

US EPA ARCHIVE DOCUMENT

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

Data Requirement: PMRA Data Code:
EPA DP Barcode: 280800
OECD Data Point:
EPA Guideline: 162-1

Test material:

Common name: Iodomethane.

Chemical name

IUPAC: Not reported.

CAS name: Iodomethane.

CAS No: 74-88-4.

synonyms: Methyl iodide.

TM-425.

SMILES string: CI

Primary Reviewer: Lynne Binari
Dynamac Corporation

Signature:

Date:

QC Reviewer: Kathleen Ferguson
Dynamac Corporation

Signature:

Date:

Secondary Reviewer: Faruque Khan
EPA

Signature: *Faruque Khan*

Date: 6/10/03

Company Code: [for PMRA]
Active Code: [for PMRA]
Use Site Category: [for PMRA]
EPA PC Code: 000011

CITATION: Wujcik, C. 2001. Aerobic soil metabolism of [¹⁴C]iodomethane (TM-425). Unpublished study performed by Metabolism Division, Ricera, LLC, Concord, OH, and submitted by Arvesta Corporation, San Francisco, CA. Ricera Project ID No.: 012520 and Document No.: 012520-1. Study initiated November 2, 2000, and final report issued October 17, 2001 (pp. 1, 14).



2008518

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

EXECUTIVE SUMMARY:

The biotransformation of [^{14}C]methyl iodide (iodomethane) was studied in sandy loam soil (pH 6.5, organic matter 1.48%) from California for 12 days under aerobic conditions in darkness at 19.3-21.6°C with a soil moisture of 75% of 1/3 bar. [^{14}C]Iodomethane was applied at the rate of 31 mg a.i./kg soil, equivalent to 35 kg a.i./ha. This experiment was conducted in accordance with USEPA Subdivision N Guideline §162-1 and in compliance with the 40 CFR Part 160 GLP standards. The test system consisted of sealed glass columns containing treated soil incubated in darkness under temperature-controlled conditions; each soil column was connected to a flow-through system for the continuous collection of CO_2 and volatile organics. Duplicate treated samples were collected after 0, 1, 2, 3, 4, 5, 6, 8, 24, 96, 168 and 288 hours of incubation. Soil samples were initially cooled, then heated and purged with nitrogen. Nitrogen purge trapping solutions, purged soil and volatiles trapping solutions from the incubation were analyzed for total radioactivity using LSC. Nitrogen purge and volatiles trapping solutions (2% tripropylamine in dimethyl sulfoxide) were qualitatively analyzed for [^{14}C]methyltripropylammonium ion, the derivatize of iodomethane formed via reaction with tripropylamine, using reverse-phase HPLC and identified by comparison to derivatized reference standard. Identification of derivatized iodomethane was confirmed using LC/MS-ESI.

Test conditions outlined in the study protocol were maintained throughout the study.

Overall material balance averaged $95.0 \pm 2.6\%$ (range 91.2-101.7%, $n = 24$) of the applied radioactivity; there was no decline in material balances during the 12-day study.

[^{14}C]Iodomethane (as total radioactivity in 2% TPA in DMSO solutions) rapidly dissipated from the soil decreasing from 92.7-97.9% of the applied at time 0 posttreatment to 43.1-56.4% at 2 hours, 19.9-24.9% at 4 hours, 5.5-9.8% at 6-8 hours and was <1.0% by 24 hours.

No major transformation products of [^{14}C]iodomethane were detected in the soil. Minor products detected following the heated nitrogen purge were $^{14}\text{CO}_2$ and other unidentified volatile [^{14}C]organics each detected at $\leq 0.2\%$ of the applied radioactivity. Extractable (heated nitrogen purge) [^{14}C]residues rapidly decreased from 92.8-98.1% of the applied at time 0 to <1.0% at 24 hours, while nonextractable [^{14}C]residues totaled $\leq 1.3\%$ of applied at any sampling interval.

[^{14}C]Iodomethane (as total radioactivity detected in 2% TPA in DMSO solutions) rapidly volatilized from the soil layer increasing from 12.9-15.2% of the applied at 1 hour to 35.2-49.9% at 2 hours, 85.1-86.6% at 8 hours, 90.1-91.2% at 24 hours and was 94.5-94.7% at 288 hours (maximum 98.4% at 168 hours). At 288 hours (study termination), volatilized $^{14}\text{CO}_2$ and unidentified [^{14}C]organic volatiles totaled 1.1% and 2.3-2.9% of the applied, respectively.

