Data Evaluation Record on the aerobic biotransformation of clofentezine (NC 21314) in water-sediment system

PMRA Submission Number {.....} EPA MRID Numbers 47192116

Data Requirement: PMRA Data Code:
EPA DP Barcode: D342560
OECD Data Point:
EPA Guideline: 162-4

Test material:
Common name: Clofentezine.
Chemical name:
IUPAC name: 3,6-Bis(2-chlorophenyl)-1,2,4,5-tetrazine.
CAS name: 3,6-Bis(2-chlorophenyl)-1,2,4,5-tetrazine.
CAS No: 74115-24-5.
Synonyms: NC 21314, NC 21 314, AE B084866.
SMILES string: Clc1ccccc1c2nnc(c3ccccc3Cl)nn2 (EPI Suite, v3.12 SMILES).

Primary Reviewer: Lynne Binari
Cambridge Environmental
Signature:
Date: 12/19/07

Secondary Reviewer: Kathleen Ferguson
Cambridge Environmental
Signature:
Date: 12/19/07

QC/QA Manager: Joan Gaidos
Cambridge Environmental
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Date: 12/19/07

Final Reviewer: Lucy Shanaman
EPA Reviewer
Signature: Lucy Shanaman
Date: 2/21/08

Company Code:
Active Code:
Use Site Category:
EPA PC Code: 125501

CITATION: Leake, C.R. and D.J. Arnold. 1983. The degradation of NC 21314 in surface water/sediment microcosms. Unpublished study performed by FBC Limited, Chesterford Park Research Station, Essex, United Kingdom; sponsored and submitted by Makhteshim Agan of North America (MANA), Inc., Raleigh, North Carolina (pp.2-4). FBC Study No.: 46J and Report No.: METAB/83/17 (p.4). Registration Document No.: NC 21314/W37 (p.1). Experimental start and completion dates were not provided. Final report issued April 26, 1983.

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Final Reviewer: Keara Moore
EPA Reviewer
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EXECUTIVE SUMMARY

The biotransformation of [tetrazine-3,6-^{14}C]-labeled 3,6-bis(2-chlorophenyl)-1,2,4,5-tetrazine (clofentezine, NC 21314; radiochemical purity ≥97%) was studied in ditch water-sandy clay loam sediment (water not characterized; sediment pH 6.8, organic carbon 7.6%) and ditch water-clay loam sediment (water not characterized; sediment pH 6.6, organic carbon 3.5%) systems from the United Kingdom for 6 weeks under aerobic conditions in darkness at 20 ± 2°C. Based on the theoretical water volume, [^{14}C]clofentezine was applied at a rate of *ca.* 0.8 mg a.i./L. The sediment:water ratio was 1:1.3 (9 cm sediment:12 cm water, specific weights/volumes were not reported). This study was neither conducted in accordance with any specified guidelines, nor in compliance with any specific GLP regulations. The test apparatus consisted of cylindrical, silanized, glass vessels (5-cm i.d. x 30 cm) connected to a continuous flow-through (CO_2-free, humidified air, flow rate up to 10 mL/minute) system with traps for the collection of CO_2 (ethanolamine) and volatile organics (ethylene glycol, 0.1M sulfuric acid). Sediment and water were pre-incubated for 3 days, then following treatment, a single vessel per system type was collected after 0 and 2 days, and 1, 2, 3, and 6 weeks of incubation. Water layers were drawn off, partitioned with methylene chloride, acidified and partitioned again. Resulting organic phases were combined and concentrated via rotary evaporation for chromatographic analysis. Sediment was reflux extracted with methylene chloride for 18 hours, followed by methanol:water (9:1, v:v) for 18 hours. Reflux-extracted sediment was dried (40°C), ground, then Soxhlet-extracted with acetonitrile:water (8:2, v:v) for 18 hours. Aliquots of sediment extracts were separately concentrated via rotary evaporation for chromatographic analysis. The cellulose thimbles (CT) used during reflux extractions were also Soxhlet-extracted with methylene chloride and methanol for 6 hours, followed by maceration in methanol:water. Water layer extracts and remaining aqueous phases, sediment extracts, extracted sediment, CT extracts, extracted CT residue, trapping solutions and incubation vessel rinses (methylene chloride/methanol) were analyzed for total radioactivity using LSC. Water layer extracts, sediment extracts and selected vessel rinse samples were analyzed for clofentezine and its transformation products via one-dimensional, normal-phase TLC. Five reference standards, in addition to parent clofentezine, were available for identification purposes (see Table 6 below). The 0-day to 3-week water layer extracts were also analyzed for parent clofentezine by reverse-phase HPLC.

For both systems, one major nonvolatile transformation product,

- 2-chlorobenzoic-(2-chlorobenzylidene)-hydrazide (compound III, AE C593600),

and three minor products,

- 2,5-bis(2-chlorophenyl)-1,3,4-oxadiazole (NC 12940, compound II),
- N',N-bis(2-chlorobenzoyl)-hydrazine (NC 12898, compound IV), and
- 2-chlorobenzoic acid (NC 233, compound V),

were identified via TLC against reference standards; however, a second, confirmatory method was not utilized.

System parameters, such as redox potential, dissolved oxygen and pH, were not monitored in the test systems.

There were significant losses of up to 21.8% and 16.4% of the applied radioactivity for the sandy clay loam and clay loam systems, respectively. However, there were no consistent patterns of decline of applied radioactivity for either system over the 6-week incubations. Following application of [^{14}C]clofentezine to the water layers, parent and total residues quickly translocated from the water layers of both systems to the sediments. However, variable and incomplete recoveries and the limited number of sampling intervals preclude any meaningful comparison of clofentezine transformation rates and/or water:sediment residue partitioning between the two sediment types.

Vessel rinses recovered maximums of 8.7-8.9% of the applied for the two systems, with the residues consisting primarily of parent clofentezine (7.6-8.2% of applied).

Volatilized residues were significant totaling 29.9% and 32.0% of the applied for the sandy clay loam and clay loam sediment systems, respectively, at study termination. However, formation of $^{14}CO_2$ and volatile [^{14}C]organic compounds were not separately distinguished.

United Kingdom ditch water-sandy clay loam sediment systems. Overall recovery of radiolabeled material averaged 87.2 ± 5.5% (range 78.2-92.7%) of the applied. Following application of [^{14}C]clofentezine to the water layer, [^{14}C]residue distribution ratios (water:sediment, n = 1) were 33:1 at day 0, 1:3 at 2 days, 1:5 at 2 weeks and 1:10 at 6 weeks. Extractable sediment [^{14}C]residues increased from 2.2% of the applied at day 0 to 59.8% at 1 week and were 26.9% at study termination. Nonextractable [^{14}C]residues increased from 0.3% at day 0 to 16.8% at 2 weeks and were 16.9% at 6 weeks. **Clofentezine** in the total system decreased from 82.7% of the applied at day 0 to 65.4% at 2 days, 44.1% at 1 week, 27.7% at 3 weeks and was 16.5% at 6 weeks. In the water layer, clofentezine decreased from 81.0% at day 0 to 19.1% at 2 days, 3.4% at 1 week, 1.5% at 3 weeks and was 0.5% at study termination. In the sediment, clofentezine increased from 1.7% at day 0 to 46.3% at 2 days, then decreased to 26.2% at 3 weeks and was 16.0% at 6 weeks. **Observed DT_{50}** values of clofentezine were *ca.* 1 day in the water layer, *ca.* 4 weeks in the sediment and *ca.* 6 days in the total system. Calculated **linear half-lives** (r^2 = 0.7357-0.9950) were 1, 4, and 3 weeks in the water, sediment and total system, respectively, with respective **nonlinear half-lives** (r^2 = 0.9871-0.9996) of 1 day, 4 weeks and 2 weeks. **Compound III** was detected at maximums of 7.5% (1 week), 14.8% (3 weeks) and 17.3% (1 week) of the applied in the water, sediment and total system, respectively, decreasing to 0.7%, 2.0% and 2.7%, respectively, at study termination. Minor products were detected at maximums in the water layer, sediment and total system as follows: **compound II** at 1.3%, 2.1% and 2.4%, respectively, **compound IV** at 0.2%, 1.2% and 1.4%, respectively, and **compound V** at 2.4%, 2.6% and 4.5%, respectively. Unidentified TLC [^{14}C]residues, comprised of multiple components, were total maximums of 2.3%, 9.2% and 11.3% in the water layer, sediment and total system, respectively. Unanalyzed aqueous-soluble (water layer) and organo-soluble (vessel rinse) [^{14}C]residues were maximums of 2.6% and 0.7%, respectively.

United Kingdom ditch water-clay loam sediment systems. Overall recovery of radiolabeled material averaged 91.0 ± 5.8% (range 83.6-98.5%) of the applied. Following application of

[^{14}C]clofentezine to the water layer, [^{14}C]residue distribution ratios (water:sediment, n = 1) were 88:1 at day 0, 1:3 at 2 days, 1:5 at 1 week, 1:7-10 at 2-3 weeks and 1:13 at 6 weeks. Extractable sediment [^{14}C]residues increased from 0.9% of the applied at day 0 to 52.3% at 1 week and were 30.9% at study termination. Nonextractable [^{14}C]residues increased from 0.2% at day 0 to 26.3% at 2 weeks and were 24.8% at 6 weeks. **Clofentezine** in the total system decreased from 93.8% of the applied at day 0 to 54.4% at 2 days, 23.6-29.4% at 2-3 weeks and was 12.8% at 6 weeks. In the water layer, clofentezine decreased from 93.3% at day 0 to 22.8% at 2 days, 4.9% at 1 week, 1.4% at 3 weeks and was 0.2% at study termination. In the sediment, clofentezine increased from 0.5% at day 0 to 31.6% at 2 days and was 12.6% at 6 weeks. **Observed DT_{50}** values of clofentezine were *ca.* 1 day in the water layer, *ca.* 5 weeks in the sediment and *ca.* 3 days in the total system. Calculated **linear half-lives** (r^2 = 0.7552-0.8875) were 5 days, 5 weeks and 3 weeks in the water, sediment and total system, respectively, with respective **nonlinear half-lives** (r^2 = 0.9357-0.9968) of 1 day, 6 weeks and 1 week. **Compound III** was detected at maximums of 4.4%, 22.6% and 27.0% of the applied in the water, sediment and total system, respectively, at 1 week, decreasing to 0.4%, 5.9% and 6.3%, respectively, at study termination. Minor products were detected at maximums in the water layer, sediment and total system as follows: **compound II** at 0.9%, 1.7% and 1.8%, respectively, **compound IV** at 0.1%, 1.7% and 1.8%, respectively, and **compound V** at 0.3%, 2.6% and 2.7%, respectively. Unidentified TLC [^{14}C]residues, comprised of multiple components, were total maximums of 2.7%, 11.7% and 13.7% in the water layer, sediment and total system, respectively. Unanalyzed aqueous-soluble (water layer) and organo-soluble (vessel rinse) [^{14}C]residues were maximums of 1.8% and 0.4%, respectively.

Transformation pathways consistent with the products detected in this study were proposed by the study authors. The primary pathway involved cleavage and deamination of the tetrazine ring to yield 2-chlorobenzoic-(2-chlorobenzylidene)-hydrazide (III), then hydrolysis further yielding 2-chlorobenzoic acid (V, NC 233), with ultimate formation of bound sediment residues and significant levels volatilized residues (CO_2 and volatile organic compounds were not distinguished). Other minor pathways (≤4.5% in total system) included formation of 2,5-bis(2-chlorophenyl)-1,3,4-oxadiazole (II, NC 12940) and N'N-bis(2-chlorobenzoyl)-hydrazine (IV, NC 12898).

Results Synopsis:

Test system used: Ditch water-sandy clay loam sediment from United Kingdom.

Linear half-life in water:	1.0 week (r^2 = 0.7357).
Linear half-life in sediment:	3.7 weeks (r^2 = 0.9950).
Linear half-life in the total system:	2.7 weeks (r^2 = 0.9310).
Non-linear half-life in water:	1.0 day (r^2 = 0.9980).
Non-linear half-life in sediment:	3.6 weeks (r^2 = 0.9996).
Non-linear half-life in total system:	1.9 weeks (r^2 = 0.9871).
Observed DT_{50} in water:	*ca.* 1 day.

Observed DT_{50} in sediment: *ca.* 4 weeks.
Observed DT_{50} in total system: *ca.* 6 days.

Major transformation products:
2-Chlorobenzoic-(2-chlorobenzylidene)-hydrazide (compound III; maximum 7.5%, 14.8% and 17.3% of applied in water layer, sediment and total system, respectively).
Volatile residues; CO_2 + volatile organics (maximum 29.9% of applied).
Minor transformation products:
3,6-Bis(2-chlorophenyl)-1,3,4-oxadiazole (compound II, NC 12940; maximum 1.3%, 2.1% and 2.4% of applied in water layer, sediment and total system, respectively).
N'N-Bis(2-chlorobenzoyl)-hydrazine (compound IV, NC 12898; maximum 0.2%, 1.2% and 1.4% of applied in water layer, sediment and total system, respectively).
2-Chlorobenzoic acid (compound V, NC 233; maximum 2.4%, 2.6% and 4.5% of applied in water layer, sediment and total system, respectively).

Test system used: Ditch water-clay loam sediment from United Kingdom.
Linear half-life in water: 5.4 days ($r^2 = 0.8875$).
Linear half-life in sediment: 4.9 weeks ($r^2 = 0.7552$).
Linear half-life in the total system: 2.6 weeks ($r^2 = 0.7751$).

Non-linear half-life in water: 1.0 day ($r^2 = 0.9968$).
Non-linear half-life in sediment: 5.5 weeks ($r^2 = 0.9768$).
Non-linear half-life in total system: 1.1 weeks ($r^2 = 0.9357$).

Observed DT_{50} in water: *ca.* 1 day.
Observed DT_{50} in sediment: *ca.* 5 weeks.
Observed DT_{50} in total system: *ca.* 3 days.

Major transformation products:
2-Chlorobenzoic-(2-chlorobenzylidene)-hydrazide (compound III; maximum 4.4%, 22.6% and 27.0% of applied in water layer, sediment and total system, respectively).
Volatile residues; CO_2 + volatile organics (maximum 32.0% of applied).
Minor transformation products:
3,6-Bis(2-chlorophenyl)-1,3,4-oxadiazole (compound II, NC 12940; maximum 0.9%, 1.7% and 1.8% of applied in water layer, sediment and total system, respectively).
N'N-Bis(2-chlorobenzoyl)-hydrazine (compound IV, NC 12898; maximum 0.1%, 1.7% and 1.8% of applied in water layer, sediment and total system, respectively).
2-Chlorobenzoic acid (compound V, NC 233; maximum 0.3%, 2.6% and 2.7% of applied in water layer, sediment and total system, respectively).

Study Acceptability: This study is classified as **supplemental**. No deviations from good scientific practices were noted. Material balances were incomplete, with up to 16-22% of the applied unaccounted for. Volatilized residues, which comprised maximums of 30-32% of the applied, were not adequately identified. The test waters were not characterized.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was not conducted in accordance with any specified guidelines. The following significant deviations from good scientific practices or the objectives of Subdivision N guidelines were noted:

Material balances were incomplete with up to 21.8% and 16.4% of the applied unaccounted for with the sandy clay loam sediment and clay loam sediment systems, respectively.

Volatilized residues, which comprised maximums of 30-32% of the applied for the two systems, were not distinguished between $^{14}CO_2$ and volatile [^{14}C]organic compounds. Additionally, identification of $^{14}CO_2$, if present, was not confirmed.

The test waters were not characterized; therefore, it was not established that the foreign test waters used in this study are comparable to aquatic systems that would be found at intended use sites for clofentezine in the United States.

COMPLIANCE: This study was not conducted in compliance with any specified GLP regulations (p.3). Signed and dated Data Confidentiality and GLP statements were provided (pp.2-3). A Quality Assurance statement was not provided.

A. MATERIALS:

1. Test Materials		[Tetrazine-3,6-^{14}C]-labeled clofentezine (p.7).
Chemical Structure:		See DER Attachment 1.
Description:		Technical; physical state not reported (p.7).
Purity:	Radiochemical purity:	≥97% via HPLC and TLC verifying data and/or certificate of analysis were not provided.
	Lot/Batch No.	CFQ 2874.
	Analytical purity:	Not reported.
	Specific activity:	47.7 µCi/mg.
	Location of the radiolabel:	At 3-C and 6-C of tetrazine ring.
Storage conditions of test chemicals:		Not reported.

Physico-chemical properties of clofentezine:

Parameter		Value	Comment
Molecular weight		303.15 g/mol.	
Molecular formula		$C_{14}H_8Cl_2N_4$.	
Water Solubility		2.5 µg/L.	At 22°C, pH 5.
Solubility in solvents	Dichloromethane Acetone Hexane Ethanol	37 g/L. 9.3 g/L. 1 g/L. 0.5 g/L.	At 25°C.
Vapor Pressure/Volatility		Not reported.	
UV Absorption		Not reported.	
pKa		Not reported.	
K_{ow}/log K_{ow}		Not reported.	
Stability of compound at room temperature, if provided		Not reported.	

Data obtained MRID 47192107.

2. Water-sediment collection, storage and properties

Table 1: Description of water-sediment collection and storage.

Description		Lode	Sadlers Farm
Geographic location		Lode, Cambridgeshire, United Kingdom.	Sadlers Farm, Essex, United Kingdom.
Ordinance Survey Map reference		Sheet 154 1:50,000 (526641).	Sheet 154 1:50,000 (553417).
Pesticide use history at the collection site		Not reported.	
Collection procedures for	Water:	Sediment and corresponding surface water collected from ditches adjacent to agricultural land; no additional details were provided.	
	Sediment:		
Sampling depth for	Water:	Not reported.	
	Sediment:	*ca.* 8 cm.	
Storage conditions		Sediment and water were separately maintained at 20°C.	
Storage length		4 days prior to preparation of water-sediment test systems.	
Preparation	Water:	Aerated via bubbler tubes during 4-day acclimatization period.	
	Sediment:	None reported.	

Data obtained from pp.7-9 of the study report.

Table 2: Properties of the waters.

Property	Lode		Sadlers Farm	
Temperature (°C)	Not reported.			
pH	Not reported.			
Redox potential (mV)	Initial	Final	Initial	Final
	Not reported.			
Oxygen concentration (mg/L)	Initial	Final	Initial	Final
	Not reported.			
Dissolved organic carbon (mg/L)	Not reported.			
Hardness (mg $CaCO_3$/L)	Not reported.			
Electrical conductivity (mmhos/cm)	Not reported.			
Microbial biomass/population (units)	Initial	Final	Initial	Final
	Not reported.			

Table 3: Properties of the sediments.

