Data Evaluation Report on the aerobic biotransformation of prothioconazole (JAU6476) in soil

PMRA Submission Number 2004-0843 EPA MRID Number 46246511

Data Requirement:

PMRA DATA CODE:	8.2.3.4.2
EPA DP Barcode:	DP 303488
OECD Data Point:	IIA 7.1.1, IIA 7.2.1
EPA Guideline:	162-1

Test material:

Common name: Prothioconazole

chemical name:

IUPAC: 2-[2-(1-Chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole-3-thione

CAS name: 2-[2-(1-Chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole-3-thione

CAS No: 178928-70-6

Synonyms: JAU 6476 Technical

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12/9/05

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: Hellpointner, E. 2001. Proazolthion (proposed) [JAU6476]: Degradation and Metabolism of JAU6476 in Aerobic Soils. Performing Laboratory: Bayer AG Crop Protection Business Group, Germany. Bayer CropScience, North Carolina. Unpublished. Report No. MR-104/01. July 25, 2001.

EXECUTIVE SUMMARY:

The aerobic biotransformation of radiolabelled prothioconazle (JAU6476) ([phenyl-UL-^{14}C] and [triazole-3,5-^{14}C] labels) was studied in a silt soil (Höfchen, pH 7.1, organic carbon 2.14 %, 8.5% sand, 81.3% silt, 10.2% clay) from Burscheid, Germany and a loamy sand soil (Byromville, pH 6.8, organic carbon 0.79%, 86.8% sand, 7.6% silt, 5.6% clay) from Georgia, USA. [^{14}C]Prothioconazole was applied at a rate of 0.267 mg a.i./kg soil, equivalent to 600 g a.i./ha, the highest annual rate. The experiment was conducted in compliance with German and OECD GLP and in accordance with BBA, EC, and SETAC guidelines (silt soil), as well as USEPA Subdivision N guidelines (loamy sand soil). [^{14}C]Prothioconazole was applied to soils that were maintained in the dark, under aerobic conditions, at 20±1°C and 50% of the maximum water holding capacity (silt soil) or 75% of 1/3 bar moisture (loamy sand soil) for up to 365 days. The test system consisted of Erlenmeyer flasks attached with traps for the collection of CO_2 and volatile organics. Samples were taken for analysis at 0, 1, 3, 7, 14, 30, 63, 90, 120, 181, 272 and 365 days of incubation. The soil samples were extracted with acetonitrile/water (80:20 v/v), to which was added 1 g/L of cysteine hydrochloride to prevent oxidative degradation of the active ingredient. Volatile organic compounds were extracted with acetonitrile, while $^{14}CO_2$ was liberated with HCl and purged into Liquid Scintillatin Counting (LSC) cocktails with nitrogen. The [^{14}C]prothioconazole residues were analysed by Normal Phase-Thin Layer Chromatography (NP-TLC). Identification of the transformation products was done by co-chromatography, High Performance Liquid Chromatography (HPLC), Liquid Chromatography-Mass Spectrometry (LC-MS) and LC-MS/MS. The extracted soil samples were oxidized by combustion and non-extractable radioactivity was quantified by LSC. The Limit of Detection (LOD) was approximately 2.5 µg/kg (about 1% of total applied radioactivity) and the Limit of Quantification (LOQ) was 4.9 µg/kg (2% of total applied radioactivity).

Overall material balance was good in both soils and both labels, ranging from 90.2 to 102.8% of the applied radioactivity (AR) in any treatment. The concentration of [phenyl-UL-^{14}C]prothioconazole in the silt decreased from 73.4% of the AR at day 0, to <2.0% of the AR at day 365, while [triazole-3,5-^{14}C]prothioconazole concentrations decreased from 81.0% of the AR at study initiation to 5.9% of the AR at study termination. In the loamy sand, [phenyl-UL-^{14}C]- and [triazole-3,5-^{14}C]prothioconazole concentrations decreased from 89.9 and 95.5% of the AR, respectively, at day 0 to 2.3 and 4.6% of the AR, respectively, at study termination. Transformation of [^{14}C]prothioconazole in either soil was very rapid and did not differ significantly between the two radiolabels. The half-life, determined by first order non-linear regression on non-transformed data, in the silt soil are 0.3 days for both radiolabels and the corresponding $t_{9/10}$ is 1.0 day for both radiolabels. The half-lives determined by linear regression on log-transformed data in the silt are 105 and 740 days for the phenyl and triazole labels, respectively. The half-life, determined by first order non-linear regression on non-transformed data, in the loamy sand are 1.2 and 1.4 days for phenyl and triazole labels, respectively, and the corresponding $t_{9/10}$ is 4.4 days for both radiolabels. The half-lives determined by linear regression

on log-transformed data in the loamy sand are 107 and 123 days for the phenyl and triazole labels, respectively.

Two major transformation products were detected in both soils. Concentrations of JAU6476-desthio reached a maximum of 46.5-49.4% of the AR at 7 days posttreatment in the silt and 38.4-41.2% of the AR on day 90 in the loamy sand; corresponding concentrations had decreased to 6.1-6.3% and 21.9-23.7% of the AR by day 365 (study termination). JAU6476-S-methyl was detected at a maximum of 11.3-12.8% of the AR on day 1 in the silt and 13.7-14.6% of the AR on day 7 in the loamy sand; corresponding concentrations decreased to 2.8-3.1% and 7.1-7.6% of the AR by day 365. Six characterized and three uncharacterized minor transformation products were detected, none of which exceeded 5% of the AR with the exception of JAU6476-sulfonic acid, detected at a maximum of 8.3% of the AR on day 181 in the silt ([triazole-3,5-^{14}C] label). All minor transformation products were decreasing by study termination. No unique transformation products were associated with either label other than 1,2,4-triazole, detected in samples treated with [triazole-3,5-^{14}C]prothioconazole. Total unidentified radioactivity was ≤6.1% of the AR.

Non-extractable [^{14}C]residues in the silt were 7.0-7.5% of the AR on day 0, were 28.2-30.3% of the AR on day 1 and then slowly increased to 47.3-56.4% of the AR on day 365. Similarly in the loamy sand, non-extractable [^{14}C]residues increased from 2.7-3.4% of the AR at study initiation to 20.6-22.1% of the AR on day 1 and gradually increased to 38.2-42.8% of the AR at the end of incubation period. The organic matter in the nonextractable residues showed similar ratios of humin/fulvic acids/humic acids fractions for both radiolabels, approximately 23:6:10 in the silt and 16:4:17 in the loamy sand.

The rapid movement of [^{14}C]residues to the non-extractable phase by day 1 may be artificially reducing the DT_{50} and DT_{90} values. The decrease in [^{14}C]prothioconazole concentrations was not proportional to the increase in non-extractable [^{14}C]residues, and major transformation products JAU6476-desthio and JAU6476-S-methyl were detected in quantities >10% by 1-3 days posttreatment in all treatments, which indicates that at least part of the parent compound was transformed and did not simply move to the non-extractable phase.

At the end of the study, 17.9% and 5.3% of the AR was present as CO_2 in the silt samples treated with [phenyl-UL-^{14}C] and [triazole-3,5-^{14}C]prothioconazole, respectively. In the loamy sand, CO_2 represented 6.1% and 0.7% of the AR in samples treated with [phenyl-UL-^{14}C] and [triazole-3,5-^{14}C]prothioconazole, respectively, at day 365. The greater mineralization of [^{14}C]prothioconazole residues in the silt compared to the loamy sand may be due to the much higher microbial biomass in the silt soil. No volatile organics were detected in either soil throughout the entire study period.

Results Synopsis:

Silt (Höfchen soil)
Half-life, nonlinear (both labels): 0.3 days
Half-life, log-linear (phenyl label): 105 days
Half-life, log-linear (triazole label): 740 days
$t_{9/10}$: 1.0 day (both labels)
Observed DT_{50} (both labels): 0-1 day
Observed DT_{90} (both labels): 0-1 day

Loamy sand (Byromville)
Half-life, nonlinear (phenyl label): 1.2 days
Half-life, nonlinear (triazole label): 1.4 days
Half-life, log-linear (phenyl label): 107 days
Half-life, log-linear (triazole label): 123 days
$t_{9/10}$: 4.4 days (both labels)
Observed DT_{50} (both labels): 0-3 days
Observed DT_{90} (both labels): 3-7 days

When nonextractable material is added back in with parent, due to large amounts and increasing pattern of nonextractable material (29.7-56.4% of the applied from 3 days posttreatment through study termination; both labels, both soils), calculated linear half-lives on log-transformed data are statistically stable. This is likely because nonextractable material is composed of nonextracted parent in addition to non-extracted degradates. [^{14}C]Prothioconazole is degrading as evidenced by the formation of major degradates and CO_2. However, nonlinear half-lives and observed DT_{50}s may underestimate aerobic soil metabolism half-life due to the large amounts of applied radioactivity which immediately become nonextractable material (28.2-30.0% of applied in Hofchen silt and 20.6-22.1% of applied in Byrombille loamy sand at 1 day posttreatment) and may potentially still be parent.

Major transformation products (both soils, both labels):
- JAU 6476-desthio
- JAU 6476-S-methyl

Minor transformation products (both soils, both labels):
- JAU6476-sulfonic acid
- JAU6476-triazolinone
- JAU6476-6-OH-desthio
- JAU6476-3-OH-desthio
- 2-chlorobenzoic acid
- 1,2,4-triazole ([triazole-3,5-^{14}C]prothioconazole samples only)

Study Acceptability: This study is classified acceptable and satisfies the guideline requirement for an aerobic biotransformation study in soil.

I. MATERIALS AND METHODS:

GUIDELINE FOLLOWED: BBA-Guideline for the fate of crop protection agents in soil; EC-Directive 91/414/EEC Annex I, Part 7 and Annex II Part 9; SETAC Procedures for Assessing the Environmental Fate and Ecotoxicity of Pesticides; USEPA Pesticide Assessment Guidelines, Subdivision N, 162-1 (1982), Addendum 5 on Data Reporting (1988) and EPA-540/9-85-015 (1985), Environmental Fate Rejection Rate Analysis, USEPA Draft (1992).
The following deviations were noted by the study author: The test series with the German soil was incubated based on the requirements of the European Guidelines while the test series with the US soil was incubated based on the requirements of the USEPA Guidelines. The deviations do not affect the validity of the study.

