Data Evaluation Report on the hydrolysis of prothioconazole (JAU6476)

PMRA Submission Number 2004-0843 EPA MRID Number 46246505

Data Requirement:: PMRA DATA CODE: 8.2.3.2
EPA DP Barcode: DP 303488
OECD Data Point: IIA 2.9.1
EPA Guideline: 161-1, OPPTS 835.2110

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: JAU6476 Technical
SMILES string: ClC1(C(Cc2ccccc2Cl)(CN2N=CNC2=S)O)CC1.

Primary Reviewer (officer number): Émilie Larivière (#1269) **Date:** February 16, 2005
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Connie Hart 13 Jun 05
Secondary Reviewer (officer number): Connie Hart (#1158) **Date:** June 13, 2005
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Secondary Reviewer(s) (officer number): Roxolana Kashuba **Date:** August 1, 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

2050563

The hydrolysis of [phenyl-UL-^{14}C]labelled 2-[2-(1-Chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole-3-thione (prothioconazole; JAU6476; chemical purity >98%) at 3.6-3.9 mg a.i./L was studied in the dark at 50°C in sterile aqueous buffered solutions at pH 4 (0.01M acetate buffer), pH 7 (0.01M tris hydroxymethyl aminomethane buffer) and pH 9 (0.01M borate buffer) for 7 days (168 hours). The experiment was conducted in accordance with US EPA Subdivision N, Section 161-1 and EC Guidelines, and in compliance with OECD Principles of Good Laboratory Practice (GLP). Samples were analyzed at 0, 1 (pH 9 only), 2.5 (pH 9 only), 6, 24, 48, 72, 96 and 168 hours by removing aliquots, without extraction, and residues of [phenyl-UL-^{14}C]prothioconazole were analyzed by liquid scintillation counting (LSC) and high performance liquid chromatography (HPLC). Identification of transformation products was done by high performance liquid chromatography-mass spectrometry (HPLC-MS).

The radioactivity balance was 103.4 ± 2.7%, 103.0 ± 2.0%, and 102.3 ± 1.5% of the applied radioactivity at pH 4, pH 7, and pH 9, respectively. At test termination, the concentration of [phenyl-UL-^{14}C]prothioconazole decreased from 94.5% at day 0 to 93.3% of the initial at pH 4, remained at 95.0%-99.9% at pH 7, and remained at 97.4%-100.7% at pH 9. No major transformation products were detected in any pH solution. The minor transformation products were JAU6476-desthio (SXX0665; 2-[2-(1-chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole), formed at a maximum of 5.3%, 2.7%, and 2.4% of the applied at pH 4, pH 7, and pH9, respectively, and an unidentified transformation product (M1) formed at a maximum of 2.5%, 1.9%, and 1.9% of the applied at pH 4, pH 7, and pH9, respectively. Volatiles were not measured. The unidentified radioactivity (sum of unidentified transformation product 'M1' and 'other' radioactivity) was 4.2, 0.7, and 2.2% of the applied amount at study termination, at pH 4, pH 7 and pH 9, respectively.

The half-life of prothioconazole at 50°C was calculated to be 120 days at pH 4 (using linear regression on log-transformed data), and was statistically stable at pH 7 and pH 9. The half-life of prothioconaole at 25°C was extrapolated by the study author from the 50°C data to between 679 days and >10 years at pH 4. Prothioconazole is stable to hydrolysis at pH 4 at 25 °C and at pH 7 and 9 at 50 °C.

This study is classified as acceptable for a hydrolysis study.

RESULTS SYNOPSIS:

	Half-life	Major transformation products
pH 4	stable (679 days - >10 years)	None
pH 7	stable (> 1 year)	None
pH 9	stable (> 1 year)	None

I. MATERIALS AND METHODS

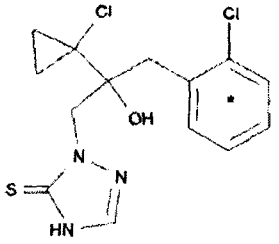
GUIDELINE FOLLOWED: EC Guidelines (Commission directive 95/36/EC (1995) and 95/37/EC (1994); Official Journal of the European Communities, No 1 383 A, EED method C7 (1992); SETAC-Europe (1995)) and US EPA Guidelines (161-1 (1982, 1985, 1989), EPA 738-R-93-010 (1993) and EPA 738-R-95-015 (1995)). No deviations were noted by the study author.

