

US EPA ARCHIVE DOCUMENT

(3-2-05)

Data Evaluation Report on the aerobic biotransformation of BAS 670H in water-sediment system

PMRA Submission Number {.....}

EPA MRID Number 45902424

Data Requirement: PMRA Data Code:
EPA DP Barcode: D290065
OECD Data Point:
EPA Guideline: 162-4

Test material:

Common name: BAS 670 H.

Chemical name

IUPAC name: Not found.

CAS name: [3-(4,5-Dihydro-3-isoxazolyl)-2-methyl-4-(methylsulfonyl)phenyl](5-hydroxy-1-methyl-1H-pyrazol-4-yl)methanone.
[3-(4,5-Dihydro-3-isoxazol-3-yl)-4-methanesulfonyl-2-methyl-phenyl](5-hydroxy-1-methyl-1H-pyrazol-4-yl)methanone.

CAS No: 210631-68-8.

SMILES string: Cc1c(c(ccc1C(=O)c1c(n(nc1)C)O)S(=O)(=O)C)C1=NOCC1.

Primary Reviewer: Lynne Binari
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Date: 3-2-05

Company Code:

Active Code:

Use Site Category:

EPA PC Code: 123009

CITATION: Fent, G. 2002. Degradation and distribution of BAS 670H in a water-sediment system under outdoor conditions. Unpublished study performed by Staatliche Lehr- und Forschungsanstalt für Landwirtschaft, Weinbau und Gartenbau (SLFA), Neustadt an der Weinstraße, Germany, and BASF Aktiengesellschaft, Limburgerhof, Germany; sponsored and submitted by BASF Agro Research, Research Triangle Park, NC. SLFA Study No.: BAS70 and BASF Report (Document) No.: 2002/1007741. Experiment initiation July 18, 2001, and completion May 22, 2002 (p. 10). Final report issued August 29, 2002.

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Administrative Conclusions: This outdoor study is classified as **unacceptable**. This study, conducted with [phenyl-U-¹⁴C]- and [pyrazol-4-¹⁴C]-labeled BAS 670H, cannot be used towards the fulfillment of the aerobic aquatic metabolism guideline, Subdivision N Guideline §162-4, data requirements for BAS 670H because the experimental design was inadequate to assess aerobic aquatic degradation. In addition, for systems treated with [pyrazole-4-¹⁴C]BAS 670H, material balances were incomplete (<90% of applied) at study termination.

Scientific Conclusions: No conclusions can be made at this time.

EXECUTIVE SUMMARY:

The biotransformation of [phenyl-U-¹⁴C]- and [pyrazol-4-¹⁴C]- labeled [3-(4,5-dihydro-isoxazol-3-yl)-4-methanesulfonyl-2-methyl-phenyl]-(5-hydroxy-1-methyl-1H-pyrazol-4-yl)methanone (BAS 670H) was studied in river water-loamy sand sediment (water pH 8.4, organic carbon not reported; sediment pH 6.0-7.0, organic matter 0.7%) from Ohio for 120 days under natural, outdoor conditions from July 31 to November 28, 2001, in Neustadt an der Weinstraße, Germany. During the 120-day study, mean water and air temperatures were 14.3°C (range 0.7 to 28.6°C) and 14.5°C (range -4.8 to 40.7°C), respectively. Based on the water volume, [¹⁴C]BAS 670H was applied at a nominal rate of *ca.* 0.033 mg a.i./L. The sediment:water ratio used was *ca.* 1:5 (*ca.* 400 g wet wt. sediment:2,000 mL water). This experiment was conducted in accordance with BBA Guidelines for the Official Testing of Plant Protectants (Part IV, 5-1, 1990) and in compliance with OECD Principles of GLP ([C(97) 186/Final], 1997) and Federal Republic of Germany GLP Regulations (Chemikaliengesetz of 1994, amended 2001). The test system consisted of 2-L glass vessels containing the water-sediment. The 2-L glass vessels were placed outdoors in larger plastic boxes containing water to simulate a larger body of water with a Plexiglas cover positioned above (not sealing) the vessels to exclude rainfall. Sediment and water were pre-incubated *ca.* 2 weeks, then following treatment, systems were collected after 0, 1, 2, 7, 14, 30, 59, 100 and 120 days of incubation; two systems per label were collected at 0 and 120 days, with a single system per label at all other intervals. The vessels were maintained open with no collection of CO₂ and volatile organic compounds. Water layers were decanted and analyzed directly. Sediment samples were extracted four times with pH 8 phosphate buffer (concentration not specified):methanol (1:1, v:v). Sediment extracts were combined and concentrated. Water layers, sediment extracts and extracted sediment were analyzed for total radioactivity using LSC. Water layers and sediment extracts were analyzed for [¹⁴C]BAS 670H and its transformation products by reverse-phase HPLC; parent BAS 670H its degradates, M670H05 and M607H01, were reportedly identified by co-chromatography with reference standards; however, supporting chromatograms were not provided. Identification of parent BAS 670H and transformation product M670H05 were reportedly confirmed using LC/MS and LC/MS/MS; however, supporting results were not provided.

Conditions in both the water and sediment layers of systems treated with unlabeled BAS 670H and incubated alongside the [¹⁴C]BAS 670H treated systems went from moderately reducing to

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moderately oxidizing during the 120-day study. In the water layers, redox potentials, oxygen saturation levels and pH averaged $+243 \pm 42$ mV, $81 \pm 8\%$ and 8.23 ± 0.19 , respectively. In the sediment layers, redox potentials averaged $+18 \pm 71$ mV during the initial 2 months of the study and $+208 \pm 38$ mV during the final two months.

Recoveries of radiolabeled material averaged $92.9 \pm 1.5\%$ (range 90.6-94.9%) of the applied and $91.1 \pm 5.7\%$ (range 80.5-96.5%) for the [phenyl-U- ^{14}C]- and [pyrazol-4- ^{14}C]-label treated systems, respectively, with declines in recoveries for both labels throughout the 120-day study. Following application of [^{14}C]BAS 670H to the water layer, [^{14}C]residues (both labels) partitioned from the water layer into the sediment with average ($n = 2$) distribution ratios (water:sediment) of 32:1 at day 0, 11:1 at 1 week, 5:1 at 1 month, then were 1:3 ($n = 1$) thereafter for the [phenyl-U- ^{14}C]-label and 1:2 at 2 months and 1:1 thereafter for the [pyrazol-4- ^{14}C]-label.

