

**Data Evaluation Report on the aerobic biotransformation of BAS 510 F in soil**

PMRA Submission Number {.....}

EPA MRID Number 45405208

**Data Requirement:** PMRA Data Code:  
EPA DP Barcode: D278387  
OECD Data Point:  
EPA Guideline: 162-1

**Test material:**

Common name: BAS 510 F

**Chemical name**

IUPAC: 2-Chloro-*N*-(4-chlorobiphenyl-2-yl)-nicotinamide.  
CAS name: 2-Chloro-*N*-(4-chloro[1,1-biphenyl]-2-yl)-3-pyridinecarboxamide.  
CAS No: 188425-85-6.  
Synonyms: 2-Chloro-*N*-(4'-chlorobiphenyl-2-yl)-nicotinamide.  
Nicobifen.  
~~BAS 516 02 F.~~

SMILES string:

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Dynamac Corporation

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**Company Code:** [for PMRA]  
**Active Code:** [for PMRA]  
**Use Site Category:** [for PMRA]  
**EPA PC Code:** 128008

**CITATION:** Stephan, A. 1999. Metabolism of BAS 510F (<sup>14</sup>C-diphenyl and <sup>14</sup>C-pyridin) in soil under aerobic conditions. Unpublished study performed BASF Aktiengesellschaft, Crop Protection Division, Limburgerhof, Germany. Sponsored by BASF Corporation, Research Triangle Park, NC. Study Code 42381; BASF Registration Document No. 1999/11807. Study initiated June 30, 1997 and completed December 21, 1999 (p. 13).



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### EXECUTIVE SUMMARY:

The biotransformation of [diphenyl- $^{14}\text{C}$ ]- and [pyridine-3- $^{14}\text{C}$ ]-labeled 2-chloro-N-(4'-chlorobiphenyl-2-yl)nicotinamide (BAS 510 F) was studied in German sandy loam soil (pH 7.4, organic carbon 1.3%) for 364 days under aerobic conditions in darkness at  $20 \pm 1^\circ\text{C}$  and a soil moisture content of 40% of the maximum water holding capacity (approximately 106% of field capacity at 1/3 bar). [Diphenyl- $^{14}\text{C}$ ]- and [pyridine-3- $^{14}\text{C}$ ]-labeled BAS 510 F were applied at the nominal rate of 1 mg/kg soil. This experiment was conducted in accordance with BBA-Guideline for the Official Testing of Plant Protection Products, Part IV. 4-1 and SETAC Procedures for assessing the environmental fate and ecotoxicity of pesticides and in compliance with Good Laboratory Practice Regulations of the Federal Republic of Germany (1994). The test system consisted of glass dishes containing treated soil that were maintained in a flow-through apparatus with traps for the collection of  $\text{CO}_2$  and volatile organics. Single treated samples were collected after 0, 7, 14, 29, 57, 93, 119, 182, 266, and 364 days of incubation. Soil samples were sequentially extracted three times with methanol and three times with methanol:water (1:1, v:v). Extracts and extracted soil were analyzed for total radioactivity using LSC. [ $^{14}\text{C}$ ]BAS 510 F and its transformation products were separated by TLC and HPLC, and identified by comparison with reference standards. The identification of the transformation products was confirmed by HPLC/MS.

Overall material balances averaged 100.3 and 93.0% of the applied (ranges 93.3-104.6% and 83.4-101.8%), respectively, in the [diphenyl- $^{14}\text{C}$ ] and [pyridine-3- $^{14}\text{C}$ ]BAS 510 F-treated soils. Material balances appeared to be decreasing in the pyridinyl label study, but were acceptable (93.9%) at the final sampling interval. The rate of dissipation of [ $^{14}\text{C}$ ]BAS 510 F was similar with the two treatments, decreasing from 99.5-99.6% of the applied at day 0 to 48.0-51.7% at 93 days posttreatment, 20.5-26.3% at 266 days, and 16.7-17.3% at 364 days (final sampling interval). The calculated half-life (first-order linear regression, 0-119 days) was 96.3 days; the DT50 (nonlinear) was 108.3 days.

Volatilized  $^{14}\text{CO}_2$  was the only major transformation product detected, and bound residues accounted for up to 50.1% and 60.0% of the applied radioactivity in the two label studies. The rate of formation of  $^{14}\text{CO}_2$  was higher with the pyridine label than the diphenyl label (25.4% compared with 15.5%, respectively, at 364 days), while the formation of soil bound residues was higher with the diphenyl label than the pyridine label (60.0% compared with 50.1%). All other transformation products were minor, with each comprising  $\leq 0.7\%$  of the applied radioactivity at any sampling interval. Minor transformation products were M510F50 ("Unknown 2"; maximum 0.2% of the applied), M510F49 [2-hydroxy-N-(4'-chlorobiphenyl-2-yl)-nicotinamide; maximum 0.1%], and "Unknown 1" (maximum 0.6-0.7%).

