

Data Evaluation Report on the phototransformation of prothioconazole (JAU6476) in water

PMRA Submission Number 2004-0839

EPA MRID Number 46246507



Data Requirement: PMRA DATA CODE: 8.2.3.3.2
 US EPA DP Barcode: DP 303488
 OECD Data Point: IIA 2.9.2
 US EPA Guideline: 161-2

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
 SMILES string: C1C1(C(Cc2ccccc2Cl)(CN2N=CNC2=S)O)CC1.

Primary Reviewer (officer number): Émilie Larivière (#1269) **Date:** March 17, 2005
 EAD, PMRA *Emilie Lariviere 3/17/05*

Secondary Reviewer (officer number): *Connie Hart 14 Jun 05*
 Connie Hart (#1158) **Date:** June 14, 2005
 EAD, PMRA

Secondary Reviewer(s) (officer number): *Roxolana Kashuba 8/10/05*
 Roxolana Kashuba **Date:** August 10, 2005
 (EPA/OPP/EFED/ERB4)

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: Gilges, W. and W. Bornatsch. 2001. Photolysis of JAU6476 in Sterile Aqueous Buffer. Performing Laboratory: Bayer AG Crop Protection Business Group, Germany. Bayer CropScience, North Carolina. Unpublished. Report No. MR-213/01.



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EXECUTIVE SUMMARY:

The aqueous phototransformation of [phenyl-UL-¹⁴C] and [triazole-3,5-¹⁴C] labelled 2-[2-(1-Chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole-3-thione (prothioconazole; JAU6476; purity >98%) was studied at 25 °C in sterile aqueous phosphate buffer solutions at pH 7 at initial concentrations of 4.09 - 4.47 mg a.i./L under continuous irradiation using a UV-filtered xenon lamp (measured intensity of 750 W/m² between 300-800 nm) for 18 days (an equivalent of 65, 93, and 92 days of summer sunlight at 33° N, 40° N, 53° N latitude, respectively). This study was conducted in accordance with US EPA Subdivision N §161-2 (1982), EC-Guideline 91/414/EEC (1991), and SETAC Procedures for Assessing the Environmental Fate and Ecotoxicity of Pesticides (1995) and in compliance with German and OECD Principles of Good Laboratory Practice (GLP). A quartz glass vessel containing 100 mL of test solution (20 mL for dark controls) were connected to passive volatile traps filled with soda lime granules for absorption of ¹⁴CO₂ and fitted with a polyurethane foam plug for absorption of volatile organic transformation products. The control vessels were placed in a cryostat while irradiated vessels were exposed to light in a Suntest cooling platform connected to a cryostat. Single irradiated samples were collected at 0, 1.5 and 4 hours, 1, 5, 11 and 18 days of irradiation; single dark control samples were collected at 0, 5 and 18 days. Samples were analyzed for total radioactivity using Liquid Scintillation Counting (LSC) and for parent and transformation products using radio-High Performance Liquid Chromatography (HPLC), without extraction.

The mass balance was 97.5 ± 5.8% and 100.3 ± 8.4 % of the applied amount in the dark and irradiated samples, respectively, for [phenyl-UL-¹⁴C]prothioconazole, and 99.7 ± 5.2% and 104.0 ± 5.3 % of the applied amount in the dark and irradiated samples, respectively, for [triazole-3,5-¹⁴C]prothioconazole.

At study termination, 91.5% and 95.9% of HPLC peak area ratio (99.5% and 103.3% of the applied radioactivity), remained as the parent in the dark samples for the phenyl and triazole labels, respectively. The radioactivity attributed to prothioconazole in dark controls on days 0 and 5 was not determined, and peak area ratios by HPLC were not provided for those days. Quantitative data for the HPLC-identified transformation product, JAU6476-desthio, and for two other peaks visible in chromatograms of the dark control samples on day 18 were not reported. At study termination, the evolved CO₂ and volatile organic compounds in the dark samples amounted to <0.1% and 0.1% of the applied radioactivity, respectively, for the phenyl label, and 2.3% and <0.1% of the applied radioactivity, respectively, for the triazole label.

In the irradiated samples, the concentration of parent compound decreased from 98.4% and 97.4% of the applied amount at study initiation for the phenyl and triazole labelled compounds, respectively, to <MDL at study termination (18 days). The major transformation products detected in the irradiated samples were **JAU6476-desthio** (SXX0665; 2-[2-(1-chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole), **JAU6476 thiazocine** (6-(1-chlorocyclopropyl)-6,7-dihydro-triazole-5H-[1,2,4]triazolo[5,1-

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b)[1,3]benzothiazon-6-ol), and **1,2,4-triazole** (1-H-1,2,4-triazole) with maximum concentrations of 55.7%, 14.1%, and 11.9% of the applied observed on the 11th, 5th, and 18th day of incubation from the phenyl, phenyl, and triazole labelled parent, respectively. After reaching the maximum, concentrations of JAU6476-desthio and JAU6476 thiazocine decreased to 53.2% and 8.4% of the applied, respectively, from the phenyl labelled parent by study termination, while 1,2,4-triazole was at maximum at study termination. The six minor transformation products in the irradiated samples were characterized but not identified and were formed at a maximum of 4.6-7.0% of the applied amount in both phenyl and triazole labelled treatments. From seven to nine additional unassigned peaks were detected in both labelled treatments, together representing 13.0-19.2% of the applied radioactivity on day 18, with the largest single peak at 3.1% of the applied radioactivity (2.9% HPLC peak area ratio) in either treatment. At test termination, in the irradiated samples, the evolved CO₂ and volatile organic compounds amounted to 3.0% and 1.7% of the applied radioactivity, respectively, for the phenyl label, and 0.5% and 0.1% of the applied radioactivity, respectively, for the triazole label. The total unidentified radioactivity eluting in the void volume of the column was a maximum of 4.5-7.1% of the applied radioactivity in the irradiated samples treated with either radiolabel. Unidentified radioactivity was not reported for the dark samples.

Comparison of transformation products formed in the dark and irradiated samples is not possible, as transformation products formed in the dark other than JAU6476-desthio were not identified, despite their presence in chromatograms of the dark control samples, and no dark sample transformation products were quantified. It cannot be determined which transformation products are formed by phototransformation only. No phototransformation pathway was proposed.

The half-life of both [phenyl-UL-¹⁴C] and [triazole-3,5-¹⁴C]prothioconazole in the irradiated samples was 1.9 days, calculated using linear regression on log-transformed data. The half-life (or statistical stability) of [phenyl-UL-¹⁴C] and [triazole-3,5-¹⁴C]prothioconazole in the dark samples could not be calculated, as raw data were not provided for [¹⁴C]prothioconazole recoveries in the dark control samples on days other than day 18. For the purpose of aqueous photolysis half-life calculation, it is assumed that all degradation can be attributed to photolysis, based on reported parent HPLC peak areas greater than 90% at study termination and on the stability of prothioconazole to hydrolysis (MRID: 46246505).