In the water layers, [phenyl-U- ^{14}C]BAS 670H decreased from 91.4% of the applied at day 0 to 49.1% at 1 month, 26.0% at 2 months and was 17.2-21.2% at 3.3-4 months, whereas [pyrazol-4- ^{14}C]BAS 670H decreased from 96.3% at day 0 to 48.6% at 2 months and was 31.0% at 4 months. In the sediment, [phenyl-U- ^{14}C]- and [pyrazol-4- ^{14}C]BAS 670H were detected at maximums of 5.0% (1 week) and 7.2% (2 months) of the applied, respectively, and was 3.5-4.9% (both labels) at study termination. Based on nonlinear/normal (2-parameter, unweighted) regression analysis, [phenyl-U- ^{14}C]- and [pyrazol-4- ^{14}C]-label BAS 670H dissipated in the water layers with reviewer-calculated half-lives of 40 and 69 days, respectively, and in the total system with half-lives of 44 and 81 days, respectively; observed DT_{50} values in the sediments were >2 months and >4 months, respectively.

In [phenyl-U- ^{14}C]-label treated systems, one major nonvolatile transformation product, 3-(4,5-dihydro-isoxazol-3-yl)-4-methanesulfonyl-2-methyl-benzoic acid (M670H05), was detected at a maximum 54.2% of the applied (51.2% in water layer, 3.0% in sediment) at 3.3 months and was 50.6% (48.1% in water, 2.5% in sediment) at study termination. For both labels, one minor product, [3-cyano-4-methane-sulfonyl-2-methyl-phenyl]-(5-hydroxy-1-methyl-1H-pyrazol-4-yl)methanone (M670H01), was detected at maximums of 3.5-3.9%, 0.4-0.5% and 3.5-4.3% in the water layer, sediment and total system, respectively. In [pyrazol-4- ^{14}C]-label treated systems, one minor unidentified [^{14}C]compound (R_t 3.9 minutes) was detected in the water layer at a maximum 6.9% of applied. Extractable [phenyl-U- ^{14}C]- and [pyrazol-4- ^{14}C]-label residues in the sediment increased from $<0.1\%$ of the applied at day 0 to maximums of 9.4% (2 months) and 11.9% (3.3 months), respectively and were 8.6% and 10.4%, respectively, at study termination. Nonextractable [phenyl-U- ^{14}C]- and [pyrazol-4- ^{14}C]-label residues increased to maximums of 14.0% and 33.6% of the applied, respectively, at study termination.

Transformation pathways proposed by the study author involved cleavage of the pyrazole moiety to yield 3-(4,5-dihydro-isoxazol-3-yl)-4-methanesulfonyl-2-methyl-benzoic acid (M670H05; maximums of 51.2%, 3.0% and 54.2% of applied in water layer, sediment and total system, respectively). A second pathway involved opening of the oxazole ring to yield [3-cyano-4-

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methanesulfonyl-2-methyl-phenyl]-(5-hydroxy-1-methyl-1H-pyrazol-4-yl)-methanone (M670H01; maximums of 3.5-3.9%, 0.4-0.5% and 3.5-4.3% in water layer, sediment and total system, respectively).

Results Synopsis:

Test system used: River water-loamy sand sediment from Ohio.

[Phenyl-U-¹⁴C]-label:

Nonlinear half-life (0- to 120-day data) in water: 39.6 days ($r^2 = 0.973$).

Half-life (observed) in sediment: >59 days.

Nonlinear half-life (0- to 120-day data) in total system: 44.0 days ($r^2 = 0.967$).

Major transformation products: 3-(4,5-Dihydro-isoxazol-3-yl)-4-methanesulfonyl-2-methyl-benzoic acid (M670H05; maximums of 51.2%, 3.0% and 54.2% of applied in water, sediment and total system, respectively).

Minor transformation products: [3-Cyano-4-methanesulfonyl-2-methyl-phenyl]-(5-hydroxy-1-methyl-1H-pyrazol-4-yl)-methanone (M670H01; maximum of 3.5% of applied in total system).

[Pyrazol-4-¹⁴C]-label:

Nonlinear half-life (0- to 120-day data) in water: 68.5 days ($r^2 = 0.978$).

Half-life (observed) in sediment: >120 days.

Nonlinear half-life (0- to 120-day data) in total system: 80.8 days ($r^2 = 0.981$).

Major transformation products: None.

Minor transformation products: [3-Cyano-4-methanesulfonyl-2-methyl-phenyl]-(5-hydroxy-1-methyl-1H-pyrazol-4-yl)-methanone (M670H01; maximum of 4.3% of applied in total system).

Unknown (R_t 3.9 minutes; maximum 6.9% in water layer).

Study Acceptability: This study is classified as **unacceptable**. This study, conducted with [phenyl-U-¹⁴C]- and [pyrazol-4-¹⁴C]-labeled BAS 670H, cannot be used towards the fulfillment of the aerobic aquatic metabolism guideline, Subdivision N Guideline §162-4, data requirements for BAS 670H because the experimental design was inadequate to assess aerobic aquatic degradation. In addition, for systems treated with [pyrazole-4-¹⁴C]BAS 670H, material balances were incomplete (<90% of applied) at study termination.

The following non-validity issues were also noted:

1. The systems were incubated outdoors under natural conditions, consequently, the systems were not maintained at a constant ($\pm 1^\circ\text{C}$) temperature between 18 and 30°C.

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2. The systems were not maintained in darkness to minimize photodegradation.
3. Volatilization was neither measured nor controlled.
4. The test substance was incompletely characterized.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with BBA Guidelines for the Official Testing of Plant Protectants (Part IV, 5-1, 1990; pp. 10, 26). The following deviations from USEPA Subdivision N Guideline §162-4 were noted:

The experimental design employed was inadequate to assess aerobic aquatic degradation because an aerobic soil/sediment was not treated and flooded at the same time so that both aerobic and anaerobic conditions exist in the soil/sediment and the initial microbial population of the soil/sediment is predominantly aerobic. This affects the validity of the study.

For the [pyrazol-4-¹⁴C]-label treated systems, material balances were incomplete with up to 19.5% of the applied unaccounted for at study termination. This affects the validity of this portion of the study.

Volatilization was neither measured nor controlled, consequently, it could not be determined if the declining recoveries of applied radioactivity were due to loss of volatilized radioactivity, or due to some other factor. This may affect the validity of the study.

The treated systems were incubated outdoors under natural conditions; during the 120-day study, mean water and air temperatures were 14.3°C (range 0.7 to 28.6°C) and 14.5°C (range -4.8 to 40.7°C), respectively. Subdivision N Guidelines §162-4 specifies that the treated systems should be maintained at a constant ($\pm 1^\circ\text{C}$) temperature

between 18 and 30°C. This does not affect the validity of the study.

The systems were incubated outdoors under natural sunlight conditions. Subdivision N Guidelines §162-4 specifies that the treated systems should be maintained in darkness to minimize photodegradation. This does not affect the validity of the study.