Total extractable [ $^{14}\text{C}$ ]residues decreased from 99.7-99.7% of the applied at day 0 to 17.8-18.4% at 364 days posttreatment. Total nonextractable [ $^{14}\text{C}$ ]residues in the [diphenyl- $^{14}\text{C}$ ]BAS 510 F-treated soil increased from 0.3% of the applied at day 0 to 31.4% at 57 days and 60.0% at 364

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days; at 364 days, 4.4% of the applied was associated with the fulvic acid fraction, 3.1% with humic acid, and 34.4% with humin. Total nonextractable [<sup>14</sup>C]residues in the [pyridine-3-<sup>14</sup>C]BAS 510 F-treated soil increased from 0.4% at day 0 to 32.7% at 119 days and 50.1% at 364 days; at 364 days, 3.1% of the applied was associated with the fulvic acid fraction, 0.9% with humic acid and 31.7% with humin.

It was proposed that BAS 510 F degrades to M510F49 [2-hydroxy-N-(4'-chlorobiphenyl-2-yl)-nicotinamide] and M510F50 (Unknown 2). All three compounds then degrade to CO<sub>2</sub> or bind to the soil. The study author could not determine where Unknown 1 appeared in the degradation pathway.

The calculated initial half-life value of BAS 510 F in aerobic sandy loam soil was 96.3 days ( $r^2 = 0.9754$ ; linear regression assuming first-order kinetics, combining concentration data from 0-119 days for both labels) and the secondary half-life was 169.1 days ( $r^2 = 0.9413$ , 93-364 days). The DT50 and DT90 were 108 and 360 days, respectively, for the combined data (p. 30; ModelMaker v.3 using Marquardt-Newton optimization).

### Results Synopsis:

Soil type: Sandy loam (German)

Half-life: 96.3 days (linear, 0-119 days; based on combined data from both label studies; affected by high level of bound residues)

DT50: 108.3 days (nonlinear)

DT90: 359.9 days (nonlinear)

Major transformation product: CO<sub>2</sub>

Minor transformation products: M510F50 (Unknown 2)

M510F49 (Reg. No. 391572; 2-hydroxy-N-(4'-chlorobiphenyl-2-yl)-nicotinamide]

Unknown 1

**Study Acceptability:** This study is scientifically valid and provides supplemental information on the aerobic soil metabolism of BAS 510 F. It does not satisfy the guideline data requirement for an aerobic biotransformation study in soil (§162-1) because a foreign soil was utilized and the soil moisture content was higher than that recommended in the guidelines (which were intended to provide for the use of sub-optimal soil conditions in soil metabolism studies). Additionally, replicate data were not obtained for use in the determination of the patterns of formation and decline of the degradates, and combined data from the two radiolabel studies had to be used to determine the half-life of the parent compound.

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## I. MATERIALS AND METHODS

**GUIDELINE FOLLOWED:** This study was conducted in accordance with BBA-Guideline for the Official Testing of Plant Protection Products, Part IV. 4-1 and SETAC Procedures for assessing the environmental fate and ecotoxicity of pesticides. The only significant deviation from USEPA Subdivision N Guideline §162-1 is:

The soil moisture content was 40% of the maximum water holding capacity, rather than the recommended 75% of field capacity at 1/3 bar. Using data provided by the study author, it was calculated that the soil was at 106% of field capacity at 1/3 bar. This does not affect the scientific validity of the study, but does not provide a half-life determination for the parent compound under sub-optimal conditions as intended by Subdivision N Guidelines.

**COMPLIANCE:** This study was conducted in compliance with the Good Laboratory Practice Regulations of the Federal Republic of Germany (1994). Signed and dated GLP, Data Confidentiality, Quality Assurance and Study Certification statements were provided (pp. 2-5).

### A. MATERIALS:

**1. Test Materials:** [Diphenyl-U-<sup>14</sup>C]- and [pyridine-3-<sup>14</sup>C]-labeled BAS 510 F

#### Chemical Structure:

**Description:** Solid (p. 17).

#### Purity:

[Diphenyl-U-<sup>14</sup>C] label: Radiochemical purity: >99% (p. 61).  
Chemical purity: 99%  
Batch No. 641-1018.  
Specific activity: 314,000 dpm/μg (5.23 MBq/mg).