COMPLIANCE: Chemikaliengesetz (attachment 1, dated 1994/1997) and OECD (1997). Signed and dated GLP, Quality Assurance and Data Confidentiality statements were provided.

A. MATERIALS:

1. Test Material [phenyl-UL-^{14}C]JAU6476 (prothioconazole, p. 6; Appendix 1, p. 18)

Chemical Structure:



* denotes ^{14}C-labelling position

Description: Technical, solid (Appendix 1, p. 18).

Purity:
Analytical purity: >98%
Radiochemical purity: 97.7% (97.3%-98.1%)
Lot: 11403/1
Batch No.: KML 2468
Specific activity: 2.97 Mbq/mg
Locations of the label: phenyl ring

Storage conditions of test chemicals: Freezer (≤-20 °C), reference JAU 6476 stored at 0-10°C; reference SXX 0665 stored at room temperature.

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

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

pH	Type and final molarity of buffer	Composition

4	0.01 M acetate buffer	1.36 g CH_3COONa x 3 H_2O in 250 mL H_2O. pH adjusted to 4.0 using acetic acid. Buffer stock solution diluted to 0.01 M with H_2O (1 + 3; v+v).
7	0.01 M TRIS buffer	50 mL of 0.1 M tris(hydroxymethyl)aminomethane solution (12.1 g/L H_2O), mixed with 46 mL of 0.1 N HCl solution (3.65 g HCl/L H_2O) and filled to 100 mL with H_2O. pH adjusted to 7.0 with 0.1N HCl or NaOH solutions. Buffer stock solution diluted to 0.01 M with H_2O (1+4; v+v)
9	0.01 M borate buffer	0.62 g boric acid (H_3BO_3) + 0.75 g KCl in 250 mL H_2O. To 125 mL of this solution, add 53 mL of 0.04 M sodium hydroxide solution (1.6 g NaOH/L H_2O) and dilute with H_2O up to 250 mL. pH adjusted to 9.0 iwth 0.4 M sodium hydroxide or boric acid. Buffer stock solution diluted to 0.01 M with H_2O (1+1; v+v)

Data were obtained from p. 8 and Appendix 4, p. 21 of the study report.

B. EXPERIMENTAL CONDITIONS

1) Preliminary Study: No preliminary study was described.

2) Experimental conditions

Table 3. Experimental parameters.

Parameters	Details
Duration of the study	168 hours (7 days)
Test concentrations (mg a.i./L) nominal: measured:	 4 mg a.i./L 3.57, 3.77, 3.93 mg a.i./L for pH 4, 7, and 9, respectively
No. of replications	1

Preparation of test medium	volume used/treatment	5 mL
	method of sterilization	Steam pressure sterilization
	co-solvent (type/concentration)	Acetonitrile: 0.1%
Test apparatus (type/material/volume)		10 mL glass vials
Details of traps for volatile, if any		No traps, as no volatilization of radioactivity from the solutions was not to be expected from preliminary tests.
If no traps were used, is the test system closed/open		Closed. The vessels were stoppered with crimp caps with Teflon-faced septa.
Is there any indication of the test material adsorbing to the walls of the test apparatus?		No, total radiocarbon recovery was 98.2-106.7% of the applied radioactivity (all pH's 4-9).
Experimental conditions Temperature (°C) Lighting		50±1°C (within 50±0.1°C) in the dark
Other details, if any		none

Data were obtained from p. 7-9 of the study report.

3). Supplementary Experiments: No supplementary experiments were described.

4). Sampling: The solutions were incubated for a maximum period of 7 days (168 hours) and the sampling intervals were 0, 6, 24, 48, 72, 96 and 168 hours. For pH 9, additional samples were collected after 1 and 2.5 hours.

Table 4. Sampling details.

Criteria	**Details**
Sampling intervals for the parent/transformation products	pH 4: 0, 6, 24, 48, 72, 96 and 168 hours pH 7: 0, 6, 24, 48, 72, 96 and 168 hours pH 9: 0, 1, 2.5, 6, 24, 48, 72, 96 and 168 hours

Sampling method	50 µL aliquots of the solutions were analyzed directly without any step of enrichment or conditioning.
Sampling methods for the volatile compounds, if any	n/a
Sampling intervals/times for: pH measurement sterility check	 0, 72 and 168 hours 0, 72 and 168 hours
Sample storage before analysis	Freezer (≤-20 °C), not more than one day
Other observation, if any (e.g.: precipitation, color change etc.)	none

Data were obtained from p. 9-10 of the study report.

