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Data Evaluation Report on the adsorption-desorption of the transformation product JAU6476-desthio (SXX0665) in soil

PMRA Submission Number 2004-0843 EPA MRID Number 46246450

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:

Common name: SXX 0665

chemical name:

IUPAC: (R,S) 2-(1-chlorocycloproyl)1-(2-chlorophenyl)-3-(1,2,4-triazol-1-yl)-propan-2-ol

CAS name: 2-(1-Chlorocyclopropyl)1-(2-chlorophenyl)-3-(1,2,4-triazol-1-yl)-propan-2-ol

CAS No: 120983-64-4

synonyms: JAU 6476-desthio

SMILES string: ClC1(C(Cc2ccccc2Cl)(CN2N=CNC2)O)CC1.

Primary Reviewer (officer number): Émilie Larivière (#1269) EAD, PMRA **Date:** April 25, 2005 4/25/05

Secondary Reviewer (officer number): Amber McCoy (#1349) EAD, PMRA **Date:** May 30, 2005

Secondary Reviewer (officer number): Dirk Young, PhD EPA/OPP/EFED/ERB4 **Date:** Aug. 12, 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: Fent, G. 1998. Adsorption/Desorption of [phenyl-UL-^{14}C]SXX0665 on Four Different Soils. Performing Laboratory: Staatliche Lehr-und Forschungsanstalt für Landwirtsxchaft, Weinbau und Gartenbau (SLFA). Bayer CropScience, North Carolina. Unpublished. Report No. FM768. August 11, 1998.

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EXECUTIVE SUMMARY:

The adsorption/desorption characteristics of [phenyl-UL-^{14}C]SXX0665 (JAU6476-desthio; purity >96%), a transformation product of prothioconazole (JAU6476), was studied on 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-^{14}C]JAU6476-desthio at 0.27, 1.20, 5.80, 28.80 mg/kg soil (0.09, 0.40, 1.93, 9.60 mg/kg soil for the loamy sand) in the dark at 20°C for 24 hours. The equilibrating solution used was 0.01M $CaCl_2$, with a soil/solution ratio of 1:6.66 for all soils except for the loamy sand, which was equilibrated with a soil/solution ratio of 1:2.22. 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 $CaCl_2$ solution and equilibrating in the dark for 24 hours 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 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. High dose [phenyl-UL-^{14}C]JAU6476-desthio residues were analysed by radio-HPLC.

[Phenyl-UL-^{14}C]JAU6476-desthio accounted for more than 96% of the applied radioactivity (AR) recovered in the high-dose adsorption supernatants, showing that JAU6476-desthio was stable throughout the study. 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 92.8-110.6% 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 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-desthio has low mobility in soils 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	63-85	12.46	0.79	617
Höfchen am Hohenseh	Silt	64-82	13.38	0.83	625
Stanley	Silty clay loam	53-74	8.9	0.83	536
Byromville	Loamy sand	60-83	12.46	0.8	523

* 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	12.55	0.77	621
Höfchen am Hohenseh	14.75	0.82	689
Stanley	9.32	0.84	561
Byromville	6.92	0.83	876

* 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-desthio. Note that the desorption portion of this study is not valid for the PMRA as only one desorption cycle was conducted. 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

A deviation was noted by the study author:

Temperatures during preliminary test II and the definitive test were between 19.6 and 21.1°C, instead of the recommended 20±1°C. The mean temperature for the two tests was 20.8 and 20.5°C, respectively. The slight difference in temperature of 0.1°C is not expected to alter the results of this study.

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

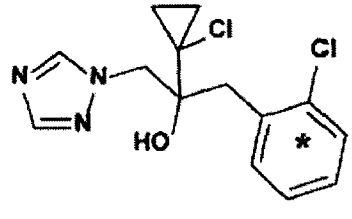
The study was conducted using only one desorption cycle rather than the three to five cycles required.

COMPLIANCE: The study was conducted in compliance with Chemicals Law (ChemG), dated 25 July, 1994, current version of Annex 1 and the current OECD standards of Good Laboratory Practice. Signed and dated GLP, Quality Assurance and Data Confidentiality statements were provided.