The predicted environmental phototransformation half-life of both [phenyl-UL-¹⁴C] and [triazole-3,5-¹⁴C]prothioconazole, derived from the measured half-life in the laboratory in a sterile buffer solution under the xenon lamp, was calculated to be 9.7 days and 9.6 days for 40° N latitude (New York, NY, USA) and 53° N latitude (Edmonton, AB, Canada), respectively, in June sunlight.

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Results Synopsis

Test medium: 0.01M phosphate buffer at pH 7
Source of irradiation: Xenon lamp NXe 1500B in a Heraeus Original Hanau Suntest unit
Half-life/DT₅₀ for dark: All data not provided. Assume no statistically significant degradation but no raw data submitted to support this conclusion.
Half-life/DT₅₀ for phototransformation: 45.4 hours (1.9 days, combined data); continuous irradiation
 [phenyl-UL-¹⁴C]prothioconazole: 45.3 hours (1.9 days)
 [triazole-3,5-¹⁴C]prothioconazole: 45.6 hours (1.9 days)

Predicted environmental half-life/DT₅₀ for phototransformation:
 9.7 days at 40° N latitude (New York, NY, USA) in the June sun
 9.6 days at 53° N latitude (Edmonton, AB, Canada) in the June sun

Major transformation products (irradiated samples, phenyl label):

JAU6476-desthio (maximum of 54.8% of applied radioactivity at 18 days)
JAU6476-thiazocine (maximum of 14.1% of applied radioactivity at 5 days)

Minor transformation products (irradiated samples, phenyl label):

Six unidentified, separately quantified metabolites (maximum of 7.0%, 2.8%, 3.5%, 3.4%, 4.5%, 3.0%, and 4.5% of applied radioactivity at days 18, 5, 11, 5, 18, 18, and 11, respectively).
Seven unidentified, not separately quantified metabolites (together maximum of 13.0% of applied radioactivity at 18 days, with the largest single peak at 2.7% HPLC peak area ratio)

Major transformation products (irradiated samples, triazole label):

JAU6476-desthio (maximum of 55.7% of applied radioactivity at 11 days)
1,2,4-triazole (maximum of 11.9% of applied radioactivity at 18 days)

Minor transformation products (irradiated samples, triazole label):

JAU6476-thiazocine (maximum of 9.5% of applied radioactivity at 11 days)
Three unidentified, separately quantified metabolites (maximum of 2.9%, 4.6%, and 2.7% of applied radioactivity at days 5, 18, and 5, respectively).
Nine unidentified, not separately quantified metabolites (together maximum of 19.2% of applied radioactivity at 18 days, with the largest single peak at 2.9% HPLC peak area ratio)

Study Acceptability: The U.S. EPA is classifying this study on phototransformation in water as supplemental because single replicates from a bulk sample were used (multiple replicates per sampling interval from separate vessels are preferable), all dark control data were not reported, and 13.0-19.2% of applied radioactivity (“unassigned metabolites”) were not separately reported. The PMRA does not use the same classification scheme as the U.S. EPA. This study is classified as acceptable to the PMRA.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with US EPA-Guidelines, Subdivision N § 161-2 (1982), related USEPA guidance (including SEPs and Pesticide Reregistration Rejection Rate Analysis; 1985, 1988, 1993), as well as EC-Guideline 91/414/EEC and SETAC Procedures for Assessing the Environmental Fate and Ecotoxicity of Pesticides (1995). No deviations were reported.

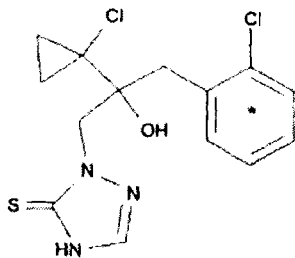
COMPLIANCE: This study was conducted in compliance with German (Chemikaliengesetz, attachment 1, dated 1994/1997) and OECD (1997) GLP. Signed and dated GLP, Quality Assurance and Data Confidentiality statements were provided.

A. MATERIALS:

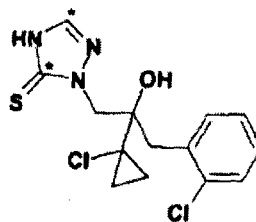
1. Test Material [phenyl-UL-¹⁴C] and [triazole-3,5-¹⁴C] radiolabelled prothioconazole (JAU6476; p. 10-11)

Chemical Structure: * denotes ¹⁴C-labelling position

[phenyl-UL-¹⁴C]JAU6476



[triazole-3,5-¹⁴C]JAU6476



Description: Technical; solid (p. 10-11)

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Purity:

[phenyl-UL-¹⁴C]JAU6476 used in main test

Analytical purity: >98%

Lot/Batch No. 12268/3, Synthesis KML 2720

Radiochemical purity: >99%

Specific activity: 3.66 MBq/mg

Locations of the radio label: [phenyl-UL-¹⁴C]JAU6476

[phenyl-UL-¹⁴C]JAU6476 used in dark controls

Analytical purity: >99%

Lot/Batch No. 13094/1, Synthesis KML 2761

Radiochemical purity: >99%

Specific activity: 1.85 MBq/mg

Locations of the radio label: [phenyl-UL-¹⁴C]JAU6476

[triazole-3,5-¹⁴C]JAU6476 used in main test

Analytical purity: 99%

Lot/Batch No. 10708/17, Synthesis THS 5018

Radiochemical purity: >99%

Specific activity: 1.94 MBq/mg

Locations of the radio label: [triazole-3,5-¹⁴C]JAU6476

[triazole-3,5-¹⁴C]JAU6476 used in dark controls

Analytical purity: >99%

Lot/Batch No. 10708/17, Synthesis THS 5018

Radiochemical purity: >99%

Specific activity: 1.94 MBq/mg

Locations of the radio label: [triazole-3,5-¹⁴C]JAU6476

Storage conditions of test chemicals:

As cool as possible until application.

Table 1: Physico-chemical properties of prothioconazole (JAU6476).

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

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Vapour pressure/volatility	<u>Temperature (°C)</u> 20 25	<u>Vapor pressure(Pa)</u> $<<4 \times 10^{-7}$ $<<4 \times 10^{-7}$	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}	<u>pH</u> 4 7 9 unbuffered	<u>log K_{ow}</u> 4.16 3.82 2.0 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) Buffer solution: Buffer solutions were made with Milli-Q water as follows:

Table 2: Description of buffer solution.

pH	Type of buffer and final molarity	Composition
7	0.01 M phosphate buffer	buffer solution was prepared using Milli-Q water, according to SOP 2107. No other details were provided.