COMPLIANCE:

This study was conducted in compliance with OECD Principles of GLP ([C(97) 186/Final], 1997) and Federal Republic of Germany GLP Regulations (Chemikaliengesetz of 1994, amended 2001; pp. 3-4; Appendix 1, p. 27). Signed and dated Data Confidentiality, GLP, Quality Assurance and Report Approval (study certification) statements were provided (pp. 2-5).

A. MATERIALS:

1. Test Materials:

[Phenyl-U-¹⁴C]- and [pyrazol-4-¹⁴C]-labeled BAS 670H (pp. 12-13).

Chemical Structures:

See DER Attachment 2.

Description:

Technical, white solid (pp. 12-13).

Purity:

[Phenyl-U-¹⁴C]:

Radiochemical purity: >97% (p. 12; neither a certification of purity nor quantitative analysis of the dosing solution were provided).

Batch No.: 714-1103 (p. 12).

Analytical purity: >95%.

Specific activity: 279,000 dpm/μg (4.65 MBq/mg).

Location of radiolabel: Uniformly in phenyl ring.

[Pyrazol-4-¹⁴C]:

Radiochemical purity: >98% (p. 13; neither a certification of purity nor quantitative analysis of the dosing solution were provided).

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Batch No.: 706-2006 (p. 13).
 Analytical purity: >97%.
 Specific activity: 343,000 dpm/μg (5.72 MBq/mg).
 Location of radiolabel: 4-C in pyrazol ring.

Storage conditions of test chemicals:

Stored frozen (<18°C) from July 5th to 24th, 2001 (pp. 12-13).
 No other storage details were provided.

Table 1: Physico-chemical properties of BAS 670H.

Parameter	Values	Comments
Molecular weight:	363.39 g/mol.	
Molecular formula:	C ₁₆ H ₁₇ N ₃ O ₅ S	
Water solubility:	Not reported.	
Vapor pressure/volatility:	Not reported.	
UV absorption:	Not reported.	
pK _a :	Not reported.	
K _{ow} /log K _{ow} :	Not reported.	
Stability of compound at room temperature:	Not reported.	

Data obtained from p. 13 of the study report.

2. Water-sediment collection, storage and properties:

Table 2: Description of water-sediment collection and storage.

Description	Details	
Geographic location:	Grand River, Ohio; sample collected between Elm Street and Route 2 bridge.	
Pesticide use history at the collection site:	Not reported.	
Collection date:	June 25, 2001.	
Collection procedures:	Water:	Samples collected into 5-gallon plastic pails; not specified if collected into same or separate pails.
	Sediment:	
Sampling depth:	Water:	Not reported. Water depth at collection site was 40 cm.
	Sediment:	Upper 8-12 cm scraped from river bottom.

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Description		Details
Storage conditions:		Upon arrival at the test facility, the water and sediment were stored separately at 1-10°C in darkness.
Storage length:		23 days prior to use. Water and sediment were collected on June 25, 2001. Test systems were prepared and allowed to pre-incubate for 13 days prior to treatment on July 31, 2001.
Preparation:	Water:	Sieved through 0.2-mm mesh screen.
	Sediment:	Sieved through 2-mm mesh screen.

Data obtained from pp. 14, 16; Table 1a, p. 28 of the study report.

Table 3: Properties of the water.

Property	Details	
Temperature (°C) ¹ :	22.1	
pH ¹ :	7.96	
pH ² :	8.4	
Redox potential (mV):	Initial ¹ :	Final ³ :
	170.8	+278, +285

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Property		Details
Oxygen saturation (%) ¹ :		71.0
Dissolved organic carbon (%):		Not reported.
Hardness (mg equivalent CaCO ₃ /L):		125
Electrical conductivity (mmhos/cm):		0.62
Sodium Absorption Ratio (SAR):		1.99
Total dissolved solids (mg/L):		162
Turbidity (NTU):		37.7
Biomass (units not specified) ⁴ :	Bacteria:	10,000
	Fungi:	26
	Actinomycetes:	78

¹ Measured at collection site at water surface (Table 1a, p. 28).

² Measured at AGVISE Laboratories, Northwood, ND (Table 1b, p. 28).

³ At 118 days posttreatment (Table 2, p. 30).

⁴ Microbial biomass was determined by the sponsor (Table 1c, p. 29).

Data obtained from Tables 1a-2, pp. 28-30 of the study report.

Table 4: Properties of the sediment.

Property	Details
Textural classification:	Loamy sand.

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Property		Details	
%sand (2000-50 µm):		80	
%silt (50-2 µm):		14	
%clay (<2 µm):		6	
pH:	soil:water (1:1):	7.0	
	1N KCl:	6.0	
Organic carbon (%):		Not reported.	
Organic matter (%):		0.7	
CEC (meq/100 g):		Not reported.	
Redox potential (mV):		Initial ¹ :	Final ² :
		+129.4	+219, +254
Moisture at 1/3 bar (%):		14.2	
Bulk density (disturbed, g/cm ³):		1.30	
Biomass (units not specified) ³ :	Bacteria:	38,000,000	
	Fungi:	240,000	
	Actinomycetes:	3,100,000	

¹Measured at collection site (Table 1a, p. 28).

²Measured at 118 days posttreatment (Table 2, p. 30).

³Microbial biomass was determined by the sponsor (Table 1c, p. 29).
Data obtained from Tables 1a-2, pp. 28-30 of the study report.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: None.

2. Experimental conditions:

Table 5: Study design.

Parameter	Both labels
Duration of the test:	120 days.
Water:	
Filtered/unfiltered water:	Filtered.
Type and size of filter used, if any:	0.2-mm mesh screen.

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Parameter		Both labels
Amount of sediment and water per treatment:	Water:	2,000 ± 50 mL; depth of <i>ca.</i> 20 cm.
	Sediment:	400 ± 20 g wet wt.; depth of <i>ca.</i> 2.0 cm.
Water/sediment ratio:		<i>ca.</i> 5:1 (mL:g wet wt.).
Nominal application rate (mg a.i./L):		0.033 mg a.i./L.
Actual application rate (mg a.i./L):	[Phenyl-U- ¹⁴ C]:	0.03277 mg a.i./L.
	[Pyrazol-4- ¹⁴ C]:	0.03287 mg a.i./L.
Control conditions, if used:		No sterile controls were used.
No. of Replications:	Controls, if used:	No sterile controls were used.
	Treatments:	For each label, twelve nonsterile water-sediment systems were treated with [¹⁴ C]BAS 670H.
Test apparatus (Type/material/volume):		Sediment and water were combined in a 2-L glass vessel (height 24 cm, diameter 11 cm). The glass vessels were placed outdoors in larger plastic boxes containing water (depth not specified) to simulate a larger body of water and pre-incubated for 13 days. The vessels were covered with aluminum foil during the pre-incubation period to exclude light and prevent algae growth, but the foil was removed the day of application. A Plexiglas cover was positioned 30 cm above the vessels to exclude rainfall.
Details of traps for CO ₂ and organic volatiles, if any:		No volatiles traps were used.
If no traps were used, is the system closed/open?		The water-sediment systems were incubated open.
Identity and concentration of co-solvent:		Methanol, final concentration <i>ca.</i> 0.05% based on water layer [1 mL test solution in <i>ca.</i> 2,000 mL of water.
Test material application:	Volume of test solution used/treatment:	1 mL of 65.53 µg/mL or 65.73 µg/mL for [phenyl-U- ¹⁴ C]- and [pyrazol-4- ¹⁴ C]-label test solutions, respectively.
	Application method:	Applied to water surface via pipette.
Any indication of the test material adsorbing to the walls of the test apparatus?		Not indicated.
Biomass (mg microbial C/100 g, CFU or other) of controls:	Initial:	
	Final:	No sterile controls were used.
Biomass of treated:	Initial:	
	Final:	Not determined.