A. <u>MATERIALS</u>:

<u>1. Test Material</u> [phenyl-UL-^{14}C]-labelled and non-radiolabelled SXX0665 (JAU6476-desthio)

Chemical Structure:



* denotes position of radiolabel

Description: [phenyl-UL-^{14}C]JAU6476-desthio: Technical, solid (p.9)

Non-radiolabelled JAU6476-desthio: Technical, solid, white (p.10)

Purity:

[phenyl-UL-^{14}C]JAU6476-desthio:
Analytical purity: Not reported
Synthesis ID: THS 3540-2
Radiochemical purity: >96.0%
Specific activity: 3.27 MBq/mg
Locations of the label: phenyl ring

Non-radiolabelled JAU6476-desthio:
Analytical purity: 99.8%
Reference Substance No.: 881201ELB02

Storage conditions of test chemicals:

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

Non-radiolabelled JAU6476-desthio: room temperature (data provided by sponsor); +1-10 °C, in the dark (at test facility)

Table 3: Physico-chemical properties of JAU6476-desthio.

Parameter	Values	Comments
Water solubility	0.051 g/L	p.9 of study report
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 since no degradation of the test substance was found (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	Laacher Hof, NRW, Germany	Versuchsgut Höfchen, Burscheid, Germany	Stilwell, KS, USA	Byromville, GA, USA
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.			
Storage length	collected in February 1998; study initiation February 17, 1998 (≤ 17 days)	collected in February 1998; study initiation February 17, 199 (≤ 17 days)	December 5, 1995 to February 17, 1998	January 26,1998 to February 17, 1998
Soil preparation	Air-dried; sieved, 2 mm.			

Data obtained from Appendix 4, p. 38; pp. 8, 12.

Table 5: Properties of the soils.

Property	Laacher Hof AXXa	Höfchen am Hohenseh 4a	Stanley	Byromville
Soil Texture	sandly 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_2O)	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
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-^{14}C]JAU6476-desthio and non-radiolabelled JAU6476-desthio were prepared using three stock solutions. Stock Solution I was prepared by dissolving a 1.1 g aliquot of $CaCl_2$ in 1000 mL of distilled water (0.01 M $CaCl_2$; p. 10). Standard Sock Solution I was prepared by dissolving [phenyl-UL-^{14}C]JAU6476-desthio 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 0.38 µg/µL and the purity was >96.0%. Standard Stock Solution II was prepared by dissolving 41.92 mg of non-radiolabelled JAU6476-desthio in 10 mL of acetonitrile. The final concentration was 4.192 mg/L.

To make the application solution for the Preliminary Test I (PRE I) (determination of appropriate soil:solution ratio), aliquots of 0.29 mL radioactive and 0.27 mL non-radioactive solution from Standard Stock Solutions I and II (equivalent to 0.11 mg of labelled and 1.13 mg of non-labelled test substance) were added to a 250-L volumetric flask. The organic solvent was evaporated and

the volumetric flask was filled with Stock Solution I. The radioactivity of the solution was measured by LSC and the purity was determined by HPLC. The purity of the test substance in the application solution for Preliminary Test I was determined to be greater than 96.0%.

The application solution for the Preliminary Test II (PRE II) (determination of equilibration time and stability) was made by combining aliquots of 0.59 mL radioactive and 0.25 mL non-radioactive solution from Standard Stock Solutions I and II (equivalent to 0.22 mg of labelled and 1.05 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 radioactivity of the solution was measured by LSC and the purity was determined by HPLC. The purity of the test substance in the application solution for PRE II was determined to be greater than 96.0%.

Due to insufficient mass balance (decrease of test substance in control vessels) during the conduction of PRE II, the test was conducted a second time with a new solution. The application solution for the repetition of PRE II was prepared in the same way as for the first test. Aliquots of 0.59 mL radioactive and 0.25 ml non-radioactive solution from Standard Stock Solutions I and II (equivalent to 0.22 mg of labelled and 1.03 mg of nonlabelled test substance) were used. Two aliquots of 100 µL were injected for HPLC analysis of radiopurity. The purity of the test substance in the application solution for the repetition of PRE II was determined to be greater than 96.0%.