Property	Lode		Sadlers Farm	
Soil texture (BBA-German).	Sandy clay loam.		Clay loam.	
% Sand (2000-63 µm):	52.1		22.4	
% silt (63-2 µm):	26.9		42.8	
% clay (<2 µm):	21.1		34.9	
pH (soil:$CaCl_2$, 1:2.5):	6.8		6.6	
Organic carbon (%)[2]	7.6		3.5	
Organic matter (%)	13.1		6.1	
CEC (meq/100 g)	35.8		22.5	
Redox potential (mV)	Initial	Final	Initial	Final
	Not reported.			
Bulk density (disturbed, g/cm^3)	Not reported.			
Microbial biomass/population (units)	Initial	Final	Initial	Final
	Not reported.			

Data obtained from Table 2, p.8 of the study report.

1 The soil texture could not be confirmed because the particle size distribution was not according to the USDA system.

2 Percent organic carbon determined using the following formula: organic carbon (%) = organic matter (%)/1.72.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: None reported.

2. Experimental conditions:

Table 4: Study design.

Parameter		Sandy clay loam systems	Clay loam systems
Duration of the test (posttreatment)		6 weeks.	
Water: Filtered/unfiltered water: Type and size of filter used, if any:		Not reported.	
Amount of sediment and water per treatment	Water:	*ca.* 12 cm; water volumes (mL) were not reported.	
	Sediment:	*ca.* 9 cm; sediment weights (g) were not reported.	
Water/sediment ratio		1.3:1 (12-cm water layer:9-cm sediment layer).	
Application rate (mg a.i./L)	Nominal:	1 mg/kg.	
	Actual:	198.8 µg a.i. per system (1.0 kg a.i./ha); application rate in terms of the water layer (mg a.i./L) was not reported. Based on a theoretical water volume of *ca.* 236 mL, the application rate was *ca.* 0.84 mg a.i./L (198.8 µg a.i./236 mL); however, this does not take into account water associated with the sediment.[1]	
Control conditions, if used		No sterile controls were used.	
No. of replications	Control, if used:	No sterile controls were used.	
	Treated:	Not specified. For each water-sediment type, a sufficient number of nonsterile systems were treated with [^{14}C]clofentezine to allow for a single vessel at each of six sampling intervals.	
Test apparatus (type/material/volume):		Glass, cylindrical vessel (5-cm i.d. x 30 cm) fitted with an impinging tube and connected to a continuous flow-through (CO_2-free, humidified air, flow rate up to 10 mL/minute) volatiles trapping system.	
Details of traps for CO_2 and organic volatiles, if any:		In sequence as follows: ethylene glycol (ethanediol, one trap), ethanolamine (one trap), and 0.1M sulfuric acid (one trap); trapping solution volumes were not reported.	
If no traps were used, is the system closed?		Continuous flow-through volatiles trapping system was used.	
Identity and final concentration of co-solvent:		Could not be determined from the information provided. An aliquot (amount not reported) of [^{14}C]clofentezine stock solution (vehicle solution not reported) was combined (1:1, w:w) with formulation blank (CR 15456/3) to yield a 50% wettable powder, which was then dispersed in 1 mL acetone and brought to a final volume of 10 mL with deionized water. An aliquot (volume not reported) of the formulated test solution containing 0.1988 mg [^{14}C]clofentezine was applied to each system.	
Test material application method	Volume of the test solution used/treatment:	Not reported.	
	Application method (eg: mixed/not mixed):	Test solution was applied to the surface of the water layer via micro-syringe.	
Any indication of the test material adsorbing to the walls of the test apparatus?		Aqueous solubility of clofentezine was not reported. Incubation vessels and impinging tubes were silanized (2% surfasil) prior to use.	

Parameter		Sandy clay loam systems		Clay loam systems	
Microbial biomass/population of sterile controls (units)		No sterile controls were used.			
Microbial biomass/population of treated (units)		Initial	Final	Initial	Final
	Water:	Not reported.			
	Sediment:	Not reported.			
Experimental conditions:	Temperature (°C):	20 ± 2°C.			
	Continuous darkness (Yes/No):	Yes; vessels covered with black plastic and maintained in darkness.			
Other details, if any		None.			

Data were obtained from pp.6, 9-11; Table 4, p.19 of the study report.

1 The study authors neither reported the application rate in terms of the water layer (mg a.i./L), nor provided specific volumes of water used to prepare the water-sediment systems. Based on the incubation vessel diameter (5 cm i.d., p.9) and height of the water layer (*ca.* 12 cm, p.10) above the sediment, the theoretical water volume was calculated using the following equation: $v = \pi r^2 \times h$ or $[(\pi)(2.5\text{ cm})^2](ca.\ 12\text{ cm}) = ca.\ 236\text{ cm}^3 = ca.\ 236\text{ mL}$.

3. Aerobic conditions: Water and sediment were combined in the incubation vessels and maintained at 20 ± 2°C in darkness for 3 days prior to treatment, during which time air was bubbled (0.5 L/minute) directly into the water layer via an impinging tube (p.9). Following treatment, CO_2-free, humidified air was continuously bubbled (up to 10 mL/minute) into the water layer (pp.9-10). Aerobic conditions, as determined via measured redox potentials and/or dissolved oxygen levels, were not monitored either prior to or following treatment.

4. Supplementary experiment: None reported.

5. Sampling:

Table 5: Sampling details.

Criteria	Sandy clay loam systems	Clay loam systems
Sampling intervals (posttreatment)	0 and 2 days, and 1, 2, 3 and 6 weeks.	
Sampling method	Single vessel per system type was collected at each interval.	
Method of collection of CO_2 and organic volatile compounds	Trapping solutions were sampled (1 mL aliquots) and replaced weekly posttreatment.	
Sampling intervals/times for:		
Sterility check, if sterile controls are used:	No sterile controls were used.	
Redox potential, dissolved oxygen and pH:	Not monitored.	
Sample storage before analysis	Not reported.	
Other observations, if any	None.	

Data were obtained from pp.9, 11; Table 4, p.19 of the study report.

C. ANALYTICAL METHODS:

Separation of the sediment and water: The water layer was drawn off via siphon, then water and sediment were processed as described below (p.11).

Extraction/clean up/concentration methods: Water layer samples were partitioned with methylene chloride (volume, replications not reported), then acidified to pH 2 (method not reported) and partitioned again (p.11; Figure 2, p.12). Organic phases were combined, then the pooled organic phase and the remaining aqueous phase were analyzed for total radioactivity by LSC (aliquot up to 1 mL, replicates not specified; pp.11, 13). For chromatographic analysis, an aliquot (volume not reported) of the organic phase was taken to dryness via rotary evaporation (*in vacuo*, 30°C), with the resulting residues reconstituted in methylene chloride (up to 5 mL, p.14). Procedural recoveries following concentration were monitored, but no quantitative results were provided (p.14).

Sediment was reflux extracted with methylene chloride for 18 hours, followed by reflux extraction with methanol:water (9:1, v:v) for 18 hours; extraction solvent volumes were not reported (p.13; Figure 2, p.12). Reflux-extracted sediment was dried (40°C), ground (mechanism not reported), then extracted via Soxhlet with acetonitrile:water (8:2, v:v; volume not reported) for 18 hours. Triplicate aliquots (1 mL) of each extract were analyzed for total radioactivity by LSC (p.13). For chromatographic analysis, an aliquot of each extract was concentrated as described above, with the residues reconstituted in the initial solvent (p.14).

Cellulose thimbles used during the reflux extractions were extracted via Soxhlet with methylene chloride and methanol for 6 hours (no additional details regarding the extraction were provided, p.13). Extracts were analyzed for total radioactivity by LSC (3 x 1 mL), and concentrated as described above for chromatographic analysis (pp.13-14). The extracted thimbles were macerated (Waring blender) in methanol:water (ratio not reported), then the resulting slurry was vacuum-filtered and the filtrate analyzed for total radioactivity by LSC (p.13).

Vessel rinse. The incubation vessels and impinging tubes were rinsed with methylene chloride and methanol (volumes not reported, p.13). Aliquots of the rinses were analyzed for total radioactivity by LSC), and concentrated as described above for chromatographic analysis (p.14; Figure 2, p.12).

Total ^{14}C measurement: Total ^{14}C residues were determined by summing the concentrations of residues measured in the water layer extracts and remaining aqueous phase, sediment extracts, extracted sediment, volatile trapping solutions, and vessel rinse (Table 4, p.19).

Determination of nonextractable residues: Extracted sediment was dried (40°C) and ground via mortar and pestle, then aliquots (0.2-0.3 g, triplicate) were combined with glucose (*ca.* 1:1, w:w), pressed into pellets (Parr pellet press) and analyzed for total radioactivity by LSC following combustion (p.16).

Cellulose thimble residue, remaining after vacuum filtration of macerate, was analyzed for total radioactivity by LSC following combustion (p.13).

Determination of volatile residues: Aliquots (1 mL, replicates not reported) of the trapping solutions were analyzed for total radioactivity by LSC (p.9).

Derivatization method, if used: None was reported.

Identification and quantification of parent compound: concentrated water layer, sediment extract, cellulose thimble extract and vessel rinse samples were analyzed using one-dimensional TLC on normal-phase plates (Machery-Nagel, silica gel F254) developed with either toluene:ethanol:ethyl acetate:glacial acetic acid (80:10:5:0.5, v:v, SS1 or TEEA) or chloroform methanol (49:1, v:v, SS2; p.14). Following development, areas of radioactivity were detected via autoradiography (LKB Ultrafilm, ≥3 days), then scraped from the plates, combined with scintillation fluid and quantified by LSC (pp.13-14). Parent [^{14}C]clofentezine was identified by co-chromatography with unlabeled reference standard which was visualized under UV light (254 nm; p.14; Figure 7, p.25).

Day 0- to 3-week water layer samples were also analyzed using reverse-phase HPLC under the following conditions: Zorbax ODS column (4.6 x 250 mm, 10 µm), isocratic mobile phase of 0.005M tetrabutylammonium hydroxide in methanol:water (76:24, v:v), injection volume not reported, flow rate 1.0 mL/minute, UV detector (268 nm), fraction collection (1-minute intervals) with LSC analysis (p.16). Method for identification of parent [^{14}C]clofentezine was not provided. Retention time of parent, LC chromatograms and/or data from LSC analysis of fraction collection also not provided.

Identification and quantification of transformation products: Transformation products were separated, quantified and identified using TLC as described for the parent compound (pp.13-14; Figure 7, p.25).

A second confirmatory method was not utilized.

Table 6: Reference compounds available for identifying transformation products of clofentezine (NC 21314).

Applicant's code	Chemical Name	Purity[1] (%)	Lot/Batch No.
NC 22505 (IB)	3,6-Bis(2-chlorophenyl)-1,2-dihydro-1,2,4,5-tetrazine	--[2]	--
NC 12940 (II)	2,5-Bis(2-chlorophenyl)-1,3,4-oxadiazole	--	--
III	2-Chlorobenzoic-(2-chlorobenzylidene)-hydrazide	--	--
NC 12898 (IV)	N',N-bis(2-Chlorobenzoyl)-hydrazine	--	--
NC 233 (V)	2-Chlorobenzoic acid	--	--

Data obtained from Figure 3, pp.15-16 of the study report.
1 Purity w/w unless otherwise designated.
2 Information not reported.

Detection limits (LOD, LOQ) for the parent compound and transformation products: No limits of detection (LOD)/quantification (LOQ) were reported.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: System parameters, such as redox potential, dissolved oxygen and pH, were not monitored in the test systems. No supporting records were provided to establish that the incubation temperature was maintained at 20 ± 2°C throughout the study (p.9).

B. MATERIAL BALANCE: For both systems, although there were no consistent patterns of decline of applied radioactivity, there were significant losses of up to 21.8% and 16.4% of the applied for the sandy clay loam and clay loam systems, respectively. Variable recoveries and the limited number of sampling intervals preclude any meaningful comparison of residue partitioning between the two sediment types.

Sandy clay loam sediment (Lode) systems. Overall recovery of radiolabeled material averaged 87.2 ± 5.5% (range 78.2-92.7%, n = 6) of the applied (DER Attachment 2. Following application of [^{14}C]clofentezine to the water layer, [^{14}C]residues partitioned from the water layer to the sandy clay loam sediment with distribution ratios (water:sediment, n = 1) of 33:1 at day 0, 1:3 at 2 days, 1:5 at 2 weeks and was 1:10 at 6 weeks (DER Attachment 2).

Clay loam sediment (Sadlers Farm) systems. Overall recovery of radiolabeled material averaged 91.0 ± 5.8% (range 83.6-98.5%, n = 6) of the applied (DER Attachment 2). Following application of [^{14}C]clofentezine to the water layer, [^{14}C]residues partitioned from the water layer to the clay loam sediment with distribution ratios (water:sediment, n = 1) of 88:1 at day 0, 1:3 at 2 days, 1:5 at 1 week, 1:7-10 at 2-3 weeks and was 1:13 at 6 weeks (DER Attachment 2).

Table 7: Biotransformation of [tetrazine-3,6-^{14}C]clofentezine, expressed as percentage of applied radioactivity (n = 1), in United Kingdom ditch water-sandy clay loam sediment under aerobic conditions.

Compound		Sampling times (posttreatment)					
		0 day	2 days	1 week	2 weeks	3 weeks	6 weeks
Clofentezine	Water	81.0	19.1	3.4	1.8	1.5	0.5
	Sediment[1]	1.7	46.3	40.7	33.9	26.2	16.0
	System	82.7	65.4	44.1	35.7	27.7	16.5
NC 12940 (Compound II)	Water	<0.1	1.3	0.3	0.3	0.2	0.2
	Sediment[1]	<0.1	0.9	1.2	2.1	0.8	<0.1
	System	<0.1	2.2	1.5	2.4	1.0	0.2
Compound III	Water	<0.1	1.6	7.5	6.3	1.1	0.7
	Sediment[1]	<0.1	5.1	9.8	6.8	14.8	2.0
	System	<0.1	6.7	17.3	13.1	15.9	2.7
NC 12898 (Compound IV)	Water	<0.1	0.1	0.2	0.2	0.2	0.2
	Sediment[1]	<0.1	1.1	1.1	1.2	0.8	1.1
	System	<0.1	1.2	1.3	1.4	1.0	1.3
NC 233 (Compound V)	Water	<0.1	0.2	1.9	1.4	2.4	0.2
	Sediment[1]	<0.1	1.7	2.6	2.2	1.0	0.6
	System	<0.1	1.9	4.5	3.6	3.4	0.8
Unidentified TLC [^{14}C]residues[2]	Water	2.3	1.2	2.4	1.9	2.0	0.9
	Sediment[1]	0.4	7.7	8.9	8.0	9.2	6.7
	System	2.7	8.9	11.3	9.9	11.2	7.6
Unanalyzed [^{14}C]residues	Water[3]	0.2	0.2	1.5	2.6	1.2	1.7
	Vessel rinse	0.6	--	--	--	0.7	0.2
Total unidentified [^{14}C]residues[4]	Water	2.5	1.4	3.9	4.5	3.2	2.6
	Sediment/vessel rinse	1.0	7.7	8.9	8.0	9.9	6.9
	System	3.5	9.1	12.8	12.5	13.1	9.5
Volatiles[5]		<0.1	0.1	3.0	5.7	5.0	29.9
Extractable sediment residues		2.2	54.4	59.8	52.3	52.6	26.9
Nonextractable sediment residues		0.3	5.8	8.1	16.8	15.1	16.9
Total recovery	Water	83.4	23.7	17.0	14.5	8.6	4.3
	Sediment	2.5	60.2	67.9	69.1	67.7	43.8
	Vessel rinse	0.6	8.7	4.5	2.0	0.7	0.2
	System	86.5	92.7	92.4	91.3	82.0	78.2

Data obtained from DER Attachment 2.

1 Includes residues detected in vessel rinses analyzed by TLC.

2 Applied radioactivity unidentified following TLC analysis consisting of one unknown (X), origin residues and additional unassigned ("Remainder") residues (DER Attachment 2).

3 Residues remaining in aqueous phase following methylene chloride partition of water layer.

4 Unidentified TLC [^{14}C]residues plus unanalyzed [^{14}C]residues (DER Attachment 2).

5 $^{14}CO_2$ and volatile [^{14}C]organics were not distinguished.

Table 8: Biotransformation of [tetrazine-3,6-^{14}C]clofentezine, expressed as percentage of applied radioactivity (n = 1), in United Kingdom ditch water-clay loam sediment under aerobic conditions.

Compound		Sampling times (posttreatment)					
		0 day	2 days	1 week	2 weeks	3 weeks	6 weeks
Clofentezine	Water	93.3	22.8	4.9	3.2	1.4	0.2
	Sediment[1]	0.5	31.6	25.4	20.4	28.0	12.6
	System	93.8	54.4	30.3	23.6	29.4	12.8
NC 12940 (Compound II)	Water	0.9	0.1	0.3	0.1	0.2	0.1
	Sediment[1]	<0.1	1.1	1.5	1.7	0.9	0.5
	System	0.9	1.2	1.8	1.8	1.1	0.6
Compound III	Water	0.2	0.7	4.4	0.7	1.9	0.4
	Sediment[1]	0.1	10.7	22.6	8.5	5.1	5.9
	System	0.3	11.4	27.0	9.2	7.0	6.3
NC 12898 (Compound IV)	Water	<0.1	<0.1	0.1	0.1	0.1	0.1
	Sediment[1]	<0.1	0.8	1.2	1.7	0.7	1.3
	System	<0.1	0.8	1.3	1.8	0.8	1.4
NC 233 (Compound V)	Water	0.1	<0.1	0.2	0.1	0.2	0.3
	Sediment[1]	<0.1	1.2	2.2	2.6	1.6	1.2
	System	0.1	1.2	2.4	2.7	1.8	1.5
Unidentified TLC [^{14}C]residues[2]	Water	2.5	0.6	1.7	2.0	2.7	1.7
	Sediment[1]	0.3	7.9	8.4	11.7	7.8	9.5
	System	2.8	8.5	10.1	13.7	10.5	11.2
Unanalyzed [^{14}C]residues	Water[3]	<0.1	1.3	1.7	1.1	1.8	1.6
	Vessel rinse	0.4	--	--	--	--	0.2
Total unidentified [^{14}C]residues[5]	Water	2.5	1.9	3.4	3.1	4.5	3.3
	Sediment/vessel rinse	0.7	7.9	8.4	11.7	7.8	9.7
	System	3.2	9.8	11.8	14.8	12.3	13.0
Volatiles[5]		<0.1	<0.1	3.5	3.6	12.0	32.0
Extractable sediment residues		0.9	49.1	52.3	43.8	39.9	30.9
Nonextractable sediment residues		0.2	18.0	12.7	26.3	19.1	24.8
Total recovery	Water	97.0	25.5	13.3	7.2	8.2	4.3
	Sediment	1.1	67.1	65.0	70.1	59.0	55.7
	Vessel rinse	0.4	4.5	8.9	3.0	4.4	0.2
	System	98.5	97.1	90.7	83.9	83.6	92.2

Data obtained from DER Attachment 2.