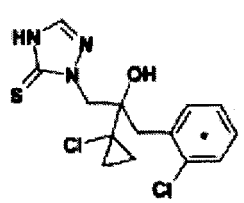
COMPLIANCE: Chemikaliengesetz, dated 1994-07-25, attachment 1 dated 1997-05-14; OECD-GLP, dated 1997-11-26. Signed and dated GLP, Quality Assurance and Data Confidentiality statements were provided.

A. MATERIALS:

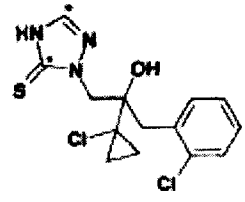
1. Test Material Radiolabelled prothioconazole (JAU6476)

Chemical Structure:

[phenyl-UL-^{14}C] JAU6476



[triazole-3,5-^{14}C] JAU6476



* indicates position of radio labeling

Description: Technical pure ^{14}C labeled products, solid, dried in a vacuum

Purity:

[phenyl-UL-^{14}C] JAU6476

Analytical purity: >99% Lot/Batch No.: ECW 11145
Radiochemical purity: >99%
Specific activity: 2.97 MBq/mg (80 µCi/mg)
Locations of the radio label: phenyl ring

[triazole-3,5-^{14}C] JAU6476

Analytical purity: >99% Lot/Batch No.: 10708/1
Radiochemical purity: >99%
Specific activity: 1.94 MBq/mg (52 µCi/mg)
Locations of the radio label: triazole ring

Storage conditions of test chemicals: Test substances were kept cool and in the dark, no temperature was provided (p. 17). Reference substances were stored in the refrigerator (p. 18).

Table 1: Physico-chemical properties of prothioconazole.

Parameter	Values		Comments
Water solubility (20°C)	pH	Solubility (mg/L)	Low solubility at acidic pH, very soluble at alkaline pHs.
	4	5	
	8	300	
	9	2000	

Vapour pressure/volatility	Temperature (°C) Vapor pressure (Pa) 20 $<<4 \times 10^{-7}$ 25 $<<4 \times 10^{-7}$	Relatively non-volatile under field conditions.
UV absorption	Peak maxima at 275 nm. No absorption at > 300 nm.	Phototransformation is not expected to be an important route of transformation
pK_a	$pK_a = 6.9$	Weak acid, anion at neutral and alkaline pHs
log K_{ow}	pH log K_{ow} 4 4.16 7 3.82 9 2.0 log K_{ow} in water = 4.05	Potential for bioaccumulation at neutral and acidic pH.
Stability of compound at room temperature, if provided	Thermally stable at room temperature under air. Stable to most metals. Colour changes observed in the presence of copper materials.	Thermally stable at room temperature under air.

Data were obtained from Chemistry Review.

2. Soil Characteristics

Table 2: Description of soil collection and storage.

Description	Höfchen Silt	Byromville loamy sand
Geographic location	Höfchen, Burscheid, Germany (soil HF)	Byromville, Georgia, USA (soil BV)
Pesticide use history at the collection site	Not reported	Not reported
Collection procedures	About 10 kg fresh weight with about 16% soil moisture were sampled.	About 18 kg (40 lbs) fresh weight with about 3% soil moisture were sampled.
Sampling depth (cm)	20 cm (top 8 inches)	15 cm (top 6 inches)
Storage conditions	At about 4°C, not closed air-tight	At about 4°C, not closed air-tight
Storage length	From November 4, 1997 to February 12, 1998	From January 26, 1998 to February 12, 1998
Soil preparation (eg: 2 mm sieved; air dried etc.)	5 days prior to start of study, the soil was gently air dried and screened to ≤2 mm.	5 days prior to start of study, the soil was gently air dried and screened to ≤2 mm.

Table 3: Properties of the soils.

Property	Höfchen	Byromville
Soil texture	Silt	Loamy sand
% sand	8.5	86.8
% silt	81.3	7.6
% clay	10.2	5.6
pH	7.1	6.8
Organic carbon (%)	2.14	0.79
CEC (meq/100 g)	15	4.3
Moisture at 1/3 atm (%)	35.56	4.8
Bulk density (g/cm^3)	2.09	1.59
Soil Taxonomic classification	Loamy, mixed, mesic Typic Argudalfs	Loamy, siliceous, thermic Arenic Kandiudults
Soil Mapping Unit (for EPA)		

B. EXPERIMENTAL CONDITIONS:

1) Preliminary experiments: No preliminary experiments were described.

2) Experimental conditions:

Table 4: Experimental design.

Parameter		**Höfchen silt**	**Byromville loamy sand**
Duration of the test		365 days	
Soil condition: (Air dried/fresh)		Fresh sampled soil, gently air dried in order to get it seived, then pre-incubated at test conditions for 5 days	
Soil (g/replicate)		100 g dry weight/replicate	
Test concentrations (mg a.i./kg soil) and equivalent g a.i./ha		0.267 mg a.i./kg soil, equivalent to 600 g a.i./ha	
Control conditions, if used (present differences from other treatments, i.e., sterile/non-sterile, experimental conditions)		Controls were used for microbial biomass determinations.	
No. of Replication	Controls, if used	No replication (1 flask per label, for each sampling interval) (Tables 1-2, 4-5, pp.38-40, 42-43)	
	Treatments	No replication (1 flask per label, for each sampling interval)	
Test apparatus (Type/material/volume)		300 mL Erlenmeyer glass flask .	
Details of traps for CO_2 and organic volatile, if any		Solid trap attachment containing soda lime and polyurethane foam to trap CO_2 and organic volatiles, respectively. The attachments are permeable to oxygen.	
If no traps were used, is the system closed/open		N/A	
Identity and concentration of co-solvent		Mill-Q-water + acetonitrile; 95 + 5 (v/v); The addition of a small portion of co-solvent was regarded necessary for getting 26.7 µg of test substance well diluted in 500 µL of application solution.	
Test material application	volume of test solution used/treatment	Phenyl label: 500 µL Triazole label: 479 µL	

Parameter		Höfchen silt		Byromville loamy sand	
	application method (eg: applied on surface, homogeneous mixing etc.)	Manually distributed by a pipette (Eppendorf)			
	Is the co-solvent evaporated:	Not reported			
Microbial biomass/microbial population of control soil (mg C microbial/kg dry weight)		Initial	Final	Initial	Final
		1400	356	23	<20
Microbial biomass/microbial population of treated soil, if provided		Initial	Final	Initial	Final
		1432	356	25	<20
Any indication of the test material adsorbing to the walls of the test apparatus		No			
Experimental conditions	Temperature (°C)	20±1°C			
	Moisture content	50% of WHC_{max} (31.55 g water/100 g soil)		75% of 1/3 bar (3.6 g water/100 g soil)	
	Moisture maintenance method:	Periodic re-weighing of test vessels and addition of loss by pipetting of Milli-Q water			
	Continuous darkness (Yes/No):	Yes			
Other details, if any					

3. Aerobic conditions: So-called bio-meter flask system with solid trap permeable for air (passive exchange of air), incubated in a large air-conditioned room. No other information was provided.

4. Supplementary experiments: No supplementary experiments were described.

5. Sampling:

Table 5: Sampling details.

Parameters	Details
Sampling intervals	0 (2 hours), 1, 3, 7, 14, 30, 63, 90, 120, 181, 272 and 365 days
Sampling method for soil samples	Soil was extracted immediately after sampling of vessels. The total soil portion of each test vessel was transferred (using a portion of the 1st extraction solvent) into a centrifuging beaker. The extraction solvent contained 1 g/L cysteine hydrochloride as a protecting agent to prevent oxidative degradation of the active ingredient.
Method of collection of CO_2 and volatile organic compounds	Solid trap containing soda lime for absorption of $^{14}CO_2$ and polyurethane foam for volatile organics
Sampling intervals/times for:	
microbial biomass determinations:	0, 120 and 365 days
moisture content:	0 (2 hours), 14, 28, 42, 56, 70, 112, 142, 181, 217, 244, 272, 295, 321, 343 and 365 days (Tables 4-5, pp. 42-43)
redox potential/other:	N/A
Sample storage before analysis	N/A for soil samples and polyurethane foam of the solid traps which were processed immediately. The traps containing the soda lime and the quartz wool were not always processed immediately and were stored in a freezer, if applicable.
Other observations, if any	

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods: The soil was extracted immediately after sampling. The total soil portion of each test vessel was transferred into a centrifuging beaker and extracted 3 times with acetonitrile/water (80:20 v/v) on a shaker. The extraction solvent contained 1 g/L cysteine hydrochloride as a protecting agent to prevent oxidative degradation of the active ingredient. After each shaking procedure, the solution was centrifuged for 20 minutes and the clear supernatant was decanted through a paper filter.

The soil was then subjected to a hot extraction procedure by refluxing for 1 hour. Each filter paper was pressed into pellets which were combusted in an oxidizer. For an overall evaluation and calculation of material balances the radioactivity of the filters was added to the non-extracted (bound) residues of soil.

Volatile organic compounds were extracted with acetonitrile using an ultrasonic bath while $^{14}CO_2$ was liberated with 18% HCl and purged into ice-cooled scintillation cocktail with nitrogen.

Non-extractable residue determination: Non-extracted radioactivity was determined by combusting aliquots of air-dried homogenised soils in an oxidizer. The resulting carbon dioxide was absorbed in Oxysolve C400 and measured in an LS counter.

Total ^{14}C measurement: The radioactivity in solution was measured by LSC.

Identification and quantification of the parent and transformation products: [^{14}C]Prothioconazole residues in the soil extracts were analysed by normal phase radio-thin-layer chromatography (NP-TLC). Aliquots of extracts/solutions were spotted on either silica gel Si60 or reversed phase RP-18 plates using an automatic plate spotter (Linomat IV, Camag) at 20 mm distance from the edge. The plates were developed in a saturated glass tank using either of two solvent systems: SS1: dichloromethane/methanol/25% aqueous NH_3 (90/10/1 v/v/v) containing 1 g/L ionol; SS2: acetonitrile/water/methanol/acetic acid (70/25/5/1 v/v/v/v) and containing 1 g/L ionol. SS1 was used for quantification of the parent compound and its transformation products, while SS2 was used mainly for confirmation.

The distribution of radioactive zones on the plates was measured using a Bio-Imaging Analyser (BAS 2000, Fuji Co.) and radioactive regions were quantified with TINA® software (Version 2.09G, Raytest). The co-chromatographed spots of the non-radioactively labelled references were detected by means of a UV chamber (Camag) at 254 nm.

Identification of the transformation products was made by co-chromatography, HPLC, LC/MS and LC/MS/MS methods.