C. ANALYTICAL METHODS:

Radioactivity in solution was determined by LSC (two 500 µL aliquots) using Quicksafe A or Quickszint 401 (Zinsser Analytic). The samples were measured using LS 6500 (Beckman instruments) or LKB-Wallac 1219 Spectral (Wallac Oy). Identification and quantification of parent compound and transformation products was done by HPLC/MS with a radioactivity flow through detector (Ramona 2000, Raytest) with solid scintillator cell (CaF, Raytest). Aliquots of the solutions were analyzed directly without any step of enrichment or conditioning. The limit of detection was about 1% of the applied radioactivity (p. 11-13).

II. RESULTS AND DISCUSSION:

A. TEST CONDITIONS: The pH, sterility, temperature and other experimental conditions were maintained throughout the study (p. 12-13).

B. MASS BALANCE: Total radiocarbon recovery ranged from 97.7 to 106.7% of the applied radioactivity at pH 4, 99.4 to 105.8 % of the applied at pH 7, and 98.8 to 105.0 % of the applied at pH 9, in replicate samples (calculated from Appendices 8-10, p. 25-27).

Table 5. Hydrolysis of prothioconazole, expressed as percentage of the applied radioactivity (mean ± s.d.) at pH 4 at 50 °C.

Compound	Sampling times (hours)						
	0	6	24	48	72	96	168

prothioconazole	94.5 ±0.7	95.9 ±1.0	101.1 ±0.2	98.6 ±0.3	99.3 ±0.0	102.1 ±0.8	93.3 ±0.4
SXX 0665	2.1 ±0.9	2.5 ±0.3	3.0 ±0.0	3.2 ±0.0	3.3 ±0.2	3.4 ±0.2	5.3 ±0.5
M 1	1.5 ±0.8	2.5 ±0.7	1.5 ±0.1	1.7 ±0.4	1.9 ±0.4	1.2 ±0.5	0.8 ±0.0
Others	n.d.	1.5 ±0.1	n.d.	n.d.	n.d.	n.d.	3.4 ±0.4
Volatiles	Not measured.						
Total % recovery	98.1 ±0.6	102.4 ±0.0	105.6 ±0.1	103.5 ±0.1	104.5 ±0.2	106.7 ±0.0	102.8 ±0.4

Data obtained from Appendices 8, 11 and 14, pp. 25, 28, and 31.

Table 6. Hydrolysis of prothioconazole, expressed in relative values (mean % peak area ± s.d.) of HPLC analysis of samples at pH 4 at 50°C.[1]

Compound	**Sampling times (hours)**						
	0	**6**	**24**	**48**	**72**	**96**	**168**
prothioconazole	96.3 ±0.1	93.7 ±1.0	95.8 ±0.1	95.3 ±0.3	95.0 ±0.1	95.7 ±0.7	90.8 ±0.0
SXX 0665	2.2 ±0.9	2.4 ±0.2	2.9 ±0.0	3.1 ±0.0	3.2 ±0.2	3.2 ±0.2	5.2 ±0.5
M 1	1.5 ±0.8	2.5 ±0.7	1.4 ±0.1	1.7 ±0.4	1.8 ±0.4	1.2 ±0.5	0.8 ±0.0
Others	n.d.	1.5 ±0.1	n.d.	n.d.	n.d.	n.d.	3.3 ±0.4
Volatiles	Not measured.						
Total % recovery	100	100	100	100	100	100	100

Data obtained from Appendix 11, p.28.

[1] These values were used in estimation of the hydrolysis half-life for prothioconazole at pH 4.

Table 7. Hydrolysis of prothioconazole, expressed as percentage of the applied radioactivity (mean ± s.d.) at pH 7 at 50 °C.