Half-life of dissipation, based on first order linear regression analysis, of iodomethane was 2 hours. DT_{50} and DT_{90} values, based on nonlinear regression analysis, were 2 and 7 hours, respectively.

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

Iodomethane rapidly dissipated from the soil (*ca.* 10-inch, 25-cm depth) via volatilization with minor formation of CO₂, unidentified organic volatiles and soil-bound residues.

Results Synopsis:

Soil type: California sandy loam.

Half-life: 2.1 hours ($r^2 = 0.915$).

DT₅₀: 2.0 hours ($r^2 = 0.9837$).

DT₉₀: 6.8 hours ($r^2 = 0.9837$).

Major transformation products:

None.

Minor transformation products:

CO₂.

Unidentified organic volatiles.

Study Acceptability: This study is classified as **acceptable** and satisfies the guideline requirement for an aerobic soil biotransformation study. The rapid degradation of iodomethane in the aerobic soil study is primarily the result of volatilization rather than microbial degradation. However, carbon dioxide was detected in the study. This indicates that some microbial degradation of iodomethane took place in this study.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with USEPA Subdivision N Guideline §162-1 (p. 16). No significant deviations from USEPA Subdivision N Guideline §162-1 that affect the acceptability of the study were noted.

COMPLIANCE: This study was conducted in compliance with USEPA GLP Standards (40 CFR, Part 160; p. 3). Signed and dated Data Confidentiality, GLP (Compliance) and Quality Assurance statements and a Certificate of Authenticity were provided (pp. 2, 3, 6, 8).

A. MATERIALS:

1. Test Material: [¹⁴C]Iodomethane (p. 17).

Chemical Structure: H₃C*-I

Description: Technical, clear colorless liquid (p. 17; p. C 232 of Farm Chemicals Handbook 2002).

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

Purity: Radiochemical purity: >99% (p. 42).
 Lot No.: 110K9407 (p. 17).
 Analytical purity: Not reported.
 Specific activity: 6.1 mCi/mMol.

Storage conditions of test chemicals: Stored at <10°C (p. 81).

Table 1: Physico-chemical properties of iodomethane (TM-425).

Parameter	Values	Comments
Molecular weight:	141.94 g/mol	
Molecular formula:	CH ₃ I	
Water solubility:	14.2 mg/mL at 25°C	
	1.4 g/100 mL at 20°C	International Chemical Safety Cards - Methyl Iodide at http://www.cdc.gov/niosh/ipcsneng/neng0509.html
	14 g/100 g at 20°C	p. C232 of Farm Chemicals Handbook 2002.
Vapor pressure/volatility (kPa):	50 at 20°C	International Chemical Safety Cards - Methyl Iodide
UV absorption:	Not reported.	
pK _a :	Not reported.	
K _{ow} /log K _{ow} :	Not reported.	
Henry's law K _H :	0.22	
Octanol/water partition coefficient (log P _{ow}):	1.51-1.69	International Chemical Safety Cards - Methyl Iodide
Boiling point:	42.4 ⁷⁶⁰ °C	
Melting point:	-66.5°C	International Chemical Safety Cards - Methyl Iodide
Relative density (water = 1):	2.3	International Chemical Safety Cards - Methyl Iodide
Relative vapor density (air = 1)	4.9	International Chemical Safety Cards - Methyl Iodide
Relative density of vapor/air mixture at 20°C (air = 1):	2.9	International Chemical Safety Cards - Methyl Iodide
Stability of compound at room temperature:	Not reported.	

Data obtained from pp. 17, 18, 21 of the study report and where noted in the Comments column.

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

2. Soil Characteristics:

Table 2: Description of soil collection and storage.

Description	Details
Geographic location:	Nakano property adjacent to Plant Sciences, Inc., Watsonville, California.
Pesticide use history at the collection site:	No pesticides had been applied to the collection site since 1998, and the site had not been treated with the same class of compound as iodomethane for the previous 5 years.
Collection date:	January 25, 2001.
Collection procedures:	Not reported.
Sampling depth:	Not reported.
Storage conditions:	Stored in greenhouse at Plant Sciences, Inc., for 4 days following collection, then transferred to Ricera and stored in an environmental chamber at 20°C until use; maintained moist.
Storage length:	Soil received at test facility 1/30/01 and experimental start date 4/26/01 (day of application).
Preparation:	2-mm sieved.