[Pyridine-3-<sup>14</sup>C] label: Radiochemical purity: >99% (p. 62).  
Chemical purity: 97-99%  
Batch No. 640-1026.  
Specific activity: 349,000 dpm/μg (5.81 MBq/mg).

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### Storage conditions of test chemicals:

In darkness at a low (unspecified) temperature (pp. 61-62).

Table 1: Physico-chemical properties of BAS 510 F.

Parameter	Values	Comments
Water solubility:	4.64 mg/L at 20°C <sup>1</sup>	MRID 45405210
Vapor pressure/volatility:	Not reported	
UV absorption:	Not reported.	
pK <sub>a</sub> :	Not reported.	
K <sub>ow</sub> /log K <sub>ow</sub> :	Not reported.	
Stability at room temperature:	Not reported.	

<sup>1</sup>Was reported as 6.0 mg/L @ 20°C (pH not reported) in MRID 45405216.

## 2. Soil Characteristics:

Table 2: Description of soil collection and storage.

Description	Details
Geographic location:	Limburgerhof, Germany
Collection date:	1997 (? , p. 71)
Pesticide use history at the collection site	Not reported.
Collection procedures	Not reported.
Sampling depth (cm)	Not reported.
Storage length	Not reported.
Storage conditions:	Not reported
Soil preparation:	2 mm sieved.

Data obtained from pp. 16-17 of the study report.

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Table 3: Properties of the soil.

Property	Details
Texture:	Sandy loam.
sand (%)	77
silt (%)	17
clay (%)	6
pH (CaCl <sub>2</sub> )	7.4
Organic carbon (%)	1.3
CEC (meq/100 g)	12.7
Maximum water holding capacity (g/100 g dry soil)	43
Moisture at 1/3 Bar (g/100 g dry soil)	16.1
Bulk density (g/cm <sup>3</sup> )	Not provided
Soil Taxonomic classification:	Not provided.
Soil Mapping Unit (for EPA):	Not provided.

Data obtained from p. 71 of the study report.

### B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: None.

2. Experimental conditions:

Table 4: Experimental design.

Parameter		[Diphenyl-U- <sup>14</sup> C]BAS 510 F	[Pyridine-3- <sup>14</sup> C]BAS 510 F
Duration of the test		364 days.	
Soil condition (air dried/fresh)		Not specified.	
Soil (g/replicate)		100 g dry wt.	
Application rates		0.933 mg/kg; 0.700 kg a.i./ha.*	1.022 mg/kg; 0.767 kg a.i./ha.*
Control conditions, if used		No controls were used.	
No. of Replications	Controls, if used	No controls were used.	
	Treatments	Single samples were collected at each sampling interval. Samples from the two different radiolabel studies served as replicates for the determination of the parent half-life.	

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Parameter		[Diphenyl-U- <sup>14</sup> C]BAS 510 F	[Pyridine-3- <sup>14</sup> C]BAS 510 F
Test apparatus (Type/material/volume)		Treated soil samples (100 g) were weighed into glass dishes (not described). The dishes were placed on metal trays (5-6 per tray), and the trays were placed in stainless steel incubation tubes. There were 4-5 tubes used for each label. Each tube was equipped with inlet/outlet ports. The tubes were housed within an incubation chamber. The test apparatus is illustrated in Attachment 12, p. 72.	
Details of traps for CO <sub>2</sub> and organic volatiles, if any:		Humidified CO <sub>2</sub> -free air was drawn (flow rate not specified) through each incubation tube, then sequentially through 0.5 M sodium hydroxide, 0.5 M sulfuric acid, and ethylene glycol trapping solutions (50 mL/solution).	
If no traps were used, is the system closed/open?		Volatiles traps were used.	
Co-solvent	Identity	Methanol	
	Final concentration	0.05%	0.06%
Test material application.	Volume of test solution used/treatment	2 mL of 2.027 mg/mL test solution per 4.054 kg soil (dry wt).	2 mL of 1.455 mg/mL test solution per 2.91 kg soil (dry wt).
	Application method	The test solution was pipetted onto soil surface, then the soil was mixed. The mixing procedure was not described.	
	Is the co-solvent evaporated?	No.	
Microbial biomass/Microbial population of test soil		Initial: 35.1 mg C/100 g dry soil. Final: 12.7 mg C/100 g dry soil	
	Actinomycetes	Individual CFUs were not measured.	
	Fungi	Individual CFUs were not measured.	
	Bacteria	Individual CFUs were not measured.	
Any indication of the test material adsorbing to the walls of the test apparatus?		Not determined.	
Experimental conditions.	Temperature (°C):	20 ± 1°C.	
	Moisture content:	40% of maximum water holding capacity; 106% of field capacity at 1/3 bar.	
	Moisture maintenance method:	Soil samples weighed periodically (interval not specified) and moistened as needed.	
	Continuous darkness (Yes/No):	Yes.	