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Parameter		Both labels
Experimental conditions:	Temperature (°C):	Systems were incubated outdoors under natural environmental conditions.
	Continuous darkness (Yes/No):	No, natural light conditions.
Other details, if any:		For each label, two water-sediment systems, to be used to measure system parameters (temperature, pH, oxygen saturation, redox potential) during the study, were treated with unlabeled BAS 670H (purity 99.9%, Lot No. 01586-177).

Data obtained from pp. 8, 14-16; Figures 1a-1b, p. 34 of the study report.

3. Aerobic conditions: Open, water-sediment systems were incubated outdoors under natural environmental conditions, with the exceptions that aluminum foil was used to exclude light during the 13-day pre-incubation period and a Plexiglas cover was used to exclude rainfall during the pre-incubation and following treatment (p. 15; Figures 1a-1b, p. 34). In water-sediment systems at 1 day prior to treatment, redox potentials and oxygen saturation levels in the water layers were +122 to +128 mV and 63-65%, respectively, and redox potentials in the sediment were -25 to -18 mV (Table 2, p. 30).

4. Supplementary experiments: None.

5. Sampling:

Table 6: Sampling details.

Criteria	Both labels
Sampling intervals:	0 (1-2 hours), 1, 2, 7, 14, 30, 59, 100 and 120 days.
Sampling method:	For each label, duplicate systems (vessels) were collected at the 0- and 120-day intervals, with a single vessel collected at all remaining intervals.
Method of collection of CO ₂ and volatile organic compounds:	Volatiles were not collected.
Sampling intervals/times for: Sterility check, if sterile controls are used: Redox potential/oxygen saturation/pH:	No sterile controls were used. Measured at 2- to 5-day intervals throughout the 120-day incubation.
Sample storage before analysis:	Water and sediment were separated the day of sampling and stored frozen (≤-18°C) until processed (storage intervals not specified). Water samples and sediment extracts were stored refrigerated or frozen (temperatures not specified) until analysis. Sediment

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Criteria	Both labels
	extracts were stored up to 1 month after sampling prior to HPLC analysis; storage intervals prior to HPLC analysis of water samples were not reported.
Other observations, if any:	None.

Data obtained from pp. 15-17; Table 2, p. 30 of the study report.

C. ANALYTICAL METHODS:

Separation of the sediment and water: Upon collection, the water layer was decanted and aliquots (volume, replicates not specified) were analyzed for total radioactivity by LSC (p. 16). The sediment was transferred to centrifuge tubes.

Extraction/clean up/concentration methods: Aliquots (volume, replicates not specified) of the water layer were analyzed directly by HPLC (p. 17).

Sediment samples were extracted four times with pH 8 phosphate buffer (concentration not specified):methanol (1:1, v:v); all extraction solvent volumes were 300 mL (p. 17). Each extraction was done using a horizontal shaker (200 rpm, 30 minutes), after which sediment and extract were separated by centrifugation (speed, interval not specified). Extracts were combined and aliquots (volume, replicates not specified) were analyzed for total radioactivity by LSC. The methanol phase was removed from the extract via rotary evaporation (temperature not specified), then the remaining aqueous phase was acidified to pH 2 with HCl and partitioned three times with ethyl acetate (100 mL x 3). Organic (ethyl acetate) phases were combined, then aliquots (volume, replicates not specified) of the combined organic extract and the remaining aqueous phase were analyzed by LSC. The combined organic extract was evaporated to dryness (method not specified), with the resulting residues reconstituted in either methanol or methanol:water (1:1, v:v, 2-5 mL) using an ultrasonic bath. Aliquots of the concentrated sediment sample were analyzed by LSC and HPLC.

Nonextractable residue determination: Extracted sediments were combined with cellulose (ca. 0.4 g cellulose/g sediment), air-dried in a drying chamber at 30°C and homogenized (method not specified), then aliquots (weight, replicates not specified) were analyzed for total radioactivity by LSC following combustion (p. 17).

Volatile residue determination: Volatiles were not collected.

Total ¹⁴C measurement: Total ¹⁴C residues were determined by summing the concentrations of residues measured in the water layers, sediment extracts and extracted sediment (Table 3, p. 31).

Derivatization method, if used: A derivatization method was not employed.

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Identification and quantification of parent compound: Water layer samples were analyzed by reverse-phase HPLC under the following conditions: Phenomenex Columbus column (10 x 250 mm, 10 μ m, packing not specified, Reviewer's Comment No. 6), Phenomenex Columbus pre-column (10 x 50 mm, 10 μ m, packing not specified), gradient mobile phase combining (A) 0.01M ammonium acetate and (B) methanol:0.01M ammonium acetate (950:50, v:v) [percent A:B at 0 min. 95:5 (v:v), 10 min. 95:5, 60 min. 5:95, 61 min. 0:100, 65 min. 0:100, 70 min. 95:5], injection volume 5 mL, flow rate 4 mL/minute, Jasco UV/VIS detector (254 nm), Canberra Packard Flow-One-Beta, A-525 AX radioactivity detector (pp. 18-19).

Sediment extracts were analyzed by reverse-HPLC as described above with the following differences: Phenomenex Columbus column (4.6 x 250 mm, 5 μ m, packing not specified), Phenomenex Security Guard 2 C-18 pre-column (3.0 x 4, units and particle size not specified), injection volume not specified, flow rate 1 mL/minute (p. 18).

[¹⁴C]BAS 670H was identified by co-chromatography with unlabeled reference standard (purity 99.9%, Lot No.: 01586-177); however, supporting chromatograms were not provided (pp. 13-14, 24; Figures 4-7, pp. 37-40).

Identification of [¹⁴C]BAS 670H was reportedly confirmed using LC/MS and LC/MS/MS with electrospray ionization; however, those results were referenced and not provided with this study report for review (pp. 19, 24-26).