1 Includes residues detected in vessel rinses analyzed by TLC.

2 Applied radioactivity unidentified following TLC analysis consisting of one unknown (X), origin residues and additional unassigned ("Remainder") residues (DER Attachment 2).

3 Residues remaining in aqueous phase following methylene chloride partition of water layer.

4 Unidentified TLC [^{14}C]residues plus unanalyzed [^{14}C]residues (DER Attachment 2).

5 $^{14}CO_2$ and volatile [^{14}C]organics were not distinguished.

C. TRANSFORMATION OF PARENT COMPOUND: Parent clofentezine quickly translocated from the water layers of both systems to the sediments. However, variable and incomplete recoveries of applied radioactivity prevent any meaningful comparison of transformation rates between the sediment types.

In sandy clay loam sediment (Lode) systems, [^{14}C]clofentezine in the total system decreased from 82.7% of the applied at day 0 to 65.4% at 2 days, 44.1% at 1 week, 27.7% at 3 weeks and was 16.5% at 6 weeks (DER Attachment 2). In the water layer [^{14}C]clofentezine decreased from 81.0% at day 0 to 19.1% at 2 days, 3.4% at 1 week, 1.5% at 3 weeks and was 0.5% at 6 weeks. In the sediment, [^{14}C]clofentezine increased from 1.7% at day 0 to a maximum 46.3% at 2 days, then decreased to 26.2% at 3 weeks and was 16.0% at 6 weeks.

In clay loam sediment (Sadlers Farm) systems, [^{14}C]clofentezine in the total system decreased from 93.8% of the applied at day 0 to 54.4% at 2 days, 23.6-29.4% at 2-3 weeks, and was 12.8% at 6 weeks (DER Attachment 2). In the water layer [^{14}C]clofentezine decreased from 93.3% at day 0 to 22.8% at 2 days, 4.9% at 1 week, 1.4% at 3 weeks and was 0.2% at 6 weeks. In the sediment, [^{14}C]clofentezine increased from 0.5% at day 0 to a maximum 31.6% at 2 days, then decreased to 12.6% at 6 weeks.

Levels of parent [^{14}C]clofentezine in the water layers of both systems as determined by reverse-phase HPLC analyses were comparable to the one-dimensional, normal-phase TLC analyses (Table 3, p.18).

HALF-LIFE/DT50/DT90: In sandy clay loam sediment (Lode) systems, observed DT_{50} values for clofentezine were *ca.* 1 day in the water layer, *ca.* 4 weeks in the sediment and *ca.* 6 days in the total system. First-order linear regression analysis (Excel 2007) yielded half-lives for clofentezine of 1 week in the water layer (0- to 6-week intervals), 4 weeks in the sediment (2-day to 6-week intervals) and 3 weeks in the total system (all intervals), with respective nonlinear (SigmaPlot v 9.0) half-lives of 1 day, 4 weeks and 2 weeks (DER Attachment 2).

In clay loam sediment (Sadlers Farm) systems, observed DT_{50} values for clofentezine were *ca.* 1 day in the water layer, *ca.* 5 weeks in the sediment and *ca.* 3 days in the total system. First-order linear regression analysis yielded half-lives for clofentezine of 5 days in the water layer (0- to 6-week intervals), 5 weeks in the sediment (2-day to 6-week intervals) and 3 weeks in the total system (all intervals), with respective nonlinear (SigmaPlot v 9.0) half-lives of 1 day, 6 weeks and 1 week (DER Attachment 2).

Half-lives/DT_{50}/DT_{90}

Phase	Half-life/DT_{50}[1] (weeks)	First-order linear regression equation	r^2	DT_{50} (days)	DT_{90} (days)
United Kingdom ditch water-sandy clay loam sediment systems					
Ditch water					
Linear/natural log	1.0	y = -0.7165x + 2.9451	0.7357	--	--
Nonlinear/normal	1.0 day	--	0.9980	--	--
Observed DT50	*ca.* 1 day	--	--	--	--
Sandy clay loam sediment					
Linear/natural log	3.7	y = -0.1882x + 3.8830	0.9950	--	--
Nonlinear/normal	3.6	--	0.9996	--	--
Observed DT50	*ca.* 4	--	--	--	--
Total system					
Linear/natural log	2.7	y = -0.2528x + 4.1979	0.9310	--	--
Nonlinear/normal	1.9	--	0.9871	--	--
Observed DT50	*ca.* 6 days	--	--	--	--
United Kingdom ditch water-clay loam sediment systems					
Ditch water					
Linear/natural log	0.8 (5.4 days)	y = -0.9050x + 3.3768	0.8875	--	--
Nonlinear/normal	1.0 day	--	0.9968	--	--
Observed DT50	*ca.* 1 day	--	--	--	--
Clay loam sediment					
Linear/natural log	4.9	y = -0.1410x + 3.4603	0.7552	--	--
Nonlinear/normal	5.5	--	0.9768	--	--
Observed DT50	*ca.* 5	--	--	--	--
Total system					
Linear/natural log	2.6	y = -0.2715x + 4.0627	0.7751	--	--
Nonlinear/normal	1.1	--	0.9357	--	--
Observed DT50	*ca.* 3 days	--	--	--	--

1 Determined using Excel 2007 (linear, first-order) and SigmaPlot v 9.0 (nonlinear, one-compartment/two-parameter) and individual sample data obtained from Tables 5-6, pp.21-22 of the study report (DER Attachment 2). Observed DT_{50} values assume time 0 application as 100% to water layer.

TRANSFORMATION PRODUCTS: For both systems, one major nonvolatile transformation product,

- 2-chlorobenzoic-(2-chlorobenzylidene)-hydrazide (compound III),

and three minor products,

- 2,5-bis(2-chlorophenyl)-1,3,4-oxadiazole (NC 12940, compound II),
- N',N-bis(2-chlorobenzoyl)-hydrazine (NC 12898, compound IV), and
- 2-chlorobenzoic acid (NC 233, compound V),

were detected. Products were identified via one-dimensional, normal-phase TLC against reference standards; a confirmatory method was not utilized.

In sandy clay loam sediment (Lode) systems, compound III was detected at maximums of 7.5% (1 week) in the water layer, 14.8% (3 weeks) in the sediment and 17.3% (1 week) in the total system, decreasing to 0.7%, 2.0% and 2.7%, respectively, at 6 weeks (DER Attachment 2). The minor products were detected at maximums in the water layer, sediment and total system as follows: compound II at 1.3%, 2.1% and 2.4%, respectively, compound IV at 0.2%, 1.2% and 1.4%, respectively, and compound V at 2.4%, 2.6% and 4.5%, respectively. Unidentified TLC [^{14}C]residues, comprised of Unknown X, origin residues and additional unassigned residues, were total maximums of 2.3%, 9.2% and 11.3% in the water layer, sediment and total system, respectively (DER Attachment 2). Unanalyzed aqueous-soluble (water layer) and organo-soluble (vessel rinse) [^{14}C]residues were maximums of 2.6% and 0.7%, respectively (DER Attachment 2).

In clay loam sediment (Sadlers Farm) systems, compound III was detected at maximums of 4.4%, 22.6% and 27.0% in the water layer, sediment and total system, respectively, at 1 week, decreasing to 0.7%, 8.5% and 9.2%, respectively, at 2 weeks, and was 0.4%, 5.9% and 6.3%, respectively, at 6 weeks (DER Attachment 2). The minor products were detected at maximums in the water layer, sediment and total system as follows: compound II at 0.9%, 1.7% and 1.8%, respectively, compound IV at 0.1%, 1.7% and 1.8%, respectively, and compound V at 0.3%, 2.6% and 2.7%, respectively. Unidentified TLC [^{14}C]residues, comprised of Unknown X, origin residues and additional unassigned residues, were total maximums of 2.7%, 11.7% and 13.7% in the water layer, sediment and total system, respectively (DER Attachment 2). Unanalyzed aqueous-soluble (water layer) and organo-soluble (vessel rinse) [^{14}C]residues were maximums of 1.8% and 0.4%, respectively (DER Attachment 2).

Half-lives/DT_{50}/DT_{90} for product 2-chlorobenzoic-(2-chlorobenzylidene)-hydrazide (III)

Phase	Half-life/DT_{50}[1] (weeks)	First-order linear regression equation	r^2	DT_{50} (days)	DT_{90} (days)
United Kingdom ditch water-sandy clay loam sediment systems					
Ditch water					
Linear/natural log	ND[2]	--	--	--	--
Nonlinear/normal	ND	--	--	--	--
Observed DT50	*ca.* 2.5	--	--	--	--
Sandy clay loam sediment					
Linear/natural log	ND[3]	--	--	--	--
Nonlinear/normal	ND	--	--	--	--
Observed DT50	*ca.* 4.5	--	--	--	--
Total system					
Linear/natural log	1.8	y = -0.3782x + 3.4302	0.8695	--	--
Nonlinear/normal	3.0	--	0.9569	--	--
Observed DT50	*ca.* 4.5	--	--	--	--
United Kingdom ditch water-clay loam sediment systems					
Ditch water					
Linear/natural log	ND[2]	--	--	--	--
Nonlinear/normal	ND	--	--	--	--
Observed DT50	--	--	--	--	--
Clay loam sediment					
Linear/natural log	3.2	y = -0.2179x + 2.8194	0.4933	--	--
Nonlinear/normal	6.2 days	--	0.9490	--	--
Observed DT50	*ca.* 1.5	--	--	--	--
Total system					
Linear/natural log	3.0	y = -0.2349x + 3.0302	0.5801	--	--
Nonlinear/normal	6.1 days	--	0.9512	--	--
Observed DT50	*ca.* 1.5	--	--	--	--

1 Determined using Excel 2007 (linear, first-order) and SigmaPlot v 9.0 (nonlinear, one-compartment/two-parameter) and individual sample data obtained from Tables 5-6, pp.21-22 of the study report (DER Attachment 2).

2 Not determined; compound III detected at ≤7.5% of the applied in water layer of either system (Tables 5-6, pp.21-2).

3 Not determined due to insufficient number of sampling intervals following detection of maximum level of compound III at 3 weeks posttreatment (Table 6, p.22).

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: In sandy clay loam sediment (Lode) systems, extractable sediment [^{14}C]residues increased from 2.2% of the applied at day 0 to 59.8% at 1 week, then decreased to 26.9% at 6 weeks (DER Attachment 2). Nonextractable sediment [^{14}C]residues increased from 0.3% at day 0 to 16.8% at 2 weeks and were 16.9% at 6 weeks.

In clay loam sediment (Sadlers Farm) systems, extractable sediment [^{14}C]residues increased from 0.9% of the applied at day 0 to 52.3% at 1 week, then decreased to 30.9% at 6 weeks (DER Attachment 2). Nonextractable sediment [^{14}C]residues increased from 0.2% at day 0 to 26.3% at 2 weeks and were 24.8% at 6 weeks.

For both systems, vessel rinses recovered maximums of 8.7-8.9% of the applied, comprised primarily of parent [^{14}C]clofentezine (7.6-8.2% of applied; Tables 5-6, pp.21-22).

VOLATILIZATION: Formation of $^{14}CO_2$ and volatile [^{14}C]organic compounds were not separately distinguished. At study termination (6 weeks), total volatile [^{14}C]compounds were maximums of 29.9% and 32.0% of the applied for the sandy clay loam sediment (Lode) and clay loam sediment (Sadlers Farm) systems, respectively, (DER Attachment 2).

TRANSFORMATION PATHWAY: The study authors provided transformation pathways that were consistent with the transformation products detected in this study, with the exception that compound IB [3,6-bis(2-chlorophenyl)-1,2-dihydro-1,2,4,5-tetrazine] was not detected in this study (p.18; Figure 5, p.23). The primary pathway involved cleavage and deamination of the tetrazine ring to yield 2-chlorobenzoic-(2-chlorobenzylidene)-hydrazide (III), then hydrolysis further yielding 2-chlorobenzoic acid (V, NC 233), with ultimate formation of bound sediment residues and significant levels of volatilized residues (CO_2 and volatile organic compounds were not distinguished). Other minor pathways (≤4.5% in total system) included formation of 2,5-bis(2-chlorophenyl)-1,3,4-oxadiazole (II, NC 12940) and N'N-bis(2-chlorobenzoyl)-hydrazine (IV, NC 12898).

Table 9: Chemical names and CAS numbers for the transformation products of clofentezine.[1]

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	MW (g/mol)	Smiles String
NC 12940, II	--[2]	2,5-Bis(2-chlorophenyl)-1,3,4-oxadiazole	--	--	--
AE C593600; III[3]	--	2-Chlorobenzoic-(2-chlorobenzylidene)-hydrazide	--	--	--
NC 12898, IV	--	N',N-Bis(2-chlorobenzoyl)-hydrazine	--	--	--
NC 233, V	--	2-Chlorobenzoic acid	--	--	--

Information obtained from pp.15-16 of the study report.
1 Identifications via TLC co-chromatography against reference standards.
2 Information not provided.
3 Code name AE C593600 obtained from MRID 47192104.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: None reported.

III. STUDY DEFICIENCIES

1. Material balances were incomplete, with up to 16-22% of the applied unaccounted for.

2. Volatilized residues were not adequately identified.

3. The test waters were not characterized.

IV. REVIEWER'S COMMENTS

1. All mean results and standard deviations presented in this review were determined using Microsoft Excel 2007 (12.0.6024.5000) MSO (12.0.6017.5000) software (DER Attachment 2). Standard deviations were determined using the "biased" or "n" method which determines the standard deviation of the entire sample population. Material balance summations reported by the study author (Table 4, p.19) were verified and, with the following exceptions, there was consistent agreement (within ± 0.1% of applied) between the study authors' reported values and those determined by the reviewer (DER Attachment 2). Summations of clofentezine and transformation products in the total system were not provided by the study author and were determined by the reviewer (DER Attachment 2).

   The following discrepancies between results determined by the reviewer and those reported by the study authors were noted:

   a) For the 1-week sandy clay loam sediment system, the study authors reported "Total Recovered" as 92.7% of applied (Table 4, p.19), whereas, the reviewer determined a result of 92.4% (DER Attachment 2).

   b) Similarly for the 2-day and 1-week clay loam sediment systems, the study authors reported "Total Recovered" as 93.1% and 91.4%, respectively (Table 4, p.19), whereas, the reviewer determined results of 97.1% and 90.7%, respectively (DER Attachment 2).

2. Material balances were incomplete with up to 21.8% and 16.4% of the applied unaccounted for with the sandy clay loam sediment (Lode) and clay loam sediment (Sadlers Farm) systems, respectively. The study authors contended that "an adequate balance of radioactivity was maintained throughout the experiment" (p.17). Of twelve systems that were analyzed, five of the twelve had material balance recoveries <90% of the applied, with four of the five "low balance" systems having recoveries <85% of applied.

3. Volatilized residues, which comprised maximums of 29.9-32.0% of the applied for the two systems, were not distinguished between $^{14}CO_2$ and volatile [^{14}C]organic compounds. Additionally, identification of $^{14}CO_2$, if present, was not confirmed.

4. A U.S.A. soil/sediment was not used, and it was not established that the foreign test sediments used in this study are comparable to soils/sediments that would be found at intended use sites for clofentezine in the United States. Two sediments from the United Kingdom, classified as a sandy clay loam and a clay loam according to German BBA textural classifications, were used in this study. However, FAO soil classifications were not provided to allow for adequate comparisons.

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 162-4, Aerobic Aquatic Metabolism Studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.

2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.

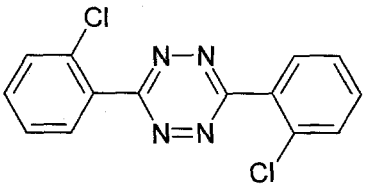
3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

Attachment 1: Structures of Parent Compound and Transformation Products

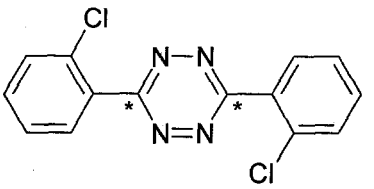
Clofentezine [NC 21314, NC 21 314, AE B084866]

IUPAC Name: 3,6-Bis(2-chlorophenyl)-1,2,4,5-tetrazine.
CAS Name: 3,6-Bis(2-chlorophenyl)-1,2,4,5-tetrazine.
CAS Number: 74115-24-5.
SMILES String: Clc1ccccc1c2nnc(c3ccccc3Cl)nn2 (EPI Suite, v3.12 SMILES).

Unlabeled



[Tetrazine-3,6-^{14}C]Clofentezine

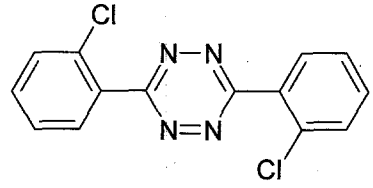


* = Location of the radiolabel.

Identified Compounds

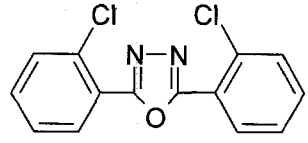
Clofentezine [NC 21314, NC 21 314, AE B084866]

IUPAC Name: 3,6-Bis(2-chlorophenyl)-1,2,4,5-tetrazine.
CAS Name: 3,6-Bis(2-chlorophenyl)-1,2,4,5-tetrazine.
CAS Number: 74115-24-5.
SMILES String: Clc1ccccc1c2nnc(c3ccccc3Cl)nn2 (EPI Suite, v3.12 SMILES).



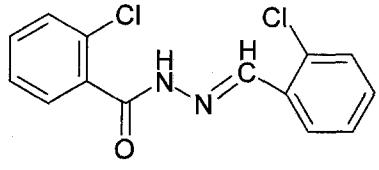
NC 12 940 [Compound II]

IUPAC Name: 2,5-Bis (2-chlorophenyl) 1,3,4 oxadiazole.
CAS Name: Not reported.
CAS Number: Not reported.



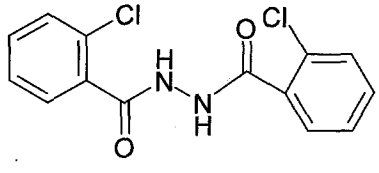
AE C593600 [R1, M1, Compound III]

IUPAC Name: 2-Chlorobenzoic (2-chlorobenzylidene) hydrazide.
2-Chlorobenzoic acid (2-chlorobenzylidene)hydrazide.
CAS Name: 2-Chlorobenzoic acid {(2-chlorophenyl)methylene}hydrazide.
CAS Number: Not reported.