Application Solution A (5.0 mg/L) for the definitive test was prepared by adding approximately 3.32 mL of Standard Stock Solution I (1.26 mg of [phenyl-UL-^{14}C]JAU6476-desthio) to a 250 mL volumetric flask. 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 (1.00, 0.20 and 0.04 mg/L, respectively) were prepared by mixing 40, 8.0 and 2.0 mL of Application Solution A to 200, 200 and 250 mL of Stock Solution I, respectively. Four 100 µL aliquots of each solution were taken for LSC analysis (p. 11).

To determine the soil:solution ratio to be used in the definitive study, 9-, 6- and 3-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 5.0 mg/L (p. 12). The samples were shaken in the dark at 20 ± 1°C for 24 hours. The samples were centrifuged and duplicate 100 µL 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 1:6.66 (corresponding to 3 g soil and 20 mL solution) for the sandy loam, the silt and the silty clay loam and a soil: ratio of 1:2.22 (corresponding to 9 g soil and 20 mL solution) for the loamy sand was selected.

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 -g portions (dry weight equivalent) of each test soil were added to 20-mL aliquots of

Application Solution A, at a nominal concentration of 5.038 mg/L (p. 10). The samples were shaken in the dark at 20 ± 1°C for 1, 3, 6, 24, 48 and 72 hours (p. 13). The samples were centrifuged and 100-µL aliquots of the supernatants were analyzed for total radioactivity using LSC. The 24-, 48- and 72-hour samples were also analyzed by HPLC to investigate the stability of the test substance. Duplicate soil-less control samples were also prepared and were shaken for 72 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 24 hours of shaking (pp. 16-17; Figure 1, p.26). No adsorption of the test substance to the surface of the test vessels was observed (mean recovery was 98.8%; p. 17).

Based on the results of this preliminary test, a soil:solution ratio of 1:6.66 (corresponding to 3 g soil and 20 mL solution) for the sandy loam, the silt and the silty clay loam and a soil: ratio of 1:2.22 (corresponding to 9 g soil and 20 mL solution) for the loamy sand was selected. and an equilibrium time of 24 hours were selected for use in the definitive study (pp. 15-16).

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**
Condition of soil (air dried/fresh)	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)	3	3	3	9
Equilibrium solution used (name and concentration; eg: 0.01N $CaCl_2$)	0.01 M $CaCl_2$			
Control used (with salt solution only) (Yes/No)	yes			

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Test material concentrations [1]	Nominal application rates	0.04, 0.20, 1.00, 5.00 mg/L, equivalent to 0.27, 1.33, 6.67, 33.33 mg/kg soil	0.04, 0.20, 1.00, 5.00 mg/L, equivalent to 0.27, 1.33, 6.67, 33.33 mg/kg soil	0.04, 0.20, 1.00, 5.00 mg/L, equivalent to 0.27, 1.33, 6.67, 33.33 mg/kg soil	0.04, 0.20, 1.00, 5.00 mg/L, equivalent to 0.09, 0.44, 2.22, 11.11 mg/kg soil
	Analytically measured concentrations	0.04, 0.18, 0.87, 4.32 mg/L, equivalent to 0.27, 1.20, 5.80, 28.80 mg/kg soil	0.04, 0.18, 0.87, 4.32 mg/L, equivalent to 0.27, 1.20, 5.80, 28.80 mg/kg soil	0.04, 0.18, 0.87, 4.32 mg/L, equivalent to 0.27, 1.20, 5.80, 28.80 mg/kg soil	0.04, 0.18, 0.87, 4.32 mg/L, equivalent to 0.09, 0.40, 1.93, 9.60 mg/kg soil
Identity and concentration of co-solvent, if any		Acetonitrile (evaporated)			
Soil:solution ratio		1:6.66	1:6.66	1:6.66	1:2.22
Initial pH of the equilibration solution, if provided		Not reported			
No. of replications	Controls	2			
	Treatments	2			
Equilibration	Time (hours)	24			
	Temperature (°C)	20 ± 1			
	Darkness (Yes/No)	Yes			
	Shaking method	Rotary shaker			
	Shaking time (hours)	24			
Method of separation of supernatant		Centrifugation			
Centrifugation	Speed (rpm)	≈5000			
	Duration (min)	≈20			
	Method of separation of soil and solution	Decanted			