The agreement of the R_f-value of the radioactive zone in the soil extracts with that of the cochromatographed reference was considered to be indicative of the identity of a substance in a radioactive zone. Then the major radiolabelled zones were isolated from crude soil extracts by HPLC and the isolates were investigated by LC-MS and/or LC-MS/MS.

The conditions for HPLC analysis were the following: HP LC 1090 coupled to a Ramona-92 RA monitor with a solid scintillation flow-through cell (Raytest); LiChrospher 100 RP18e column (5µm, 250 x 4mm); gradient mobile phase (A) 1% acetic acid in water or (B) 1% acetic acid in acetonitrile [percent A:B at 0-1 min. 100:0 (v:v), 10 min. 60:40, 35 min. 40:60, 40 min. 0:100, 45 min, 0:100], flow rate 1.2 mL/minute (p.26).

The electro-spray inonization MS spectra were obtained with a TSQ 7000 instrument by Finnigan. For the MS/MS experiments, argon gas was used as the collision gas. The chromatographic conditions for the MS experiments are provided on page 27 of the study report. The radioactivity detector (Ramona 90, Raytest) was either coupled via a flow splitter between the HPLC instrument (HP 1050, Hewlett Packard) and the mass spectrometer, or it was put in line between the HPLC and the mass spectrometer.

As the portion of bound residues increased with incubation time and accounted for more than 30% of the AR, aliquots of selected soil samples were further extracted (over night) with 0.01M sodium pyrophosphate to characterize bound residues. However, the method described is so harsh that it would have chemically altered prothioconazole and its transformation products. Extracts and solids were separated by centrifugation. Soil residues were air-dried and radio-assayed by combustion/LSC to determine the portion which remained unextracted ("humin"). The sodium pyrophosphate extract was acidified to pH 2 with concentrated sulfuric acid and left to stand overnight at room temperature. The clear supernatant ("fulvic acids")was separated from the dark brown to black precipitate. Radioactivity in the supernatant was determined by LSC. The black precipitate ("humic acids") was dissolved in 0.1 N NaOH and then radio-assayed by LSC.

Detection limits (LOD, LOQ) for the parent compound and transformation products: Detection limits (LOD, LOQ) for the parent compound and transformation products were approximately 1% (about 2.5 µg/kg) and 2% (about 4.9 µg/kg) of the applied radioactivity, respectively (pp. 25, 28).

II. RESULTS AND DISCUSSION:

A. TEST CONDITIONS: Aerobicity was not measured but the study author claims that it was achieved via the use of a so-called bio-meter flask system with a solid trap permeable to air (passive exchange of air), incubated in a large air-conditioned room. No other information was provided.

The anticipated standardized soil moisture was maintained during the study. The moisture in the Höfchen soil (silt) decreased from 50% to a mean of 49% of WHCmax. Because of the rather low water holding capacity of the Byromville soil (loamy sand), the moisture decreased from 75% to a mean of 61% of the 1/3 bar moisture over the course of the study. This was regarded as inevitable between two sampling intervals and as usual for that type of soil, either under laboratory or field conditions.

Soil temperature was maintained at 20±1°C (range of 20.3-20.9°C) throughout the study.

The measured values for microbial biomass were in the usual range expected of soils taken from agricultural fields, according to the study author. According to the author, the decrease in

biological activity in the isolated soil is inevitable, under the conditions of a laboratory experiment. Similar microbial biomass determinations were observed between soils treated and not treated with prothioconazole. The parent compound did not affect microbial biomass in the test soil.

B. MATERIAL BALANCE:

In silt (Höfchen soil), total recovery of radiolabelled material averaged 94.2±3.6% of the applied radioactivity (AR) (range: 90.2-102.8% of the AR) in the samples treated with [phenyl-UL-^{14}C]prothioconazole and 97.8±2.4% of the AR (range: 94.2-102.3% of the AR) in the samples treated with [triazole-3,5-^{14}C]prothioconazole (reviewer-calculated).

In loamy sand (Byromville soil), total recovery of radiolabelled material averaged 95.1±2.4% of the AR (range: 92.2-101.4% of the AR) in samples treated with [phenyl-UL-^{14}C]prothioconazole and 97.5±2.3% of the AR (range: 94.4-102.0% of the AR) in samples treated with [triazole-3,5-^{14}C]prothioconazole (reviewer-calculated).

Table 6: Biotransformation of [phenyl-UL-^{14}C]prothioconazole (JAU6476), expressed as percentage of applied radioactivity, in silt (Höfchen soil) under aerobic conditions (n=1).

Compound	Sampling times (days)											
	0	1	3	7	14	30	63	90	120	181	272	365
Parent compound	73.4	7.9	6.1	2	4.2	2.9	2.2	<2.0	<2.0	<2.0	<2.0	<2.0
JAU6476-desthio	15.9	39.8	38.6	46.5	35.8	35	35	33.8	17.5	16.8	8.8	6.3
JAU6476-S-methyl	<2.0	11.3	10.7	10.3	8.4	7.5	6.4	6.6	6	4.9	2.6	2.8
JAU6476-triazolinone	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
JAU6476-6-OH-desthio	n.d.	<2.0	<2.0	<2.0	3.1	3.4	3.2	2.2	4.2	2.0	2.9	2.9
JAU6476-3-OH-desthio	n.d.	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	n.d.	<2.0	n.d.	<2.0	<2.0
JAU6476-sulfonic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	3.2	3.7	3.1	3.1
2-chlorobenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
Z2	<2.0	2.2	2.3	<2.0	2.7	2.9	2.5	<2.0	n.d.	n.d.	<2.0	n.d.
Z4	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0
Z17	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0
Origin	1.4	1.1	2.4	0.9	2.4	2.7	1.2	0.9	2.6	2.0	2.5	2.2
Unidentified radioactivity	2.4	3.8	2.4	<2.0	2.8	<2.0	<2.0	<2.0	<2.0	<2.0	3.1	3.0
Total extractable residues	95.8	68.4	66.5	63.8	61.4	58.4	52.1	48.2	39.8	32.3	28.2	25.0
CO_2	--	0.2	0.7	1.5	2.5	3.1	4.6	6.5	10.7	14.0	15.9	17.9
Total volatile organics	--	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Non-extractable residues	7.0	28.2	30.8	28.4	30.5	32.5	37.4	37.0	42.0	45.2	46.5	47.3
Total % recovery	102.8	96.8	98.0	93.7	94.4	94.0	94.1	91.8	92.5	91.5	90.6	90.2

n.d = not detected; LOQ = 2% of applied radioactivity (4.9 µg/kg)

Table 7: Biotransformation of [triazole-3,5-^{14}C]prothioconazole (JAU6476), expressed as percentage of applied radioactivity, in silt (Höfchen soil) under aerobic conditions (n=1).

Compound	Sampling times (days)											
	0	1	3	7	14	30	63	90	120	181	272	365
Parent compound	81.0	9.0	6.7	<2.0	4.6	3.1	<2.0	<2.0	5.6	<2.0	6.6	5.9
JAU6476-desthio	10.2	38.8	39.4	49.4	39.5	37.7	35.9	34.8	15.1	16.6	7.9	6.1
JAU6476-S-methyl	<2.0	12.8	11.8	10.7	10.3	9.0	7.4	6.3	6.4	5.2	3.1	3.1
JAU6476-triazolinone	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0
JAU6476-6-OH-desthio	n.d.	<2.0	<2.0	<2.0	2.4	3.3	3.3	2.1	4.6	2.4	2.6	2.3
JAU6476-3-OH-desthio	n.d.	<2.0	<2.0	n.d.	2.1	<2.0	<2.0	n.d.	<2.0	n.d.	<2.0	n.d.
JAU6476-sulfonic acid	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0	2.4	3.3	8.3	3.5	3.3
2-chlorobenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	2.2	<2.0
1,2,4-triazole	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	n.d.
Z2	<2.0	<2.0	2.5	<2.0	2.7	3.0	3.3	3.0	n.d.	<2.0	<2.0	n.d.
Z4	n.d.	n.d.	<2.0	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0
Z17	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0
Origin	<2.0	<2.0	2.4	<2.0	2.1	2.9	<2.0	<2.0	2.8	3.2	3.3	2.9
Unidentified radioactivity	<2.0	3.5	2.6	2.2	2.2	2.3	<2.0	<2.0	3.6	3.1	4.6	6.1
Total extractable residues	94.8	68.7	69.2	67.2	65.9	63.7	57.1	52.7	46.7	40.1	36.1	33.4
CO_2	--	<0.1	<0.1	<0.1	0.1	0.2	0.7	1.1	2.0	2.9	4.9	5.3
Total volatile organics	--	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Non-extractable residues	7.5	30.3	31.3	32.0	32.5	34.7	40.2	41.7	48.3	52.7	53.3	56.4
Total % recovery	102.3	99.0	100.6	99.2	98.4	98.6	98.0	95.5	97.0	95.7	94.2	95.1

n.d = not detected; LOQ = 2% of applied radioactivity (4.9 µg/kg)

Table 8: Biotransformation of [phenyl-UL-^{14}C]prothioconazole (JAU6476), expressed as percentage of applied radioactivity, in loamy sand (Byromville soil) under aerobic conditions (n=1).

Compound	Sampling times (days)											
	0	1	3	7	14	30	63	90	120	181	272	365
Parent compound	89.9	46.3	20.5	8.5	8.2	5.2	4.3	4.8	2.5	2.4	4.1	2.3
JAU6476-desthio	7.5	14.3	21.0	31.7	28.8	28.3	32.6	41.2	23.9	29.5	23.5	21.9
JAU6476-S-methyl	<2.0	6.6	11.3	13.7	12.9	12.3	11.7	8.3	9.8	9.2	7.0	7.1
JAU6476-triazolinone	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0
JAU6476-6-OH-desthio	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0	<2.0	<2.0
JAU6476-3-OH-desthio	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
JAU6476-sulfonic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0	<2.0	<2.0
2-chlorobenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
Z2	n.d.	<2.0	<2.0	n.d.	<2.0	<2.0	<2.0	n.d..	<2.0	<2.0	n.d.	n.d.
Z4	n.d.	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0
Origin	<2.0	3.0	3.9	3.2	3.6	4.5	3.0	<2.0	2.9	3.2	4.4	3.8
Unidentified radioactivity	<2.0	2.8	3.6	<2.0	2.4	3.2	<2.0	<2.0	2.2	2.3	3.7	4.6
Total extractable residues	98.7	74.3	63.1	59.4	58.8	56.4	55.2	58.3	49.9	49.1	50.6	47.9
CO_2	--	0.1	0.2	0.3	0.4	0.8	2.0	0.4	3.0	3.1	4.3	6.1
Total volatile organics	--	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Non-extractable residues	2.7	20.6	29.7	36.0	35.2	38.0	39.1	36.9	40.1	41.4	40.2	38.2
Total % recovery	101.4	95.1	93.0	95.8	94.4	95.1	96.4	95.7	93.0	93.6	95.1	92.2

n.d = not detected; LOQ = 2% of applied radioactivity (4.9 µg/kg)

Table 9: Biotransformation of [triazole-3,5-^{14}C] prothioconazole (JAU6476), expressed as percentage of applied radioactivity, in loamy sand (Byromville soil) under aerobic conditions (n=1).