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Parameter	[Diphenyl-U- <sup>14</sup> C]BAS 510 F	[Pyridine-3- <sup>14</sup> C]BAS 510 F
Other details, if any:	None.	

Data obtained from pp. 16-18, 71, 72 of the study report.

\* Field application rate equivalents determined by the study author assuming a soil depth of 5 cm and a bulk density of 1.5 g/cm<sup>3</sup> (p. 17).

**3. Aerobic conditions:** It was reported that the metal tubes containing the treated soil samples were purged with humidified CO<sub>2</sub>-free air during the study (p. 19). No measurements were made to establish the oxygen content of the soils.

**4. Supplementary experiments:** In order to facilitate identification of degradates, additional soil samples (100 g) were treated with [pyridine-3-<sup>14</sup>C]BAS 510 F at 48.5 mg/kg (p. 20). The soils were incubated under the conditions described for the definitive study. Samples were collected at 86 and 114 days posttreatment.

### 5. Sampling:

Table 5: Sampling details.

Parameters	[Diphenyl-U- <sup>14</sup> C]BAS 510 F	[Pyridine-3- <sup>14</sup> C]BAS 510 F
Sampling intervals:	0, 7, 14, 29, 57, 93, 119, 182, 266 and 364 days	
Sampling method for soil samples:	One dish (100 g soil) was collected for each label at each interval; 50 g of each sample was extracted and 50 g was frozen.	
Method of collection of CO <sub>2</sub> and volatile organic compounds:	Trapping solutions were collected and replaced at each sampling interval.	
Sampling intervals/times for: Sterility check, if sterile controls are used: Moisture content: Redox potential/other:	Sterile controls were not used. Not reported. Not determined.	
Sample storage before analysis:	Soil samples were extracted the day of collection. Extracts solutions were stored frozen and analyzed within 6 days.	
Other observations, if any:	None.	

Data obtained from pp. 18-19, 70 of the study report.

### C. ANALYTICAL METHODS:

**Extraction/clean up/concentration methods:** Each soil sample (50 g) was sequentially extracted three times with 90 mL of methanol and three times with 90 mL of methanol:water (1:1, v:v) by shaking on a rotary shaker at room temperature (p. 18). Following each extraction,

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samples were centrifuged, then decanted through a filter. Aliquots were analyzed for total radioactivity by LSC. Like extracts were combined and concentrated (not described), and the resulting residues redissolved in methanol for TLC analysis or acetonitrile:water (1:1; v:v) for HPLC analysis (methanol:water extracts only).

**Nonextractable residue determination:** Portions of the extracted soils were analyzed for total radioactivity using LSC following combustion. Additional portions (20 g) of the 14 through 364 day extracted soils were further extracted three times with water and three times with 0.5 M sodium hydroxide. Aliquots of the extracts were analyzed for total radioactivity by LSC. The alkaline extracts were acidified and stored, and the resulting precipitate was removed by centrifugation. The supernatant (fulvic acid) was analyzed by LSC; the precipitate (humic acid) was redissolved in sodium hydroxide and analyzed using LSC. [<sup>14</sup>C]Residues remaining in the extracted soil (humin) were quantified by LSC following combustion. For samples collected between 182 and 364 days, the fulvic acid fraction was extracted with methylene chloride and ethyl acetate, and each fraction was analyzed using LSC.

**Volatile residue determination:** Aliquots of each trapping solution were analyzed for total radioactivity by LSC (p. 18).

**Total <sup>14</sup>C measurement:** Total <sup>14</sup>C residues were determined by summing the concentration of residues measured in the soil extracts, extracted soil, and volatile trapping solutions.

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

**Identification and quantification of parent compound:** Samples were analyzed using TLC and HPLC. Normal-phase one-dimensional TLC was conducted on silica gel plates developed with diisopropyl ether:methanol:formic acid (80:20:1, v:v) (p. 22). Following development, areas of radioactivity were detected using a Phosphor Imaging Plate. Aliquots of the organic and aqueous extracts were analyzed by HPLC under the following conditions: Waters Spherisorb ODS-2 column (4.6 x 250 mm, 10 µm particle size), gradient mobile phase combining (A) water:acetonitrile:formic acid (950:50:1) and (B) acetonitrile:water:formic acid (950:50:1) [percent A:B at 0 min. 100:0 (%), 10 min. 100:0, to 95:5, 70 min. 5:95 to 0:100, 80 min. 0:100, 85 min. 100:0], injection volume (not specified), flow rate 1 mL/minute, Kontron UV detector 430 and Berthold 507 A radiodetector (p. 22). BAS 510F was identified by comparison with a reference standard.