Data were obtained from Table 2, p. 12 and 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); e.g., (0.04 mg/L x 0.02 L) ÷ 0.003 kg = 0.27 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			
Amount of test material present in the adsorbed state/adsorbed amount (mg a.i./kg soil)	0.27 or 0.09 for Byromville soil	0.201	0.194	0.176	0.066
	1.20 or 0.40 for Byromville	0.944	0.936	0.843	0.317
	5.80 or 1.93 for Byromville	4.089	4.175	3.582	1.407
	28.80 or 9.60 for Byromville	18.182	18.531	15.387	5.833
No. of desorption cycles		1			
Equilibration solution and quantity used per treatment for desorption (eg., 0.01M $CaCl_2$)		0.01M $CaCl_2$ 20 mL			
Soil:solution ratio		1:6.66	1:6.66	1:6.66	1:2.22
Replications	Controls	0			
	Treatments	2			
Desorption equilibration	Time (hours)	24			
	Temperature (°C)	20 ± 1			
	Darkness	Yes			
	Shaking method	Rotary shaker			
	Shaking time (hours)	24			
Centrifugation	Speed (rpm)	≈5000			
	Duration (min)	≈20			
	Method of separation of soil and solution	Decanted			

Data were obtained from pp.12, 14, and Tables 11-14, pp. 21-24 of the study report.

3. Description of analytical procedures:

Extraction/clean up/concentration methods: Extraction/clean up/concentration methods were not employed in this study.

Total ^{14}C 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 compbusted 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 [^{14}C]residues measured in the supernatants after equilibrium (adsorption) and after desorption, and the [^{14}C]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 (28.80 mg/kg soil, or 9.60 mg/kg soil for the loamy sand) adsorption and desorption supernatants were analyzed for [phenyl-UL-^{14}C]JAU6476-desthio 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) acetonitrile + 0.2% H_3PO_4 (40:60, w/w) or (B) acetonitrile [percent A:B at 0 min. 100:0 (v:v), 10 min.100:0, 15 min. 0:100, 20 min. 0:100], flow rate 1.70 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-desthio.

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 ± 1°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 6.4 to 7.6 for all test soils (Table 17 of study report, p. 2). Based on HPLC analysis, [phenyl-UL-^{14}C]JAU6476-desthio accounted for more than 96% of the radioactivity recovered in the high-dose adsorption supernatants (p. 17; Figure 2, p. 27).

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 94.8-100.3%, 95.7-98.9%, 92.8-97.5% and 95.8-110.6% of the AR in the sandy loam, the silt, the silty clay loam and the loamy sand, respectively (Tables 11-14, pp. 21-24 of study report).

Table 8: Recovery of [phenyl-UL-^{14}C]JAU6476-desthio, expressed as percentage of applied radioactivity, in soil after adsorption/desorption (mean ± 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	0.04 mg/L	15.4 ± 0.5	18.4 ± 0.1	26.0 ± 0.3	17.0 ± 0.1
	0.18 mg/L	21.0 ±0.0	21.7 ± 0.1	29.5 ± 0.4	20.5 ± 0.5
	0.87 mg/L	29.1 ± 0.9	27.6 ± 0.3	37.9 ± 0.0	26.8 ± 0.7
	4.32 mg/L	36.9 ± 0.5	35.7 ± 0.2	46.6 ± 0.3	39.2 ± 0.2
Solid phase (total ^{14}C)		Not analyzed			
Non-extractable residues in soil, if measured		Not measured			
Total recovery		Not determined			
At the end of the desorption phase					
Supernatant solution	0.04 mg/L	10.5 ± 0.4	11.9 ± 0.2	16.5 ± 0.1	9.5 ± 0.1
	0.18 mg/L	13.5 ± 0.1	13.8 ± 0.1	17.6 ± 0.2	11.0 ± 0.3
	0.87 mg/L	17.2 ± 0.3	16.6 ± 0.3	20.0 ± 0.1	13.2 ± 0.3
	4.32 mg/L	19.4 ± 0.2	19.3 ± 0.1	21.3 ± 0.1	16.7 ± 0.1
Solid phase (total ^{14}C)[1]	0.04 mg/L	74.4 ± 7.7	68.0 ± 1.8	51.4 ± 0.5	78.0 ± 0.1
	0.18 mg/L	61.3 ± 0.7	60.2 ± 0.5	45.7 ± 0.3	64.3 ± 0.3
	0.87 mg/L	48.5 ± 1.2	51.6 ± 0.1	37.3 ± 0.2	60.4 ± 0.3
	4.32 mg/L	39.1 ± 1.0	43.9 ± 0.1	29.6 ± 0.4	54.7 ± 4.5