Compound	Sampling times (days)											
	0	1	3	7	14	30	63	90	120	181	272	365
Parent compound	95.5	52.1	24.6	8.4	9.2	5.1	3.4	2.6	2.1	2.3	3.8	4.6
JAU6476-desthio	2.4	11.7	20.9	31.7	29.9	30.0	34.0	38.4	25.1	29.1	23.2	23.7
JAU6476-S-methyl	n.d.	6.4	12.4	14.6	14.4	13.2	13.2	11.7	10.8	10.2	7.2	7.6
JAU6476-triazolinone	n.d.	n.d.	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0
JAU6476-6-OH-desthio	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0	<2.0	<2.0
JAU6476-3-OH-desthio	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
JAU6476-sulfonic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0	2.0	2.3
2-chlorobenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
1,2,4-triazole	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0
Z2	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0	<2.0	n.d.	<2.0	<2.0	<2.0	n.d.
Z4	n.d.	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0
Origin	<2.0	3.0	2.9	2.9	4.2	4.9	2.4	<2.0	3.3	4.3	4.6	4.0
Unidentified radioactivity	<2.0	2.6	2.7	<2.0	<2.0	3.2	2.4	<2.0	2.9	2.9	4.4	3.7
Total extractable residues	98.6	76.3	66.3	60.1	62.5	58.6	56.5	55.2	52.7	51.6	51.7	54.1
CO_2	--	<0.1	<0.1	<0.1	0.1	0.1	0.1	0.2	0.3	0.4	0.5	0.7
Total volatile organics	--	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Non-extractable residues	3.4	22.1	32.6	34.4	37.6	38.3	42.1	40.5	42.6	44.7	42.5	42.8
Total % recovery	102.0	98.5	98.9	94.4	100.2	96.9	98.8	95.9	96.7	95.5	94.7	97.7

n.d = not detected; LOQ = 2% of applied radioactivity (4.9 µg/kg)

C. TRANSFORMATION OF PARENT COMPOUND:

The concentration of [^{14}C]prothioconazole in silt (Höfchen soil) decreased from 73.4% of the applied radioactivity (AR) at day 0, to <2.0% of the AR at the end of the study period in the soil treated with [phenyl-UL-^{14}C] prothioconazole, while it decreased from 81.0% of the AR at study initiation to 5.9% of the AR at study termination in the soil treated with [triazole-3,5-^{14}C]prothioconazole.

In loamy sand (Byromville soil), [^{14}C]prothioconazole concentrations decreased from 89.9% of the AR at day 0 to 2.3% of the AR at study termination in the soil treated with [phenyl-UL-^{14}C] prothioconazole while they decreased from 95.5% of the AR at day 0, to 4.6% of the AR after 365 days of exposure in the soil treated with [triazole-3,5-^{14}C]prothioconazole.

Transformation of the parent compound was very rapid, with less than 10% of the parent compound remaining after 1-7 days for both labels in both soils.

HALF-LIFE: The study author used values of percent of applied radioactivity (%AR) to determine the DT_{50} (50% decline time) and DT_{90} (90% decline time) for prothioconazole, as opposed to expressing the values as percent of initial radioactivity (%IR), the latter of which adjusts %AR values to set 100% at time 0. The EAD-reviewer used SigmaPlot to recalculate the half-lives with values of %IR following a first order non-linear regression model of exponential decay (**Table 10**). The USEPA-reviewer used Excel 2002 to calculate half-lives via non-linear and log-transformed linear regression on values of %AR, finding that DT_{50}s did not differ significantly whether values of %AR or %IR were used. Log-linear half-life values were calculated to characterize degradation across time periods considered for chronic exposure (**Table 11**).

The study author combined the data for both labels to estimate the DT50s in the two soils (**Table 12**). Reviewers calculated half-lives for both radiolabels separately. When values were below the limit of quantification (LOQ; 2% of the AR), the study author used the 'exact' values ranging from 0.6-1.9% of the AR in the calculations of transformation kinetics for prothioconazole in silt soil (Table 23 of study report, p. 61). Due to the uncertainty of values below the LOQ, reviewers assigned a value equal to the limit of detection (LOD; 1% of the AR) in calculations when values were reported to be below the LOQ.

For silt, the DT_{50} and DT_{90} empirically observed from the transformation curves of either radiolabel are both 0-1 day . Based on first order nonlinear regression on non-transformed data, the half-lives and $t_{9/10}$s in the silt for both radiolabels are 0.3 and 1.1 days, respectively. The half-lives calculated using linear regression on natural log-tranformed data in the silt are 105 days for the phenyl label and 740 days for the triazole label.
For loamy sand, the DT_{50} and DT_{90}s determined by PMRA via curvilinear interpolation of both radiolabel curves are approximately 1 and 6.5 days, respectively for the phenyl label and 1.2 days and 6.8 days, respectively for the triazole label. The DT_{50} and DT_{90} empirically observed from

the transformation curves of either radiolabel were both 0-1 day. Based on first order nonlinear regression on non-transformed data, the half-lives and $t_{9/10}$s in the loamy sand are 1.2 and 4.2 days, respectively, for the phenyl label and 1.4 days and 4.7 days, respectively, for the triazole label. The half-lives calculatd using linear regression on natural log-tranformed data in the loamy sand are 107 days for the phenyl label and 123 days for the triazole label.

Table 10: Half-lives and DT_{50}s for [^{14}C]prothioconazole, calculated by EAD-reviewer.

Soil type	**First order non-linear regression model**			**observed DT_{50} from curvilinear interpolation (days)**	**observed DT_{90} from curvilinear interpolation (days)**
	half-life ($t_{1/2}$) and $t_{9/10}$ (days)	**Regression equation y = a*exp(-b*x)**	**r^2**		
silt (Höfchen soil)					
phenyl label	$t_{1/2}$ = 0.3 $t_{9/10}$ = 1.1	a = 99.9769 b = 2.1971	0.982	~0.5	~1
triazole label	$t_{1/2}$ = 0.3 $t_{9/10}$ = 1.1	a = 99.9749 b = 2.1690	0.96	~0.5	~1
loamy sand (Byromville soil)					
phenyl label	$t_{1/2}$ = 1.2 $t_{9/10}$ = 4.2	a = 97.6223 b = 0.5379	0.964	~1	~6.5
triazole label	$t_{1/2}$ = 1.4 $t_{9/10}$ = 4.7	a = 97.4081 b = 0.4814	0.97	~1.2	~6.8

Table 11: Log-linear half-lives for [^{14}C]prothioconazole, calculated by USEPA-reviewer.

Soil type	Log-linear model		
	Half-life (days)	Regression equation ln(y) = -kx + ln(b)	r^2
silt (Höfchen soil)			
phenyl label	105	k = 0.00662, b = 5.18	0.3850
triazole label	740	k = 0.00094, b = 4.34	0.0076
loamy sand (Byromville soil)			
phenyl label	107	k = 0.00648, b = 14.08	0.4311
triazole label	123	k = 0.00563, b = 12.97	0.2893

TRANSFORMATION PRODUCTS: JAU6476-desthio (SXX 0665) and JAU6476-S-methyl were the two major transformation products. The data indicate that these transformation products seem to further transform and do not accumulate in the soil. Minor transformation products which were characterized were JAU6476-sulfonic acid, JAU6476-triazolinone, JAU6476-6-OH-desthio, JAU6476-3-OH-desthio, 2-chlorobenzoic acid and 1,2,4-triazole ([triazole-3,5-^{14}C]prothioconazole samples only).

Concentrations of JAU6476-desthio reached a maximum of 46.5-49.4% of the AR at 7 days posttreatment in the silt and 38.4-41.2% of the AR at 90 days posttreatment in the loamy sand; corresponding concentrations had decreased to 6.1-6.3% and 21.9-23.7% of the AR by day 365 (study termination). JAU6476-S-methyl was detected at a maximum concentration of 11.3-12.8% of the AR on day 1 in the silt and 13.7-14.6% of the AR on day 7 in the loamy sand; corresponding concentrations decreased to 2.8-3.1% and 7.1-7.6% of the AR at study termination. Six characterized (JAU6476-sulfonic acid, JAU6476-6-OH-desthio, JAU6476-triazolinone, JAU6476-3-OH-desthio, 2-chlorobenzoic acid and 1,2,4-triazole ([triazole-3,5-^{14}C] label only)) and three uncharacterized minor transformation products were detected, none of which exceeded 5% of the AR with the exception of JAU6476-sulfonic acid, detected at a maximum of 8.3% of the AR on day 181 in the silt ([triazole-3,5-^{14}C] label). All minor transformation products were decreasing by study termination. No unique transformation product were associated with either label,other than 1,2,4-triazole detected in samples treated with [triazole-3,5-^{14}C]prothioconazole. Total unidentified radioactivity was ≤6.1% of the AR.

NON-EXTRACTABLE AND EXTRACTABLE RESIDUES:

Extractable [^{14}C]residues in the silt decreased from 95.8% ([phenyl-UL-^{14}C] label) and 94.8% ([triazole-3,5-^{14}C] label) of the AR at day 0 to 25.0% ([phenyl-UL-^{14}C] label) and 33.4% ([triazole-3,5-^{14}C] label) of the AR, at study termination. In the loamy sand, extractable [^{14}C]residues in samples treated with [phenyl-UL-^{14}C]prothioconazole decreased from 98.7% of the AR on day 0 to 47.9% of the AR on day 365, while those in samples treated with [triazole-3,5-^{14}C]prothioconazole decreased from 98.6% of the AR to 54.1% of the AR over the same time period.