**Identification and quantification of transformation products:** Transformation products were quantified as described for BAS 510 F. The procedure used to identify the transformation products was not clearly described, but appears to have involved the comparison with reference standards (M10F49 only) and HPLC/MS. Extracts from the high dose samples were used to obtain sufficient material for identification.

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To confirm the presence of  $^{14}\text{CO}_2$  in the NaOH trapping solution, an aliquot was reacted with barium chloride and centrifuged. The supernatant was analyzed by LSC.

**Detection limits (LOD, LOQ) for the parent compound:** Detection limits were not reported..

**Detection limits (LOD, LOQ) for the transformation products:** Detection limits were not reported. The study author noted that using HPLC,  $^{14}\text{C}$  compounds present at  $<0.001$  mg/kg were still detectable (p. 24).

## II. RESULTS AND DISCUSSION:

**A. TEST CONDITIONS:** It was reported that aerobicity, moisture, temperature and other environmental conditions were maintained throughout the study. No supporting records were provided.

**B. MATERIAL BALANCE:** Overall recoveries of radiolabeled material averaged  $100.3 \pm 3.7\%$  (range 93.3-104.6%) of the applied during the 364 day incubation of [diphenyl- $^{14}\text{C}$ ]BAS 510 F-treated soil. Overall recoveries of radiolabeled material averaged  $93.0 \pm 6.1\%$  (83.4-101.8%) during the 364 day incubation of [pyridine-3- $^{14}\text{C}$ ]BAS 510 F-treated soil (pp. 27, 32). In the latter samples, material balances appeared to be decreasing but were acceptable (93.9%) at the final sampling interval.

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Table 6: Biotransformation of [diphenyl-U-<sup>14</sup>C]BAS 510 F, expressed as percentage of applied radioactivity (mean ± s.d.), in sandy loam under aerobic conditions.\*

Compound	Sampling times (days)									
	0	7	14	29	57	93	119	182	266	364
BAS 510 F	99.7	95.5	93.0	81.6	61.4	51.7	44.2	32.7	26.3	16.7
M510F49 2-Hydroxy-N-(4'-chlorobiphenyl-2-yl)-nicotinamide)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0
M510F50 (Unknown 2)	0.0	0.0	0.0	0.0	0.2	0.2	0.2	0.1	0.2	0.2
Unknown 1	0.0	0.0	0.0	0.0	0.0	0.1	0.2	0.2	0.6	0.4
Others	0.0	0.0	0.1	0.1	0.2	0.2	0.2	0.4	0.4	0.4
Total extractable residues	99.7	95.5	93.1	81.7	61.8	52.2	44.8	33.4	27.7	17.8
Total volatile organics	---	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO <sub>2</sub>	---	0.1	0.6	1.5	3.9	6.5	8.3	11.5	13.6	15.5
Nonextractable residues	0.3	6.1	10.8	19.7	31.4	43.1	48.6	50.8	62.7	60.0
Total % recovery	100.0	101.7	104.6	102.9	97.1	101.8	101.6	95.7	104.0	93.3

Data obtained from Table 1, p. 32 and Table 7, p. 35 of the study report.

\* Only one sample was collected at each sampling interval.

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Table 7: Biotransformation of [pyridine-3-<sup>14</sup>C]BAS 510 F, expressed as percentage of applied radioactivity (mean ± s.d.), in sandy loam under aerobic conditions.\*

Compound	Sampling times (days)									
	0	7	14	29	57	93	119	182	266	364
BAS 510 F	99.6	95.5	85.6	77.9	62.7	48.0	42.0	28.8	20.5	17.3
M510F49 2-Hydroxy-N-(4'-chlorobiphenyl-2-yl)-nicotinamide)	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.1	0.1
M510F50 (Unknown 2)	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.2	0.1	0.1
Unknown 1	0.0	0.1	0.0	0.1	0.2	0.3	0.4	0.6	0.7	0.6
Others	0.0	0.0	0.1	0.1	0.3	0.5	0.6	0.3	0.2	0.3
Total extractable residues	99.6	95.6	85.7	78.1	63.2	49.1	43.2	29.8	21.5	18.4
CO <sub>2</sub>	---	0.6	1.8	3.9	7.7	12.5	15.0	19.1	23.2	25.4
Total volatile organics	---	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Nonextractable residues	0.4	5.6	8.6	14.6	22.5	28.3	32.7	35.2	38.6	50.1
Total % recovery	100.0	101.8	96.1	96.6	93.4	89.9	90.8	84.1	83.4	93.9

Data obtained from Table 2, p. 32 and Table 8, p. 35 of the study report.