Identification and quantification of transformation products: Transformation products were separated, quantified and identified by HPLC as described for the parent (pp. 13-14, 18-19, Figures 4-7, pp. 37-40). Identification of one transformation product, M670H05, was reportedly confirmed by MS analysis (pp. 19, 24-26).

Table 7: Reference compounds available for identifying transformation products of BAS 670H.

Applicant's code	Chemical Name	Formula	m.w.	Purity
M670H01	[3-Cyano-4-methanesulfonyl-2-methyl-phenyl]-(5-hydroxy-1-methyl-1H-pyrazol-4-yl)-methanone ¹	C ₁₄ H ₁₃ N ₃ O ₄ S	319.34	96.9%
M670H05	3-(4,5-Dihydro-isoxazol-3-yl)-4-methanesulfonyl-2-methyl-benzoic acid ¹	C ₁₆ H ₁₇ N ₃ O ₆ S	379.39	99.9%

¹Chemical name obtained from MRID 45902423 (Figure 1, pp. 53-54) submitted concurrently with this study. Data, other than chemical name, obtained from p. 14 of the study report.

Detection limits (LOD, LOQ) for the parent compound and transformation products: The limit of quantitation (LOQ) for LSC analyses was reported as twice background (dpm not specified) or <0.1% of the applied radioactivity (p. 17; Table 3, p. 31). The LOD/LOQ for HPLC analyses was taken to be <0.1% of the applied radioactivity based on the reported results (Table 4, p. 32).

II. RESULTS AND DISCUSSION:

A. TEST CONDITIONS: During the 120-day study, the mean water temperature was 14.3°C (range 0.7 to 28.6°) and mean air temperature was 14.5°C (range -4.8 to 40.7°C; p. 23; Figure 2, p. 35). Conditions in both the water and sediment layers of systems treated with unlabeled BAS 670H and incubated alongside the [¹⁴C]BAS 670H treated systems went from moderately reducing (-50 to +200 mV) to moderately oxidizing (+200 to +400 mV) during the 120-day study (Reviewer's Comment No. 7). Redox potentials in the water layers increased from +100 to +183 mV at 2-14 days to +190 to +297 mV thereafter, while redox potentials in the sediment layers were -62 to +229 mV at 2-58 days and +100 to +255 mV for the remainder of the study (Table 2, p. 30). Oxygen saturation levels in the water layers were 60-95% during the 120-day study, while pH levels were 7.46-7.94 at 2-9 days and 8.06-8.52 thereafter.

B. MATERIAL BALANCE: Recoveries of radiolabeled material averaged $92.9 \pm 1.5\%$ (range 90.6-94.9%, n = 9) for the [phenyl-U-¹⁴C]-label treated systems and $91.1 \pm 5.7\%$ (range 80.5-96.5%, n = 9) for the [pyrazole-4-¹⁴C]-label treated systems, with declines in recoveries for both labels throughout the incubations (Table 3, p. 31; Attachment 1; Reviewer's Comment No. 1). Following application of [¹⁴C]BAS 670H to the water layer, [¹⁴C]residues (both labels) partitioned from the water layer into the sediment with average (n = 2) distribution ratios (water:sediment) of 32:1 at day 0, 11:1 at 7 days, 5:1 at 30 days, then were 1:3 (n = 1) thereafter for the [phenyl-U-¹⁴C]-label and 1:2 at 56 days and 1:1 thereafter for the [pyrazol-4-¹⁴C]-label (Attachment 1).

Table 8: Biotransformation of [phenyl-U-¹⁴C]BAS 670H, expressed as percentage of applied radioactivity (mean, n = 2 at 0 and 120 days¹; n = 1 at all other intervals), in Ohio river water-loamy sand sediment under aerobic, outdoor conditions.

Compound		Sampling times (days)								
		0	1	2	7	14	30	59	100	120
BAS 670H	water	91.4	89.4	90.0	81.4	78.6	49.1	26.0	17.2	21.2
	sediment	n.d. ²	2.5	3.3	5.0	4.3	3.4	4.2	2.4	3.5
	system ³	91.4	91.9	93.3	86.4	82.9	52.5	30.2	19.6	24.7
M670H05	water	n.d.	n.d.	n.d.	2.0	3.7	26.8	41.1	51.2	48.1
	sediment	n.d.	n.d.	n.d.	n.d.	n.d.	0.8	2.3	3.0	2.5
	system	n.d.	n.d.	n.d.	2.0	3.7	27.6	43.4	54.2	50.6
M670H01	water	3.5	2.3	n.d.	2.4	2.6	2.2	1.7	0.8	n.d.
	sediment	n.d.	0.1	0.1	0.2	0.2	0.2	0.4	0.3	0.2
	system	3.5	2.4	0.1	2.6	2.8	2.4	2.1	1.1	0.2
Unidentified residues ⁴	sediment	<0.1	0.1	0.2	0.5	0.9	1.6	2.5	2.1	2.4
Total extractable sediment residues ⁵		<0.1	2.7	3.6	5.7	5.4	6.1	9.4	7.7	8.6
Total CO ₂		-- ⁶	--	--	--	--	--	--	--	--
Total volatile organics		--	--	--	--	--	--	--	--	--
Nonextractable sediment residues		<0.1	0.2	0.6	1.6	3.2	8.1	12.4	13.8	14.0
Total % recovery	water	94.8	91.7	90.0	85.8	85.0	78.0	68.8	69.2	69.3
	sediment ⁵	<0.1	2.9	4.2	7.3	8.6	14.2	21.8	21.5	22.6
	system	94.9	94.7	94.1	93.1	93.6	92.3	90.6	90.8	92.0

¹Reviewer's Comment No. 1.

²Not detected; based on reported results, the LOD was <0.1% of applied (Table 4, p. 32).

³Entire system; water + sediment; value determined by primary reviewer (Attachment 1).

⁴[¹⁴C]Residues remaining in aqueous phase following ethyl acetate partitioning (Table 3, p. 31).

⁵Determined by primary reviewer (Attachment 1).

⁶Not collected.

Data obtained from Tables 3-4, pp. 31-32 of the study report and Attachment 1.

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Table 9: Biotransformation of [pyrazol-4-¹⁴C]BAS 670H, expressed as percentage of applied radioactivity (mean, n = 2 at 0 and 120 days¹; n = 1 at all other intervals), in Ohio river water-loamy sand sediment under aerobic, outdoor conditions.