Data were obtained from p. 11 of the study report.

3) Details of light source:

Table 3: Artificial light source.

Property	Details
Nature of light source	Xenon lamp NXe 1500B in a Heraeus Original Hanau Suntest unit
Emission wavelength spectrum	280-830 nm

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Light intensity	Based on the radiometer, 750 W/m ² in the range of 300-800 nm; based on the actinometer, 1.424 x 10 ¹⁶ photons x s ⁻¹ x cm ⁻² or 78.5 W/m ² in the relevant range of 295-400 nm.
Filters used	UV glass filter system to eliminate radiation < 290 nm
Relationship to natural sunlight	The study authors stated that 1 day (24 hours) of artificial light (4.66 MJ/m ²) was comparable to 3.6 days of natural sunlight in June in Phoenix, Arizona, USA (33.26°N; 31 MJ/m ² /day) and 5.1 days in Edmonton, Alberta, Canada (53.33°N; 22 MJ/m ² /day). Additionally, New York, New York (40.47°N) is reported to have solar radiation in June equivalent to 70% of that in Phoenix, Arizona (which equals 21.7 MJ/m ² /day). Between 270 and 800 nm, the artificial light was similar in wavelength distribution to global radiation.

Data were obtained from p. 14 and Appendices 10, 13, 14, and 16, p. 38, 41, 42, and 44 of the study report.

B. EXPERIMENTAL CONDITIONS:

1) **Preliminary Study:** No preliminary studies were described.

2) **Experimental Conditions**

Table 4: Experimental Parameters

Parameters		Details
Duration of the study		18 days
Test concentrations (mg a.i./L)		
nominal:		approximately 4.5 mg a.i./L (1/20th of water solubility)
measured:		irradiated phenyl label: 4.22 mg a.i./L irradiated triazole label: 4.09 mg a.i./L dark control phenyl label: 4.47 mg a.i./L dark control triazole label: 4.19 mg a.i./L
Dark controls used (Yes/No)		yes, but not all reported
Replication	Dark:	1 sample collected at each interval
	Irradiated:	1 sample collected at each interval from one bulk sample
Preparation of the test medium:	volume used/treatment:	100 mL; 5 mL removed per sampling interval (20 mL for dark controls)

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	method of sterilization:	steam pressure sterilization
	co-solvent	acetonitrile (0.35-0.61% by volume)
Test apparatus (Type/Material/Volume)		quartz glass vessel containing 100 mL of test solutions (20 mL for dark controls) with trap attachments for volatile organic products and CO ₂ . The vessel was exposed to light in the Suntest cooling platform connected to a cryostat at 25±1°C. The solutions were stirred by magnetic stirrers beneath the Suntest apparatus. The control samples were placed in a cryostat at 25°C.
Details of traps for volatile compounds, if any		Traps were filled with soda lime granules for absorption of ¹⁴ CO ₂ and fitted with a polyurethane foam plug for absorption of any volatile organic transformation products.
If no traps were used, is the test system closed/open		closed.
Is there any indication of the test material adsorbing to the walls of the test apparatus?		No
Experimental Conditions		
Temperature;		25±1°C
Duration of light/darkness:		continuous light
Other details, if any		None

Data were obtained from p. 15 of the study report.

3) Supplementary experiments: No supplementary experiments were described.

4) Sampling:

Table 5: Sampling details

Observations	Details
Sampling intervals for the parent/transformation products	irradiated: 0, 1.5 and 4 hours, 1, 5, 11 and 18 days dark controls: 0, 5 and 18 days
Sampling method	Aliquots of 5 mL were sampled under sterile conditions for LSC measurements (3 x 100 µL), chromatographic analyses, pH measurements and sterility tests if necessary. After sampling, a new trap attachment was put on the vessel and the vessel was returned to the Suntest apparatus. An aliquot of 1 mL of each sample was mixed with 100 µL 1 mol/L NaOH and stored in a freezer for determinations of CO ₂ in solution if required.

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Method of sampling volatile compounds, if any	Prior to opening a test vessel, radioactive volatile compounds were drawn into the trap by vacuum produced by placing the vessels in an exsiccator for about 10 minutes. The trap attachments were stored in a freezer until analysis.
Sampling intervals/times for: sterility check pH measurement	Irradiated: 0, 1, 5, 11 and 18 days performed on agar plates according to SOP 2500. No details on the SOP were provided. Dark controls: 0, 5 and 18 days Irradiated: 0, 5, 11 and 18 days Dark controls: 0, 5 and 18 days
Sample storage before analysis, if any	Freezer An aliquot of each sample was mixed with 100 µL 1 mol/L NaOH and stored in a freezer for determinations of CO ₂ in solution if required. The trap attachments were stored in a freezer until analysis of volatile organic compounds.
Other observation, if any	None

Data were obtained from p. 13-15 of the study report.

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods, if used: Aliquots of the test solutions were analyzed by LSC and radio-HPLC without extraction (p. 16).

Identification and quantification of the parent and transformation products: Parent and transformation products were quantified by reversed phase HPLC with a radioactivity flow-through detector, without extraction (p. 16).

The identity of JAU6476-thiazocine was determined from radio-HPLC as well as NMR and MS. The identity of transformation product 1,2,4-triazole was determined from radio-HPLC as well as LC-MS and LC-MS/MS (p. 17-18).

Volatile residue determination: The polyurethane foam plug of each trap for the absorption of volatile organic transformation products was extracted with ethylacetate. Two aliquots of the extract were used for radioactivity determinations.

The ¹⁴CO₂ bound to the soda lime was liberated with HCl and trapped in an absorption / scintillation cocktail which was measured by LSC. To determine the content of dissolved volatile radioactivity in the buffer solution, 100 µL aliquots of all solutions were mixed with 1 M NaOH. These aliquots were stored in a deep freezer. Only the aliquots of the last sampling interval were analysed as described above with ¹⁴CO₂ dissolved in water being liberated with HCl, trapped in a cocktail of which aliquots were measured by LSC (p. 15).

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Total radioactivity measurements: The radioactivity in solution was measured by LSC. Total material balances for the entire test were calculated as the sum of radioactivity leaving the systems i.e., radioactivity removed by taking the two 5 mL samples at time 0 (to determine applied radioactivity, leaving 90 mL for irradiation), the amount detected in the soda lime granules and the polyurethane foam plug, as well as the activity measured in the remaining 60 mL of test solutions at test termination. All these were related to the radioactivity in the original volume of 90 mL at commencement of irradiation (considered 100% applied radioactivity) (p. 20).