Data obtained from pp. 19, 32, 38 of the study report.

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

Table 3: Properties of the soil.

Property		Details
Soil texture:		Sandy loam.
% sand:		76.8
% silt:		11.6
% clay:		11.6
pH:		6.5
Organic carbon (%):		Not reported.
Organic matter (%):		1.48
CEC (meq/100 g):		9.62
Moisture (%) at	1/3 bar:	10.6
	15 bar:	5.04
	saturation:	18.9
Bulk density (g/cm ³):		1.41
Soil Taxonomic classification:		Coarse-loamy, mixed, thermic Cumulic Haploxerolls.
Soil Mapping Unit (for EPA):		Not reported.

Data obtained from p. 37 of the study report.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: A preliminary experiment to establish methodology and obtain information on the rate of degradation and formation of potential transformation products of iodomethane in aerobic soil was conducted, but not included in the study report (pp. 65, 67, 88).

2. Experimental conditions:

Table 4: Study design.

Criteria	Sandy loam soil
Duration of the test:	288 hours (12 days).
Soil condition (air dried/fresh):	Prior to use, the soil moisture content was determined to be 8.0%; waterholding capacity of the soil at 1/3 bar was 7.95%. Aliquots (ca. 120 g) of the soil were placed in the test vessels, then the vessels were placed within upright flow-through chambers and the soil pre-incubated at 20 ± 1°C for 8 days prior to treatment. During the pre-incubation, humidified air was drawn (flow rate not specified) through the chambers.

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

Criteria		Sandy loam soil		
Soil (g/replicate):		120 g (wet/dry wt. not specified).		
Test concentrations (mg a.i./kg soil and equivalent kg a.i./ha):	Nominal:	31 mg/kg (35 kg/ha).		
	Actual:	31.4-31.6 mg/kg (35.5-35.7 kg/ha).		
Control conditions, if used:		Untreated soil samples to be used for microbial evaluations were incubated under the same conditions as the treated samples.		
No. of Replications:	Controls, if used:	Not reported.		
	Treatments:	Duplicate samples at each collection interval.		
Test apparatus (Type/material/volume):		Cylindrical glass tubes (2.5-cm i.d. x 25 cm) pre-conditioned with AquaSil Siliconizing Fluid. Polytetrafluoroethylene (PTFE)-lined silicone septum caps were used to seal both ends of each tube.		
Details of traps for CO ₂ and organic volatiles, if any:		Excluding the time 0 samples, humidified air was continuously drawn (5-7 mL/minute) through the headspace of each vessel via inlet/outlet 18-gauge 1½ Precision Glide Needles in the septum cap, then sequentially through single tubes of 2% tripropylamine (TPA) in dimethyl sulfoxide (DMSO), 1 N NaOH and coconut charcoal (10 g).		
If no traps were used, is the system closed/open?		Volatile traps were used.		
Identity and concentration of co-solvent:	Identity:	Water.		
	Final concentration:	Not applicable.		
Test material application:	Vol. of test solution used/treatment:	0.84-0.87 mL of 4.35-4.48 mg/mL test solution per 120 g soil.		
	Application method:	Following pre-incubation, the top of the vessel was capped, the vessel was inverted, [¹⁴ C]iodomethane test solution was applied through the septum cap evenly over the "bottom" surface of the soil column, then the vessel was re-inverted and attached to the air-flow system for incubation.		
	Co-solvent evaporated:	Not applicable.		
Any indication of the test material adsorbing to the walls of the test apparatus?		Not reported.		
Microbial biomass/population of the control (x 10 ⁵ CFU/g soil dry wt.):		Initial (time 0):	24 hours:	Final (288 hours):
	bacteria:	69	76	85
	fungi:	1.8	2.0	2.8

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

Criteria		Sandy loam soil		
Microbial biomass/population of the treated (x 10 ⁵ CFU/g soil dry wt.):		Initial (time 0):	24 hours:	Final (288 hours):
	bacteria:	81	70	70
	fungi:	1.7	0.98	2.4
Experimental conditions:	Temperature (°C):	20 ± 1°C in an environmental chamber.		
	Moisture content: Moisture maintenance method:	75% of 1/3 bar. At 8 days posttreatment, moisture monitored by weight and adjusted, as needed.		
	Continuous darkness (Yes/No):	Yes.		
Other details, if any:		None.		

Data obtained from pp. 15, 20-23, 38, 43, 65, 66 of the study report.