Non-extractable residues in soil, if measured		Not measured			
Total recovery	0.04 mg/L	100.3 ± 8.6	98.3 ± 1.7	93.9 ± 1.1	104.5 ± 0.1
	0.18 mg/L	95.8 ± 0.8	95.7 ± 0.3	92.8 ± 0.1	95.8 ± 0.9
	0.87 mg/L	94.8 ± 0.0	95.8 ± 0.4	95.2 ± 0.0	100.4 ± 0.7
	4.32 mg/L	95.4 ± 1.6	98.9 ± 0.3	97.5 ± 0.1	110.6 ± 4.6

Data were obtained from Tables 11-14, pp. 21-24 of the study report.
[1] All soils were combusted following desorption.

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

Concentration (mg a.i./kg soil)[1]	Laacher Hof AXXa sandy loam			Höfchen am Hohenseh 4a silt		
	on soil (mg a.i./kg)[2]	in solution (µg a.i./mL)[3]	% adsorbed	on soil (mg a.i./kg)[2]	in solution (µg a.i./mL)[3]	% adsorbed
0.27 (0.09)	0.201 ± 0.001	0.005 ± 0.002	84.6 ± 3.4	0.194 ± 0.000	0.006 ± 0.000	81.6 ± 0.3
1.20 (0.40)	0.944 ± 0.000	0.038 ± 0.000	79.0 ± 0.1	0.936 ± 0.001	0.039 ± 0.000	78.3 ± 0.5
5.80 (1.93)	4.089 ± 0.054	0.252 ± 0.008	70.9 ± 3.2	4.175 ± 0.015	0.239 ± 0.002	72.4 ± 1.0
28.8 (9.60)	18.182±0.137	1.592 ± 0.020	63.1 ± 1.3	18.531 ± 0.071	1.540 ± 0.011	64.3 ± 0.7

Concentration (mg a.i./kg soil)[1]	Stanley silty clay loam			Byromville loamy sand		
	on soil (mg a.i./kg)[2]	in solution (µg a.i./mL)[3]	% adsorbed	on soil (mg a.i./kg)[2]	in solution (µg a.i./mL)[3]	% adsorbed
0.27 (0.09)	0.176 ± 0.001	0.009 ± 0.000	74.0 ± 1.3	0.066 ± 0.000	0.006 ± 0.000	83.0 ± 0.5
1.20 (0.40)	0.843 ± 0.004	0.053 ± 0.001	70.5 ± 1.3	0.317 ± 0.002	0.037 ± 0.001	79.5 ± 2.2
5.80 (1.93)	3.582 ± 0.001	0.328 ± 0.000	62.1 ± 0.1	1.407 ± 0.014	0.232 ± 0.006	73.2 ± 2.7
28.8 (9.60)	15.387 ± 0.078	2.012 ± 0.012	53.4 ± 0.6	5.833 ± 0.024	1.695 ± 0.011	60.8 ± 0.6

Data were obtained from Tables 11-14, pp. 21-24 of the study report.
[1]Values in parentheses are for Byromville loamy sand

[2] Amount on soil was calculated by the reviewer by dividing the amount in soil at equilibrium by the initial amount of soil; e.g. 0.60301µg ÷ 3.0 g soil = 0.201 µg/g soil; equivalent to 0.201 mg/kg soil.
[3]Amount 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 µg ÷ 20 mL = 0.00549 µg/mL.