Detection limits (LOD and LOQ) for the parent and transformation products: The limits of quantification (LOQ) and detection (LOD) of the radio-HPLC were approximately 0.4% and 0.2% of applied radioactivity, respectively (LOQ and LOD were reported by the applicant, in a response to a clarifax received on September 8, 2004). The LOQ and LOD were not reported for LSC.

II. RESULTS AND DISCUSSION:

A. TEST CONDITIONS: The incubation temperatures remained at $25 \pm 1^\circ\text{C}$ throughout the study (Appendix 9, p. 37). The pH of the irradiated solutions (phenyl and triazole label) ranged from 6.96 to 7.03 while the pH in the dark control solutions ranged from 7.00 to 7.12 (phenyl label) and 6.95 to 7.18 (triazole label) (Table 4, p. 19). The samples remained sterile throughout the study; no supporting sterility data were provided.

B. MASS BALANCE: The mass balance was $97.5 \pm 5.8\%$ and $100.3 \pm 8.4\%$ of the applied amount in the dark and irradiated samples, respectively, for [phenyl-UL- ^{14}C]prothioconazole, and $99.7 \pm 5.2\%$ and $104.0 \pm 5.3\%$ of the applied amount in the dark and irradiated samples, respectively, for [triazole-3,5- ^{14}C]prothioconazole (Appendices 17 and 20, p. 45 and 48).

Table 6: Phototransformation of phenyl-labelled prothioconazole ([phenyl-UL- ^{14}C]JAU6476) in irradiated samples in pH 7 phosphate buffer, expressed as percentage of the applied radioactivity (n=1).

Compound	Sampling times (days)						
	0	0.06 (1.5 hrs)	0.17 (4 hrs)	1	5	11	18
Prothioconazole (JAU 6476)	98.4	97	89.7	70.2	13.3	0.7	n.d.
JAU 6476-desthio	1.6	1.7	3.4	12.6	43.1	54.1	54.8
JAU 6476-thiazocine	n.d.	n.d.	1.2	2.5	14.1	12.8	8.4
Met 2B	n.d.	n.d.	n.d.	0.8	4.6	5.7	7

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Met 3	n.d.	n.d.	0.5	0.8	2.8	2.2	1.5
Met 4	n.d.	n.d.	n.d.	n.d.	2.3	3.5	3
Met 5	n.d.	n.d.	n.d.	n.d.	3.4	1.4	n.d.
Met 6	n.d.	n.d.	n.d.	n.d.	2.4	3.6	4.5
Met 7	n.d.	n.d.	n.d.	n.d.	n.d.	2.6	3
Unassigned transformation products ¹	n.d.	0.7	1.9	n.d.	6.8	8.9	13
Unidentified radioactivity ²	n.d.	n.d.	n.d.	n.d.	n.d.	4.5	4
CO ₂	n.m.	<0.1	<0.1	<0.1	0.4	1.2	3
Volatile organics	n.m.	<0.1	<0.1	<0.1	0.3	0.9	1.7
Total % recovery	100	99.4	96.7	86.9	93.5	102.1	103.9

¹ Sum of seven unassigned peaks with the largest single peak at 2.7% peak area ratio.

² Unidentified radioactivity eluting in the void volume of the column.

n.m.= not measured; n.d. = not detected; LOD and LOQ are ~0.2% and ~0.4% of applied radioactivity, respectively. Data obtained from Appendices 17 and 22, p. 45 and 52 of the study report.

Table 7: Phototransformation of triazole-labelled prothioconazole ([triazole-3,5-¹⁴C]JAU6476) in irradiated samples in pH 7 phosphate buffer, expressed as percentage of the applied radioactivity (n=1).

Compound	Sampling times (days)						
	0	0.06 (1.5 hrs)	0.17 (4 hrs)	1	5	11	18
Prothioconazole (JAU 6476)	97.4	93.3	93.9	71.1	19.3	0.8	n.d.
JAU 6476-desthio	1.1	2.3	3.2	10.8	43	55.7	53.2
JAU 6476-thiazocine	n.d.	n.d.	1.3	3.1	9.2	9.5	9.1
1,2,4-triazole	n.d.	n.d.	n.d.	n.d.	2.6	7.4	11.9
Met 3	n.d.	n.d.	0.4	1.1	2.9	2	1.7
Met 4	n.d.	n.d.	n.d.	0.4	2.9	4.3	4.6
Met 5	n.d.	n.d.	n.d.	1.7	2.7	0.9	n.d.
Unassigned transformation products ¹	1.6	2.7	1.5	2.9	12.4	18.6	19.2

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Unidentified radioactivity ²	n.d.	n.d.	n.d.	n.d.	1.7	4.3	7.1
CO ₂	n.m.	<0.1	<0.1	<0.1	0.1	0.3	0.5
Volatile organics	n.m.	<0.1	<0.1	<0.1	<0.1	<0.1	0.1
Total % recovery	100	98.3	100.3	91.1	96.8	103.8	107.4

¹ Sum of nine unassigned peaks with the largest single peak at 2.9% peak area ratio.

² Unidentified radioactivity eluting in the void volume of the column.

n.m.= not measured; n.d. = not detected; LOD and LOQ = ~0.2% and ~0.4% of applied radioactivity, respectively. Data obtained from Appendices 17 and 22, p. 45 and 52 of the study report.

Table 8: Transformation of phenyl-labelled prothioconazole ([phenyl-UL-¹⁴C]JAU6476) in dark control samples in pH 7 phosphate buffer, expressed as percentage of the applied radioactivity (n=1).

Compound	Sampling times (days)		
	0	5	18
prothioconazole	n.r.	n.r.	99.51
Other radioactivity in solution	n.r.	n.r.	9.21
CO ₂	n.m.	<0.1	<0.1
Volatile organics	n.m.	0.1	0.1
Total % recovery	100	92	108.8

¹ Percentage of AR calculated by the reviewer by multiplying a value of 91.5% peak area ratio by HPLC reported by the study authors (p. 21) by a value of 1.087 (108.7%) of applied radioactivity in solution (Appendix 20, p. 48). The % AR for the 'other radioactivity in solution' was calculated as the remaining 8.5% (100% peak area ratio - 91.5%) peak area ratio by HPLC multiplied by 1.087.

n.m.= not measured

n.r.= not reported

Table 9: Transformation of phenyl-labelled prothioconazole ([triazole-3,5-¹⁴C]JAU6476) in dark control samples in pH 7 phosphate buffer, expressed as percentage of the applied radioactivity (n=1).