Compound		Sampling times (days)								
		0	1	2	7	14	30	59	100	120
BAS 670H	water	96.3	93.7	89.8	82.4	81.8	60.9	48.6	36.2	31.0
	sediment	n.d. ²	2.2	3.0	5.7	5.0	4.8	7.2	6.4	4.9
	system ³	96.3	95.9	92.8	88.1	86.8	65.7	55.8	42.6	35.9
M670H01	water	n.d.	n.d.	2.1	1.0	0.8	2.6	3.9	2.3	2.8
	sediment	n.d.	0.1	0.1	0.1	0.1	0.2	0.4	0.5	0.4
	system	n.d.	0.1	2.2	1.1	0.9	2.8	4.3	2.8	3.2
UNK (R, 3.9 min) ⁴	water	n.d.	n.d.	n.d.	2.2	2.4	6.9	3.7	2.5	2.8.
Unidentified residues ⁵	sediment	<0.1	0.2	0.2	0.5	1.0	2.1	3.8	5.0	5.1
Total extractable sediment residues ⁶		<0.1	2.5	3.3	6.3	6.1	7.1	11.4	11.9	10.4
Total CO ₂		-- ⁷	--	--	--	--	--	--	--	--
Total volatile organics		--	--	--	--	--	--	--	--	--
Nonextractable sediment residues		<0.1	0.4	0.6	2.0	3.9	12.2	21.4	30.1	33.6
Total % recovery	water	96.3	93.7	91.9	85.6	85.0	70.4	56.2	41.0	36.6
	sediment ⁶	<0.1	2.9	3.9	8.3	10.0	19.3	32.8	42.0	44.0
	system	96.4	96.5	95.8	93.8	95.1	89.7	88.9	82.9	80.5

¹Reviewer's Comment No. 1.

²Not detected; based on reported results, the LOD was <0.1% of applied (Table 5, p. 33).

³Entire system; water + sediment; value determined by primary reviewer (Attachment 1).

⁴Detected only in water layer.

⁵[¹⁴C]Residues remaining in aqueous phase following ethyl acetate partitioning (Table 3, p. 31).

⁶Determined by primary reviewer (Attachment 1).

⁷Not collected.

Data obtained from Table 3, p. 31; Table 5, p. 33 of the study report and Attachment 1.

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C. TRANSFORMATION OF PARENT COMPOUND: [Phenyl-U-¹⁴C]BAS 670H in the water layer decreased from 91.4% of the applied at day 0 to 49.1% at 30 days, 26.0% at 59 days and was 17.2-21.2% at 100-120 days, while in the sediment [phenyl-U-¹⁴C]BAS 670H was detected at maximum 5.0% at 7 days and was 3.5% at 120 days (Table 4, p. 32). [Pyrazol-4-¹⁴C]BAS 670H in the water layer decreased from 96.3% at day 0 to 48.6% at 59 days and was 31.0% at 120 days, while in the sediment [pyrazol-4-¹⁴C]BAS 670H was detected at a maximum 7.2% at 59 days and was 4.9% at 120 days (Table 5, p. 33).

HALF-LIFE/DT₅₀: Half-life values for the dissipation of [¹⁴C]BAS 670H from the water and total system of the treated water-sediment systems were determined by the primary reviewer using linear/natural log regression analysis as calculated by Corel Quattro Pro version 8 and nonlinear/normal (single, 2 parameter, unweighted) regression analysis as calculated by SigmaPlot version 8 (Attachment 1).

DT₅₀, and DT₉₀ values (50% and 90% decline times, respectively) for [¹⁴C]BAS 670H in the total system (both labels plotted together) and for [phenyl-U-¹⁴C]BAS 670H in the water layer and sediment were determined by the study author utilizing overall (total system) and compartment (water and sediment) model nonlinear analysis (Marquardt method) as calculated by Modelmaker version 4.0 (pp. 19-23, 25; Figures 8-9, pp. 41-42).

Table 10: Half-life ($t_{1/2}$) and DT50 values for the dissipation of BAS 670H in aerobic water-loamy sand sediment.

OH Grand River water-loamy sand sediment	Regression type	Half-life (days)	3 x half-life (days) and/or DT ₉₀	y-intercept	p-value	r ²
[Phenyl-U-¹⁴C]-label						
Water:	Empirical data	DT ₅₀ = 30-59	DT ₉₀ = >120	--	--	--
	Linear/Natural log ¹	47.9	143.7	4.46	--	0.921
	Nonlinear/Normal ¹	39.6	118.8	92.12	<0.0001	0.973
	Nonlinear/compartment ²	39.8	119.4, DT ₉₀ = 132.2	--	--	0.989
Sediment:	Empirical data	DT ₅₀ = >59	DT ₉₀ = >120	--	--	--
	Linear/Natural log	NC ³	--	--	--	--
	Nonlinear/Normal	NC	--	--	--	--
	Nonlinear/compartment ²	4.4	13.2, DT ₉₀ = 14.7	--	--	0.989
Total system:	Empirical data	DT ₅₀ = 30-59	DT ₉₀ = >120	--	--	--
	Linear/Natural log ¹	51.9	155.7	4.49	--	0.919
	Nonlinear/Normal ¹	44.0	132.0	94.39	<0.0001	0.967
[Pyrazol-4-¹⁴C]-label						
Water:	Empirical data	DT ₅₀ = 30-59	DT ₉₀ = >120	--	--	--
	Linear/Natural log ¹	74.4	223.2	4.50	--	0.981
	Nonlinear/Normal ¹	68.5	205.5	92.17	<0.0001	0.978
Sediment:	Empirical data	DT ₅₀ = >120	DT ₉₀ = >120	--	--	--
	Linear/Natural log	NC	--	--	--	--
	Nonlinear/Normal	NC	--	--	--	--
Total system:	Empirical data	DT ₅₀ = 59-100	DT ₉₀ = >120	--	--	--
	Linear/Natural log ¹	85.1	255.3	4.54	--	0.984
	Nonlinear/Normal ¹	80.8	242.4	94.69	<0.0001	0.981
Both labels plotted together⁴						
Total system:	Nonlinear/overall model	60.3	180.9, DT ₉₀ = 200.4	--	--	0.917

¹Determined by primary reviewer using data obtained from Table 4, p. 32 of the study report (Attachment 1).
²Determined by study author (pp. 22-23, 25; Figure 9, p. 42).

³Not calculated since parent [¹⁴C]BAS 670H was detected at ≤7.2% of the applied at any sampling interval (Tables 4-5, pp. 32-33).

⁴Determined by study author (pp. 20-21, 25; Figure 8, p. 41).

TRANSFORMATION PRODUCTS: One major nonvolatile transformation product, 3-(4,5-dihydro-isoxazol-3-yl)-4-methanesulfonyl-2-methyl-benzoic acid (M670H05), was reportedly identified by LC/MS and LC/MS/MS and one minor product, [3-cyano-4-methane-sulfonyl-2-methyl-phenyl]-(5-hydroxy-1-methyl-1H-pyrazol-4-yl)methanone (M670H01, p. 16), was reportedly identified by HPLC co-chromatography (pp. 24-25; Reviewer's Comments No. 3 and 10).