Compound	**Sampling times (hours)**						
	0	**6**	**24**	**48**	**72**	**96**	**168**
prothioconazole	95.0 ±3.1	99.4 ±0.0	101.8 ±0.6	99.1 ±1.8	102.5 ±1.6	101.3 ±1.1	99.9 ±0.3

SXX 0665	2.7 ±2.8	1.5 ±0.1	1.3 ±0.2	2.1 ±1.0	1.6 ±0.1	2.0 ±0.3	1.9 ±0.1
M 1	1.9 ±0.6	1.5 ±0.1	1.2 ±0.4	1.2 ±0.5	1.1 ±0.7	1.9 ±0.7	0.7 ±0.1
Others	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Volatiles	Not measured.						
Total % recovery	99.6 +0.3	101.4 +0.7	104.4 +0.1	102.4 +0.3	105.2 +0.8	105.2 +0.7	102.5 +0.2

Data obtained from Appendices 9, 12 and 14, pp. 26, 29, and 31.

Table 8. Hydrolysis of prothioconazole, expressed as percentage of the applied radioactivity (mean ± s.d.) at pH 9 at 50 °C.

Compound	**Sampling times (hours)**								
	0	**1**	**2.5**	**6**	**24**	**48**	**72**	**96**	**168**
prothioconazole	97.7 ±0.1	97.9 ±0.3	98.2 ±0.4	97.3 ±1.2	99.6 ±0.5	99.4 ±0.6	100.6 ±0.9	100.7 ±0.9	98.3 ±0.5
SXX 0665	1.5 ±0.5	2.2 ±0.2	1.8 ±0.1	2.3 ±0.2	2.1 ±0.2	2.2 ±0.6	2.4 ±0.3	2.3 ±0.2	2.3 ±0.4
M 1	1.0 ±0.0	1.2 ±0.3	1.5 ±0.5	1.6 ±0.3	1.1 ±0.5	1.1 ±0.3	1.2 ±0.8	1.9 ±0.9	1.4 ±0.6
Others	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.4 ±0.2
Volatiles	Not measured.								
Total % recovery	99.7 +1.3	101.4 +0.2	101.5 +0.2	101.3 +1.3	102.8 +0.2	102.7 +1.5	104.2 +0.4	104.9 +0.2	102.4 +0.6

Data obtained from Appendices 10, 13 and 14, pp. 27, 30, and 31.

C. TRANSFORMATION OF PARENT COMPOUND: Most of the applied ^{14}C was associated with the parent compound at test termination (Tables 5-8). At the end of the study, the concentration of the [phenyl-UL-^{14}C]prothioconazole decreased from 94.5% of the applied radioactivity at day 0 to 93.3% of the applied at pH 4, remained at 95.0%-99.9% at pH 7, and remained at 97.4%-100.7% at pH 9.

The relative values obtained by the HPLC analysis were used to estimate the hydrolysis half-life of the parent compound, in order to suppress an influence by the mass balances found at pH 4 (p. 14). Based on these figures, the parent compound decreased from 96.3% at study intiation to 90.8% after 7 days (Table 6) at pH 4.

TRANSFORMATION PRODUCTS: No major transformation products were detected in any pH solution (Tables 5-8). The minor transformation products were JAU6476-desthio (SXX0665; 2-[2-(1-chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2-dihydro-3H-1,2,4-triazole) formed at a maximum of 5.3%, 2.7%, and 2.4% of the applied at pH 4, pH 7, and pH 9, respectively, and an unidentified transformation product 'M1' formed at a maximum of 2.5%, 1.9%, and 1.9% of the applied amount, at pH 4, pH 7 and pH 9, respectively. At pH 4, the decline in parent concentration was matched by an increase of the amount of JAU6476-desthio (reaching 5.3% of the applied radioactivity at test termination).

Volatiles were not measured; however, the complete material mass balances found at all sampling times suggested that no radioactivity dissipated from the solutions by means of volatilization. The unidentified radioactivity (sum of unidentified transformation product 'M1' and 'other' radioactivity) was 4.2, 0.7, and 2.2% of the applied radioactivity at study termination, at pH 4, pH 7 and pH 9, respectively.

PATHWAYS: n/a

Table 8. Chemical names and CAS numbers for the transformation products of prothioconazole.