Compound	Sampling times (days)		
	0	5	18
prothioconazole	n.r.	n.r.	103.31
Other radioactivity in solution	n.r.	n.r.	4.41
CO ₂	n.m.	2.4	2.3

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Volatile organics	n.m.	<0.1	<0.1
Total % recovery	100	101.9	110

¹ Percentage of AR calculated by the reviewer by multiplying a value of 95.9% peak area ratio by HPLC reported by the study authors (p. 21) by a value of 1.077 (107.7%) of applied radioactivity in solution (Appendix 20, p. 48). The % AR for the 'other radioactivity in solution' was calculated as the remaining 4.1% (100% peak area ratio - 95.9%) peak area ratio by HPLC multiplied by 1.077.

n.m.= not measured

n.r.= not reported

C. TRANSFORMATION OF PARENT COMPOUND: At study termination, 91.5% and 95.9% of HPLC peak area ratio (99.5% and 103.3% of the applied radioactivity, calculated by correcting for material balance recoveries in solution), remained as the parent in the dark samples for the phenyl and triazole labels, respectively (p. 21; Appendix 20, p. 48). The radioactivity attributed to prothioconazole in dark controls on days 0 and 5 was not determined, and peak area ratios by HPLC were not provided for those days. Quantitative data for the HPLC-identified transformation product, JAU6476-desthio, and for two other peaks visible in chromatograms of the dark control samples on day 18 were not reported. Therefore, there is no quantitative raw data submitted to support the conclusion that no statistically significant transformation occurred in the dark samples, as the reviewer is not able to confirm reported results. At study termination, the evolved CO₂ and volatile organic compounds in the dark samples amounted to <0.1% and 0.1% of the applied radioactivity, respectively, for the phenyl label, and 2.3% and <0.1% of the applied radioactivity, respectively, for the triazole label (Appendix 20, p. 48).

In the irradiated samples, [¹⁴C]prothioconazole decreased from 98.4% and 97.4% of the applied amount at study initiation for the phenyl and triazole labelled compounds, respectively, to <MDL at study termination (18 days).

TRANSFORMATION PRODUCTS: The major transformation products detected in the irradiated samples were **JAU6476-desthio** (SXX0665; 2-[2-(1-chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole), **JAU6476 thiazocine** (6-(1-chlorocyclopropyl)-6,7-dihydro-triazole-5H-[1,2,4]triazolo[5,1-b][1,3]benzothiazon-6-ol), and **1,2,4-triazole** (1-H-1,2,4-triazole) with maximum concentrations of 55.7%, 14.1%, and 11.9% of the applied observed on the 11th, 5th, and 18th day of incubation from the phenyl, phenyl, and triazole labelled parent, respectively. After reaching the maximum, concentrations of JAU6476-desthio and JAU6476 thiazocine decreased to 53.2% and 8.4% of the applied, respectively, from the phenyl labelled parent by study termination, while 1,2,4-triazole was at maximum at study termination. The six minor transformation products in the irradiated samples were characterized but not identified and were formed at a maximum of 4.6-7.0% of the applied amount in both phenyl and triazole labelled treatments. From seven to nine additional unassigned peaks were detected in both labelled treatments, together representing 13.0-19.2% of the applied radioactivity on day 18, with the largest single peak at 3.1% of the applied radioactivity (2.9% HPLC peak area ratio) in either treatment, although the reviewer is not able to confirm these

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reported results, as there was no raw data submitted to support this conclusion. At test termination, in the irradiated samples, the evolved CO₂ and volatile organic compounds amounted to 3.0% and 1.7% of the applied radioactivity, respectively, for the phenyl label, and 0.5% and 0.1% of the applied radioactivity, respectively, for the triazole label. The total unidentified radioactivity eluting in the void volume of the column was a maximum of 4.5-7.1% of the applied radioactivity in the irradiated samples treated with either radiolabel. Unidentified radioactivity was not reported for the dark samples.

Comparison of transformation products formed in the dark and irradiated samples is not possible, as transformation products formed in the dark other than JAU6476-desthio were not identified, despite their presence in chromatograms of the dark control samples, and no dark sample transformation products were quantified. It cannot be determined which transformation products are formed by phototransformation only. No phototransformation pathway was proposed.

PATHWAY: No phototransformation pathway was proposed by the study author.

Table 10: Chemical names and CAS numbers for the transformation products of prothioconazole (JAU6476).

Applicant's Code Name	CAS Number	CAS and/or IUPAC Chemical Name(s)	Chemical formula	Molecular weight
JAU6476-desthio (SXX0665)	NA	2-[2-(1-Chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxy-propyl]-1,2-dihydro-3H-1,2,4-triazole	C ₁₄ H ₁₅ Cl ₂ N ₃ O	312.2
JAU6476-thiazocine	NA	6-(1-Chlorocyclopropyl)-6,7-dihydro-triazole-5H-[1,2,4]triazolo[5,1-b][1,3]benzothiazon-6-ol	C ₁₄ H ₁₄ N ₃ ClOS	307.8
1,2,4-triazole	NA	1-H-1,2,4-triazole	C ₂ H ₃ N ₃	69.1

HALF-LIFE:

The half-life of both [phenyl-UL-¹⁴C] and [triazole-3,5-¹⁴C]prothioconazole in the irradiated samples was 1.9 days, calculated using linear regression on log-transformed data, including the <MDL point at 18 days at MDL (0.2). The half-life (or statistical stability) of [phenyl-UL-¹⁴C] and [triazole-3,5-¹⁴C]prothioconazole in the dark samples could not be calculated, as raw data were not provided for [¹⁴C]prothioconazole recoveries in the dark control samples on days other than day 18.

Table 11: Half-lives (t_{1/2}) calculated by the reviewers.

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Test system	First order linear regression on log-transformed data		
	$t_{1/2}$	Regression equation	r^2
Combined labels			
Irradiated	45.4 hours (1.9 days)	$y = -0.3662x + 4.5274$ (time unit of days)	0.9778
Phenyl label			
Irradiated	45.3 hours (1.9 days)	$y = -0.3675x + 4.4970$ (time unit of days)	0.9764
Triazole label			
Irradiated	45.6 hours (1.9 days)	$y = -0.3649x + 4.5577$ (time unit of days)	0.9798

Data obtained from Appendix 22, p. 52 of the study report.

Because the half-life of dark samples could not be calculated, for the purpose of aqueous photolysis half-life calculation, it is assumed that all degradation can be attributed to photolysis, based on reported parent HPLC peak areas greater than 90% at study termination and on the stability of prothioconazole to hydrolysis (MRID: 46246505). Therefore, the phototransformation half-life of prothioconazole is equal to the half-life of prothioconazole in the irradiated samples.

The study authors stated that 1 day (24 hours) of artificial light (4.66 MJ/m²) was comparable to 3.6 days of natural sunlight in June in Phoenix, Arizona, USA (33.26°N; 31 MJ/m²/day) and 5.1 days in Edmonton, Alberta, Canada (53.33°N; 22 MJ/m²/day) (Appendix 14, p. 42). EPA uses a predicted environmental half-life at 40° N latitude. New York, New York (40.47°N; 21.7 MJ/m²/day) is reported to have 70% of the solar radiation conditions of Phoenix, Arizona in June (Appendix 16, p. 44). This means that 1 hour of Suntest artificial light is equivalent to 5.15 hours of irradiation at 40° N latitude.