3. Aerobic conditions: Humidified air was continuously drawn (5-7 mL/minute) through the headspace of the vessels containing the treated soil samples. No determinations were made, such as redox potentials, to verify that aerobic conditions were maintained.

4. Supplementary experiments: No supplementary experiments were conducted.

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

5. Sampling:

Table 5: Sampling details.

Criteria	Details
Sampling intervals:	0, 1, 2, 3, 4, 5, 6, 8, 24, 96, 168 and 288 hours.
Sampling method:	Duplicate samples were collected at each interval.
Method of collection of CO ₂ and volatile organic compounds:	Trapping solutions/materials were collected with respective soil samples.
Sampling intervals/times for: Sterility check, if sterile controls are used: Moisture content: Redox potential/other:	Sterile controls were not used. Checked once at 8 days (192 hours) posttreatment. Not determined.
Sample storage before analysis:	All samples were reportedly analyzed within 15 days after sampling. Time 0 treated soil samples were stored frozen (<-10°C) prior to extraction (heated nitrogen purge) and analysis. All remaining treated soil samples were purged the day of collection. Nitrogen purge trapping solutions were analyzed for total radioactivity, then subsamples (30-35 mL) were stored at <10°C in amber vials until HPLC analysis. Similarly, aliquots of the liquid trapping solutions from volatiles collection during incubation were analyzed for total radioactivity upon collection, then subsamples (30-35 mL) were stored at <10°C in amber vials until further analysis. Purged soil and coconut charcoal tubes were homogenized, then stored frozen (<-10°C) until analysis.
Other observations, if any:	None.

Data obtained from pp. 20, 22-25, 30 of the study report.

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods: At each sampling interval except time 0, duplicate soil tubes were taken and cooled in a freezer ($<-10^{\circ}\text{C}$) for *ca.* 30 minutes (pp. 23, 24). Time 0 soil tubes were placed in frozen storage immediately posttreatment. After cooling, the upper septum seal was replaced with a new septum, then the outside of the soil tube was wrapped first with heating tape followed by several layers of aluminum foil for insulation. The prepared soil tube was connected to a nitrogen-flow system in which nitrogen was purged (35-40 mL/minute) through the soil tube from bottom to top, then sequentially through duplicate tubes containing 2% TPA in DMSO and a single tube of 1N NaOH (p. 44). The heating tape was set at 45°C during the 45-minute purge. A vacuum set at a rate slightly greater than the nitrogen flow was connected at the end of the system to ensure complete draw-through. Following the purge, triplicate aliquots (1-2 mL x 3) of the trapping solutions were analyzed for total radioactivity by LSC. Subsamples (30-35 mL) of the trapping solutions were stored in amber vials at $<10^{\circ}\text{C}$ until further analysis; all 2% TPA in DMSO trapping solutions containing $\geq 1\%$ of the applied radioactivity were analyzed by HPLC (p. 26).

Nonextractable residue determination: Purged soil was air-dried overnight, homogenized by grinding to a powder with a mortar and pestle, then stored at $<-10^{\circ}\text{C}$ in high-density polyethylene (HDPE) bottles until analysis (p. 24). Triplicate subsamples (0.5 g x 3) were analyzed for total radioactivity by LSC following combustion (p. 25).

Volatile residue determination: Aliquots (1-2 mL x 3) of the trapping solutions were analyzed for total radioactivity using LSC (p. 24). All 2% TPA in DMSO solutions containing $\geq 1\%$ of the applied radioactivity were analyzed by HPLC. All NaOH trapping solutions containing $>0.25\%$ of the total applied radioactivity were analyzed for $^{14}\text{CO}_2$ by barium chloride precipitation (p. 25). Upon collection, the coconut charcoal tube was homogenized by grinding to a powder with a mortar and pestle, then stored at $<-10^{\circ}\text{C}$ in an amber bottle until analysis. Triplicate subsamples (0.1 g x 3) of the coconut charcoal were analyzed for total radioactivity by LSC following combustion.

Total ^{14}C measurement: Total ^{14}C residues were determined by summation of the concentrations of [^{14}C]residues measured in the nitrogen purge trapping solutions, purged soil and volatiles trapping materials (solutions and coconut charcoal; pp. 25, 39).