Applicant's Code Name	CAS Number	CAS and/or IUPAC Chemical Name(s)	Chemical formula	Molecular weight
JAU6476-desthio (SXX 0665)	NA	2-[2-(1-Chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxy-propyl]-1,2-dihydro-3H-1,2,4-triazole	$C_{14}H_{15}Cl_2N_3O$	312.2
M1	NA	not identified	not identified	not identified

HALF-LIFE: The half-life of prothioconazole at 50°C was 120 days at pH 4, and was statistically stable at pH 7 and pH 9, calculated by EPA using linear regression on log-transformed data from HPLC % peak areas (Appendices 11-13, p. 28-30). The half-life of [phenyl-UL-^{14}C]prothioconazole at 25°C and pH 4 was extrapolated from the 50°C data by the study author using Van't Hoff's law, which says that the reaction velocity increases by a factor of 2 to 4 with an increasing temperature increment of 10°C. Using this law and the lower empirical factor of 2 , the calculated half-life (at 50°C/pH4) was extrapolated to obtain a half-life of 679 days at 25°C. If the empirical factor of 4 is used for extrapolation, a theoretical half-life of more than 10 years will result for 25°C and pH 4. Therefore, prothioconazole is stable to hydrolysis at pH 4 at 25 °C and at pH 7 and 9 at 50 °C.

PMRA estimated the hydrolysis half-life of the parent compound with linear regression of the natural logarithm of the percent of initial applied over time (using values based on the % of the AR as opposed to HPLC relative figures), and obtained a half-life of 413 days. The regression (equation: $y = -0.00007x + 4.5873$, $r^2$0.0164) was not significant ($p > 0.05$). The reviewer

accepts the half-life of prothioconazole at pH 4 reported by the study author, as all results indicate that hydrolysis is not an important route of transformation for prothioconazole. Only a half-life at pH 7 is used for modelling purposes; in this case, 'stable, >1 year' will be provided to the modellers.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: No supplementary experiments were described.

III. STUDY DEFICIENCIES:

(1) Volatiles were not measured, but the complete material mass balances found at all sampling times demonstrated that no radioactivity dissipated from the solutions by means of volatilization.

(2) A test at 25°C was not conducted, as results at 50°C showed that less than 10% of the applied test substance was hydrolysed within 5 days at all tested pH values. This is consistent with the guidance provided in the US EPA OPPTS 835.2110 and in the OECD Guideline 111 (adopted April 14, 2004).
(3) All material balances except at time zero were >100%.

These deficiencies are considered minor and, therefore, this study is acceptable.

IV. REVIEWER'S COMMENTS:

These results indicate that [phenyl-UL-^{14}C]prothioconazole is stable to hydrolysis at environmentally-relevant acidic, neutral and alkaline pH in environmentally-relevant temperatures.

V. REFERENCES:

OECD. 2004. OECD Guidelines for the testing of chemicals. Hydrolysis as a Function of pH. Guideline 111. Adopted 13 April 2004.

US EPA. 1998. Fate, Transport and Transformation Test Guidelines, OPPTS 835.2110 Hydrolysis as a Function of pH. Prevention, Pesticides and Toxic Substances. United States Environmental Protection Agengy, Washington. EPA 712-C-98-057.

Chemical: Prothioconazole
PC Code: 113961
MRID: 46246505
Guideline No: 161-1

Tables 5-8

pH	4	4	4	4	4
Time (hours)	Parent	JAU6476 -desthio	Unidentified M1*	Unidentified Others	Total
0	93.98	2.78	0.95	<MDL	97.72
0	94.92	1.50	2.09	<MDL	98.50
AVG	94.45	2.14	1.52	<MDL	98.11
STDEV	0.66	0.91	0.81	N/A	0.56
6	95.17	2.66	3.00	1.57	102.40
6	96.61	2.31	2.03	1.42	102.38
AVG	95.89	2.49	2.51	1.49	102.39
STDEV	1.02	0.25	0.69	0.10	0.02
24	101.01	2.98	1.56	<MDL	105.55
24	101.26	3.03	1.38	<MDL	105.68
AVG	101.13	3.00	1.47	<MDL	105.61
STDEV	0.18	0.04	0.13	N/A	0.09
48	98.37	3.17	1.98	<MDL	103.52
48	98.78	3.22	1.43	<MDL	103.42
AVG	98.57	3.19	1.70	<MDL	103.47
STDEV	0.28	0.03	0.39	N/A	0.07
72	99.28	3.54	1.61	<MDL	104.42
72	99.29	3.21	2.13	<MDL	104.63
AVG	99.28	3.38	1.87	<MDL	104.53
STDEV	0.01	0.23	0.37	N/A	0.15
96	101.55	3.51	1.62	<MDL	106.68
96	102.68	3.21	0.85	<MDL	106.74
AVG	102.11	3.36	1.24	<MDL	106.71
STDEV	0.79	0.21	0.54	N/A	0.04
168	93.01	4.94	0.80	3.74	102.49
168	93.52	5.65	0.76	3.12	103.05
AVG	93.26	5.29	0.78	3.43	102.77
STDEV	0.36	0.50	0.03	0.44	0.39
AVR					**103.47**
STDEV					**2.90**