The **predicted environmental phototransformation half-life** estimated for both [phenyl-UL-¹⁴C] and [triazole-3,5-¹⁴C]prothioconazole, derived from the measured half-life in the laboratory in a sterile buffer solution under the xenon lamp, was calculated to be 9.7 days and 9.6 days for 40° N latitude (New York, NY, USA) and 53° N latitude (Edmonton, AB, Canada), respectively, in June sunlight.

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

III. STUDY DEFICIENCIES:

Single samples were collected at each sampling interval from one bulk sample. It is preferred that two or more samples be collected from each treatment interval, using individual vessels for each sample, so that between sample variation can be quantified and to minimize the possibility of contamination of the test solution (and, therefore, cause the parent to metabolize due to microbe contamination and not photolysis). In this case, sterility appears to have been maintained (although supporting raw data was not provided), despite the greater risk for contamination.

The raw data (peak area ratios by HPLC) were not provided for day 18 in dark controls (for degradates) and for days 0 and 5 in dark controls (for prothioconazole and degradates). Additionally, 13.0-19.2% of applied radioactivity ("unassigned metabolites") were not separately reported in the irradiated samples. If raw data is not submitted to support study conclusions, then the reviewer is not able to confirm reported results.

The U.S. EPA is classifying this study on phototransformation in water supplemental because single replicates from a bulk sample were used (multiple replicates per sampling interval from separate vessels are preferable), all dark control data were not reported, and 13.0-19.2% of applied radioactivity ("unassigned metabolites") were not separately reported. The PMRA does not use the same classification scheme as the U.S. EPA. This study is classified acceptable to the PMRA.

IV. REVIEWER'S COMMENTS:

1. Small peaks of JAU6476-desthio appeared on sample chromatographs for dark controls (p. 54 of study report) but the percent area associated with prothioconazole and JAU64765-desthio (or percent of applied radioactivity attributed to each compound present in solution) was not provided, except for % of HPLC peak area attributed to parent at study termination (p.21). It is difficult to interpret the reported % peak areas, without the context of the % peak areas for rest of dark control sampling intervals. And, if there is even a small amount of prothioconazole-desthio degradate in the dark controls, this means that not all prothioconazole degradation can be attributed to photolysis. Without the data on the dark controls, there is no way to know how large a deviation there is between the true photolysis-only degradation rate and the rate not corrected for hydrolysis.

2. Despite the fact that raw data on degradation in dark controls was not reported, the hydrolysis study submitted for prothioconazole (Riegner, 1998) showed that it was stable to hydrolysis, with extrapolated half-lives of greater than 1 year at pH 7. Based on this information, the EAD reviewer agrees with the study authors that the contribution from hydrolysis can be neglected and that phototransformation is the main route of transformation of prothioconazole in this study. The phototransformation half-life will not be corrected for hydrolysis. EPA concurs for aqueous

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photolysis half-life calculation purposes, but notes that this conclusion cannot be verified from the data submitted with this study and adds uncertainty to the aqueous photolysis half-life.

3. From 13.0-19.2% of applied radioactivity was unidentified as unassigned metabolites. Even though the study reports that this radioactivity is made up of seven separate metabolites for phenyl-labelled prothioconazole and nine separate metabolites for triazole-labelled prothioconazole, it does not give data on each metabolite. The only quantitative information reported concerning these metabolites is reported in the text (ie., that an individual metabolite within those seven and nine was at a max of 2.7% and 2.9% of applied, respectively, per label). Again, without raw data submitted to support this conclusion, the reviewer is not able to confirm the reported results and the uncertainty associated with this study increases.

4. Although quantitative data for JAU6476-desthio was not provided for the dark samples, the proportion of JAU6476-desthio in the irradiated samples compared to the parent prothioconazole in the chromatograms for the dark and irradiated samples on day 18 appears much higher than in the dark samples. In addition, the study author states that the remaining a.i. detected in the dark control samples amounted to 91.5-95.9% of the HPLC peak area ratio (both labels) (p. 21). Although not explicitly stated, the EAD reviewer assumes the 'remaining a.i.' refers to day 18. Assuming this to be the case, JAU6476-desthio could therefore only account for a maximum of 4.1-8.5% HPLC peak area ratio ($100-95.9=4.1$; $100-91.5=8.5$). Taking into account that the mass balance recovery in solution on day 18 was 108.7% of AR in the dark controls (Appendix 20, p. 48), 91.5-95.9% of HPLC peak area ratios for the parent prothioconazole amount to 99.5-103.3% of the AR ($108.7*0.915=99.5$; $108.7*95.9=103.3$). Similarly, 4.1-8.5% HPLC peak area ratios for JAU6476-desthio correspond to 4.4-9.2% of the AR ($108.7*0.041=4.4$; $108.7*0.085=9.2$). Considering that JAU6476-desthio was formed at 55.7% of the AR in the irradiated samples, it is reasonable to assume that JAU6476-desthio is a major transformation product of phototransformation. Upon inspection of the chromatograms provided for the dark and irradiated samples, the retention time of the unidentified peaks in the dark controls do not seem to correspond with those of JAU6476-thiazocine or 1,2,4-triazole in the irradiated samples, suggesting that these compounds may be formed by phototransformation alone. However, quantitative data were not submitted to support this. No phototransformation pathway was proposed.

5. The co-solvent acetonitrile is used at 0.35-0.61% by volume, and should not affect the photolysis rate.

6. The study author used single first order nonlinear regression on non-transformed data to calculate a half-life of 44.3 hours ($k = 0.0157 \text{ h}^{-1}$, $r^2 = 0.999$) and 51.4 hours ($k = 0.0135 \text{ h}^{-1}$, $r^2 = 0.999$), respectively, for the [phenyl-UL- ^{14}C] and [triazole-3,5- ^{14}C]-treated continuously irradiated samples. The half-life for the combined labels, calculated using the same methodology, was 47.7 hours ($k= 0.0145$, $r^2=1.000$). Taking the stability of prothioconazole in the dark controls into account, the study authors concluded that contributions by hydrolysis can

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be neglected and that phototransformation is the main process of transformation of prothioconazole in water exposed to sunlight (p. 21).

Table 12: Half-lives ($t_{1/2}$) calculated by the study author.