\* Only one sample was collected at each sampling interval.

**C. TRANSFORMATION OF PARENT COMPOUND:** The rate of dissipation of [diphenyl-U-<sup>14</sup>C]- and [pyridine-3-<sup>14</sup>C]-labeled BAS 510 F were identical. [<sup>14</sup>C]BAS 510 F decreased from 99.6-99.7% at day 0 to 48.0-51.7% at 93 days posttreatment, 28.8-32.7% at 182 days, 20.5-26.3% at 266 days, and 16.7-17.3% at 364 days (Tables 7 and 8, p. 35).

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**HALF-LIFE:** The half-life for BAS 510 F was determined by the reviewer using linear regression analysis based on first-order kinetics as calculated by Excel 97 SR-2. DT50 and DT90 values were determined by the study author using a non-linear analysis based on multi-compartment models as calculated by ModelMaker v. 3 (pp. 23, 60, 104).

Table 8: Half-life and DT 50/DT90 values of BAS 510 F in aerobic sandy loam soil.

Soil type	First order Linear			DT50 (days)	DT90 (days)
	Half-life (days)	Regression equation	r <sup>2</sup>		
Sandy loam	0-119 days: 96.3	Linear form $y = mx + b$ as $\ln C = -kt + \ln C_0$ ; $\ln C_0$ is initial concentration ( $b = y$ intercept), $\ln C$ is concentration at time $t$ ( $y$ ), $k$ is the slope ( $m$ ), $t$ is time ( $x$ ) or $kt = \ln C_0 - \ln C$ . Half-life ( $t_{1/2}$ ) = $-(\ln 2/k)$ .	0.9754	108.3	359.9
	93-364 days: 169.1		0.9413		

<sup>1</sup>Half-lives calculated using data obtained from data obtained from Tables 7 and 8, p. 35. DT50 and DT90 data were calculated by the study author using a nonlinear model.

**TRANSFORMATION PRODUCTS:** Three nonvolatile transformation products were isolated from both sets of samples, each comprising  $\leq 0.7\%$  of the applied radioactivity at any sampling interval. M510F50 ("Unknown 2") was a maximum 0.2% of the applied in both soils. M510F49 [2-hydroxy-N-(4'-chlorobiphenyl-2-yl)-nicotinamide] was a maximum 0.1% in both soils. "Unknown 1" was a maximum 0.6% in the [diphenyl-U-<sup>14</sup>C]BAS 510 F-treated soil and 0.7% in the [pyridine-3-<sup>14</sup>C]BAS 510 F-treated soil. All three compounds appear to be increasing with time; however, there was insufficient concentration of any compound to establish a valid pattern of formation.

**NONEXTRACTABLE AND EXTRACTABLE RESIDUES:** Extractable [<sup>14</sup>C]residues decreased from 99.7% of the applied at day 0 to 17.8% at 364 days in [diphenyl-U-<sup>14</sup>C]BAS 510 F-treated soil and from 99.6% at day 0 to 18.4% at 364 days in [pyridine-3-<sup>14</sup>C]BAS 510 F-treated soil (p. 32). Nonextractable [<sup>14</sup>C]residues in [diphenyl-U-<sup>14</sup>C]BAS 510 F-treated soil increased from 0.3% of the applied at day 0 to 43.1% at 93 days and 60.0% at 364 days. At 364 days, 4.4% of the applied was associated with the fulvic acids, 3.1% with humic acid and 34.4% with humins (p. 33). Nonextractable [<sup>14</sup>C]residues in [pyridine-3-<sup>14</sup>C]BAS 510 F-treated soil increased from 0.4% at day 0 to 28.3% at 93 days and were 50.1% at 364 days. At 364 days, 3.1% of the applied was associated with the fulvic acids, 0.9% with humic acid and 31.7% with humins. HPLC analysis of the fulvic acid from both treatments found that BAS 510 F and Others were each  $\leq 2.0\%$  of the applied (p. 39).

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**VOLATILIZATION:** Volatilization of  $^{14}\text{CO}_2$  was significant for both labels, increasing to 15.5% and 25.4% of applied for [diphenyl- $^{14}\text{C}$ ]- and [pyridine-3- $^{14}\text{C}$ ]-BAS 510 F treated soils, respectively, by the final sampling interval (p. 32).