7	7	7	7	7
Parent	JAU6476 -desthio	Unidentified M1*	Unidentified Others	Total
92.85	4.61	2.36	<MDL	99.82
97.18	0.72	1.48	<MDL	99.38
95.02	2.66	1.92	<MDL	99.60
3.06	2.76	0.62	N/A	0.32
99.40	1.55	<MDL	<MDL	100.96
99.40	1.41	1.09	<MDL	101.90
99.40	1.48	1.05	<MDL	101.43
0.00	0.10	0.06	N/A	0.67
102.26	1.16	0.99	<MDL	104.41
101.35	1.50	1.48	<MDL	104.33
101.80	1.33	1.24	<MDL	104.37
0.64	0.24	0.35	N/A	0.06
97.82	2.76	1.54	<MDL	102.12
100.39	1.40	0.82	<MDL	102.60
99.10	2.08	1.18	<MDL	102.36
1.82	0.96	0.51	N/A	0.34
103.71	1.46	0.60	<MDL	105.77
101.38	1.63	1.59	<MDL	104.61
102.54	1.55	1.10	<MDL	105.19
1.64	0.12	0.70	N/A	0.82
100.58	1.78	2.36	<MDL	104.72
102.09	2.26	1.35	<MDL	105.71
101.34	2.02	1.85	<MDL	105.21
1.07	0.34	0.71	N/A	0.70
99.70	2.01	0.63	<MDL	102.34
100.15	1.81	0.72	<MDL	102.68
99.93	1.91	0.68	<MDL	102.51
0.32	0.14	0.06	N/A	0.24
				103.03
				2.21

Data were obtained from Appendices 11-12, p. 28-29 of the study report. MDL=1% of applied radioactivity.
*M1= Unidentified degradate.

Chemical: Prothioconazole
PC Code: 113961
MRID: 46246505
Guideline No: 161-1

Tables 4-6

pH	9	9	9	9	9	
Time (hours)	Parent	JAU6476 -desthio	Unidentified M1	Unidentified Others	Total	
0	97.81	1.84	0.94	<MDL	100.59	
0	97.65	1.15	<MDL	<MDL	98.79	
AVG	97.73	1.49	0.96	<MDL	99.69	0.96
STDEV	0.12	0.49	0.04	N/A	1.27	
1	97.72	2.38	1.42	<MDL	101.52	
1	98.13	2.08	1.03	<MDL	101.24	
AVG	97.92	2.23	1.23	<MDL	101.38	1.23
STDEV	0.29	0.21	0.27	N/A	0.20	
2.5	97.92	1.86	1.79	<MDL	101.57	
2.5	98.54	1.67	1.12	<MDL	101.34	
AVG	98.23	1.77	1.46	<MDL	101.45	1.46
STDEV	0.44	0.13	0.47	N/A	0.16	
6	96.51	2.41	1.39	<MDL	100.31	
6	98.22	2.13	1.86	<MDL	102.21	
AVG	97.36	2.27	1.63	<MDL	101.26	1.63
STDEV	1.21	0.20	0.33	N/A	1.34	
24	99.26	1.96	1.41	<MDL	102.62	
24	99.96	2.21	0.71	<MDL	102.88	
AVG	99.61	2.09	1.06	<MDL	102.75	1.06
STDEV	0.50	0.18	0.49	N/A	0.18	
48	99.84	2.58	1.30	<MDL	103.72	
48	98.95	1.77	0.90	<MDL	101.63	
AVG	99.40	2.18	1.10	<MDL	102.67	1.10
STDEV	0.63	0.58	0.28	N/A	1.48	
72	99.89	2.24	1.76	<MDL	103.89	
72	101.20	2.61	0.69	<MDL	104.51	
AVG	100.55	2.43	1.22	<MDL	104.20	1.22
STDEV	0.93	0.26	0.75	N/A	0.44	
96	101.27	2.48	1.23	<MDL	104.98	
96	100.07	2.19	2.50	<MDL	104.76	
AVG	100.67	2.33	1.87	<MDL	104.87	1.87
STDEV	0.85	0.20	0.90	N/A	0.15	
168	97.96	2.65	1.49	0.70	102.80	
168	98.66	2.03	1.23	<MDL	101.93	
AVG	98.31	2.34	1.36	0.86	102.37	2.22
STDEV	0.50	0.44	0.18	0.23	0.62	
AVR					**102.57**	
STDEV					**1.95**	