Test system	Values reported by the study authors			
	$t_{1/2}$	$t_{9/10}$	k	r^2
Combined labels				
Irradiated	47.7 hours	158 hours	0.01	1
Phenyl label				
Irradiated	44.3 hours	147 hours	0.02	0.999
Triazole label				
Irradiated	51.4 hours	171 hours	0.01	0.999

7. The **predicted environmental phototransformation half-lives** calculated by the study author of prothioconazole in Phoenix and Edmonton are 7.1 and 10.1 days, respectively.
8. Sterility was asserted (p. 19) without accompanying raw data.
9. The LOQ and LOD were not reported for LSC.

V. REFERENCES:

Riegner, K. 1998. Hydrolysis of [Phenyl-UL-¹⁴C]JAU 6476 in Sterile Aqueous Buffer Solutions. Performing Laboratory: Bayer AG Crop Protection Business Group, Germany. Bayer CropScience, North Carolina. Unpublished. Report No. MR-623/98. November 16, 1998.

Chemical: Prothioconazole
 PC Code: 113961
 MRID: 46246507
 Guideline No: 161-2

Table 6 Phototransformation of [phenyl-UL-¹⁴C]prothioconazole in pH 7 buffer (irradiated samples), expressed as percentage of the applied radioactivity

Time (hours)	Time (days)	Parent	-desthio	-thiazocine triazole	Met 2B	Met 3	Met 4	Met 5	Met 6	Met 7	Void	Unidentified	VOC	CO2	Total	
0	0.00	98.4	1.6	<MDL	N/A	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	N/S	N/S	100.0	
1.5	0.06	97.0	1.7	<MDL	N/A	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.7	<0.1	<0.1	99.4	
4	0.17	89.7	3.4	1.2	N/A	<MDL	0.5	<MDL	<MDL	<MDL	<MDL	1.9	<0.1	<0.1	96.7	
24	1.00	70.2	12.6	2.5	N/A	0.8	0.8	<MDL	<MDL	<MDL	<MDL	<MDL	<0.1	<0.1	86.9	
120	5.00	13.3	43.1	14.1	N/A	4.6	2.8	2.3	3.4	2.4	<MDL	<MDL	6.8	0.3	0.4	93.5
264	11.00	0.7	54.1	12.8	N/A	5.7	2.2	3.5	1.4	3.6	2.6	4.5	8.9	0.9	1.2	102.1
432	18.00	<MDL	54.8	8.4	N/A	7.0	1.5	3.0	<MDL	4.5	3.0	4.0	13.0	1.7	3.0	103.9
															AVR	97.5
															STDEV	5.8

LOQ and LOD of the radio-HPLC were approximately 0.4% and 0.2% of applied radioactivity.

LOQ and LOD were not reported for LSC.

Data were obtained from Appendices 17 and 22, pp. 45 and 52 of the study report.

N/A= Not Applicable

N/S= Not Sampled

Table 7 Phototransformation of [3,5-triazole-¹⁴C]prothioconazole in pH 7 buffer (irradiated samples), expressed as percentage of the applied radioactivity

Time (hours)	Time (days)	Parent	-desthio	-thiazocine triazole	Met 2B	Met 3	Met 4	Met 5	Met 6	Met 7	Void	Unidentified	VOC	CO2	Total	
0	0.00	97.4	1.1	<MDL	N/A	<MDL	<MDL	<MDL	N/A	N/A	<MDL	1.6	N/S	N/S	100.1	
1.5	0.06	93.3	2.3	<MDL	N/A	<MDL	<MDL	<MDL	N/A	N/A	<MDL	2.7	<0.1	<0.1	98.3	
4	0.17	93.9	3.2	1.3	N/A	0.4	<MDL	<MDL	N/A	N/A	<MDL	1.5	<0.1	<0.1	100.3	
24	1.00	71.1	10.8	3.1	N/A	1.1	0.4	1.7	N/A	N/A	<MDL	2.9	<0.1	<0.1	91.1	
120	5.00	19.3	43.0	9.2	N/A	2.9	2.9	2.7	N/A	N/A	1.7	12.4	<0.1	0.1	96.8	
264	11.00	0.8	55.7	9.5	N/A	2.0	4.3	0.9	N/A	N/A	4.3	18.6	<0.1	0.3	103.8	
432	18.00	<MDL	53.2	9.1	N/A	1.7	4.6	<MDL	N/A	N/A	7.1	19.2	0.1	0.5	107.4	
															AVR	99.7
															STDEV	5.2

LOQ and LOD of the radio-HPLC were approximately 0.4% and 0.2% of applied radioactivity.

LOQ and LOD were not reported for LSC.

Data were obtained from Appendices 17 and 22, pp. 45 and 52 of the study report.

N/A= Not Applicable

N/S= Not Sampled

Chemical: Prothioconazole
 PC Code: 113961
 MRID: 46246507
 Guideline No: 161-2

Table 6 Material balance of [phenyl-UL-¹⁴C]prothioconazole in pH 7 buffer (irradiated samples), expressed as percentage of the applied radioactivity

Time (hours)	Time (days)	Aqueous	CO2	VOC	Total
0	0.00	100.0	N/S	N/S	100.0
1.5	0.06	99.4	<0.1	<0.1	99.4
4	0.17	96.7	<0.1	<0.1	96.7
24	1.00	87.0	<0.1	<0.1	87.0
120	5.00	92.8	0.4	0.3	93.5
264	11.00	100.1	1.2	0.9	102.2
432	18.00	99.2	3.0	1.7	103.9
AVR					97.5
STDEV					5.8

LOQ and LOD were not reported for LSC.
 Data were obtained from Appendix 17, p. 45 of the study report.

Table 7 Material balance of [3,5-triazole-¹⁴C]prothioconazole in pH 7 buffer (irradiated samples), expressed as percentage of the applied radioactivity

Time (hours)	Time (days)	Aqueous	CO2	VOC	Total
0	0.00	100.0	N/S	N/S	100.0
1.5	0.06	98.3	<0.1	<0.1	98.3
4	0.17	100.2	<0.1	<0.1	100.2
24	1.00	91.1	<0.1	<0.1	91.1
120	5.00	96.7	0.1	<0.1	96.8
264	11.00	103.6	0.3	<0.1	103.9
432	18.00	106.7	0.5	0.1	107.3
AVR					99.7
STDEV					5.2

LOQ and LOD were not reported for LSC.
 Data were obtained from Appendix 17, p. 45 of the study report.

Table 8 Material balance of [phenyl-UL-¹⁴C]prothioconazole in pH 7 buffer (dark samples), expressed as percentage of the applied radioactivity

Time (hours)	Time (days)	Aqueous	CO2	VOC	Total
0	0.00	100.0	N/S	N/S	100.0
120	5.00	91.9	<0.1	0.1	92.0
432	18.00	108.7	<0.1	0.1	108.8
AVR					100.3
STDEV					8.4

LOQ and LOD were not reported for LSC.
 Data were obtained from Appendix 20, p. 48 of the study report.