**TRANSFORMATION PATHWAY:** A biotransformation pathway (p. 58) for the degradation of BAS 510 F in aerobic soil was proposed by the registrant. BAS 510 F degrades to M510F49 and/or M510F50 (Unknown 2). The parent and these transformation products are degraded to  $\text{CO}_2$  and are converted to soil bound residues.

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

Applicant's Code Name	CAS Number	CAS and/or IUPAC Chemical Name(s)	Chemical formula	Molecular weight	SMILES string
M510F49		2-hydroxy-N-(4'-chlorobiphenyl-2-yl)-nicotinamide		324.77	
M510F50 Unknown 2					
Unknown 1					

**D. SUPPLEMENTARY EXPERIMENT-RESULTS:** The high dose samples were used to obtain sufficient material to allow the HPLC/MS analysis of transformation products.

**III. STUDY DEFICIENCIES:** This study was conducted in accordance with BBA-Guideline for the Official Testing of Plant Protection Products, Part IV. 4-1 and SETAC Procedures for assessing the environmental fate and ecotoxicity of pesticides. The study author stated that it also fulfills the requirements of USEPA Subdivision N Guideline §162-1. However, a foreign soil was used rather than a domestic one, and the soil moisture content was 40% of the maximum water holding capacity, rather than the recommended 75% of field capacity at 1/3 bar. The study author provided both the maximum water holding capacity of the soil (43 g water/100 g soil) and the field capacity at 1/3 bar (16.1 g/100 g). Using this data, it was calculated that the soil was at 106% of field capacity at 1/3 bar. Therefore, the soil contained more water and less oxygen in its pore space than recommended by Subdivision N Guidelines which were intended to provide for sub-optimal conditions in the soil. However, this moisture level likely had only a minimal effect on the microbial metabolic rate, and should not have affected the chemical degradation rate since BAS 510 F is not subject to hydrolysis. Thus, this deviation should not have had a significant impact on the study results. Since the study is scientifically valid and no other deviations from Subdivision N Guidelines were noted, this study can be used to provide supplemental information on the aerobic soil metabolism of BAS 510 F. It is noted, however, that replicate samples were not utilized within the two radiolabel studies. While the combined data from the two studies were able to serve as replicate data for the determination of the parent half-life (since similar patterns of degradation were observed between the two data sets), it is also necessary that,

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in future studies, replicate data be obtained for use in the determination of the patterns of formation and decline of the degradates.

### IV. REVIEWER'S COMMENTS:

1. The soil used was obtained in Germany. It was classified according to the USDA Soil Textural Classification system. The physical, chemical, and microbiological properties of this soil are reportedly similar to soils from the US. However, Subdivision N Guidelines require that domestic soils be utilized in soil metabolism studies.
2. The study author stated that the samples were "purged" with humidified air in order to collect volatiles. Purged usually describes a volatile trapping system in which air is drawn intermittently through the samples, often just before sample collection. However, the volatile trapping system illustrated in this study is sophisticated and appears to be designed for continuous aeration. It should be noted that several terms were misused in the study writeup. Whether continuous or intermittent, the system appears to have been adequate for trapping volatiles.
3. Only one sample was collected for each treatment at each sampling interval. Replicate sampling is necessary, so that normal variability can be quantified and outliers can be identified. While, in the current study, the combined data from the two studies were able to serve as replicate data for the determination of the parent half-life (since similar patterns of degradation were observed between the two data sets), in future studies, replicate data should also be obtained for use in the determination of the patterns of formation and decline of the degradates.
4. The author stated that the water content of the soil was checked periodically, but did not specify the intervals.
5. The treated soils were reported to have been incubated at  $20 \pm 1^\circ\text{C}$  during the study. Supporting data were not provided.
6. BAS 510 F chemical name 2-chloro-*N*-(4'-chlorobiphenyl-2-yl)-nicotinamide, as presented in the study report, was identified as the IUPAC name by the Compendium of Pesticide Common Names (<http://www.hclrss.demon.co.uk/nicobifen.html>). The CAS name 2-chloro-*N*-(4-chloro[1,1-biphenyl]-2-yl)-3-pyridinecarboxamide was also obtained from the Compendium of Pesticide Common Names. The following BAS 510 F synonyms were obtained from USEPA/OPP Chemical Databases (<http://www.cdpr.ca.gov/cgi-bin/epa/chemidetriris.pl?pccode=128008> and ([http://www.cdpr.ca.gov/cgi-bin/mon/bycode.pl?p\\_chemcode=5790](http://www.cdpr.ca.gov/cgi-bin/mon/bycode.pl?p_chemcode=5790)): 2-chloro-*N*-(4'-chlorobiphenyl-2-yl)-nicotinamide, nicobifen, and BAS 516 02 F.