Table 10: Concentration of [phenyl-UL-^{14}C]JAU6476-desthio 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)[1]	Laacher Hof AXXa sandy loam			Höfchen am Hohenseh 4a silt		
	on soil (mg a.i./kg)[2]	in solution (µg a.i./mL)[3]	% desorbed as % of the adsorbed	on soil (mg a.i./kg)[2]	in solution (µg a.i./mL)[3]	% desorbed as % of the adsorbed
0.27 (0.09)	0.177 ± 0.018	Not reported	12.0 ± 9.1	0.162 ± 0.004	Not reported	16.7 ± 2.2
1.20 (0.40)	0.732 ± 0.009	Not reported	22.4 ± 1.0	0.719 ± 0.006	Not reported	23.2 ± 0.6
5.80 (1.93)	2.798 ± 0.070	Not reported	31.6 ± 1.7	2.976 ± 0.006	Not reported	28.7 ± 0.1
28.8 (9.60)	11.269 ± 0.277	Not reported	38.0 ± 1.5	12.640 ± 0.022	Not reported	31.8 ± 0.1

Concentration (mg a.i./kg soil)[1]	Stanley silty clay loam			Byromville loamy sand		
	on soil (mg a.i./kg)[2]	in solution (µg a.i./mL)[3]	% desorbed as % of the adsorbed	on soil (mg a.i./kg)[2]	in solution (µg a.i./mL)[3]	% desorbed as % of the adsorbed
0.27 (0.09)	0.122 ± 0.001	Not reported	30.6 ± 0.7	0.062 ± 0.000	Not reported	6.1 ± 0.1
1.20 (0.40)	0.546 ± 0.004	Not reported	35.2 ± 0.4	0.256 ± 0.001	Not reported	19.1 ± 0.4
5.80 (1.93)	2.149 ± 0.007	Not reported	40.0 ± 0.2	1.162 ± 0.007	Not reported	17.4 ± 0.5
28.8 (9.60)	8.519 ± 0.112	Not reported	44.6 ± 0.7	5.252 ± 0.433	Not reported	10.0 ± 7.4

Data were obtained from Tables 11-14, pp. 21-24 of the study report.
[1]Values in parentheses are for Byromville loamy sand
[2] Amount on soil was calculated by the reviewer by dividing the amount in soil at equilibrium by the initial amount of

soil; e.g. 54.546 µg ÷ 3 g soil = 18.182 µg/g.

[3] 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-desthio in the soils. K values are in mL/g. (Note: The desorption portion of the study is not acceptable to the PMRA and desorption constants reported by the study author are therefore not shown).

Soil	Adsorption[1]			
	$K_{F\ ads}$	1/n	r^2	K_{oc}
Laacher Hof AXXa sandy loam	12.46	0.79	1.0000	616.8
Höfchen am Hohenseh 4a silt	13.38	0.83	0.9997	625.3
Stanley silty clay loam	8.90	0.83	0.9996	536.4
Byromville loamy sand	4.13	0.80	0.9990	523.0

Data were obtained from Table 15, p. 25 of the study report.

$K_{F\ ads}$ - 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).

r^2 - 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. 21-24) using the following equation (p. 17):

$\ln (x/m) = \ln K_d + 1/n * \ln C$ 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. <u>ADSORPTION</u>: Adsorption decreased with increasing concentration. After 24 hours of equilibration, 63.1-84.6%, 64.3-81.6%, 53.4-74.0% and 60.8-83.0% of the applied [^{14}C]JAU6476-desthio was adsorbed to the sandy loam, the silt, the silty clay loam and the loamy sand, respectively (Tables 11-14, pp. 21-24 of the study report). Freundlich K_{ads} values were 12.46, 13.38, 8.90 and 4.13 mL/g for the sandy loam, the silt, the silty clay loam and the loamy sand, respectively; corresponding Freundlich K_{oc} values were 616.8, 625.3, 536.4 and 523.0 mL/g (Table 15, p. 25 of the study report).

The PMRA reviewer has verified the adsorption contants reported by the study author and obtained identical results. 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= 6.812, $r^2 = 0.971$, $p = 0.010$, n=4). No significant relationships was found between the Freundlich adsorption value and pH, % clay or CEC (in all cases: $r^2 = 0.000$, $p \geq 0.536$, n=4).

D. <u>DESORPTION</u>: The desorption phase of this study was only conducted with one desorption

cycle; however guidelines suggest three to five cycles (based on Guideline 106, OECD; T-1-255 Agriculture Canada). New desorption data are not required.

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).

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 February 17, 1998), but the microbial biomass was not reported. There does not seem to be an effect related to storage for this soil.

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

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.