXXa sandy loam			Höfchen am Hohenseh 4a silt		
	on soil (mg a.i./kg)	in solution ($\mu\text{g a.i./mL}$) ¹	% desorbed as % of the adsorbed	on soil (mg a.i./kg)	in solution ($\mu\text{g a.i./mL}$) ¹	% desorbed as % of the adsorbed
0.6	0.493 \pm 0.001	Not reported	15.2 \pm 0.2	0.502 \pm 0.005	Not reported	14.8 \pm 0.9
1.2	0.923 \pm 0.004	Not reported	12.7 \pm 0.4	0.935 \pm 0.011	Not reported	12.2 \pm 1.1
4.2	2.867 \pm 0.004	Not reported	14.5 \pm 0.1	2.925 \pm 0.006	Not reported	15.0 \pm 0.2
13.4	8.486 \pm 0.031	Not reported	20.1 \pm 0.2	8.690 \pm 0.113	Not reported	20.0 \pm 1.0

Concentration (mg a.i./kg soil)	Stanley silty clay loam			Byromville loamy sand		
	on soil (mg a.i./kg)	in solution ($\mu\text{g a.i./mL}$) ¹	% desorbed as % of the adsorbed	on soil (mg a.i./kg)	in solution ($\mu\text{g a.i./mL}$) ¹	% desorbed as % of the adsorbed
0.6	0.406 \pm 0.016	Not reported	21.4 \pm 3.2	0.254 \pm 0.024	Not reported	38.7 \pm 5.7
1.2	0.773 \pm 0.004	Not reported	17.8 \pm 0.4	0.479 \pm 0.014	Not reported	32.7 \pm 2.0
4.2	2.282 \pm 0.055	Not reported	24.5 \pm 1.8	1.405 \pm 0.065	Not reported	36.2 \pm 2.9
13.4	7.321 \pm 0.193	Not reported	22.8 \pm 2.0	3.462 \pm 0.050	Not reported	46.3 \pm 0.8

Data were obtained from Tables 11-14, pp. 20-23 of the study report.

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¹ Amount in solution after desorption were only reported in terms of mean % of the applied radioactivity and are therefore not reported here.

Table 11: Adsorption isotherm parameters of JAU6476-S-methyl the soils. K values are in mL/g.

Soil	Adsorption ¹			
	K _{F ads}	1/n	r ²	K _{oc}
Laacher Hof AXXa sandy loam	56.0	0.87	0.9998	2772.4
Höfchen am Hohenseh 4a silt	64.1	0.88	0.9998	2995.0
Stanley silty clay loam	41.2	0.91	1.0000	2484.0
Byromville loamy sand	15.6	0.85	0.9998	1973.6

Data were obtained from Table 15, p. 24 of the study report.

K_d - Adsorption coefficients; K_{F ads} - Freundlich adsorption coefficient; 1/n - Slope of Freundlich adsorption/desorption isotherms.

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

r² - Regression coefficient of Freundlich equation.

¹ Freundlich K values were calculated by the study author and verified by the reviewer (using data from Tables 11-14, pp. 20-23) using the following equation (p. 17):

$$\ln (x/m) = \ln K_d + 1/n * \ln C \text{ where}$$

x/m = amount of test substance adsorbed to the soil;

K_d = adsorption coefficient;

1/n = slope of the adsorption isotherm; and

C = concentration of compound in solution at equilibrium.

C. ADSORPTION: As indicated by the Freundlich exponent, the effective sorption coefficient decreased with increasing concentration. After 27 hours of equilibration (51 hours for Byromville loamy sand), 78.8-85.1%, 80.6-86.4%, 70.3-75.8% and 47.8-60.6% of the applied [¹⁴C]JAU6476-S-methyl was adsorbed to the sandy loam, the silt, the silty clay loam and the loamy sand, respectively (Tables 11-14, pp. 20-23). Freundlich K_{ads} values were 56.0, 64.1, 41.2 and 15.6 mL/g for the sandy loam, the silt, the silty clay loam and the loamy sand, respectively; corresponding Freundlich K_{oc} values were 2772.4, 2995.0, 2484.0 and 1973.6 mL/g (Table 15, p. 24).

The reviewer has verified the adsorption constants reported by the study author and obtained identical results, except for insignificant differences in the K_{oc} for the loamy sand (1972.8 instead of 1973.6 mL/g).

The PMRA reviewer investigated the relationship between K_{F ads} and % organic carbon, pH, % clay, and CEC by using linear regression with SigmaStat. K_{F ads} was significantly related only to % organic carbon (slope=34.641, r² = 0.976, p = 0.008, n=4). No significant relationship was found between the Freundlich adsorption value and pH, % clay or CEC (in all cases: r² = 0.000, p ≥ 0.483, n=4).

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D. DESORPTION: The desorption phase of this study was only conducted with one desorption cycle but guidelines suggest three to five cycles (Guideline 106, OECD; T-1-255 Agriculture Canada). New desorption data are not required, but the desorption values reported are not accepted by the PMRA.

III. STUDY DEFICIENCIES: The desorption phase of this study was only conducted with one desorption cycle but should have been conducted with three to five cycles (based on Guideline 106, OECD; T-1-255 Agriculture Canada). The desorption values reported are not accepted by the PMRA. New desorption data are not required.

IV. REVIEWER'S COMMENTS: The identity of the test substance was only examined at the test facility by means of visual criteria and accompanying documents. All data concerning the test substance were provided by the sponsor. (p.8)

Raw data were not provided.

The Stanley silty clay loam soil was stored for a very long time (December 5, 1995 to January 5, 1999), but the microbial biomass was not reported. There does not seem to be an effect related to storage for this soil.

JAU6476-S-methyl has slight mobility in the sandy loam, the silt and the silty clay loam and low mobility in the the loamy sand tested, according to the classification scheme of McCall *et al.* (1981).

V. REFERENCES:

McCall, J.P., D.A. Laskowski, R.L. Swann, and H.J. Dishburger. 1981. Measurement of sorption coefficients of organic chemicals and their use in environmental fate analysis. Pages 89-109 In *Test protocols for environmental fate & movement of toxicants*. Proceedings of a symposium. Association of Official Analytical Chemists. 94th Annual Meeting, October 21-22, 1980. Washington, DC.