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7. Attachment 9 (p. 69) of the study indicates that the compound designated M510F49 is synonymous with the compound denoted by Reg. No. 391572. However, Table 7 (p. 35) indicates that M510F49 is "Unknown 2," while M510F50 is listed as 391572. Clarification by the registrant is necessary. In this review, M510F50 is reported as "Unknown 2." A similar discrepancy was noted in other MRIDs included with this submission.

### V. REFERENCES: The following reference was cited in the study:

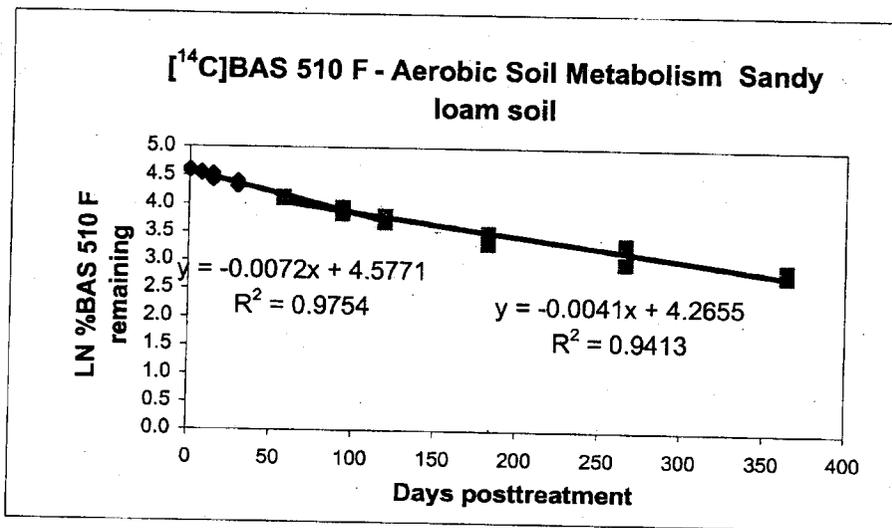
1. Walker, A. and N. Crout. 1997. ModelMaker User Manual, Version 3. Cherwell Scientific Publishing, Limited, Oxford.

Attachment 1  
Excel Spreadsheets

Chemical Name BAS 510 F      Diphenyl Ring and Pyridine ring  
 PC Code 128008  
 MRID 45405208  
 Study No. 162-1  
 Sandy loam soil

	1st	2nd
Half-life (days) =	96.3	169.1

Days posttreatment	%BAS 510 F remaining	LN (%remaining)
0	99.7	4.6022
0	98.3	4.5880
7	95.5	4.5591
7	92.8	4.5304
14	93.1	4.5337
14	83.0	4.4188
29	81.7	4.4031
29	74.8	4.3148
57	61.8	4.1239
57	60.4	4.1010
93	52.2	3.9551
93	46.3	3.8351
119	44.8	3.8022
119	40.3	3.6964
182	33.4	3.5086
182	27.5	3.3142
266	27.7	3.3214
266	19.6	2.9755
364	17.8	2.8792
364	16.2	2.7850



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Material Balance

Diphenyl Ring	Pyridine Ring
100	100
101.7	101.8
104.6	96.1
102.9	96.6
97.1	93.4
101.8	89.9
101.6	90.8
95.7	84.1
104	83.4
93.3	93.9
100.27	93
3.73156208	6.108282174

**Attachment 2**

**Structures of Parent and Transformation Products**

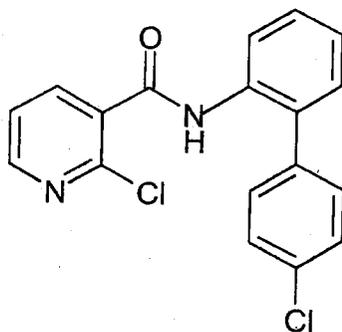
BAS 510 F

IUPAC name: 2-Chloro-*N*-(4-chlorobiphenyl-2-yl)-nicotinamide.

CAS name: 2-Chloro-*N*-(4-chloro[1,1-biphenyl]-2-yl)-3-pyridinecarboxamide.

CAS No: 188425-85-6.

Synonyms: 2-Chloro-*N*-(4'-chlorobiphenyl-2-yl)-nicotinamide, Nicobifen. BAS 516 02 F.



ERROR: stackunderflow  
OFFENDING COMMAND: exch

STACK:

-savelevel-