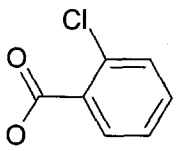
NC 12 898 [Compound IV]

IUPAC Name: N', N-Bis (2-chlorobenzoyl) hydrazine.
CAS Name: Not reported.
CAS Number: Not reported.



NC 233 [R3, Compound V]

IUPAC Name: 2-Chlorobenzoic acid.
CAS Name: Not reported.
CAS Number: Not reported.



Carbon Dioxide

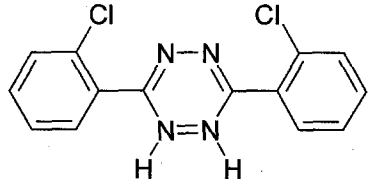
IUPAC Name: Carbon dioxide.
CAS Name: Carbon dioxide.
CAS Number: 124-38-9.

O=C=O

Unidentified Reference Compounds

NC 22 505 [Compound IB]

IUPAC Name: 3,6-Bis (2-chlorophenyl)-1,2-dihydro-1,2,4,5 tetrazine.
CAS Name: Not reported.
CAS Number: Not reported.



Attachment 2: Excel and SigmaPlot Spreadsheets

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

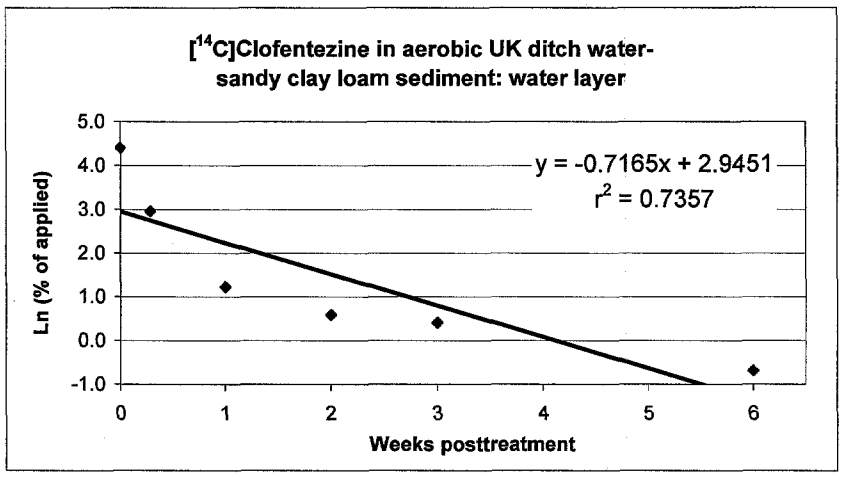
Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Half-life determination.

Sandy clay loam sediment (Lode) systems: water layer.

Half-life (weeks) 1.0 (0- to 6-week data)

	Clofentezine	
Weeks Posttreatment	(% of Applied)	Ln (% applied)
0	81.0	4.394449155
0.3	19.1	2.949688335
1	3.4	1.223775432
2	1.8	0.587786665
3	1.5	0.405465108
6	0.5	-0.693147181

Results from Table 6, p. 22 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.857719042
R Square	0.735681955
Adjusted R Square	0.669602443
Standard Error	1.072059657
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	12.79561568	12.796	11.13328383	0.0289256
Residual	4	4.597247632	1.1493		
Total	5	17.39286331			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.945106204	0.620388162	4.7472	0.008989411	1.2226325	4.6675799	1.22263253	4.667579879
X Variable 1	-0.716492302	0.214733542	-3.337	0.028925648	-1.312688	-0.1202964	-1.31268819	-0.12029641

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

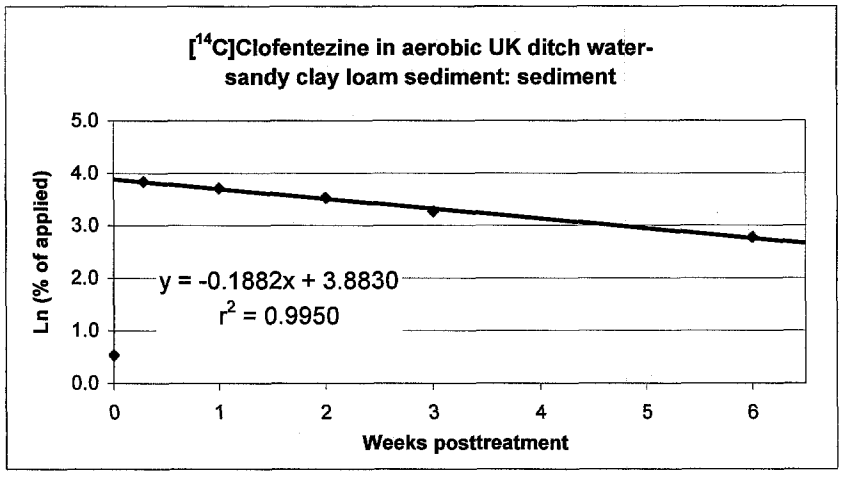
Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Half-life determination.

Sandy clay loam sediment (Lode) systems: sediment.

Half-life (weeks) 3.7 (2-day to 6-week data)

	Clofentezine	
Weeks Posttreatment	(% of Applied)	Ln (% applied)
0	1.7	0.530628251
0.3	46.3	3.835141961
1	40.7	3.706228092
2	33.9	3.523415014
3	26.2	3.265759411
6	16.0	2.772588722

Results from Table 6, p. 22 of the study report; clofentezine in sediment extract + vessel rinse.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.997473611
R Square	0.994953605
Adjusted R Square	0.993271474
Standard Error	0.034507537
Observations	5

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.704321282	0.7043	591.483835	0.0001524
Residual	3	0.00357231	0.0012		
Total	4	0.707893593			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.882960917	0.024485472	158.58	5.52898E-07	3.8050372	3.9608846	3.80503722	3.960884617
X Variable 1	-0.188159299	0.007736673	-24.32	0.000152377	-0.212781	-0.1635378	-0.21278085	-0.16353775

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

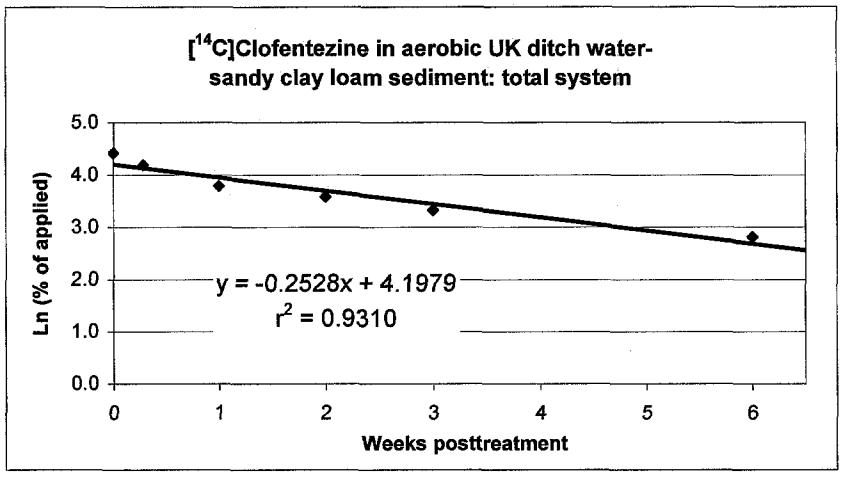
Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Half-life determination.

Sandy clay loam sediment (Lode) systems: total system.

Half-life (weeks) **2.7** ***(0- to 6-week data)***

Weeks Posttreatment	Clofentezine (% of Applied)	Ln (% applied)
0	82.7	4.415219602
0.3	65.4	4.180522258
1	44.1	3.786459782
2	35.7	3.575150689
3	27.7	3.321432413
6	16.5	2.803360381

Results imported from **Profile SCL** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.964885677
R Square	0.931004371
Adjusted R Square	0.913755463
Standard Error	0.171766244
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	1.592449857	1.5924	53.97468665	0.0018279
Residual	4	0.11801457	0.0295		
Total	5	1.710464427			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4.197920232	0.099399081	42.233	1.87898E-06	3.9219441	4.4738963	3.92194414	4.473896322
X Variable 1	-0.252763184	0.034404777	-7.347	0.001827875	-0.348286	-0.1572402	-0.34828616	-0.15724021

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

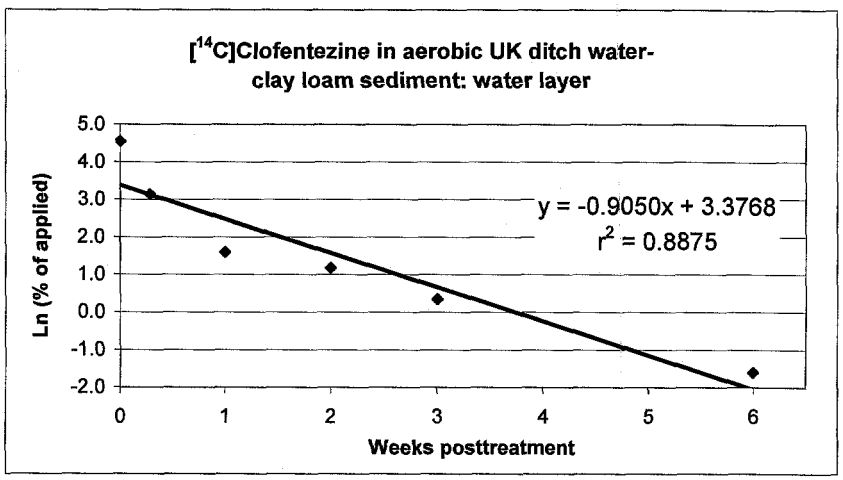
Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Half-life determination.

Clay loam sediment (Sadlers Farm) systems: water layer.

Half-life (weeks) 0.8 (0- to 6-week data)

Weeks Posttreatment	Clofentezine (% of Applied)	Ln (% applied)
0	93.3	4.535820108
0.3	22.8	3.126760536
1	4.9	1.589235205
2	3.2	1.16315081
3	1.4	0.336472237
6	0.2	-1.609437912

Results from Table 5, p. 21 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.942068114
R Square	0.887492331
Adjusted R Square	0.859365414
Standard Error	0.804365685
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	20.41500752	20.415	31.55313201	0.0049369
Residual	4	2.588016621	0.647		
Total	5	23.00302414			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.376792483	0.465476847	7.2545	0.001916993	2.0844216	4.6691634	2.08442157	4.669163395
X Variable 1	-0.905014853	0.161114441	-5.617	0.004936942	-1.35234	-0.4576895	-1.35234026	-0.45768945

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

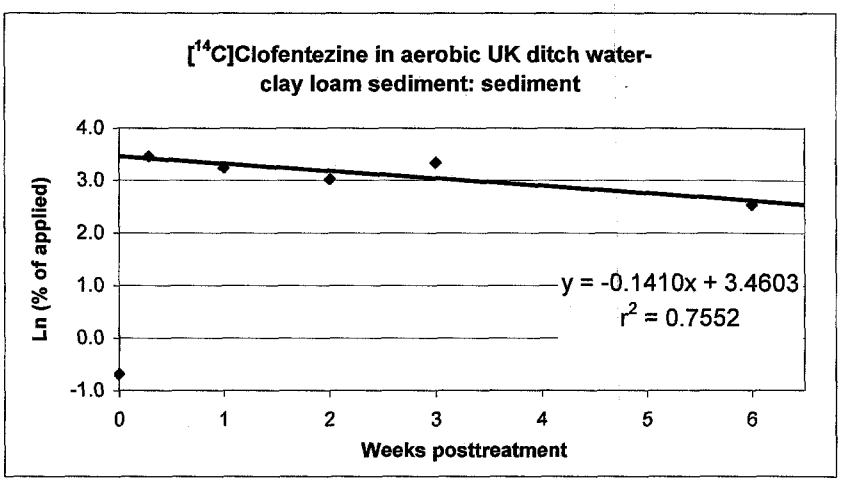
Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Half-life determination.

Clay loam sediment (Sadlers Farm) systems: sediment.

Half-life (weeks) 4.9 (2-day to 6-week data)

	Clofentezine	
Weeks Posttreatment	(% of Applied)	Ln (% applied)
0	0.5	-0.693147181
0.3	31.6	3.453157121
1	25.4	3.234749174
2	20.4	3.015534901
3	28.0	3.33220451
6	12.6	2.533696814

Results from Table 5, p. 21 of the study report; clofentezine in sediment extract + vessel rinse.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.86900999
R Square	0.755178363
Adjusted R Square	0.673571151
Standard Error	0.206724701
Observations	5

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.395462895	0.3955	9.253818885	0.0557787
Residual	3	0.128205306	0.0427		
Total	4	0.523668201			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.460304936	0.1466854	23.59	0.000166911	2.9934865	3.9271233	2.99348653	3.927123345
X Variable 1	-0.140991571	0.046348177	-3.042	0.055778707	-0.288492	0.006509	-0.28849215	0.006509012

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

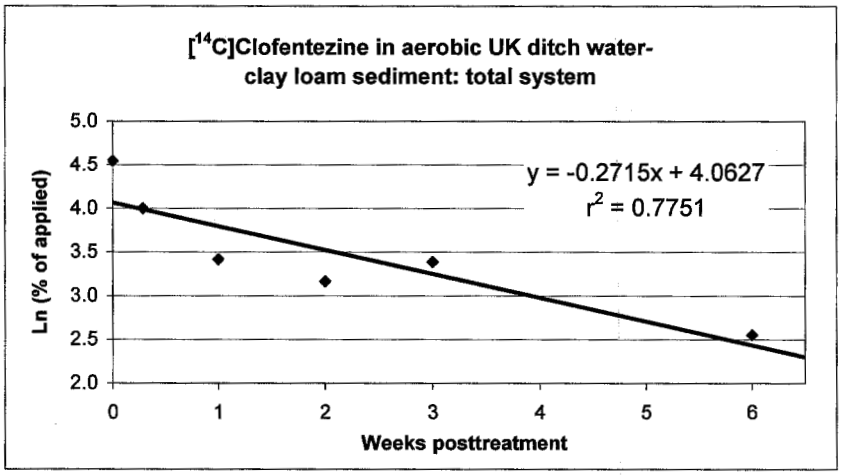
Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Half-life determination.

Clay loam sediment (Sadlers Farm) systems: total system.

Half-life (weeks) 2.6 (0- to 6-week data)

	Clofentezine	
Weeks Posttreatment	(% of Applied)	Ln (% applied)
0	93.8	4.541164856
0.3	54.4	3.996364154
1	30.3	3.411147713
2	23.6	3.161246712
3	29.4	3.380994674
6	12.8	2.549445171

Results imported from **Profile CL** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.880423918
R Square	0.775146276
Adjusted R Square	0.718932845
Standard Error	0.365039283
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	1.837480657	1.8375	13.78934291	0.0205928
Residual	4	0.533014711	0.1333		
Total	5	2.370495368			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4.062684573	0.211243887	19.232	4.30773E-05	3.4761775	4.6491916	3.47617752	4.64919163
X Variable 1	-0.271514059	0.073117366	-3.713	0.020592783	-0.47452	-0.0685077	-0.47452041	-0.06850771

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Half-life determination.

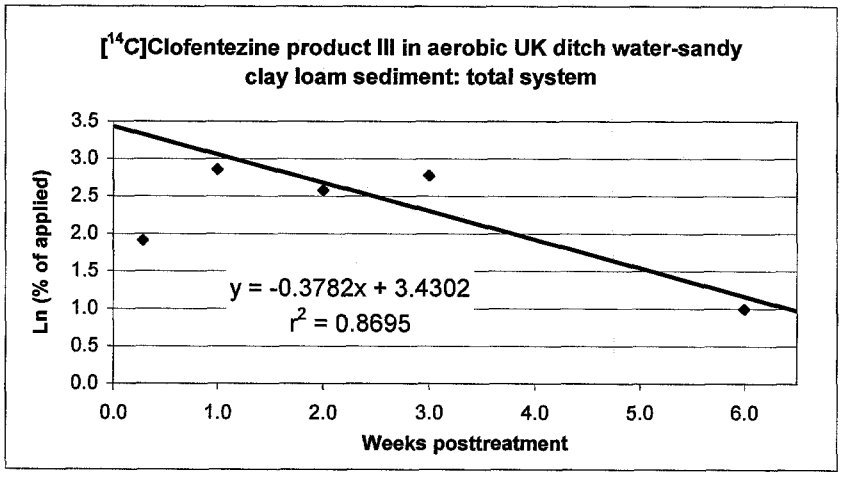
Sandy clay loam sediment (Lode) systems: total system.

Half-life (weeks) 1.8 (1- to 6-week data)

Weeks Posttreatment	Compound III[1] (% of Applied)	Ln (% applied)
0	<0.1	(not detected)
0.3	6.7	1.902107526
1	17.3	2.850706502
2	13.1	2.57261223
3	15.9	2.766319109
6	2.7	0.993251773

1 2-Chlorobenzoic-(2-chlorobenzylidene)-hydrazide.

Results imported from **Profile SCL** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.932472401
R Square	0.869504778
Adjusted R Square	0.804257167
Standard Error	0.387604118
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	2.002092423	2.0021	13.32623161	0.0675276
Residual	2	0.300473905	0.1502		
Total	3	2.302566328			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.430208814	0.366251466	9.3657	0.011209016	1.8543559	5.0060617	1.85435595	5.006061682
X Variable 1	-0.378162137	0.103591558	-3.651	0.067527599	-0.823881	0.0675564	-0.82388064	0.067556363

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Half-life determination.

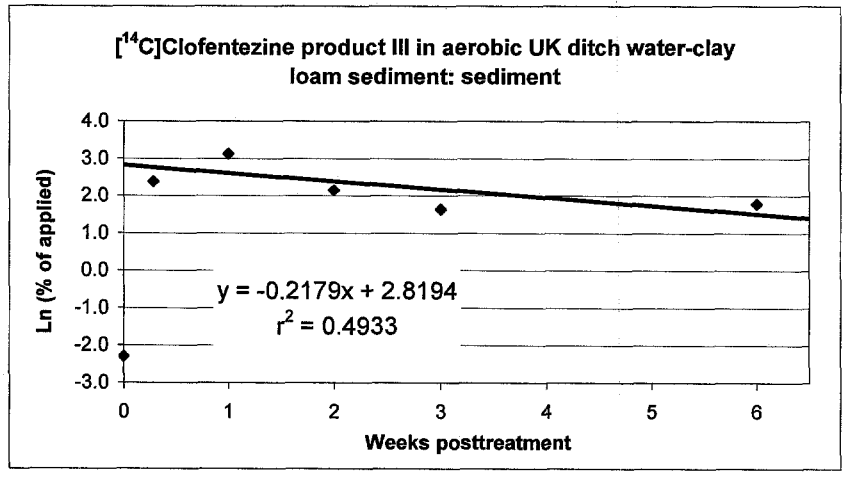
Clay loam sediment (Sadlers Farm) systems: sediment.