Non-extractable [^{14}C]residues in the silt were 7.0% and 7.5% of the AR on day 0 in the vessels treated with [phenyl-UL-^{14}C]prothioconazole and [triazole-3,5-^{14}C]prothioconazole, respectively, were 28.2 and 30.3% of the AR on day 1 and then slowly increased to 47.3% and 56.4% of the AR on day 365. Similarly in the loamy sand, non-extractable [^{14}C]residues increased from 2.7% and 3.4% of the AR at study initiation ([phenyl-UL-^{14}C] and [triazole-3,5-^{14}C] prothioconazole, respectively) to 20.6 and 22.1% of the AR on day 1 and gradually increased to 38.2 % and 42.8% of the AR at the end of incubation period.

The rapid movement of [^{14}C]residues to the non-extractable phase by day 1 may be artificially reducing the DT_{50} and DT_{90}s. The decrease in [^{14}C]prothioconazole concentrations is not proportional to the increase in non-extractable [^{14}C]residues, and major transformation products JAU6476-desthio and JAU6476-S-methyl are detected in quantities >10% by 1-3 days posttreatment in all treatments which indicates that at least part of the parent compound is transforming and not simply moving to the non-extractable phase.

The organic matter in the nonextractable residues showed similar ratios of humin/fulvic acids/humic acids fractions for both radiolabels, approximately 23:6:10 in the silt and 16:4:17 in the loamy sand.

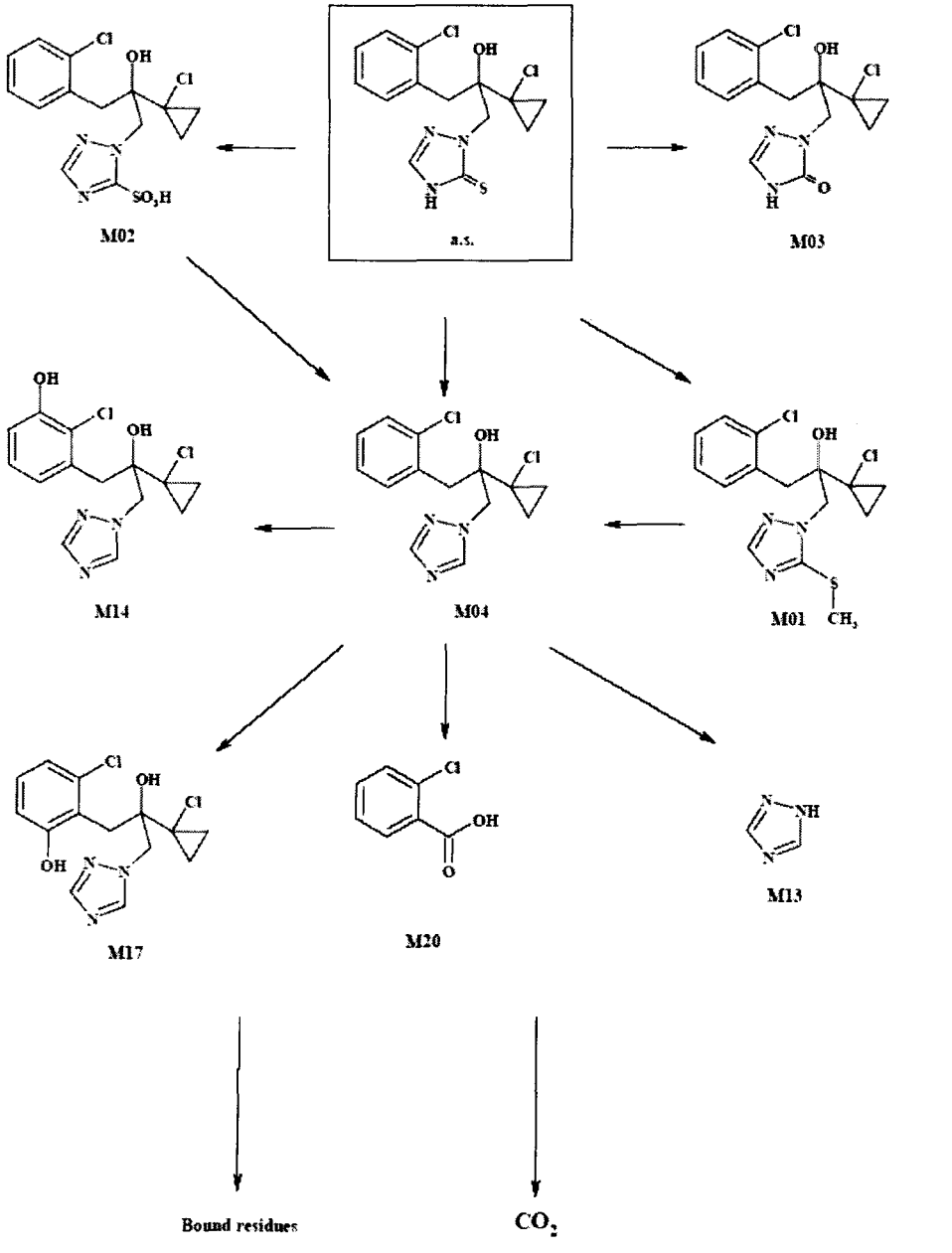
VOLATILIZATION: Mineralization of [^{14}C]prothioconazole residues occurred to a greater extent in the silt, compared to the loamy sand, possibly due to the much higher microbial biomass in the silt soil (approximately 1400 mg C microbial/kg dry weight compared to approximately 25 mg C microbial/kg dry weight in silt versus loamy sand at study initiation). In addition, mineralization of [phenyl-UL-^{14}C]prothioconazole residues was greater than that of [triazole-3,5-^{14}C]prothioconazole. This indicates that CO_2 is more likely to be formed from carbons in the triazole ring of prothioconazole than from carbons in the phenyl ring.

At the end of the study, 17.9% and 5.3% of the AR was present as CO_2 in the silt samples treated with [phenyl-UL-^{14}C] and [triazole-3,5-^{14}C]prothioconazole, respectively. In the loamy sand, CO_2 represented 6.1% and 0.7% of the AR in samples treated with [phenyl-UL-^{14}C] and [triazole-3,5-^{14}C]prothioconazole, respectively, at study termination.

No volatile organics were detected in either soil throughout the entire study period.

TRANSFORMATION PATHWAY: According to the study author, a comparison of the analytical results from the test series with the different radiolabels, does not appear to show an important difference related to product formation in the soil extracts. The predominant portion of transformation products contained both the phenyl and triazole ring. The profile of products found within this study indicates that the cleavage of the prothioconazole molecule forming other transformation products (e.g., containing just the 1-chlorocyclopropyl moiety) does not occur to a relevant extent. Thus, the proposed pathway of transformation of prothioconazole is dominated by reactions at the sulphur of the triazole ring. The biotransformation pathway proposed by the study author is shown in **Figure 1**.

Figure 1. Proposed biotransformation pathway of prothioconazole (JAU 6476) in soil (from summary of study submitted under DACO 8.2.3.4.2).



a.s. = JAU 6476
M01 = JAU 6476-S-methyl
M02 = JAU 6476-sulfonic acid
M03 = JAU 6476-triazolinone
M04 = JAU 6476-desthio
M13 = 1,2,4-triazole
M14 = JAU 6476-3-hydroxy-desthio
M17 = JAU 6476-6-hydroxy-desthio
M20 = 2-chlorobenzoic acid

Table 12: Chemical names and CAS numbers for the transformation products of prothioconazole (JAU647).

Applicant's Code Name	CAS Number	CAS and/or IUPAC Chemical Name(s)	Chemical formula	Molecular weight
JAU6476-desthio (SXX0665)	120983-64-4	2-(1-chlorocyclopropyl)1-(2-chlorophenyl)-3-(1,2,4-triazol)-1-yl)-propan-2-ol	$C_{14}H_{15}Cl_{12}N_3O$	312 g/mol
JAU6476-S-methyl (WAK7861 or HUPP0658)	178928-71-7	not provided	$C_{15}H_{17}Cl_2N_3OS$	358 g/mol
JAU6476-triazolinone (JAU7002 or WAK7860 or KTS9484)		not provided	$C_{14}H_{15}Cl_2N_3O_2$	328 g/mol
JAU6476-sulfonic acid (JAU6726)		not provided	$C_{14}H_{15}Cl_2N_3O_4S$	392 g/mol
JAU6476-6-OH-desthio (HO210898)		not provided	$C_{14}H_{15}Cl_2N_3O_2$	328 g/mol
JAU6476-3-OH-desthio (HO240898)		not provided	$C_{14}H_{15}Cl_2N_3O_2$	328 g/mol
2-chlorobenzoic acid (FHW0106C)	118-91-2	not provided	$C_7H_5ClO_2$	157 g/mol
1,2,4-triazole	288-88-0	not provided	$C_2H_3N_3$	69 g/mol

D. SUPPLEMENTARY EXPERIMENT-RESULTS: No supplementary experiment was described.

III. STUDY DEFICIENCIES:

Replicates consisted of one flask dosed with one label and a second flask dosed with the other label. These are not true replicates.

IV. REVIEWER'S COMMENTS:

1. Although recoveries remain between 110 and 90% of applied, there is a slight pattern of decline in material balance with time, starting with recovery of 102.8-101.4% of applied at time 0 for both labels in both soils and declining to recovery of 90-95% of applied for the phenyl label and 95.1-97.7% of the applied for the triazole label by study termination in both soils.

2. Nonextractable residues are at 20.6-30.3% of the applied at 1 day posttreatment, reaching 38.2-56.4% of applied by study termination in both soils with both labels. Samples were only extracted three times with acetonitrile/water (80:20 v:v). It is difficult to know whether the radioactive material unextracted from the soil has become a bound, organic part of the soil or whether it has not been harshly enough extracted. The amount of parent bound to the soil should not be considered degraded due to aerobic soil metabolism, as this will artificially increase the calculated aerobic soil metabolism half-life. Additionally, even if parent residues are not extractable under the conditions of this study, they may unbind from the soil under other conditions (different pH or redox, for example) and be present and available for metabolism in the environment. However, as mentioned above, the decrease in [^{14}C]prothioconazole concentrations was not proportional to the increase in non-extractable [^{14}C]residues, and major transformation products JAU6476-desthio and JAU6476-S-methyl were detected in quantities >10% by 1-3 days posttreatment in all treatments, which indicates that at least part of the parent compound was transformed and did not simply move to the non-extractable phase.

3. The DT_{50}s for prothioconazole were calculated by the study author in the following way: The degradation curve and regression analysis was calculated with the evaluation program ®ModelManager (Environmental Kinetics), Version 1.1, developed and published by Cherwell cientific Ltd. Oxford, UK. The model was run in the mode "use standard data" as well as "use existing parameter estimates". For determination of the degradation kinetics of JAU6476 in soil, the mean values of both labels were calculated for each soil and the Simple First Order Model (SFO) and the well fitting Hockey Stick Model were used.