Table 9 Material balance of [3,5-triazole-¹⁴C]prothioconazole in pH 7 buffer (dark samples), expressed as percentage of the applied radioactivity

Time (hours)	Time (days)	Aqueous	CO2	VOC	Total
0	0.00	100.0	N/S	N/S	100.0
120	5.00	99.5	2.4	<0.1	101.9
432	18.00	107.7	2.3	<0.1	110.0
AVR					104.0
STDEV					5.3

LOQ and LOD were not reported for LSC.
 Data were obtained from Appendix 20, p. 48 of the study report.

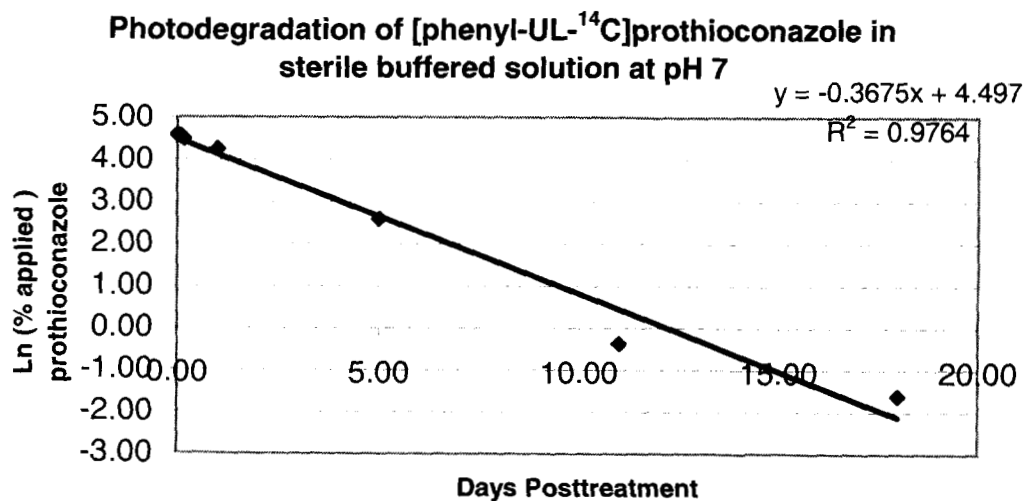
Chemical: Prothioconazole
PC Code: 113961
MRID: 46246507
Guideline No: 161-2

Table 11

Days	Hours	% applied	Ln (% applied)
0.00	0	98.4	4.59
0.06	1.5	97.0	4.57
0.17	4	89.7	4.50
1.00	24	70.2	4.25
5.00	120	13.3	2.59
11.00	264	0.7	-0.36
18.00	432	<MDL	-1.61

Data were obtained from Appendix 22, p. 52 of the study report.
MDL=0.2% of applied.

First order linear Half life = 1.9 days
First order linear Half life = 45.3 hours



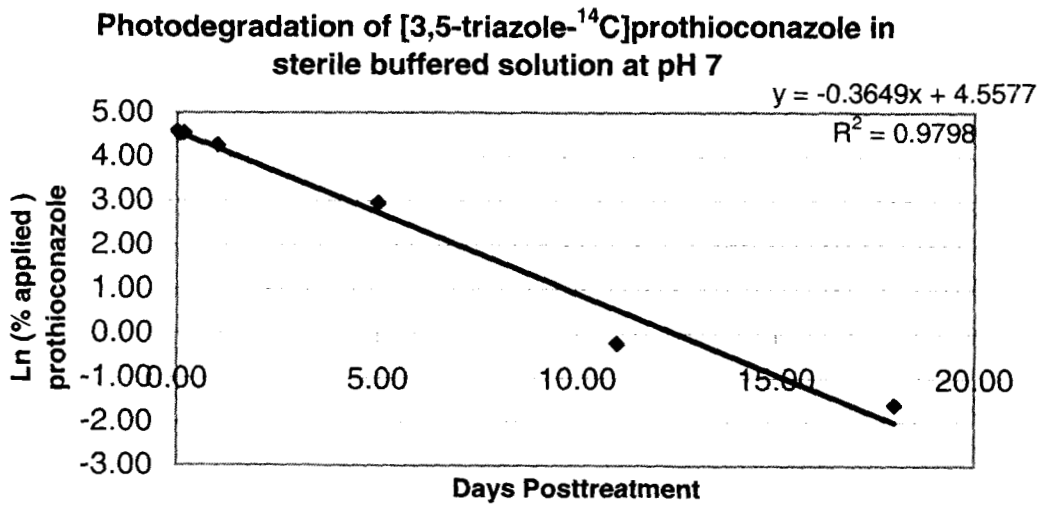
Chemical: Prothioconazole
 PC Code: 113961
 MRID: 46246507
 Guideline No: 161-2

Table 11

Days	Hours	% applied	Ln (% applied)
0.00	0	97.4	4.58
0.06	1.5	93.3	4.54
0.17	4	93.9	4.54
1.00	24	71.1	4.26
5.00	120	19.3	2.96
11.00	264	0.8	-0.22
18.00	432	<MDL	-1.61

Data were obtained from Appendix 22, p. 52 of the study report.
 MDL=0.2% of applied.

First order linear Half life = 1.9 days
 First order linear Half life = 45.6 hours



Chemical: Prothioconazole
 PC Code: 113961
 MRID: 46246507
 Guideline No: 161-2

Table 11

Days	Hours	NY-equivalent days	Ed-equivalent days	Label	% applied	Ln (% applied)
0.00	0	0.00	0.00	phenyl	98.4	4.59
0.06	1.5	0.32	0.32	phenyl	97.0	4.57
0.17	4	0.86	0.85	phenyl	89.7	4.50
1.00	24	5.15	5.08	phenyl	70.2	4.25
5.00	120	25.77	25.42	phenyl	13.3	2.59
11.00	264	56.69	55.92	phenyl	0.7	-0.36
18.00	432	92.77	91.51	phenyl	<MDL	-1.61
0.00	0	0.00	0.21	triazole	97.4	4.58
0.06	1.5	0.32	0.32	triazole	93.3	4.54
0.17	4	0.86	0.85	triazole	93.9	4.54
1.00	24	5.15	5.08	triazole	71.1	4.26
5.00	120	25.77	25.42	triazole	19.3	2.96
11.00	264	56.69	55.92	triazole	0.8	-0.22
18.00	432	92.77	91.51	triazole	<MDL	-1.61

Data were obtained from Appendix 22, p. 52 of the study report.
 MDL=0.2% of applied.

Experimental First order linear Half life = 1.9 days
 Predicted NY environmental First order linear Half life = 9.7 days
 Predicted Ed environmental First order linear Half life = 9.6 days