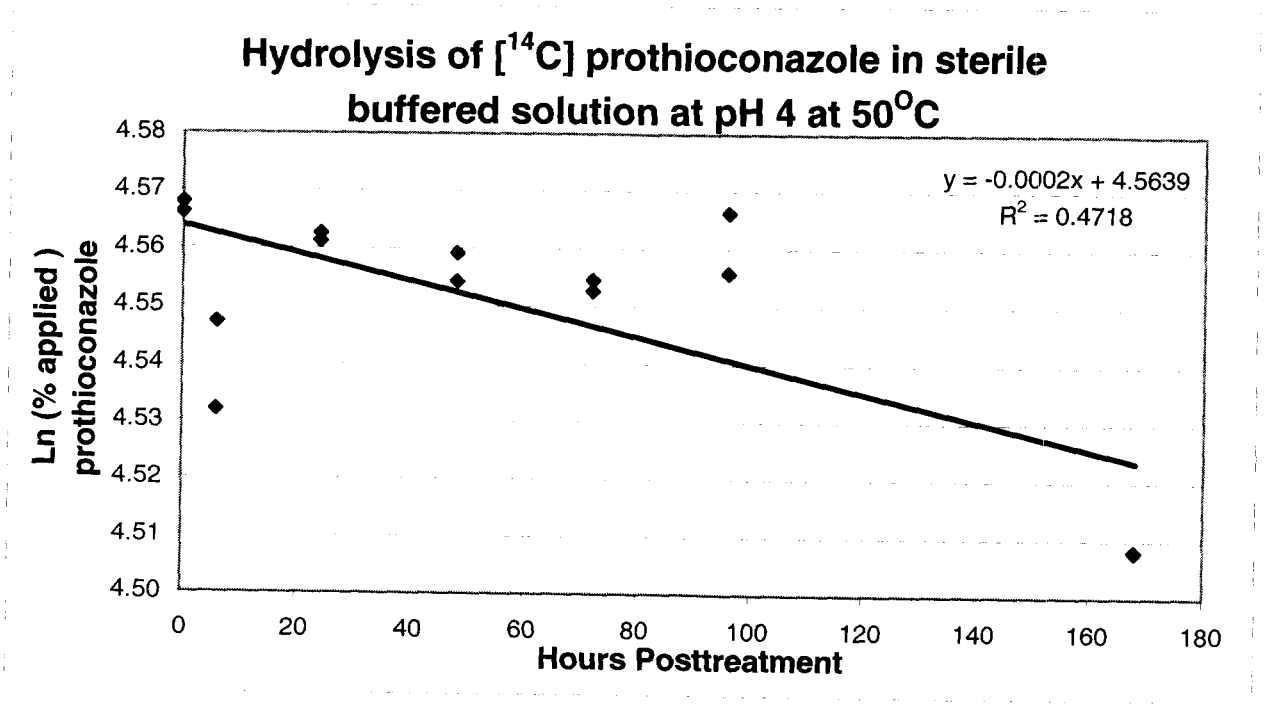
Data were obtained from Appendix 13, p. 28-29 of the study report. MDL=1% of applied radioactivity.

Chemical: Prothioconazole
PC Code: 113961
MRID: 46246505
Guideline No: 161-1

pH= 4

Hours	Prothioconazole % applied	Prothioconazole Ln (% applied)
0	96.18	4.57
0	96.35	4.57
6	92.94	4.53
6	94.37	4.55
24	95.70	4.56
24	95.83	4.56
48	95.04	4.55
48	95.51	4.56
72	95.07	4.55
72	94.89	4.55
96	95.19	4.56
96	96.19	4.57
168	90.74	4.51
168	90.76	4.51

First order linear Half life = 2888.1 hours; 120.3 days
(Slope significantly different from zero; t= -3.27; p= 0.0067)