In [phenyl-U-¹⁴C]-label treated systems, M670H05 in the total system increased to a maximum 54.2% of applied (51.2% in water layer, 3.0% in sediment) at 100 days and was 50.6% (48.1% in water, 2.5% in sediment) at 120 days (Table 4, p. 32; Attachment 1). M670H01 was detected at a maximum 3.5% at day 0 in the water layer and was ≤0.4% in the sediment at any interval.

In [pyrazol-4-¹⁴C]-label treated systems, M670H01 was detected at maximums of 3.9% and 4.3% in the water layer and total system, respectively, at 59 days, and was ≤0.5% in the sediment at any interval (Table 5, p. 33; Attachment 1). One unknown (R_t 3.9 min.) was detected at a maximum of 6.9% in the water layer at 30 days decreasing to 2.5-2.8% at 100-120 days.

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: In [phenyl-U-¹⁴C]-label treated sediment, extractable [¹⁴C]residues in the sediment increased from <0.1% of the applied at day 0 to 9.4% at 59 days and were 7.7-8.6% at 100-120 days, while nonextractable [¹⁴C]residues increased to a maximum 14.0% at 120 days (Table 3, p. 31; Attachment 1).

In [pyrazol-4-¹⁴C]-label treated sediment, extractable [¹⁴C]residues in the sediment increased from <0.1% of the applied at day 0 to 11.9% at 100 days and were 10.4% at 120 days, while nonextractable [¹⁴C]residues increased to a maximum 33.6% at 120 days (Table 3, p. 31; Attachment 1).

VOLATILIZATION: Formation of volatilized of ¹⁴CO₂ and volatile [¹⁴C]organic compounds was not monitored.

TRANSFORMATION PATHWAY: Transformation pathways were proposed by the study author involving cleavage of the pyrazole moiety to yield 3-(4,5-dihydro-isoxazol-3-yl)-4-methanesulfonyl-2-methyl-benzoic acid (M670H05). A second pathway involved opening of the oxazole ring to yield [3-cyano-4-methanesulfonyl-2-methyl-phenyl]-(5-hydroxy-1-methyl-1H-pyrazol-4-yl)-methanone (M670H01; Figure 10, p. 43).

Table 11: Chemical names for identified transformation products of BAS 670H in aerobic water-sediment¹.

Applicant's code	CAS Number	Chemical Name(s) ²	Chemical formula	Molecular weight	SMILES string ²
		[3-Cyano-4-methanesulfonyl-2-			CC1=C(C(C2C=N

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Applicant's code	CAS Number	Chemical Name(s) ²	Chemical formula	Molecular weight	SMILES string ²
M670H01	- ³	methyl-phenyl]-(5-hydroxy-1-methyl-1H-pyrazol-4-yl)-methanone	C ₁₄ H ₁₃ N ₃ O ₄ S	319.34	N(C)C2O=O)C=C C(S(=O)(C)=O)=C 1C#N
M670H05	--	3-(4,5-Dihydro-isoxazol-3-yl)-4-methanesulfonyl-2-methyl-benzoic acid	C ₁₂ H ₁₃ NO ₅ S	302.35	CC1=C(C(O)=O)C =CC(S(=O)(C)=O) =C1C2=NOCC2

¹Results supporting identifications were not provided (Reviewer's Comment No. 3).

²Reviewer's Comment No. 10.

³Not reported.

Data obtained from p. 14 of the study report.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: None.

III. STUDY DEFICIENCIES: This study, conducted with [phenyl-U-¹⁴C]- and [pyrazol-4-¹⁴C]-labeled BAS 670H, cannot be used towards the fulfillment of the aerobic aquatic metabolism guideline, Subdivision N Guideline §162-4, for BAS 670H due to the following:

1. For both labels, the soil/sediment was not flooded and treated at the same time. For an aerobic aquatic metabolism study, an aerobic soil/sediment should be treated and flooded at the same time so that both aerobic and anaerobic conditions exist in the soil/sediment and the initial microbial population of the soil/sediment is predominantly aerobic. In this study, water-sediment/soil systems were prepared and pre-incubated for ca. 2 weeks prior to application of BAS 670H to the water layer.
2. For [pyrazol-4-¹⁴C]-label treated systems, material balances were incomplete with up to 19.5% of the applied unaccounted for at study termination.

Additional deficiencies to Subdivision N Guideline §162-4 include the following:

3. For both labels, the systems were incubated outdoors under natural conditions, consequently, the systems were not maintained at a constant ($\pm 1^\circ\text{C}$) temperature between 18 and 30°C. During the 120-day study, the mean water and air temperatures were 14.3°C (range 0.7 to 28.6°C) and 14.5°C (range -4.8 to 40.7°C), respectively.
4. For both labels, the systems were not maintained in darkness to minimize photodegradation.

5. For both labels, volatilization was neither measured nor controlled.
6. For both labels, the test substance was incompletely characterized; physico-chemical characteristics including the aqueous solubility, vapor pressure/volatility, UV absorption, dissociation constant (pK_a), octanol-water partition coefficient ($K_{ow}/\log K_{ow}$) and stability at room temperature should have been reported.

IV. REVIEWER'S COMMENTS:

1. Total recoveries of applied radioactivity by the study author were verified by the primary reviewer, and there was consistent agreement (within $\pm 0.1\%$ of applied) between the study author's reported values and those determined by the primary reviewer (Tables 3, p. 31; Attachment 1).
2. The study author used the mean of the [phenyl- ^{14}C]- and [pyrazol-4- ^{14}C]-labeled BAS 670H detected at the 0- and 120-day sampling intervals in the regression analyses for determination of DT_{50} values. It is always preferred that the individual replicate results be used for regression analysis to provide a more accurate determination of the rate of degradation.
3. The study author reported that identifications of parent [^{14}C]BAS 670H and its degradate M670H05 were confirmed via LC/MS and LC/MS/MS; however, those results were not provided for review (pp. 24-25).

Similarly, the study author reported that identification of parent [^{14}C]BAS 670H and its degradates M670H05 and M670H01 in the water layers and sediment extracts were identified by co-chromatography with unlabeled reference standards, but no supporting chromatogram were provided for review (pp. 24-25).
4. Duplicate water-sediment systems treated with unlabeled BAS 670H were incubated alongside the [^{14}C]BAS 670H treated systems and used to measure system parameters (pH, oxygen saturation and redox potential) throughout the 120-day study. It is preferred that system parameters be determined in the actual systems taken for sample analysis.
5. All quantitative results obtained during HPLC analyses should have accompanied the respective chromatograms.
6. Phenomenex Columbus HPLC preparative and analytical columns contain either C-8 or C-18 packing material

(www.phenomenex.com); the study author only specified the packing material for one of the four columns used.