Table 13: DT50 values combining both labels reported by the study author.

Parameter	Silt (Höfcher soil)		Loamy sand (Byromville soil)	
	Simple First Order	Hockey Stick[1)]	Simple First Order	Hockey Stick[2)]
K (1/days)	2.34	2.34 / 0.028	0.545	0.567 / 0.005
DT_{50} (days)	0.3	0.3	1.27	1.22
DT_{75} (days)	0.59	0.59	2.54	2.45
DT_{90} (days)	0.99	0.99	4.22	4.06

r^2	0.99	0.99	0.981	0.994

[1] k1 = rate constant for t<4.58 days / k2 = rate constant for t>4.58 days
[2] k1 = rate constant for t<90 days / k2 = rate constant for t>90 days

4. An inconsistency was noted when comparing the dates moisture was checked with those of sample processing. Tables 4 and 5 (pp. 43-44) indicate that vessels for time intervals T7 (#1 and #2) and T8 were checked for moisture on days 112 and 140, while it is stated in Section 3.5.3 (p. 22) that T7 and T8 vessels were collected for analysis on days 90 and 120. Even though this is not possible, the vessels can not be checked for moisture if they have been emptied 20 days earlier, the DT50 and DT90 estimates are not affected by this inconsistency, as more than 90% of the parent compound had dissipated by day 7 in both soils (both labels).

V. REFERENCES:

Goring, C.A.I., D.A. Laskowki, J.H. Hamaker, and R.W. Meikle. 1975. Principles of pesticide degradation in soil. Pages 135-172 in (R. Haque and V.H. Freed, eds.) *Environmental dynamics of pesticides*. Plenum Press, New York.

Chemical name: JAU6476 **MRID 46246511**
PC Code 113961 **Soil: Hofchen silt**

Day posttreatment	**0**	**1**	**3**	**7**	**14**	**30**	**63**	**90**	**120**	**181**	**272**	**365**
Label 1												
Parent compound	**73.4**	**7.9**	**6.1**	**2**	**4.2**	**2.9**	**2.2**	**<2.0**	**<2.0**	**<2.0**	**<2.0**	**<2.0**
JAU6476-desthio	15.9	39.8	38.6	46.5	35.8	35	35	33.8	17.5	16.8	8.8	6.3
JAU6476-S-methyl	<2.0	11.3	10.7	10.3	8.4	7.5	6.4	6.6	6	4.9	2.6	2.8
JAU6476-triazolinone	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
JAU6476-6-OH-desthio	n.d.	<2.0	<2.0	<2.0	3.1	3.4	3.2	2.2	4.2	2	2.9	2.9
JAU6476-3-OH-desthio	n.d.	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	n.d.	<2.0	n.d.	<2.0	<2.0
JAU6476-sulfonic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	3.2	3.7	3.1	3.1
2-chlorobenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
Z2	<2.0	2.2	2.3	<2.0	2.7	2.9	2.5	<2.0	n.d.	n.d.	<2.0	n.d.
Z4	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0
Z17	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0
Origin	1.4	1.1	2.4	0.9	2.4	2.7	1.2	0.9	2.6	2	2.5	2.2
Unidentified radioactivity	2.4	3.8	2.4	<2.0	2.8	<2.0	<2.0	<2.0	<2.0	<2.0	3.1	3
Total extractable residues	95.8	68.4	66.5	63.8	61.4	58.4	52.1	48.2	39.8	32.3	28.2	25
CO2	--	0.2	0.7	1.5	2.5	3.1	4.6	6.5	10.7	14	15.9	17.9
Total volatile organics	--	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Non-extractable residues	7	28.2	30.8	28.4	30.5	32.5	37.4	37	42	45.2	46.5	47.3
Total % recovery	102.8	96.8	98	93.7	94.4	94	94.1	91.8	92.5	91.5	90.6	90.2
Label 2												
Parent compound	**81**	**9**	**6.7**	**<2.0**	**4.6**	**3.1**	**<2.0**	**<2.0**	**5.6**	**<2.0**	**6.6**	**5.9**
JAU6476-desthio	10.2	38.8	39.4	49.4	39.5	37.7	35.9	34.8	15.1	16.6	7.9	6.1
JAU6476-S-methyl	<2.0	12.8	11.8	10.7	10.3	9	7.4	6.3	6.4	5.2	3.1	3.1
JAU6476-triazolinone	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0
JAU6476-6-OH-desthio	n.d.	<2.0	<2.0	<2.0	2.4	3.3	3.3	2.1	4.6	2.4	2.6	2.3
JAU6476-3-OH-desthio	n.d.	<2.0	<2.0	n.d.	2.1	<2.0	<2.0	n.d.	<2.0	n.d.	<2.0	n.d.
JAU6476-sulfonic acid	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0	2.4	3.3	8.3	3.5	3.3
2-chlorobenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	2.2	<2.0
1,2,4-triazole	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	n.d.
Z2	<2.0	<2.0	2.5	<2.0	2.7	3	3.3	3	n.d.	<2.0	<2.0	n.d.
Z4	n.d.	n.d.	<2.0	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0
Z17	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0
Origin	<2.0	<2.0	2.4	<2.0	2.1	2.9	<2.0	<2.0	2.8	3.2	3.3	2.9
Unidentified radioactivity	<2.0	3.5	2.6	2.2	2.2	2.3	<2.0	<2.0	3.6	3.1	4.6	6.1
Total extractable residues	94.8	68.7	69.2	67.2	65.9	63.7	57.1	52.7	46.7	40.1	36.1	33.4
CO2	--	<0.1	<0.1	<0.1	0.1	0.2	0.7	1.1	2	2.9	4.9	5.3
Total volatile organics	--	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Non-extractable residues	7.5	30.3	31.3	32	32.5	34.7	40.2	41.7	48.3	52.7	53.3	56.4
Total % recovery	102.3	99	100.6	99.2	98.4	98.6	98	95.5	97	95.7	94.2	95.1

Chemical name: JAU6476
PC Code 113961

MRID 46246511
Soil: Hofchen silt
Label 1: [phenyl-UL-^{14}C]JAU 6476

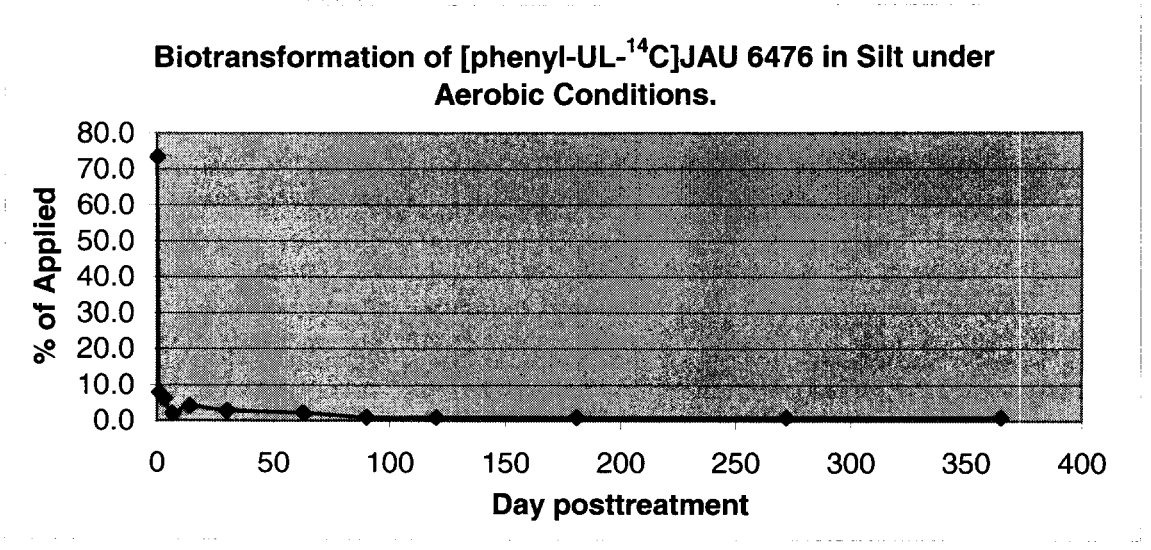
Non-linear Regression

Day	%		Est.	SE	Y^2
0	73.4		73.38374	0.000265	5387.56
1	7.9		8.120458	0.048602	62.41
3	6.1		0.099436	36.00677	37.21
7	2.0		1.49E-05	3.99994	4
14	4.2		3.03E-12	17.64	17.64
30	2.9		1.53E-27	8.41	8.41
63	2.2		4.33E-59	4.84	4.84
90	1.0		6.67E-85	1	1
120	1.0		1.4E-113	1	1
181	1.0		6.7E-172	1	1
272	1.0		6.7E-259	1	1
365	1.0		0	1	1

t 1/2	**0.314879**
C0	73.38374
k	2.201316
SSE	75.94558
R^2	0.9836

ANOVA

Source	Df	SS	MS	F	p
Reg	1	4554.984	4554.984	599.7694	2.93942E-10
Error	10	75.94558	7.594558		
Total	11	4630.929			



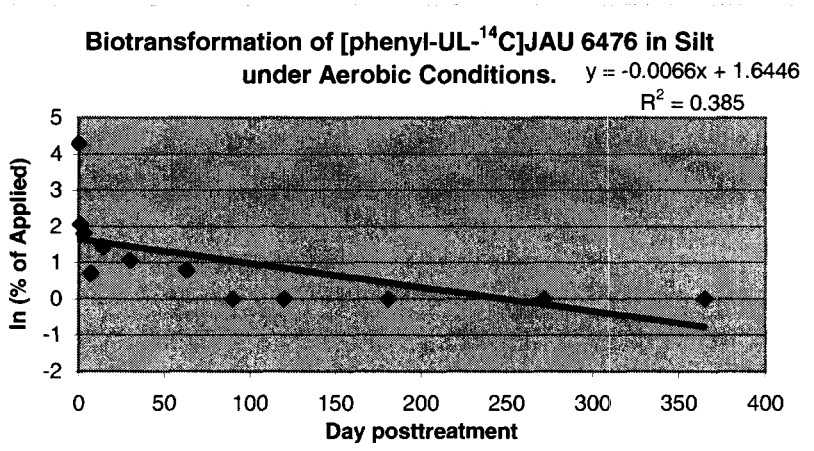
Chemical name: JAU6476
PC Code 113961

MRID 46246511
Soil: Hofchen silt
Label 1: [phenyl-UL-^{14}C]JAU 6476

Log-linear Regression

Day	%	Ln %
0	73.4	4.295924
1	7.9	2.066863
3	6.1	1.808289
7	2.0	0.693147
14	4.2	1.435085
30	2.9	1.064711
63	2.2	0.788457
90	1.0	0
120	1.0	0
181	1.0	0
272	1.0	0
365	1.0	0

t 1/2	**105**
C0	5.18
k	0.006617
R^2	0.3850



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.620515
R Square	0.385038
Adjusted R	0.323542
Standard E	1.051672
Observatio	12