Half-life (weeks) 3.2 (1- to 6-week data)

Weeks Posttreatment	Compound III[1] (% of Applied)	Ln (% applied)
0	0.1	-2.302585093
0.3	10.7	2.370243741
1	22.6	3.117949906
2	8.5	2.140066163
3	5.1	1.62924054
6	5.9	1.774952351

1 2-Chlorobenzoic-(2-chlorobenzylidene)-hydrazide.

Results from Table 5, p. 21 of the study report; clofentezine in sediment extract + vessel rinse.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.702365787
R Square	0.493317699
Adjusted R Square	0.239976548
Standard Error	0.58436368
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.664947547	0.6649	1.947246616	0.2976342
Residual	2	0.682961821	0.3415		
Total	3	1.347909368			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.819361295	0.552171776	5.1059	0.036282517	0.4435579	5.1951647	0.4435579	5.195164693
X Variable 1	-0.217936352	0.156177763	-1.395	0.297634213	-0.889915	0.4540423	-0.88991503	0.454042326

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

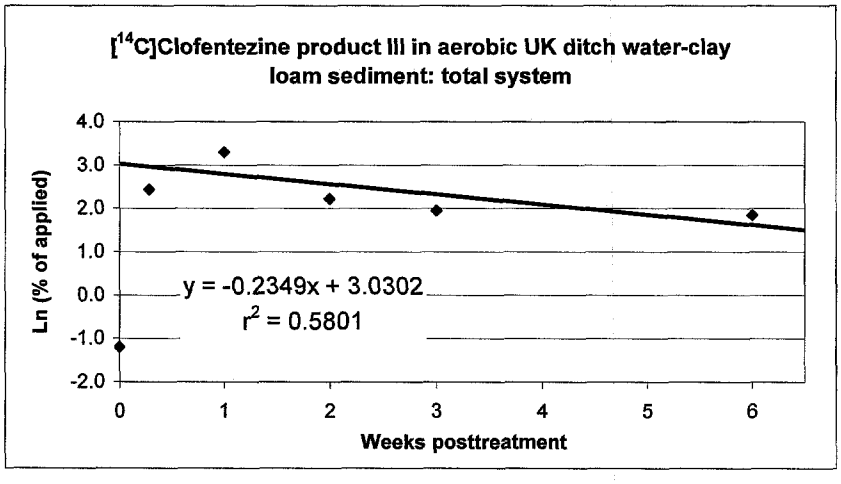
Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Half-life determination.

Clay loam sediment (Sadlers Farm) systems: total system.

Half-life (weeks) 3.0 (1- to 6-week data)

Weeks Posttreatment	Compound III[1] (% of Applied)	Ln (% applied)
0	0.3	-1.203972804
0.3	11.4	2.433613355
1	27.0	3.295836866
2	9.2	2.219203484
3	7.0	1.945910149
6	6.3	1.840549633

1 2-Chlorobenzoic-(2-chlorobenzylidene)-hydrazide.
Results imported from **Profile CL** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.761655673
R Square	0.580119365
Adjusted R Square	0.370179047
Standard Error	0.52883385
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.772787351	0.7728	2.763258486	0.2383443
Residual	2	0.559330482	0.2797		
Total	3	1.332117833			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3.030209672	0.499701019	6.064	0.026132841	0.8801697	5.1802496	0.88016972	5.180249625
X Variable 1	-0.23494488	0.141336792	-1.662	0.238344326	-0.843068	0.3731783	-0.84306801	0.373178252

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems.
Nonlinear half-lives (exponential decay/single compartment, 2 parameter):

Clofentezine:
UK ditch water-sandy clay loam sediment systems.

Phase	water	sediment	system
Half-life (weeks)	0.14	3.6	1.9
Half-life (days)	0.97		
R squared	0.9980	0.9996	0.9871

UK ditch water-clay loam sediment systems.

Phase	water	sediment	system
Half-life (weeks)	0.14	5.5	1.1
Half-life (days)	1.00		
R squared	0.9968	0.9768	0.9357

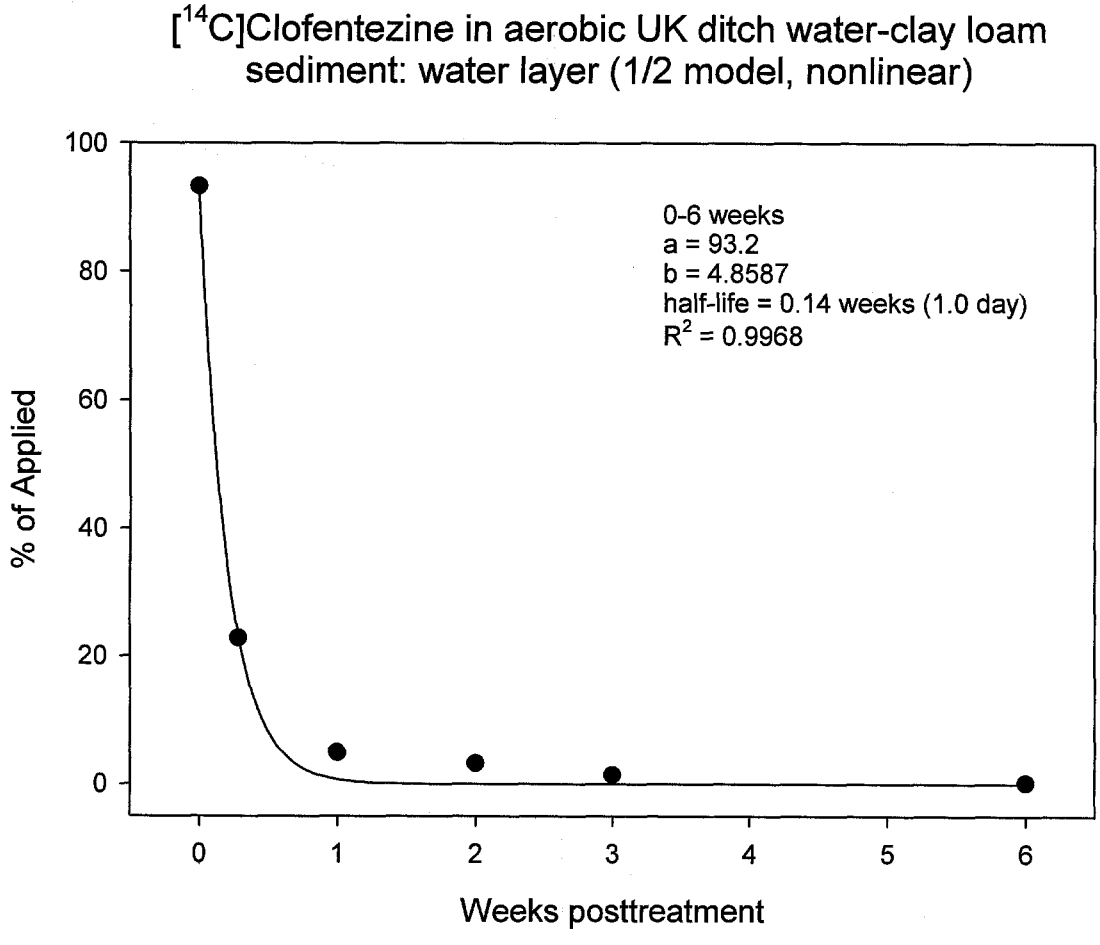
Clofentezine product III:
UK ditch water-sandy clay loam sediment systems.

Phase	water	sediment	system
Half-life (weeks)	ND	ND	3.0
R squared			0.9569

UK ditch water-clay loam sediment systems.

Phase	water	sediment	system
Half-life (weeks)	ND	0.89	0.88
Half-life (days)		6.2	6.1
R squared		0.9490	0.9512

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4)



Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-clay loam sediment: water layer
[Tetrazine-3,6-^{14}C]-label
Nonlinear Regression

Data Source: Data 1 in 125501 47192116 162-4 CL H2O.JNB
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9984	0.9968	0.9952	2.7325

	Coefficient	Std. Error	t	P	VIF
a	93.2178	2.7320	34.1208	<0.0001	1.0619
b	4.8587	0.4212	11.5349	0.0003	1.0619

Analysis of Variance:

	DF	SS	MS
Regression	2	9231.1138	4615.5569
Residual	4	29.8662	7.4666
Total	6	9260.9800	1543.4967

Statistical Tests:

PRESS 50393.2682

Durbin-Watson Statistic 0.9180 Failed

Normality Test Passed (P = 0.2168)

K-S Statistic = 0.4030 Significance Level = 0.2168

Constant Variance Test Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	93.2178	0.0822	0.0301	1.5596	2.1574<
2	23.2601	-0.4601	-0.1684	-1.5560	-2.1448<
3	0.7234	4.1766	1.5285	1.5378	2.0829<
4	0.0056	3.1944	1.1690	1.1690	1.2478
5	4.3569E-005	1.4000	0.5123	0.5123	0.4590
6	2.0364E-011	0.2000	0.0732	0.0732	0.0634

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	3267.9875<	0.9996	111.8350<
2	102.1728<	0.9883	-19.7042
3	0.0145	0.0121	0.2303

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-clay loam sediment: water layer
[Tetrazine-3,6-^{14}C]-label

4	2.0152E-006	2.9491E-006	0.0021
5	5.2712E-011	4.0163E-010	9.1990E-006
6	9.4500E-025	3.5279E-022	1.1914E-012

95% Confidence:

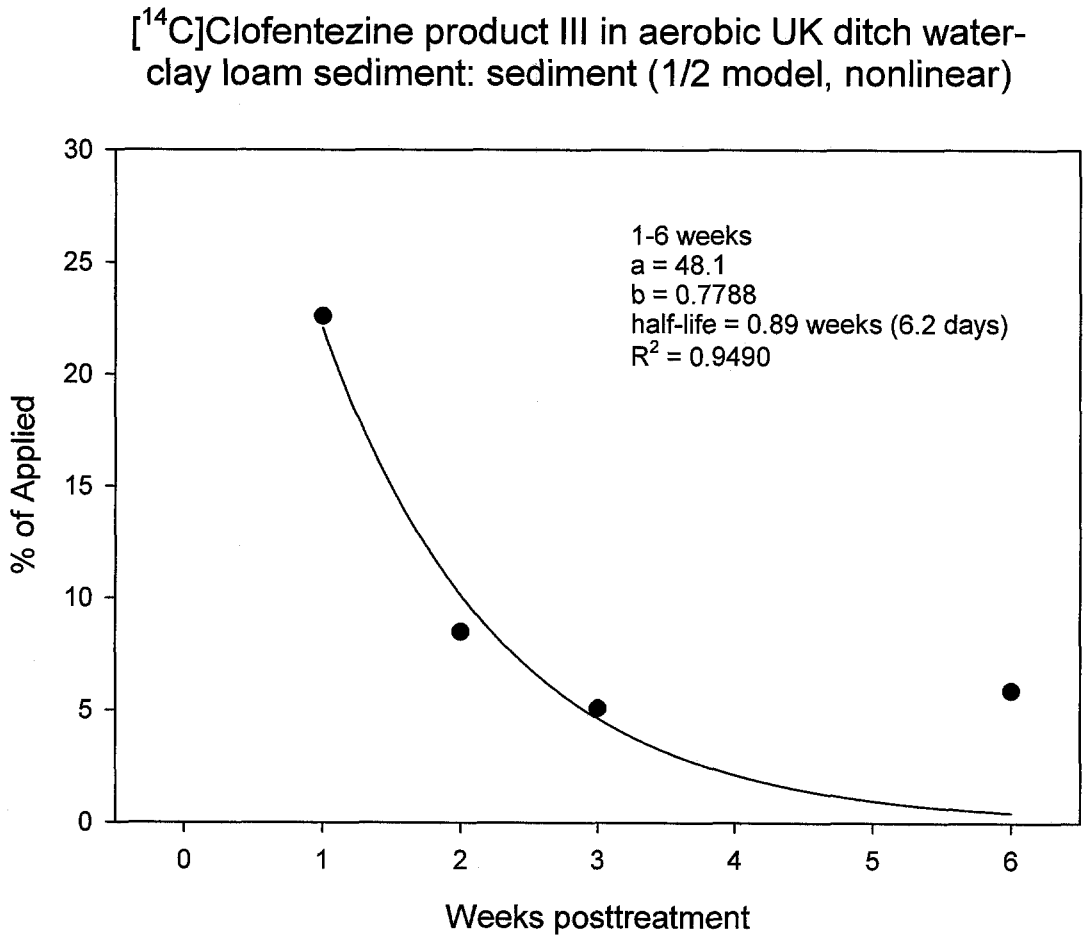
Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	93.2178	85.6326	100.8030	82.4897	103.9459
2	23.2601	15.7180	30.8022	12.5624	33.9577
3	0.7234	-0.1104	1.5572	-6.9089	8.3557
4	0.0056	-0.0074	0.0186	-7.5810	7.5923
5	4.3569E-005	-0.0001	0.0002	-7.5866	7.5867
6	2.0364E-011	-1.2213E-010	1.6286E-010	-7.5866	7.5866

Fit Equation Description:

```
[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto
{{previous: 93.2178}}
b = if(x50(x,y)-min(x)=0, 1,  -ln(.5)/(x50(x,y)-min(x)))  "Auto {{previous: 4.8587}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200
```

Number of Iterations Performed = 7

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4)



Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-clay loam sediment: sediment
[Tetrazine-3,6-^{14}C]-label
Clofentezine product III
Nonlinear Regression

Data Source: Data 1 in 125501 47192116 162-4 CL III Sed.JNB
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9742	0.9490	0.8980	4.0526

	Coefficient	Std. Error	t	P	VIF
a	48.0654	20.7309	2.3185	0.1463	6.9204<
b	0.7788	0.3217	2.4209	0.1365	6.9204<

Analysis of Variance:

	DF	SS	MS
Regression	2	610.9827	305.4914
Residual	2	32.8473	16.4236
Total	4	643.8300	160.9575

Statistical Tests:

PRESS 454.4919

Durbin-Watson Statistic 1.0345 Failed

Normality Test Passed (P = 0.7537)

K-S Statistic = 0.3099 Significance Level = 0.7537

Constant Variance Test Failed (P = <0.0001)

Power of performed test with alpha = 0.0500: 0.5824

The power of the performed test (0.5824) is below the desired power of 0.8000.
You should interpret the negative findings cautiously.

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	22.0605	0.5395	0.1331	0.8154	0.7057
2	10.1251	-1.6251	-0.4010	-0.5917	-0.4607
3	4.6471	0.4529	0.1118	0.1516	0.1078
4	0.4493	5.4507	1.3450	1.3650	3.6919<

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	12.1421<	0.9734	4.2648<

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-clay loam sediment: sediment
[Tetrazine-3,6-^{14}C]-label
Clofentezine product III

2	0.2061	0.5407	-0.4999
3	0.0097	0.4568	0.0989
4	0.0280	0.0291	0.6397

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	22.0605	4.8575	39.2636	-2.4342	46.5553
2	10.1251	-2.6972	22.9474	-11.5188	31.7690
3	4.6471	-7.1375	16.4317	-16.3987	25.6929
4	0.4493	-2.5276	3.4262	-17.2400	18.1385

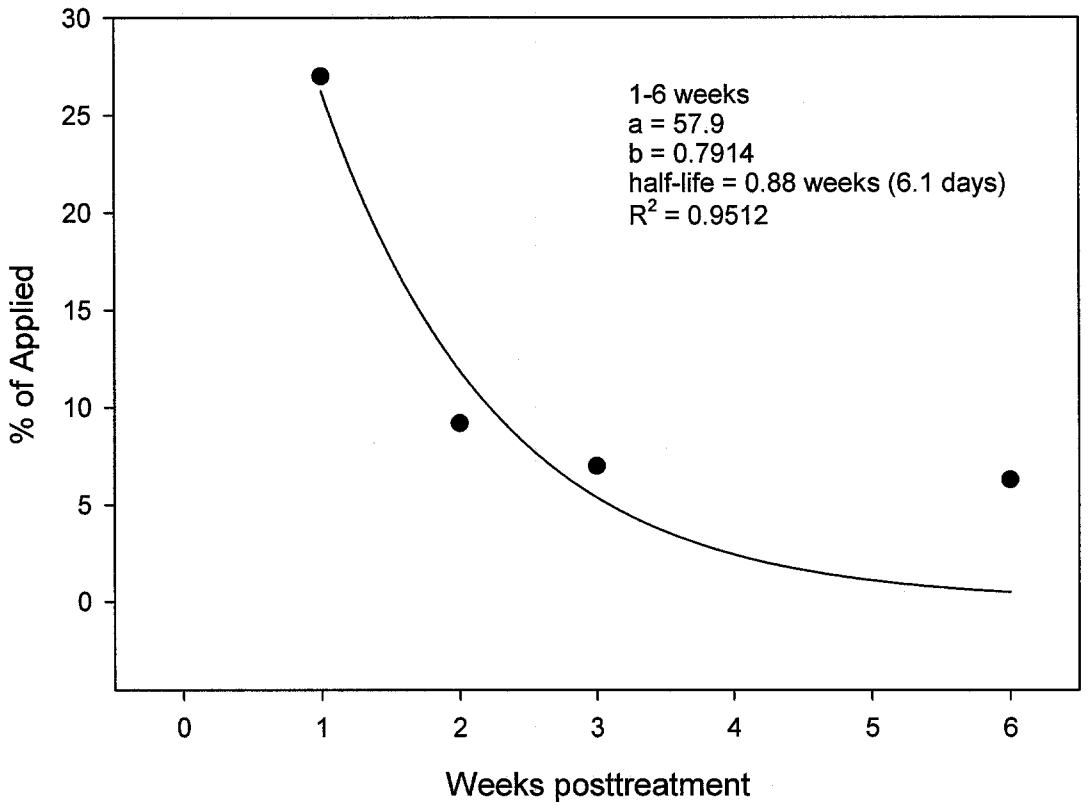
Fit Equation Description:

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto {{previous: 48.0654}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.778773}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200

Number of Iterations Performed = 17

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4)

[^{14}C]Clofentezine product III in aerobic UK ditch water-clay loam sediment: total system (1/2 model, nonlinear)



Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-clay loam sediment: total system
[Tetrazine-3,6-^{14}C]-label
Clofentezine product III
Nonlinear Regression

Data Source: Data 1 in 125501 47192116 162-4 CL III Tot sys.JNB
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9753	0.9512	0.9024	4.6925

	Coefficient	Std. Error	t	P	VIF
a	57.8648	24.5679	2.3553	0.1427	7.0265<
b	0.7914	0.3187	2.4830	0.1311	7.0265<

Analysis of Variance:

	DF	SS	MS
Regression	2	858.2914	429.1457
Residual	2	44.0386	22.0193
Total	4	902.3300	225.5825

Statistical Tests:

PRESS 1007.0044

Durbin-Watson Statistic 1.0893 Failed

Normality Test Passed (P = 0.6524)

K-S Statistic = 0.3379 Significance Level = 0.6524

Constant Variance Test Failed (P = <0.0001)

Power of performed test with alpha = 0.0500: 0.5912

The power of the performed test (0.5912) is below the desired power of 0.8000.
You should interpret the negative findings cautiously.