7. According to N. Wolfe, et al. (see reference below), redox potentials in the range of +400 to +800 mV are considered strongly oxidizing, +200 to +400 mV moderately oxidizing, -50 to +200 mV moderately reducing, -200 to -50 mV reducing, and -400 to -200 mV strongly reducing.
8. The test substance was incompletely characterized; the aqueous solubility, vapor pressure/volatility, UV absorption, dissociation constant (pK_a), octanol-water partition coefficient ($K_{ow}/\log K_{ow}$) and stability at room temperature should have been reported.
9. The study author reported that the 0.033 mg a.i./L treatment rate (68 μ g a.i./2,000 mL water) used in this study was based on the recommended maximum field application rate of 100 g a.i./ha applied to a water column 30 cm deep (p. 16).
10. The CAS Reg. No. 210631.68-8 for BAS 670H was reported in two aerobic soil metabolism studies (p. 11 in MRID 45902419; p. 12 in MRID 45902421) submitted concurrently with this study. Methanone, [3-(4,5-dihydro-3-isoxazolyl)-2-methyl-4-(methylsulfonyl)phenyl](5-hydroxy-1-methyl-1H-pyrazol-4-yl)- is listed as a common name and CAS Reg. No. 210631-68-8 was confirmed for BAS 670H at the USEPA/OPP Chemical Database (<http://www.cdpr.ca.gov/cgi-bin/epa/chemidetriris.pl?pccode=123009>).

The chemical names for degradates M670H05 and M670H01 were obtained from an additional aerobic aquatic metabolism study (MRID 45902423; Figure 1, pp. 53-54) submitted concurrently with this study.

SMILES codes for parent BAS 670H and transformation products M670H01 and M670H05 were obtained from an aerobic aquatic metabolism study (MRID 45902423; Figure 1, pp. 52-54) submitted concurrently with this study.

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The following table summarizes results from BAS 670H aerobic soil (MRIDs 45902421,), anaerobic aquatic (MRID 45902422) and aerobic aquatic (MRID 45902423, 45902424) metabolism studies:

Comparison of degradation half-lives of BAS 670H and formation of degradates between metabolism studies.

Study MRID	Study type	¹⁴ C-Label location ¹	Study length	System	BAS 670H half-life (days)		Maximum detected of transformation products (% of applied radioactivity) ⁴						CO ₂			
					Linear	Nonlinear	BAS 670H05	BAS 670H01 ⁵	BAS 670H10	BAS 670H11	BAS 670H12					
45902421	162-1	Phenyl-U	383 d	ID loam	181 (r ² =0.886)	144 (r ² =0.924)	11.72		10.32						13.81	
				IN silt loam	182 (r ² =0.958)	152 (r ² =0.918)	7.15		4.43						14.22	
				IA loam	302 (r ² =0.848)	305 (r ² =0.804)	3.20		3.84						3.28	
				MN clay loam	125 (r ² =0.924)	129 (r ² =0.933)	15.67		7.07						6.32	
				SD silt loam	196 (r ² =0.942)	157 (r ² =0.915)	10.36		4.03						6.99	
				NS sandy loam	observed: >364	observed: >364	1.34								0.75	
45902422	162-3	Phenyl-U	362 d	SD reservoir water	10.9 (r ² =0.932)	11.4 (r ² =0.994)		NA	3.63		15.39		5.29	4.14	1.61	
				silt loam	observed: 7-15				2.38		26.23		2.15	1.64	<1.0	
				total sys.	13.4 (r ² =0.917)	12.1 (r ² =0.994)			5.28		41.62		5.36	4.75	<1.0	
				SD reservoir water	18.6 (r ² =0.880)	11.5 (r ² =0.998)			3.64		15.73		4.30	4.32	<1.0	
45902423	162-4	Phenyl-U	120 d	silt loam	observed: 15-30				2.35		34.23		1.51	1.48	0.27	
				total sys.	21.8 (r ² =0.849)	13.0 (r ² =0.995)			5.27		48.05		6.15	4.32	0.27	
				OH river water	observed: >120				3.93							0.27
				loamy sand	observed: >120				1.60							0.27
				total sys.	observed: >120				5.53					0.89		
				OH river water	observed: >120				7.83					0.89		

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Study MRID	Study type	¹⁴ C-Label location ¹	Study length	System	BAS 670H half-life (days)		Maximum detected of transformation products (% of applied radioactivity) ⁴						
					Linear	Nonlinear	BAS 670H05	BAS 670H01 ⁵	BAS 670H10	BAS 670H11	BAS 670H12	CO ₂	
45902424	162-4	Phenyl-U	120 d	silt loam	observed: >120								
				total sys.	observed: >120			0.34					
				OH pond water	11.6 (r ² =0.980)	10.7 (r ² =0.976)		8.17					
				loam	55.3 (r ² =0.826)	77.7 (r ² =0.808)		ND					0.44
				total sys	29.5 (r ² =0.943)	19.0 (r ² =0.968)		10.21					
				OH pond water	12.3 (r ² =0.941)	10.9 (r ² =0.926)		2.04					
		loam		70.7 (r ² =0.705)	49.2 (r ² =0.839)		6.38					1.41	
		total sys		40.2 (r ² =0.867)	24.2 (r ² =0.968)		6.38						
		OH river water		47.9 (r ² =0.921)	39.6 (r ² =0.973)		51.2						
		loamy sand		>59			3.0						
		total sys		51.9 (r ² =0.919)	44.0 (r ² =0.967)		54.2						
		OH river water		74.4 (r ² =0.981)	68.5 (r ² =0.978)		NA						
loamy sand	>120			NA									
total sys	85.1 (r ² =0.984)	80.8 (r ² =0.981)		NA					4.3				

¹Labels: [phenyl-U-¹⁴C]- and [pyrazol-4-¹⁴C]-.
²First-order linear.
³First-order nonlinear (single, 2 parameter; unweighted).
⁴M670H01 = [3-Cyano-4-methanesulfonyl-2-methyl-phenyl]-[5-hydroxy-1-methyl-1H-pyrazol-4-yl]-methanone; aka cyano metabolite.
M670H05 = 3-(4,5-Dihydro-isoaxazol-3-yl)-4-methanesulfonyl-2-methyl-benzoic acid; aka acid metabolite.
M670H10 = 6-[5-hydroxy-1-methyl-1H-pyrazol-4-yl]carbonyl]-5-methyl-2,3-dihydro-4H-1-benzothioopyran-4-one.

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Structures proposed for M670H11 and M670H12 (MRID 45902422; Appendix 5, Figures 1-2, p. 156).
⁵M670H01 co-eluted with an unidentified product, Unknown 2, in study MRID 45902421.

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