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	6.924952	6.924952	6.261175	0.031327
Residual	10	11.06015	1.106015		
Total	11	17.9851			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 95.0%*	*Upper 95.0%*
Intercept	1.644646	0.394904	4.164668	0.001934	0.764744	2.524548	0.764744	2.52454831
X Variable	-0.006617	0.002645	-2.502234	0.031327	-0.012509	-0.000725	-0.012509	-0.0007248

Chemical name: JAU6476
PC Code 113961

MRID 46246511
Soil: Hofchen silt
Label 2: [triazole-3,5-^{14}C]JAU 6476

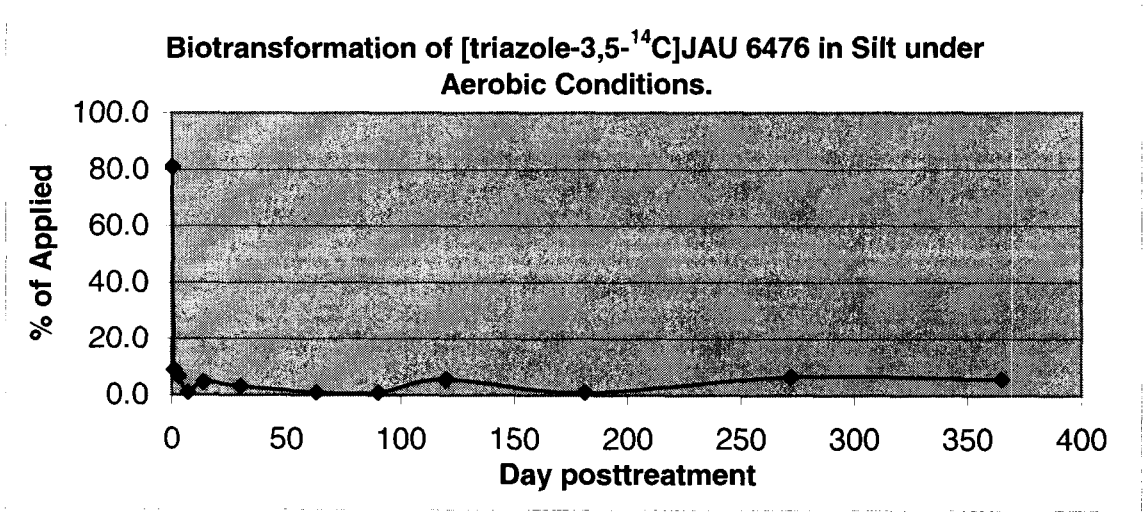
Non-linear Regression

Day	%	Est.	SE	Y^2
0	81.0	80.98034	0.000387	6561
1	9.0	9.257977	0.066552	81
3	6.7	0.121001	43.28323	44.89
7	1.0	2.07E-05	0.999959	1
14	4.6	5.28E-12	21.16	21.16
30	3.1	4.49E-27	9.61	9.61
63	1.0	3.72E-58	1	1
90	1.0	1.38E-83	1	1
120	5.6	7.7E-112	31.36	31.36
181	1.0	2.7E-169	1	1
272	6.6	5.3E-255	43.56	43.56
365	5.9	0	34.81	34.81

t 1/2	**0.319611**
C0	80.98034
k	2.168721
SSE	187.8501
R^2	0.965832

ANOVA

Source	Df	SS	MS	F	p
Reg	1	5310.019	5310.019	282.6732	1.16269E-08
Error	10	187.8501	18.78501		
Total	11	5497.869			



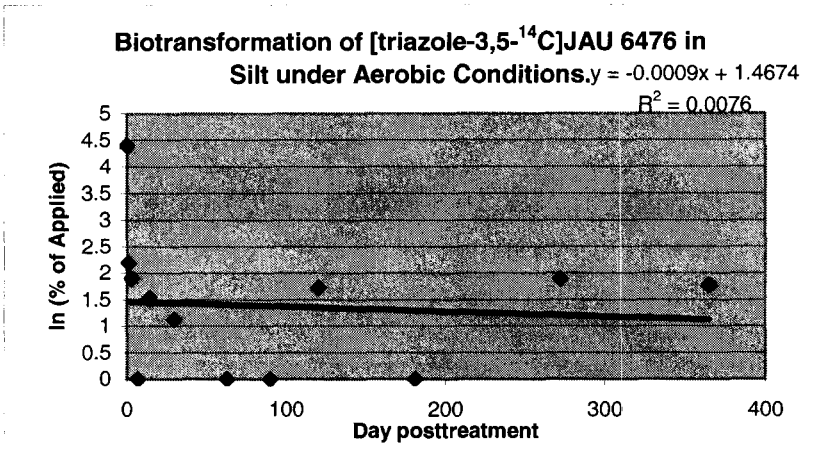
Chemical name: JAU6476
PC Code 113961

MRID 46246511
Soil: Hofchen silt
Label 2: [triazole-3,5-^{14}C]JAU 6476

Log-linear Regression

Day	%	Ln %
0	81.0	4.394449
1	9.0	2.197225
3	6.7	1.902108
7	1.0	0
14	4.6	1.526056
30	3.1	1.131402
63	1.0	0
90	1.0	0
120	5.6	1.722767
181	1.0	0
272	6.6	1.88707
365	5.9	1.774952

t 1/2	**740**
C0	4.34
k	0.000936
R^2	0.0076



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.087158
R Square	0.007597
Adjusted R	-0.091644
Standard E	1.346103
Observatio	12

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	0.138702	0.138702	0.076547	0.787667
Residual	10	18.11994	1.811994		
Total	11	18.25864			

	Coefficient	*standard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 95.0%*	*Upper 95.0%*
Intercept	1.467438	0.505464	2.903152	0.015748	0.341194	2.593681	0.341194	2.59368105
X Variable	-0.000936	0.003385	-0.276671	0.787667	-0.008478	0.006605	-0.008478	0.00660547

Chemical name: JAU6476 **MRID 46246511**
PC Code 113961 **Soil: Byromville loamy sand**

Day posttreatment	**0**	**1**	**3**	**7**	**14**	**30**	**63**	**90**	**120**	**181**	**272**	**365**
Label 1												
Parent compound	**89.9**	**46.3**	**20.5**	**8.5**	**8.2**	**5.2**	**4.3**	**4.8**	**2.5**	**2.4**	**4.1**	**2.3**
JAU6476-desthio	7.5	14.3	21	31.7	28.8	28.3	32.6	41.2	23.9	29.5	23.5	21.9
JAU6476-S-methyl	<2.0	6.6	11.3	13.7	12.9	12.3	11.7	8.3	9.8	9.2	7	7.1
JAU6476-triazolinone	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0
JAU6476-6-OH-desthio	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0	<2.0	<2.0
JAU6476-3-OH-desthio	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
JAU6476-sulfonic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0	<2.0	<2.0
2-chlorobenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
Z2	n.d.	<2.0	<2.0	n.d.	<2.0	<2.0	<2.0	n.d..	<2.0	<2.0	n.d.	n.d.
Z4	n.d.	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0
Origin	<2.0	3	3.9	3.2	3.6	4.5	3	<2.0	2.9	3.2	4.4	3.8
Unidentified radioactivity	<2.0	2.8	3.6	<2.0	2.4	3.2	<2.0	<2.0	2.2	2.3	3.7	4.6
Total extractable residues	98.7	74.3	63.1	59.4	58.8	56.4	55.2	58.3	49.9	49.1	50.6	47.9
CO2	–	0.1	0.2	0.3	0.4	0.8	2.0	0.4	3.0	3.1	4.3	6.1
Total volatile organics	--	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Non-extractable residues	2.7	20.6	29.7	36	35.2	38	39.1	36.9	40.1	41.4	40.2	38.2
Total % recovery	101.4	95.1	93	95.8	94.4	95.1	96.4	95.7	93	93.6	95.1	92.2
Label 2												
Parent compound	**95.5**	**52.1**	**24.6**	**8.4**	**9.2**	**5.1**	**3.4**	**2.6**	**2.1**	**2.3**	**3.8**	**4.6**
JAU6476-desthio	2.4	11.7	20.9	31.7	29.9	30	34	38.4	25.1	29.1	23.2	23.7
JAU6476-S-methyl	n.d.	6.4	12.4	14.6	14.4	13.2	13.2	11.7	10.8	10.2	7.2	7.6
JAU6476-triazolinone	n.d.	n.d.	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0
JAU6476-6-OH-desthio	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0	<2.0	<2.0
JAU6476-3-OH-desthio	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
JAU6476-sulfonic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	<2.0	2	2.3
2-chlorobenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0
1,2,4-triazole	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	<2.0	n.d.	n.d.	<2.0
Z2	n.d.	n.d.	<2.0	n.d.	<2.0	<2.0	<2.0	n.d.	<2.0	<2.0	<2.0	n.d.
Z4	n.d.	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0	<2.0
Origin	<2.0	3	2.9	2.9	4.2	4.9	2.4	<2.0	3.3	4.3	4.6	4
Unidentified radioactivity	<2.0	2.6	2.7	<2.0	<2.0	3.2	2.4	<2.0	2.9	2.9	4.4	3.7
Total extractable residues	98.6	76.3	66.3	60.1	62.5	58.6	56.5	55.2	52.7	51.6	51.7	54.1
CO2	--	<0.1	<0.1	<0.1	0.1	0.1	0.1	0.2	0.3	0.4	0.5	0.7
Total volatile organics	--	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Non-extractable residues	3.4	22.1	32.6	34.4	37.6	38.3	42.1	40.5	42.6	44.7	42.5	42.8
Total % recovery	102	98.5	98.9	94.4	100.2	96.9	98.8	95.9	96.7	95.5	94.7	97.7