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	26.2251	0.7749	0.1651	1.0353	1.0746
2	11.8856	-2.6856	-0.5723	-0.8506	-0.7529
3	5.3867	1.6133	0.3438	0.4642	0.3475
4	0.5015	5.7985	1.2357	1.2525	1.9074

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	20.5289<	0.9746	6.6510<

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-clay loam sediment: total system
[Tetrazine-3,6-^{14}C]-label
Clofentezine product III

2	0.4374	0.5473	-0.8279
3	0.0887	0.4515	0.3153
4	0.0215	0.0266	0.3156

95% Confidence:

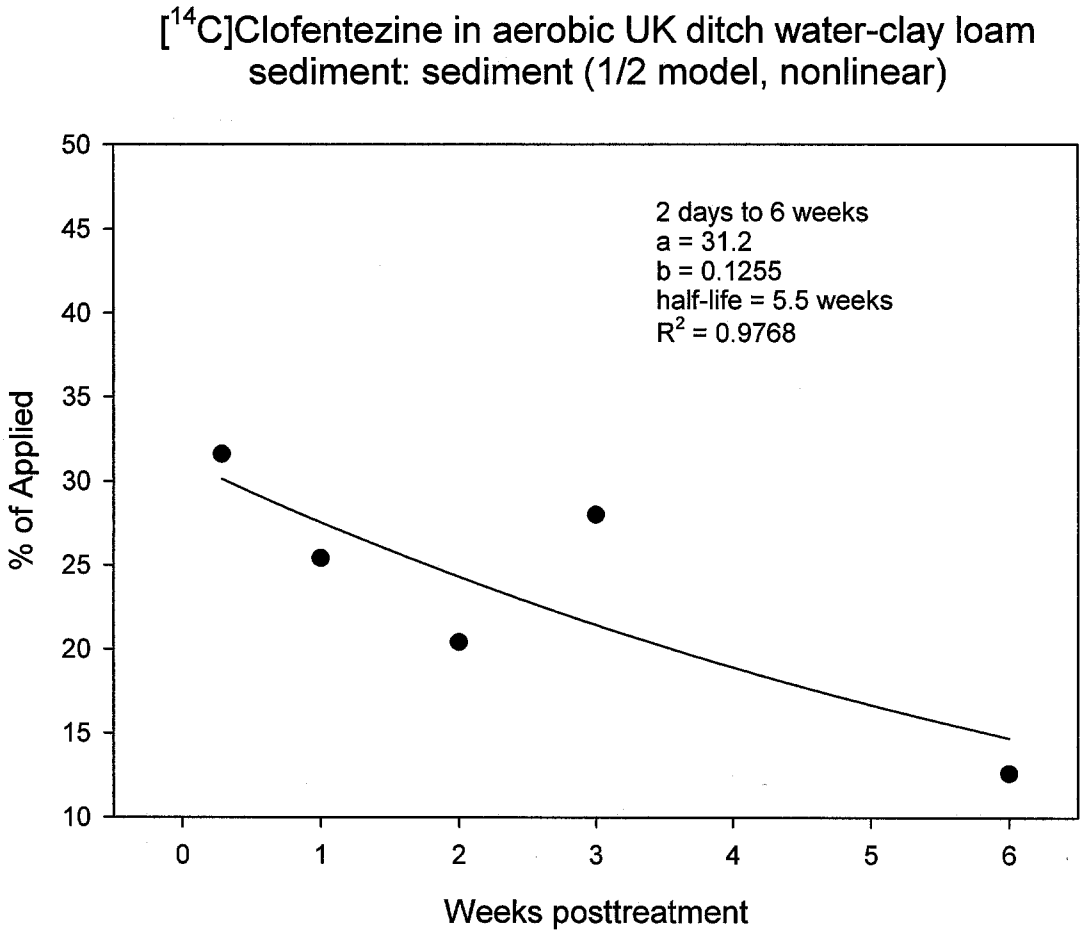
Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	26.2251	6.2935	46.1567	-2.1458	54.5960
2	11.8856	-3.0514	26.8225	-13.2292	37.0004
3	5.3867	-8.1792	18.9526	-18.9377	29.7111
4	0.5015	-2.7944	3.7973	-19.9559	20.9588

Fit Equation Description:

```
[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto
{{previous: 57.8648}}
b = if(x50(x,y)-min(x)=0, 1,  -ln(.5)/(x50(x,y)-min(x)))  "Auto {{previous: 0.791393}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200
```

Number of Iterations Performed = 17

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4)



Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-clay loam sediment: sediment
[Tetrazine-3,6-^{14}C]-label
Nonlinear Regression

Data Source: Data 1 in 125501 47192116 162-4 CL Sed.JNB
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9884	0.9768	0.9614	4.8147

	Coefficient	Std. Error	t	P	VIF
a	31.2321	4.0765	7.6616	0.0046	2.1555
b	0.1255	0.0575	2.1829	0.1170	2.1555

Analysis of Variance:

	DF	SS	MS
Regression	2	2933.0965	1466.5482
Residual	3	69.5435	23.1812
Total	5	3002.6400	600.5280

Statistical Tests:

PRESS 163.8589

Durbin-Watson Statistic 2.8895 Failed

Normality Test Passed (P = 0.7012)

K-S Statistic = 0.2935 Significance Level = 0.7012

Constant Variance Test Passed (P = 0.0500)

Power of performed test with alpha = 0.0500: 0.9530

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	30.1321	1.4679	0.3049	0.4570	0.3868
2	27.5486	-2.1486	-0.4463	-0.5358	-0.4600
3	24.2995	-3.8995	-0.8099	-0.9118	-0.8756
4	21.4337	6.5663	1.3638	1.6004	3.4176<
5	14.7093	-2.1093	-0.4381	-0.7450	-0.6738

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	0.1301	0.5549	0.4319
2	0.0633	0.3062	-0.3056
3	0.1111	0.2109	-0.4527
4	0.4830	0.2738	2.0987<

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-clay loam sediment: sediment
[Tetrazine-3,6-^{14}C]-label
5 0.5250 0.6542 -0.9268

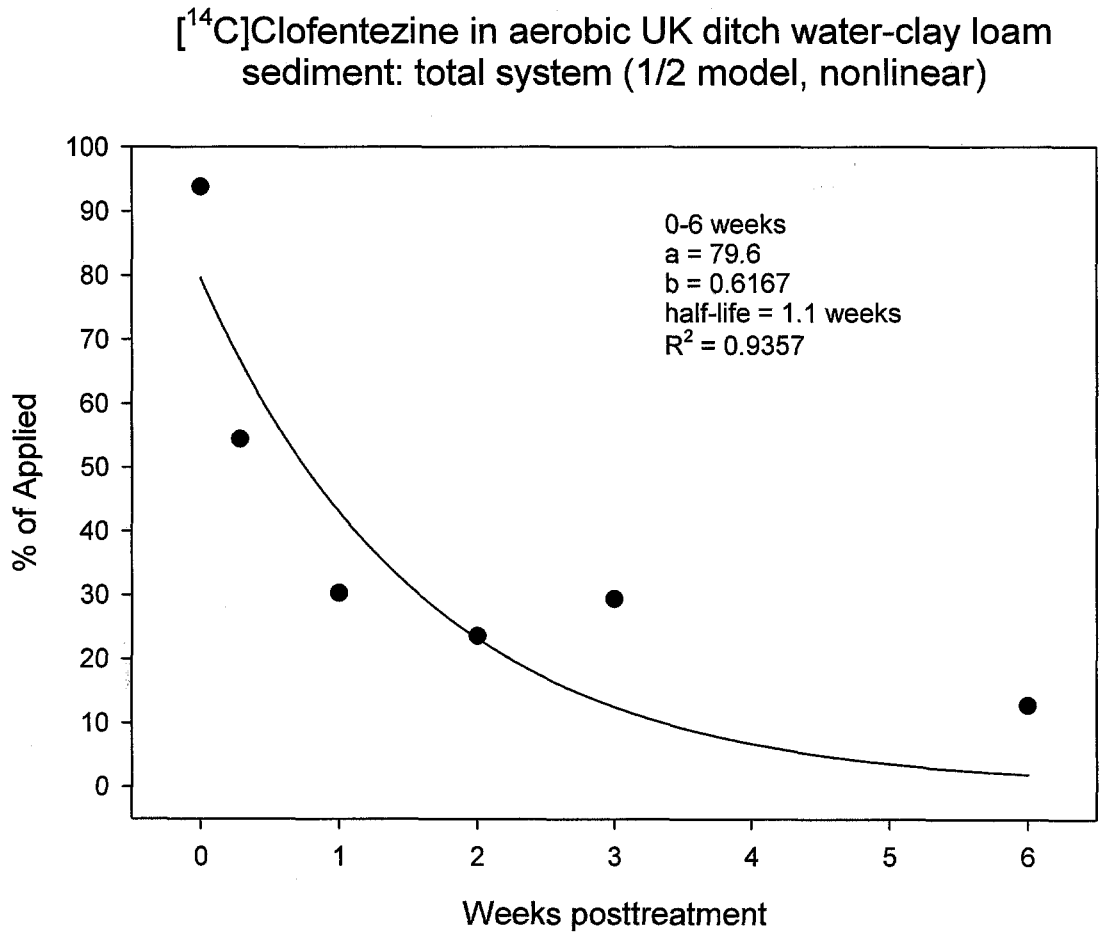
95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	30.1321	18.7186	41.5455	11.0260	49.2381
2	27.5486	19.0698	36.0274	10.0367	45.0605
3	24.2995	17.2627	31.3364	7.4385	41.1605
4	21.4337	13.4155	29.4518	4.1401	38.7272
5	14.7093	2.3162	27.1024	-4.9977	34.4163

Fit Equation Description:
[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto {{previous: 31.2321}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.125494}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200

Number of Iterations Performed = 6

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4)



Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-clay loam sediment: total system
[Tetrazine-3,6-^{14}C]-label
Nonlinear Regression

Data Source: Data 1 in 125501 47192116 162-4 CL Tot sys.JNB
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9673	0.9357	0.9036	15.1400

	Coefficient	Std. Error	t	P	VIF
a	79.6301	12.2892	6.4797	0.0029	1.3865
b	0.6167	0.2318	2.6601	0.0564	1.3865

Analysis of Variance:

	DF	SS	MS
Regression	2	13344.1761	6672.0880
Residual	4	916.8739	229.2185
Total	6	14261.0500	2376.8417

Statistical Tests:

PRESS 3082.0346

Durbin-Watson Statistic 1.2907 Failed

Normality Test Passed (P = 0.5933)

K-S Statistic = 0.2946 Significance Level = 0.5933

Constant Variance Test Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 0.9439

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	79.6301	14.1699	0.9359	1.6024	2.3192<
2	66.7654	-12.3654	-0.8167	-1.0042	-1.0057
3	42.9769	-12.6769	-0.8373	-1.0158	-1.0213
4	23.1949	0.4051	0.0268	0.0341	0.0295
5	12.5185	16.8815	1.1150	1.3046	1.4906
6	1.9680	10.8320	0.7155	0.7262	0.6749

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	2.4797	0.6589	3.2230<
2	0.2581	0.3386	-0.7195
3	0.2435	0.3206	-0.7015

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-clay loam sediment: total system
[Tetrazine-3,6-^{14}C]-label

4	0.0004	0.3832	0.0233
5	0.3140	0.2695	0.9055
6	0.0079	0.0293	0.1172

95% Confidence:

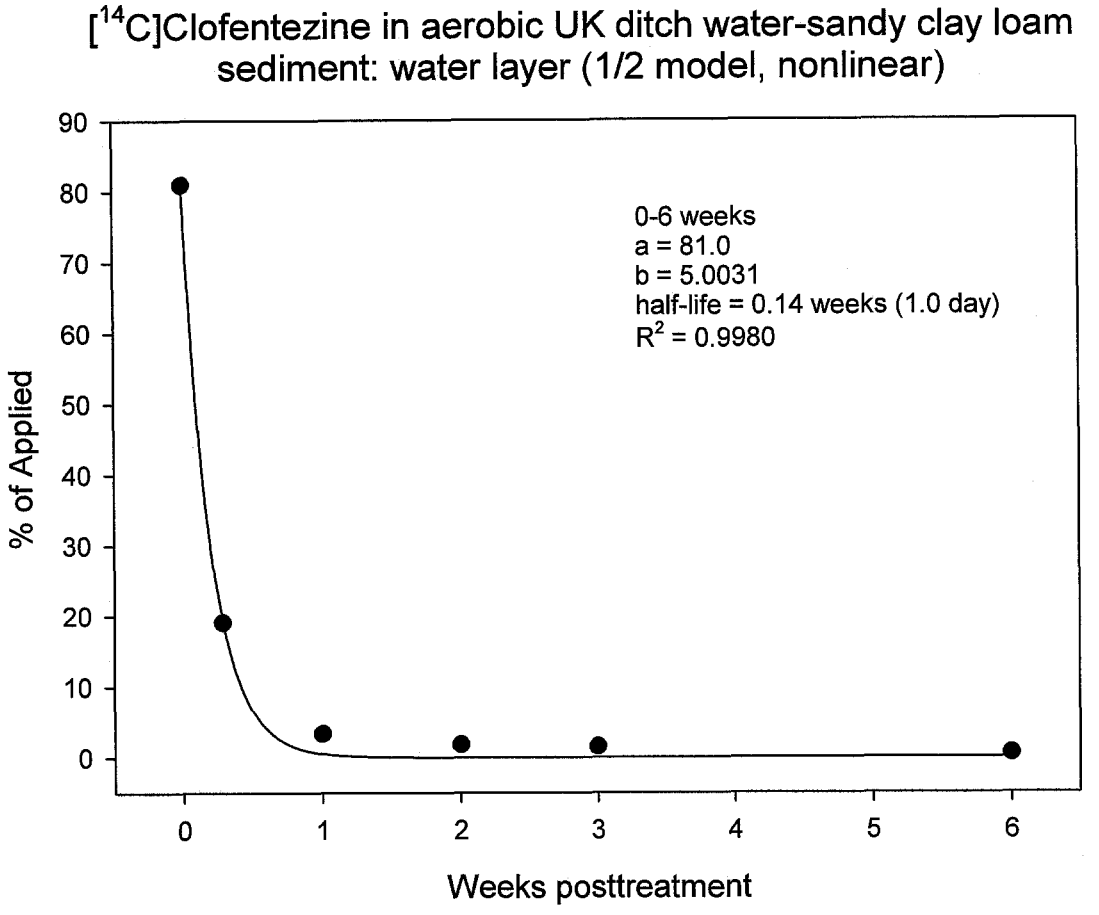
Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	79.6301	45.5099	113.7504	25.4900	133.7703
2	66.7654	42.3064	91.2243	18.1320	115.3987
3	42.9769	19.1764	66.7774	-5.3287	91.2825
4	23.1949	-2.8257	49.2156	-26.2423	72.6321
5	12.5185	-9.3046	34.3415	-34.8441	59.8810
6	1.9680	-5.2233	9.1593	-40.6780	44.6140

Fit Equation Description:

```
[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto
{{previous: 79.6301}}
b = if(x50(x,y)-min(x)=0, 1,  -ln(.5)/(x50(x,y)-min(x)))  "Auto {{previous: 0.61673}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200
```

Number of Iterations Performed = 12

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4)



Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-sandy clay loam sediment: water layer
[Tetrazine-3,6-^{14}C]-label
Nonlinear Regression

Data Source: Data 1 in 125501 47192116 162-4 SCL H2O.JNB
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9990	0.9980	0.9970	1.8686

	Coefficient	Std. Error	t	P	VIF
a	80.9515	1.8684	43.3271	<0.0001	1.0571
b	5.0031	0.3453	14.4908	0.0001	1.0571

Analysis of Variance:

	DF	SS	MS
Regression	2	6929.1427	3464.5713
Residual	4	13.9673	3.4918
Total	6	6943.1100	1157.1850

Statistical Tests:

PRESS 30991.3762

Durbin-Watson Statistic 0.8717 Failed

Normality Test Passed (P = 0.2094)

K-S Statistic = 0.4062 Significance Level = 0.2094

Constant Variance Test Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	80.9515	0.0485	0.0259	1.5516	2.1296<
2	19.3828	-0.2828	-0.1514	-1.5490	-2.1208<
3	0.5437	2.8563	1.5285	1.5361	2.0773<
4	0.0037	1.7963	0.9613	0.9613	0.9494
5	2.4533E-005	1.5000	0.8027	0.8027	0.7590
6	7.4346E-012	0.5000	0.2676	0.2676	0.2338

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	4308.8237<	0.9997	127.4118<
2	124.4628<	0.9905	-21.6007
3	0.0117	0.0098	0.2069

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-sandy clay loam sediment: water layer
[Tetrazine-3,6-^{14}C]-label

4	8.2953E-007	1.7953E-006	0.0013
5	5.8986E-011	1.8309E-010	1.0270E-005
6	2.4195E-024	6.7587E-023	1.9223E-012

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	80.9515	75.7641	86.1390	73.6149	88.2882
2	19.3828	14.2195	24.5462	12.0632	26.7025
3	0.5437	0.0295	1.0580	-4.6699	5.7574
4	0.0037	-0.0033	0.0106	-5.1845	5.1918
5	2.4533E-005	-4.5669E-005	9.4734E-005	-5.1882	5.1882
6	7.4346E-012	-3.5218E-011	5.0087E-011	-5.1882	5.1882