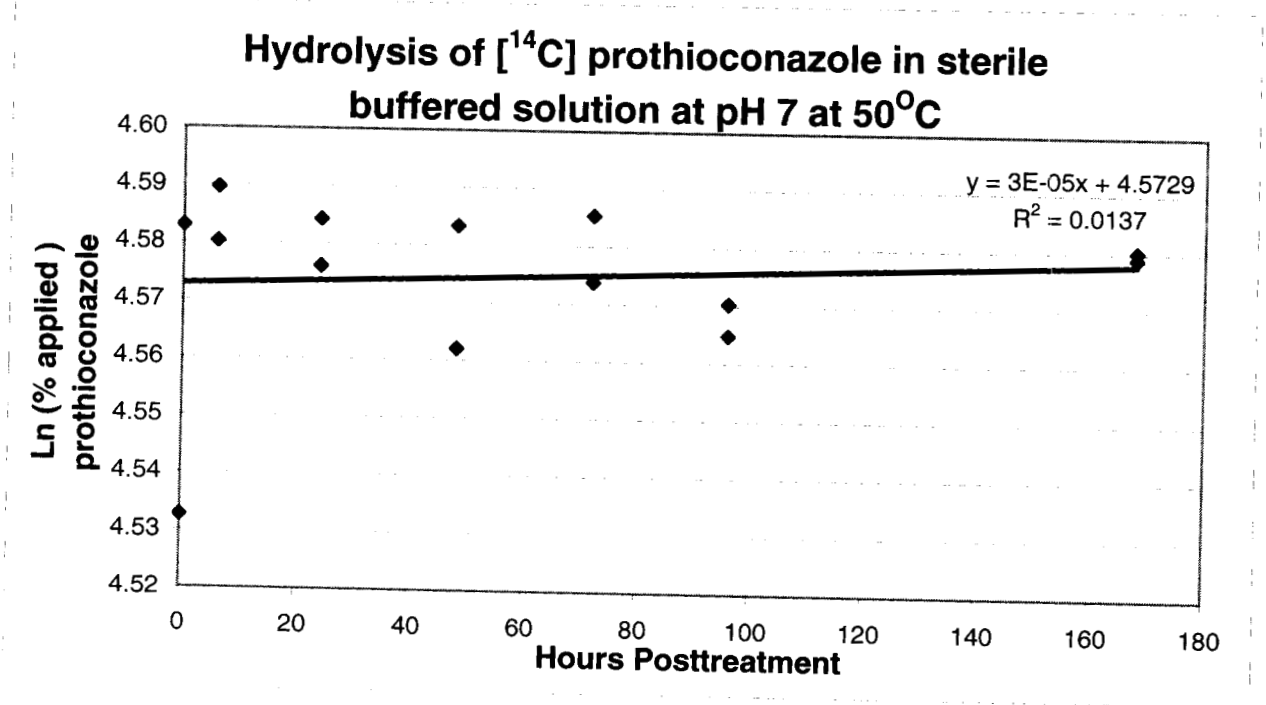


Chemical: Prothioconazole
PC Code: 113961
MRID: 46246505
Guideline No: 161-1

pH= 7

Hours	Prothioconazole % applied	Prothioconazole Ln (% applied)
0	93.01	4.53
0	97.80	4.58
6	98.46	4.59
6	97.54	4.58
24	97.93	4.58
24	97.14	4.58
48	95.78	4.56
48	97.84	4.58
72	98.04	4.59
72	96.92	4.57
96	96.05	4.56
96	96.58	4.57
168	97.42	4.58
168	97.54	4.58

First order linear Half life = No degradation; positive slope
(Slope not significantly different from zero; t= 0.41; p= 0.6901)



Chemical: Prothioconazole
PC Code: 113961
MRID: 46246505
Guideline No: 161-1

pH= 9

Hours	Prothioconazole % applied	Prothioconazole Ln (% applied)
0	97.23	4.58
0	98.84	4.59
1	96.25	4.57
1	96.93	4.57
2.5	96.41	4.57
2.5	97.24	4.58
6	96.21	4.57
6	96.10	4.57
24	96.72	4.57
24	97.16	4.58
48	96.26	4.57
48	97.37	4.58
72	96.15	4.57
72	96.83	4.57
96	96.47	4.57
96	95.52	4.56
168	95.28	4.56
168	96.80	4.57

First order linear Half life = No significant degradation
(Slope not significantly different from zero; t= -1.99; p= 0.0638)