Chemical name: JAU6476
PC Code 113961

MRID 46246511
Soil: Byromville loamy sand
Label 1: [phenyl-UL-^{14}C]JAU 6476

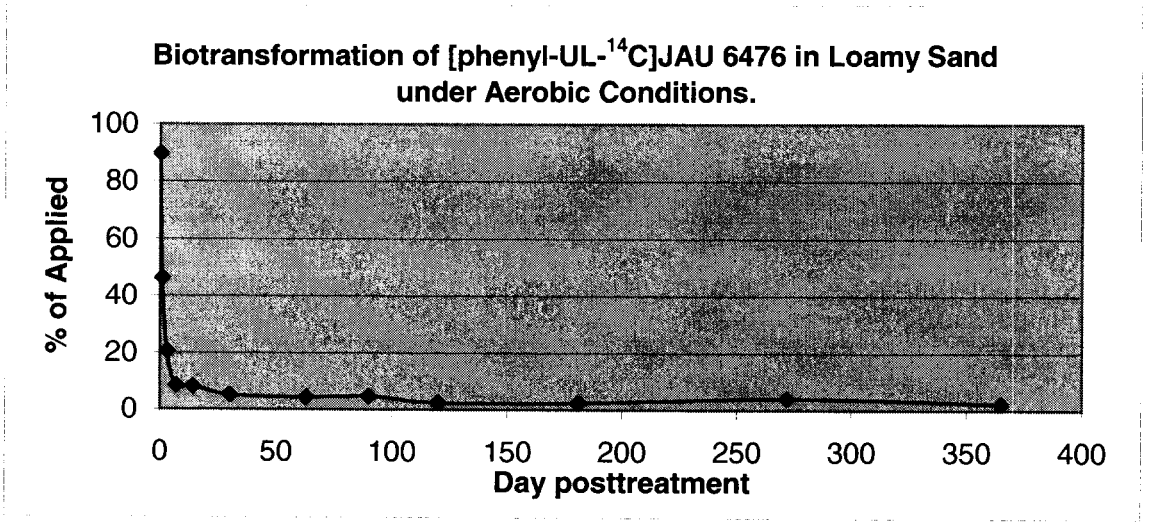
Non-linear Regression

Day	%	Est.	SE	Y^2
0	89.9	87.74662	4.637052	8082.01
1	46.3	51.27217	24.72252	2143.69
3	20.5	17.5059	8.96464	420.25
7	8.5	2.04075	41.72191	72.25
14	8.2	0.047462	66.46387	67.24
30	5.2	8.77E-06	27.03991	27.04
63	4.3	1.75E-13	18.49	18.49
90	4.8	8.75E-20	23.04	23.04
120	2.5	8.74E-27	6.25	6.25
181	2.4	5.09E-41	5.76	5.76
272	4.1	2.97E-62	16.81	16.81
365	2.3	5.9E-84	5.29	5.29

t 1/2	**1.290044**
C0	87.74662
k	0.537305
SSE	249.1899
R^2	0.96716

ANOVA

Source	Df	SS	MS	F	p
Reg	1	7338.847	7338.847	294.5082	9.53092E-09
Error	10	249.1899	24.91899		
Total	11	7588.037			



Chemical name: JAU6476
PC Code 113961

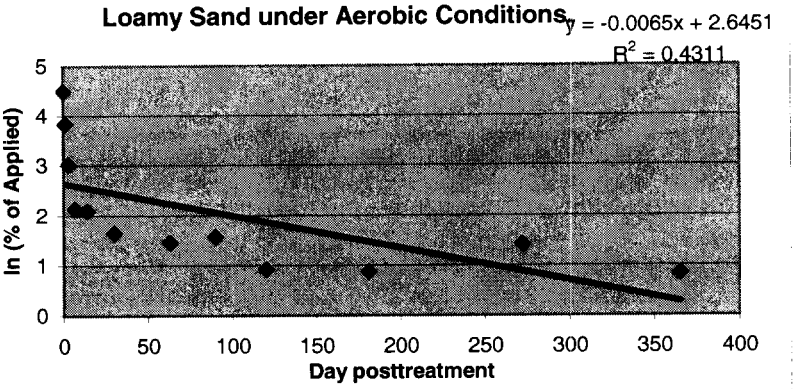
MRID 46246511
Soil: Byromville loamy sand
Label 1: [phenyl-UL-^{14}C]JAU 6476

Log-linear Regression

Day	%	Ln %
0	89.9	4.498698
1	46.3	3.835142
3	20.5	3.020425
7	8.5	2.140066
14	8.2	2.104134
30	5.2	1.648659
63	4.3	1.458615
90	4.8	1.568616
120	2.5	0.916291
181	2.4	0.875469
272	4.1	1.410987
365	2.3	0.832909

t 1/2	**107**
C0	14.08
k	0.006484
R^2	0.4311

Biotransformation of [phenyl-UL-^{14}C]JAU 6476 in Loamy Sand under Aerobic Conditions



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.656584
R Square	0.431103
Adjusted R	0.374213
Standard E	0.936782
Observatio	12

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	6.650026	6.650026	7.577862	0.02038
Residual	10	8.775597	0.87756		
Total	11	15.42562			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 95.0%*	*Upper 95.0%*
Intercept	2.645103	0.351763	7.519564	2.02E-05	1.861326	3.428879	1.861326	3.42887931
X Variable	-0.006484	0.002356	-2.752792	0.02038	-0.011733	-0.001236	-0.011733	-0.0012359

Chemical name: JAU6476
PC Code 113961

MRID 46246511
Soil: Byromville loamy sand
Label 2: [triazole-3,5-^{14}C]JAU 6476

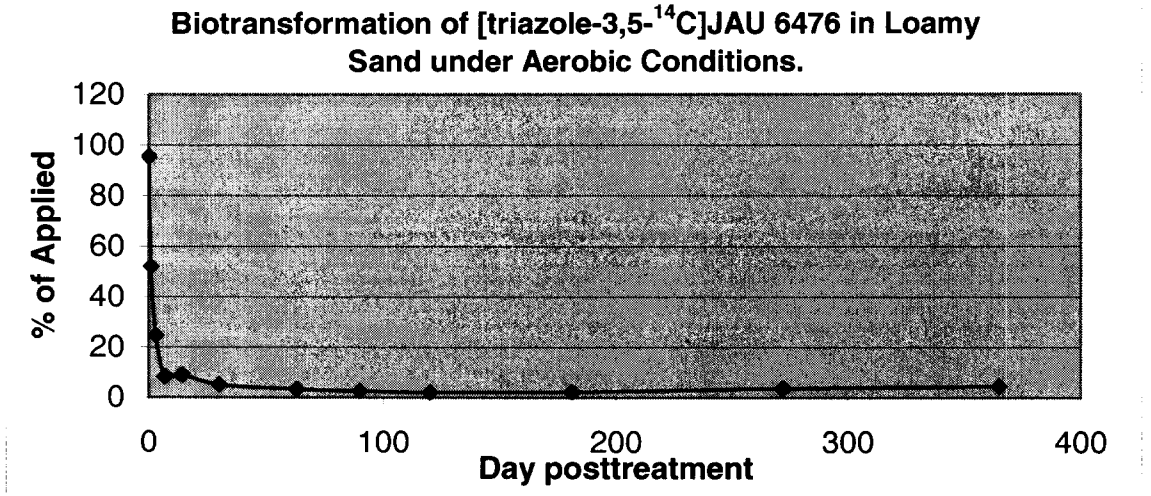
Non-linear Regression

Day	%	Est.	SE	Y^2
0	95.5	93.02182	6.141401	9120.25
1	52.1	57.44593	28.57892	2714.41
3	24.6	21.90827	7.245413	605.16
7	8.4	3.18644	27.18121	70.56
14	9.2	0.109151	82.64354	84.64
30	5.1	4.88E-05	26.0095	26.01
63	3.4	6.04E-12	11.56	11.56
90	2.6	1.35E-17	6.76	6.76
120	2.1	7.07E-24	4.41	4.41
181	2.3	1.2E-36	5.29	5.29
272	3.8	1.08E-55	14.44	14.44
365	4.6	3.67E-75	21.16	21.16

t 1/2	**1.438095**
C0	93.02182
k	0.48199
SSE	241.42
R^2	0.97281

ANOVA

Source	Df	SS	MS	F	p
Reg	1	8637.589	8637.589	357.7827	3.69933E-09
Error	10	241.42	24.142		
Total	11	8879.009			



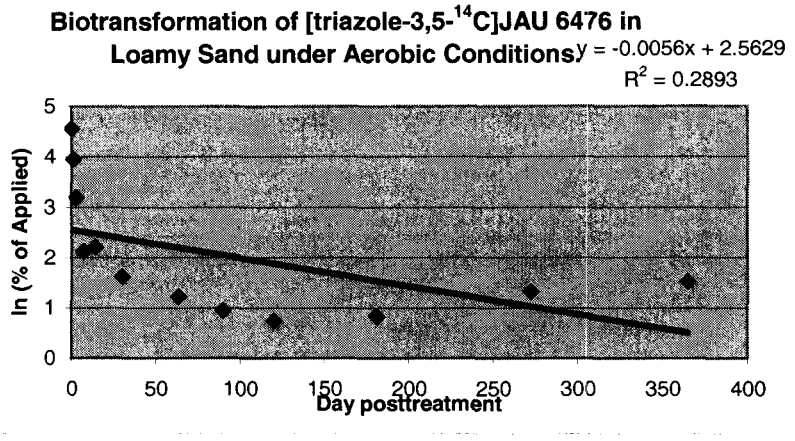
Chemical name: JAU6476
PC Code 113961

MRID 46246511
Soil: Byromville loamy sand
Label 2: [triazole-3,5-^{14}C]JAU 6476

Log-linear Regression

Day	%	Ln %
0	95.5	4.559126
1	52.1	3.953165
3	24.6	3.202746
7	8.4	2.128232
14	9.2	2.219203
30	5.1	1.629241
63	3.4	1.223775
90	2.6	0.955511
120	2.1	0.741937
181	2.3	0.832909
272	3.8	1.335001
365	4.6	1.526056

t 1/2	**123**
C0	12.97
k	0.005627
R^2	0.2893



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.537841
R Square	0.289273
Adjusted R	0.218201
Standard E	1.109169
Observatio	12

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	5.007272	5.007272	4.070104	0.071283
Residual	10	12.30256	1.230256		
Total	11	17.30984			

	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 95.0%*	*Upper 95.0%*
Intercept	2.562939	0.416495	6.153593	0.000108	1.634931	3.490947	1.634931	3.49094667
X Variable	-0.005627	0.002789	-2.01745	0.071283	-0.011841	0.000588	-0.011841	0.00058763