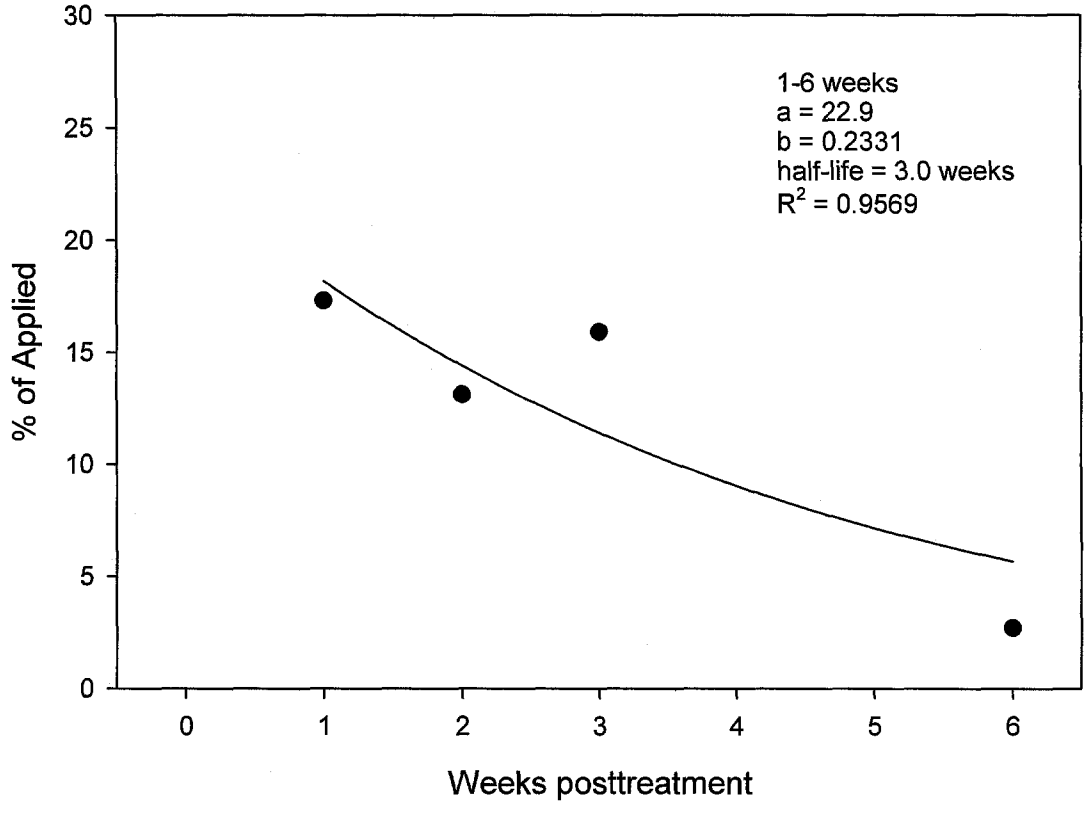
Fit Equation Description:

```
[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto
{{previous: 80.9515}}
b = if(x50(x,y)-min(x)=0, 1,  -ln(.5)/(x50(x,y)-min(x)))  "Auto {{previous: 5.00312}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200
```

Number of Iterations Performed = 7

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4)

[^{14}C]Clofentezine product III in aerobic UK ditch water-sandy clay loam sediment: total system (1/2 model, nonlinear)



Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-sandy clay loam sediment: total system
[Tetrazine-3,6-^{14}C]-label
Clofentezine product III
Nonlinear Regression

Data Source: Data 1 in 125501 47192116 162-4 SCL III Tot sys.JNB
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9782	0.9569	0.9139	3.9668

	Coefficient	Std. Error	t	P	VIF
a	22.9453	6.5346	3.5114	0.0724	3.6057
b	0.2331	0.1276	1.8270	0.2092	3.6057

Analysis of Variance:

	DF	SS	MS
Regression	2	699.5296	349.7648
Residual	2	31.4704	15.7352
Total	4	731.0000	182.7500

Statistical Tests:

PRESS 119.4693

Durbin-Watson Statistic 2.8424 Failed

Normality Test Passed (P = 0.5848)

K-S Statistic = 0.3565 Significance Level = 0.5848

Constant Variance Test Failed (P = <0.0001)

Power of performed test with alpha = 0.0500: 0.6160

The power of the performed test (0.6160) is below the desired power of 0.8000.
You should interpret the negative findings cautiously.

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	18.1735	-0.8735	-0.2202	-0.4380	-0.3258
2	14.3941	-1.2941	-0.3262	-0.3895	-0.2865
3	11.4007	4.4993	1.1343	1.4062	9.3807<
4	5.6645	-2.9645	-0.7473	-1.1889	-1.5525

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	0.2836	0.7473	-0.5601

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-sandy clay loam sediment: total system
[Tetrazine-3,6-^{14}C]-label
Clofentezine product III

2	0.0323	0.2985	-0.1869
3	0.5310	0.3494	6.8747<
4	1.0820	0.6049	-1.9209

95% Confidence:

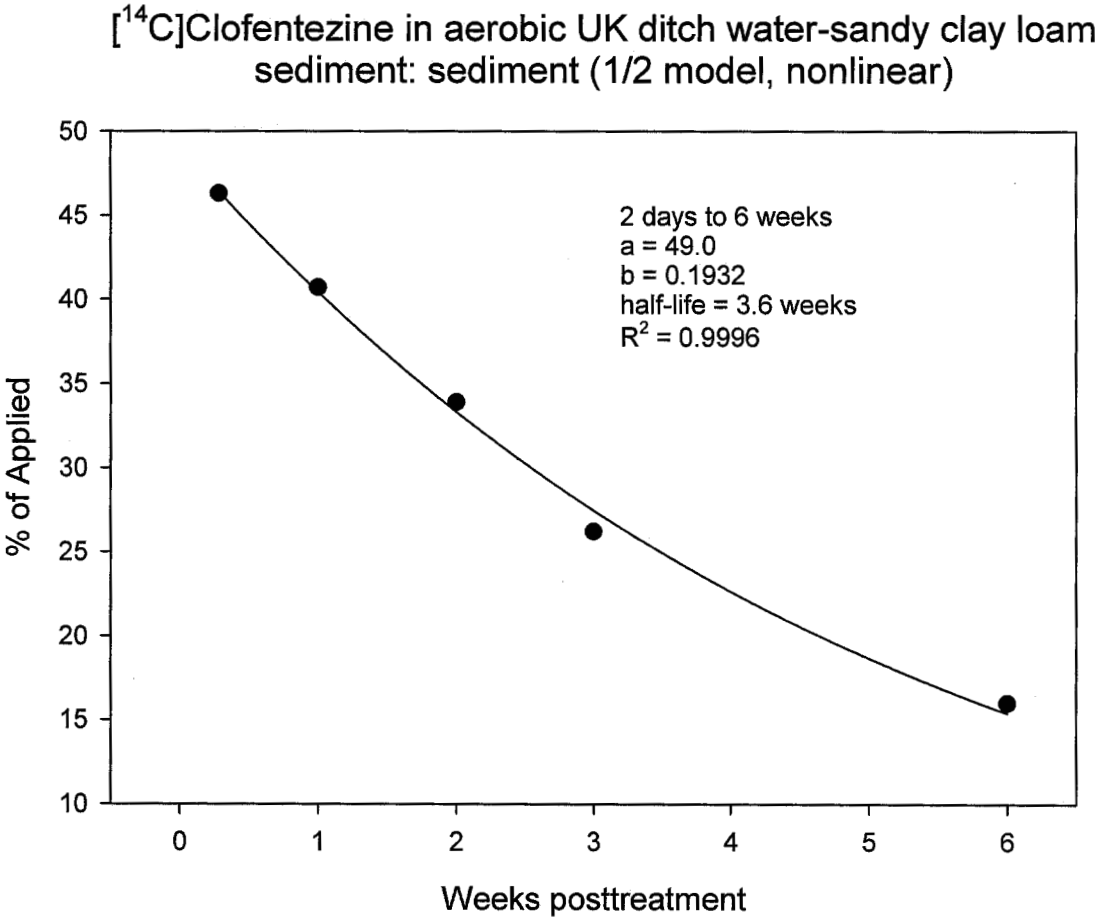
Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	18.1735	3.4196	32.9275	-4.3871	40.7341
2	14.3941	5.0699	23.7183	-5.0544	33.8426
3	11.4007	1.3118	21.4895	-8.4258	31.2271
4	5.6645	-7.6096	18.9387	-15.9573	27.2864

Fit Equation Description:

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto {{previous: 22.9453}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.233148}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200

Number of Iterations Performed = 8

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4)



Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-sandy clay loam sediment: sediment
[Tetrazine-3,6-^{14}C]-label
Nonlinear Regression

Data Source: Data 1 in 125501 47192116 162-4 SCL Sed.JNB
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9998	0.9996	0.9993	0.8957

	Coefficient	Std. Error	t	P	VIF
a	49.0383	0.8292	59.1404	<0.0001	2.0989
b	0.1932	0.0088	21.8618	0.0002	2.0989

Analysis of Variance:

	DF	SS	MS
Regression	2	5889.4232	2944.7116
Residual	3	2.4068	0.8023
Total	5	5891.8300	1178.3660

Statistical Tests:

PRESS 5.9798

Durbin-Watson Statistic 2.9861 Failed

Normality Test Passed (P = 0.8749)

K-S Statistic = 0.2461 Significance Level = 0.8749

Constant Variance Test Passed (P = 0.0500)

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	46.4051	-0.1051	-0.1174	-0.1901	-0.1562
2	40.4244	0.2756	0.3077	0.3681	0.3075
3	33.3236	0.5764	0.6436	0.7332	0.6607
4	27.4701	-1.2701	-1.4180	-1.7192	-11.5411<
5	15.3881	0.6119	0.6832	0.9977	0.9965

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	0.0293	0.6187	-0.1989
2	0.0292	0.3010	0.2018
3	0.0800	0.2295	0.3606

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-sandy clay loam sediment: sediment
[Tetrazine-3,6-^{14}C]-label

4	0.6946	0.3197	-7.9124
5	0.5636	0.5311	1.0605

95% Confidence:

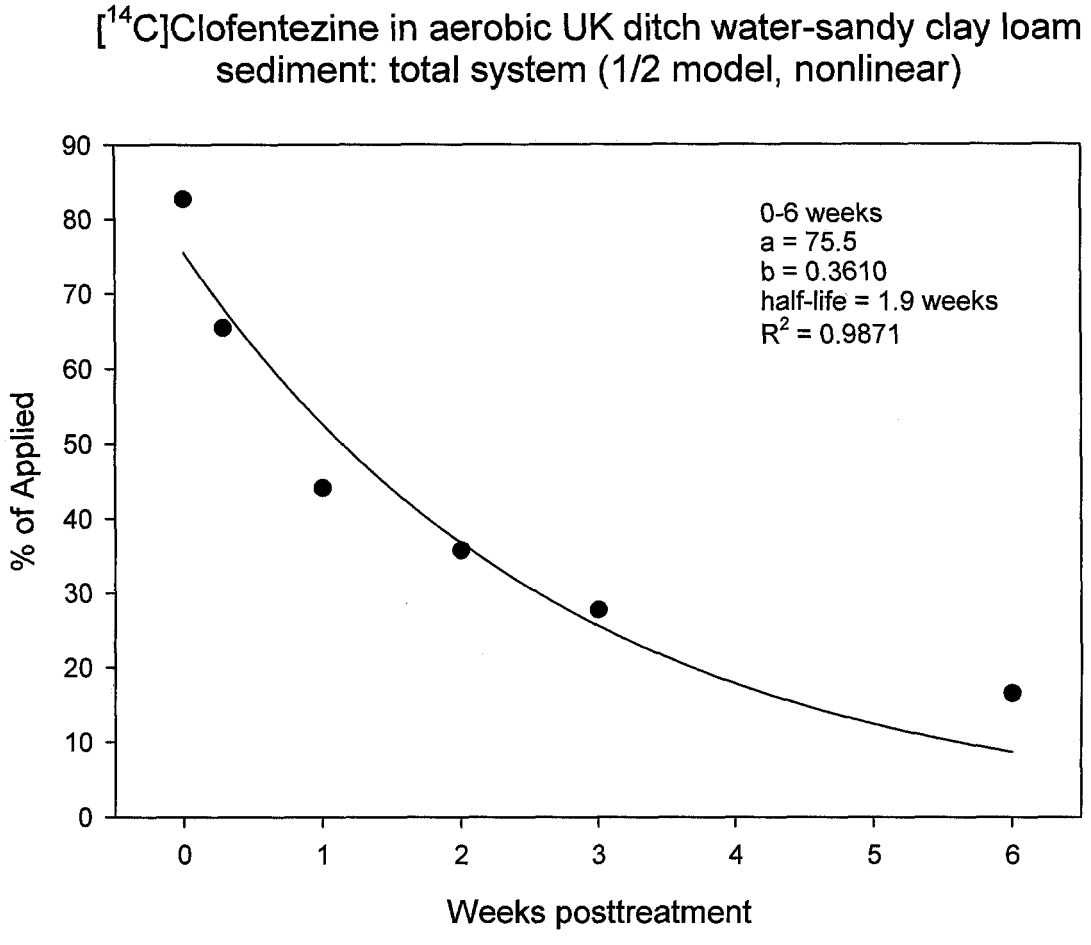
Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	46.4051	44.1630	48.6473	42.7785	50.0318
2	40.4244	38.8605	41.9883	37.1731	43.6757
3	33.3236	31.9581	34.6890	30.1629	36.4842
4	27.4701	25.8582	29.0819	24.1954	30.7447
5	15.3881	13.3108	17.4653	11.8610	18.9151

Fit Equation Description:

```
[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto
{{previous: 49.0383}}
b = if(x50(x,y)-min(x)=0, 1,  -ln(.5)/(x50(x,y)-min(x)))  "Auto {{previous: 0.193168}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200
```

Number of Iterations Performed = 7

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4)



Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-sandy clay loam sediment: total system
[Tetrazine-3,6-^{14}C]-label
Nonlinear Regression

Data Source: Data 1 in 125501 47192116 162-4 SCL Tot sys.JNB
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9935	0.9871	0.9806	7.0502

	Coefficient	Std. Error	t	P	VIF
a	75.4902	5.2605	14.3503	0.0001	1.4826
b	0.3610	0.0656	5.4992	0.0053	1.4826

Analysis of Variance:

	DF	SS	MS
Regression	2	15176.4665	7588.2332
Residual	4	198.8235	49.7059
Total	6	15375.2900	2562.5483

Statistical Tests:

PRESS 508.8364

Durbin-Watson Statistic 1.1623 Failed

Normality Test Passed (P = 0.9253)

K-S Statistic = 0.2094 Significance Level = 0.9253

Constant Variance Test Passed (P = 0.0600)

Power of performed test with alpha = 0.0500: 0.9987

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	75.4902	7.2098	1.0226	1.5360	2.0770<
2	68.0919	-2.6919	-0.3818	-0.4724	-0.4210
3	52.6147	-8.5147	-1.2077	-1.3672	-1.6223
4	36.6710	-0.9710	-0.1377	-0.1664	-0.1446
5	25.5587	2.1413	0.3037	0.3820	0.3370
6	8.6534	7.8466	1.1130	1.2396	1.3679

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	1.4816	0.5567	2.3277<
2	0.0592	0.3467	-0.3067

Chemical: Clofentezine (NC 21314)
PC: 125501
MRID: 47192116
Guideline: 162-4
UK ditch water-sandy clay loam sediment: total system
[Tetrazine-3,6-^{14}C]-label

3	0.2632	0.2197	-0.8609
4	0.0064	0.3153	-0.0982
5	0.0424	0.3677	0.2570
6	0.1847	0.1939	0.6708

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	75.4902	60.8847	90.0957	51.0671	99.9133
2	68.0919	56.5669	79.6168	45.3764	90.8073
3	52.6147	43.4389	61.7904	30.9962	74.2332
4	36.6710	25.6798	47.6623	14.2217	59.1204
5	25.5587	13.6884	37.4291	2.6662	48.4513
6	8.6534	0.0350	17.2719	-12.7345	30.0414

Fit Equation Description:

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto {{previous: 75.4902}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.361008}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200

Number of Iterations Performed = 9

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems.
Confirmation of summations (material balances) and determination of means/standard deviations for applied radioactivity.
Sandy clay loam sediment (Lode) systems.

Day/ Week	Wate layer			Sediment			Volatiles[1]	Vessel[2]	Mat bal	Study Mat bal
	Extract	Nonext.	Total	Extract	Nonext.	Total				
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR
0	83.2	0.2	83.4	2.2	0.3	2.5	0.0	0.6	86.5	86.5
2	23.5	0.2	23.7	54.4	5.8	60.2	0.1	8.7	92.7	92.7
1	15.5	1.5	17.0	59.8	8.1	67.9	3.0	4.5	92.4	92.7
2	11.9	2.6	14.5	52.3	16.8	69.1	5.7	2.0	91.3	91.3
3	7.4	1.2	8.6	52.6	15.1	67.7	5.0	0.7	82.0	82.0
6	2.6	1.7	4.3	26.9	16.9	43.8	29.9	0.2	78.2	78.2
								Mean	87.2	87.2
								std dev.	5.5	5.6
								maximum	92.7	92.7
								minimum	78.2	78.2
								n =	6	6

Clay loam sediment (Sadlers Farm) systems.

Day/ Week	Wate layer			Sediment			Volatiles[1]	Vessel[2]	Mat bal	Study Mat bal
	Extract	Nonext.	Total	Extract	Nonext.	Total				
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR
0	97.0	0.0	97.0	0.9	0.2	1.1	0.0	0.4	98.5	98.5
2	24.2	1.3	25.5	49.1	18.0	67.1	0.0	4.5	97.1	93.1
1	11.6	1.7	13.3	52.3	12.7	65.0	3.5	8.9	90.7	91.4
2	6.1	1.1	7.2	43.8	26.3	70.1	3.6	3.0	83.9	83.9
3	6.4	1.8	8.2	39.9	19.1	59.0	12.0	4.4	83.6	83.6
6	2.7	1.6	4.3	30.9	24.8	55.7	32.0	0.2	92.2	92.2
								Mean	91.0	90.5
								std dev.	5.8	5.3
								maximum	98.5	98.5
								minimum	83.6	83.6
								n =	6	6

1 Separate results for ethylene glycol, ethanolamine and sulfuric acid trapping solutions not reported.
2 Vessel rinse.
Results from Tables 4, p. 19 of the study report.
Means and standard deviations calculated using Microsoft program functions @average (A1:A2) and @stdevp (A1:A2).
Shaded block indicates result does not agree (>0.1%) with that reported by the study authors (Reviewer's Comment No. 1).

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems.
[^{14}C]Residue water phase:sediment ratios.
Sandy clay loam sediment (Lode) systems.
Total [^{14}C]residues in sediment.

Day/ Week	Sediment		
	Ext.	Nonext	Total
	% AR	% AR	% AR
0	2.2	0.3	2.5
2	54.4	5.8	60.2
1	59.8	8.1	67.9
2	52.3	16.8	69.1
3	52.6	15.1	67.7
6	26.9	16.9	43.8

[^{14}C] water phase:sediment ratios.

Day/ Week	Water	Sed	Ratio	Ratio
	% AR	% AR	W:S	S:W
0	83.4	2.5	33	0
2	23.7	60.2	0	3
1	17.0	67.9	0	4
2	14.5	69.1	0	5
3	8.6	67.7	0	8
6	4.3	43.8	0	10

Clay loam sediment (Sadlers Farm) systems.
Total [^{14}C]residues in sediment.

Day/ Week	Sediment		
	Ext.	Nonext	Total
	% AR	% AR	% AR
0	0.9	0.2	1.1
2	49.1	18.0	67.1
1	52.3	12.7	65.0
2	43.8	26.3	70.1
3	39.9	19.1	59.0
6	30.9	24.8	55.7

[^{14}C] water phase:sediment ratios.

Day/ Week	Water	Sed	Ratio	Ratio
	% AR	% AR	W:S	S:W
0	97.0	1.1	88	0
2	25.5	67.1	0	3
1	13.3	65.0	0	5
2	7.2	70.1	0	10
3	8.2	59.0	0	7
6	4.3	55.7	0	13

Results imported from **Mat bals** worksheet.
Means and standard deviations calculated using Microsoft program functions @average (A1:A2) and @stdevp (A1:A2).

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Determination of parent clofentezine and transformation products in total system. Sandy clay loam sediment (Lode) systems.

Day/ Week	Clofentezine					NC 12940 (II)					III				
	Water	Sed.	Vessel[1]	S+V[2]	System	Water	Sed.	Vessel[1]	S+V[2]	System	Water	Sed.	Vessel[1]	S+V[2]	System
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR
0	81.0	1.7		1.7	82.7				0.0	0.0				0.0	0.0
2	19.1	38.7	7.6	46.3	65.4	1.3	0.7	0.2	0.9	2.2	1.6	4.9	0.2	5.1	6.7
1	3.4	36.6	4.1	40.7	44.1	0.3	1.0	0.2	1.2	1.5	7.5	9.7	0.1	9.8	17.3
2	1.8	32.3	1.6	33.9	35.7	0.3	2.0	0.1	2.1	2.4	6.3	6.6	0.2	6.8	13.1
3	1.5	26.2		26.2	27.7	0.2	0.8		0.8	1.0	1.1	14.8		14.8	15.9
6	0.5	16.0		16.0	16.5	0.2			0.0	0.2	0.7	2.0		2.0	2.7

Day/ Week	NC 12898 (IV)					NC 233 (V)				
	Water	Sed.	Vessel[1]	S+V[2]	System	Water	Sed.	Vessel[1]	S+V[2]	System
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR
0				0.0	0.0				0.0	0.0
2	0.1	1.1		1.1	1.2	0.2	1.6	0.1	1.7	1.9
1	0.2	1.1		1.1	1.3	1.9	2.6		2.6	4.5
2	0.2	1.2		1.2	1.4	1.4	2.1	0.1	2.2	3.6
3	0.2	0.8		0.8	1.0	2.4	1.0		1.0	3.4
6	0.2	1.1		1.1	1.3	0.2	0.6		0.6	0.8

1 Vessel rinse.
2 Summation of Sediment + Vessel rinse residues.
Results from Table 6, p. 22 of the study report; blank cell = either <0.1% of applied or NA (not analyzed, <1% of applied).

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Determination of total unidentified/unaccounted for residues.
Sandy clay loam sediment (Lode) systems.

Day/ Week	Initial	Identififed					TLC Unidentified				TLC Unacct[1]	Not analyzed[2]	Total Unided[3]
		Parent	II	III	IV	V	Unk X	Origin	Rem	Total			
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR
	Water layer												
0	83.2	81.0						0.6	1.7	2.3	-0.1	0.2	2.5
2	23.5	19.1	1.3	1.6	0.1	0.2	0.3		0.9	1.2	0.0	0.2	1.4
1	15.5	3.4	0.3	7.5	0.2	1.9	1.4	0.2	0.8	2.4	-0.2	1.5	3.9
2	11.9	1.8	0.3	6.3	0.2	1.4	1.2	0.1	0.6	1.9	0.0	2.6	4.5
3	7.4	1.5	0.2	1.1	0.2	2.4	1.5	0.1	0.4	2.0	0.0	1.2	3.2
6	2.6	0.5	0.2	0.7	0.2	0.2	0.5	0.1	0.3	0.9	-0.1	1.7	2.6
	Sediment												
0	2.2	1.7						0.1	0.3	0.4	0.1		0.4
2	54.4	38.7	0.7	4.9	1.1	1.6	0.1	1.8	5.2	7.1	0.3		7.1
1	59.8	36.6	1.0	9.7	1.1	2.6	0.2	3.1	5.5	8.8	0.0		8.8
2	52.3	32.3	2.0	6.6	1.2	2.1	0.9	3.1	4.0	8.0	0.1		8.0
3	52.6	26.2	0.8	14.8	0.8	1.0	0.3	2.0	6.9	9.2	-0.2		9.2
6	26.9	16.0		2.0	1.1	0.6		1.9	4.8	6.7	0.5		6.7
	Vessel rinse												
0	0.6											0.6	0.6
2	8.7	7.6	0.2	0.2		0.1		0.1	0.5	0.6	0.0		0.6
1	4.5	4.1	0.2	0.1					0.1	0.1	0.0		0.1
2	2.0	1.6	0.1	0.2		0.1				0.0	0.0		0.0
3	0.7											0.7	0.7
6	0.2											0.2	0.2
	Total system												
0	86.0	82.7	0.0	0.0	0.0	0.0	0.0	0.7	2.0	2.7	0.6	0.8	3.5
2	86.6	65.4	2.2	6.7	1.2	1.9	0.4	1.9	6.6	8.9	0.3	0.2	9.1
1	79.8	44.1	1.5	17.3	1.3	4.5	1.6	3.3	6.4	11.3	-0.2	1.5	12.8
2	66.2	35.7	2.4	13.1	1.4	3.6	2.1	3.2	4.6	9.9	0.1	2.6	12.5
3	60.7	27.7	1.0	15.9	1.0	3.4	1.8	2.1	7.3	11.2	0.5	1.9	13.1
6	29.7	16.5	0.2	2.7	1.3	0.8	0.5	2.0	5.1	7.6	0.6	1.9	9.5

1 [^{14}C]Residues unaccounted for following TLC analysis.
2 Either [^{14}C]residues remaining after methylene chloride partition of water layer or vessel rinses not TLC analyzed.
3 **Total TLC Unidentified + Not analyzed.**
Results from Table 4, p. 19; Table 6, p. 22 of the study report and imported from **Profile SCL** worksheet.

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems.
Determination of parent clofentezine and transformation products in total system.
Clay loam sediment (Sadlers Farm) systems.

Day/ Week	Clofentezine					NC 12940 (II)					III				
	Water	Sed.	Vessel[1]	S+V[2]	System	Water	Sed.	Vessel[1]	S+V[2]	System	Water	Sed.	Vessel[1]	S+V[2]	System
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR
0	93.3	0.5		0.5	93.8	0.9			0.0	0.9	0.2	0.1		0.1	0.3
2	22.8	27.5	4.1	31.6	54.4	0.1	1.0	0.1	1.1	1.2	0.7	10.7		10.7	11.4
1	4.9	17.2	8.2	25.4	30.3	0.3	1.2	0.3	1.5	1.8	4.4	22.2	0.4	22.6	27.0
2	3.2	17.7	2.7	20.4	23.6	0.1	1.6	0.1	1.7	1.8	0.7	8.4	0.1	8.5	9.2
3	1.4	24.2	3.8	28.0	29.4	0.2	0.8	0.1	0.9	1.1	1.9	4.8	0.3	5.1	7.0
6	0.2	12.6		12.6	12.8	0.1	0.5		0.5	0.6	0.4	5.9		5.9	6.3

Day/ Week	NC 12898 (IV)					NC 233 (V)				
	Water	Sed.	Vessel[1]	S+V[2]	System	Water	Sed.	Vessel[1]	S+V[2]	System
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR
0				0.0	0.0	0.1			0.0	0.1
2		0.8		0.8	0.8		1.2		1.2	1.2
1	0.1	1.2		1.2	1.3	0.2	2.2		2.2	2.4
2	0.1	1.7		1.7	1.8	0.1	2.6		2.6	2.7
3	0.1	0.7		0.7	0.8	0.2	1.5	0.1	1.6	1.8
6	0.1	1.3		1.3	1.4	0.3	1.2		1.2	1.5

1 Vessel rinse.
2 Summation of Sediment + Vessel rinse residues.
Results from Table 5, p. 21 of the study report; blank cell = either <0.1% of applied or NA (not analyzed, <1% of applied).

Chemical: Clofentezine (NC 21314).
PC: 125501
MRID: 47192116
Guideline: 162-4

Aerobic aquatic metabolism of [tetrazine-3,6-^{14}C]clofentezine in two United Kingdom water-sediment systems. Determination of total unidentified/unaccounted for residues.
Clay loam sediment (Sadlers Farm) systems.

Day/ Week	Initial	Identififed					TLC Unidentified				TLC Unacct[1]	Not analyzed[2]	Total Unided[3]
		Parent	II	III	IV	V	Unk X	Origin	Rem	Total			
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR
	Water layer												
0	97.0	93.3	0.9	0.2		0.1		0.3	2.2	2.5	0.0		2.5
2	24.2	22.8	0.1	0.7			0.2		0.4	0.6	0.0	1.3	1.9
1	11.6	4.9	0.3	4.4	0.1	0.2	1.1	0.1	0.5	1.7	0.0	1.7	3.4
2	6.1	3.2	0.1	0.7	0.1	0.1	1.6	0.1	0.3	2.0	-0.1	1.1	3.1
3	6.4	1.4	0.2	1.9	0.1	0.2	2.1	0.2	0.4	2.7	-0.1	1.8	4.5
6	2.7	0.2	0.1	0.4	0.1	0.3	0.8	0.4	0.5	1.7	-0.1	1.6	3.3
	Sediment												
0	0.9	0.5		0.1				0.1	0.2	0.3	0.0		0.3
2	49.1	27.5	1.0	10.7	0.8	1.2	1.0	2.3	4.4	7.7	0.2		7.7
1	52.3	17.2	1.2	22.2	1.2	2.2	0.5	2.6	5.1	8.2	0.1		8.2
2	43.8	17.7	1.6	8.4	1.7	2.6	1.9	4.1	5.6	11.6	0.2		11.6
3	39.9	24.2	0.8	4.8	0.7	1.5	0.3	2.0	5.4	7.7	0.2		7.7
6	30.9	12.6	0.5	5.9	1.3	1.2	0.9	3.6	5.0	9.5	-0.1		9.5
	Vessel rinse												
0	0.4											0.4	0.4
2	4.5	4.1	0.1						0.2	0.2	0.1		0.2
1	8.9	8.2	0.3	0.4					0.2	0.2	-0.2		0.2
2	3.0	2.7	0.1	0.1					0.1	0.1	0.0		0.1
3	4.4	3.8	0.1	0.3		0.1			0.1	0.1	0.0		0.1
6	0.2											0.2	0.2
	Total system												
0	98.3	93.8	0.9	0.3	0.0	0.1	0.0	0.4	2.4	2.8	0.4	0.4	3.2
2	77.8	54.4	1.2	11.4	0.8	1.2	1.2	2.3	5.0	8.5	0.3	1.3	9.8
1	72.8	30.3	1.8	27.0	1.3	2.4	1.6	2.7	5.8	10.1	-0.1	1.7	11.8
2	52.9	23.6	1.8	9.2	1.8	2.7	3.5	4.2	6.0	13.7	0.1	1.1	14.8
3	50.7	29.4	1.1	7.0	0.8	1.8	2.4	2.2	5.9	10.5	0.1	1.8	12.3
6	33.8	12.8	0.6	6.3	1.4	1.5	1.7	4.0	5.5	11.2	0.0	1.8	13.0

1 [^{14}C]Residues unaccounted for following TLC analysis.

2 Either [^{14}C]residues remaining after methylene chloride partition of water layer or vessel rinses not TLC analyzed.

3 **Total TLC Unidentified** + **Not analyzed**.

Results from Table 4, p. 19; Table 5, p. 21 of the study report and imported from **Profile CL** worksheet.

Attachment 3: Transformation Pathway Presented by Registrant
Illustration of Test System

Figure 5

Proposed degradation pathway

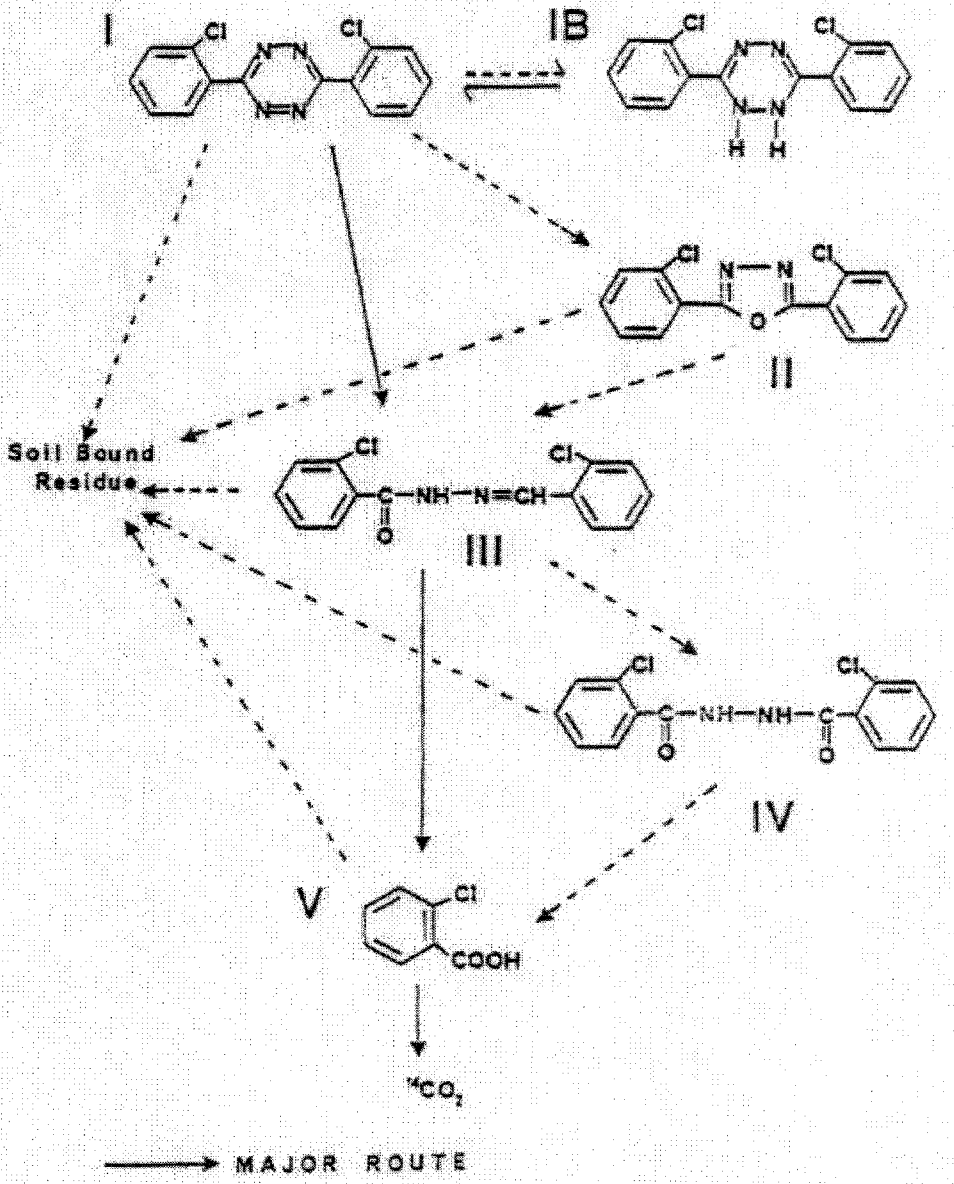


FIGURE 1

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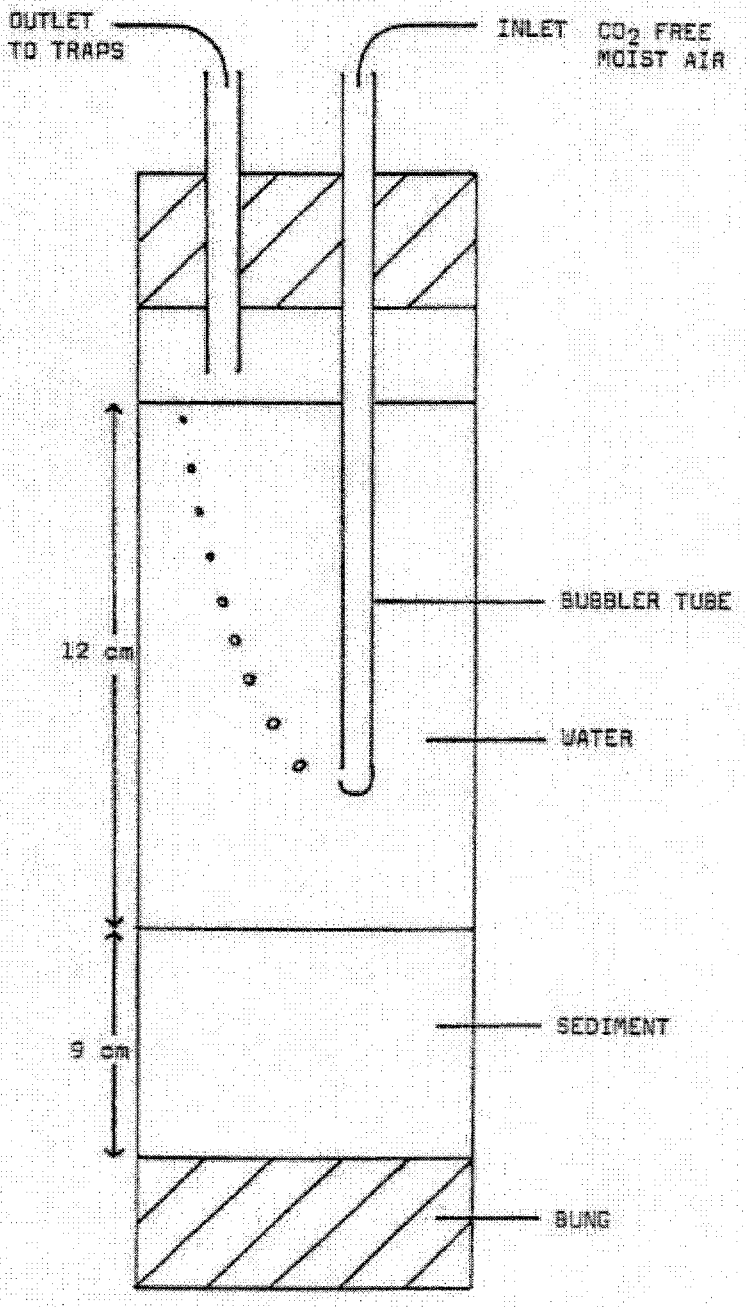

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