Derivatization method, if used: [^{14}C]Iodomethane de-methylated in the presence of the 2% TPA in DMSO trapping solution to yield [^{14}C]methyltripropylammonium ion (p. 33). An aliquot (2 mL) of the 2% TPA in DMSO solution was vortexed with cold 0.05 M 1-heptanesulfonic acid (1 mL) to ion pair the quaternary ammonium salt with 1-heptanesulfonic acid for HPLC analysis (pp. 27, 33).

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

Identification and quantification of parent compound: Nitrogen purge and volatile trapping 2% TPA in DMSO solutions were qualitatively analyzed for parent [¹⁴C]iodomethane (as [¹⁴C]methyltripropylammonium ion) using reverse-phase HPLC under the following conditions: Supelco Discovery C18 column (4.6 x 250 mm, 5 μm particle size), injection volume 500 μL, gradient mobile phase combining (A) aqueous 0.005 M 1-heptanesulfonic acid and (B) acetonitrile [percent A:B at 0 min. 90:10 (v:v), 1 min. 90:10, 20 min. 50:50, 30 min. 50:50], flow rate 1.0 mL/minute, Radiomatic FLO-ONE/Beta radioactivity detector (pp. 26, 27). HPLC recoveries of selected samples averaged 106.0 ± 2.2% (range 103.5-108.8%, n = 5) of the applied radioactivity (p. 91). Identification of parent [¹⁴C]iodomethane in the solutions was based on cochromatography with derivatized labeled reference standard (pp. 35, 51). Identification of [¹⁴C]methyltripropylammonium ion was confirmed using LC/MS in electrospray ionization (ESI) mode (pp. 29, 30, 35, 52). Consequently, all radioactivity recovered in the 2% TPA in DMSO solutions (quantified by LSC analysis) was considered parent [¹⁴C]iodomethane (pp. 33, 34).

Identification and quantification of transformation products: No transformation products, other than the [¹⁴C]methyltripropylammonium ion derivative of [¹⁴C]iodomethane, were detected.

Detection limits (LOD, LOQ) for the parent compound and transformation products: The detection limit for LSC analyses was set at 2x average system background dpm equivalent to *ca.* 0.001% of the applied radioactivity; average system background radioactivity was *ca.* 47 dpm (p. 26). The detection limit for reverse-phase HPLC analyses was established as 846 dpm (minimum peak height of 3x average background height) or a minimum of *ca.* 0.1% of the applied radioactivity; however, the detection limit was determined using a shorter column and different parameters (solvent ratios and time intervals) for the gradient mobile phase (pp. 27, 28, 90).

II. RESULTS AND DISCUSSION:

A. TEST CONDITIONS: Temperatures ranged from 19.3-20.1°C during the pre-incubation period and were 19.3-21.6°C following treatment (p. 32). At 8 days (192 hours) posttreatment, the soil moisture content deviated only 0.3% from the initial soil moisture of 8.0% (soil moisture at 75% of 1/3 bar equivalent to 7.95%). No data were provided to confirm that aerobicity was maintained throughout the study.

B. MATERIAL BALANCE: Overall recovery of radiolabeled material averaged 95.0 ± 2.6% (range 91.2-101.7%, n = 24) of the applied during the 288-hour study; there was no consistent decline in material balances during the study (p. 39).

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

Table 6: Volatilization of [¹⁴C]iodomethane, expressed as percentage of applied radioactivity (mean ± s.d.¹, n = 2), in sandy loam soil under aerobic conditions.

Compound	Sampling times (hours)												
	0	1	2	3	4	5	6	8	24	96	168	288	
Soil purged Iodomethane ²	95.3 ± 2.6	77.5 ± 0.2	49.8 ± 6.7	37.9 ± 5.3	22.4 ± 2.5	16.8 ± 1.9	8.8 ± 0.3	7.7 ± 2.2	0.8 ± 0.1	0.1 ± 0.1	0.0	0.0	
Volatilized Iodomethane ²	NA ³	14.1 ± 1.1	42.6 ± 7.4	55.4 ± 5.7	69.0 ± 2.9	76.3 ± 1.3	83.5 ± 0.5	85.9 ± 0.8	90.7 ± 0.5	90.9 ± 1.3	96.5 ± 1.9	94.6 ± 0.1	
CO ₂ ⁴	0.1-0.2	0.2	0.1-0.2	0.2	0.2-0.3	0.2-0.3	0.4	0.4	0.5-0.6	0.9-1.0	1.0-1.1	1.1	
Other volatiles ⁵	0.0	0.0	<0.2	<0.2	0.1-0.8	0.1-0.2	0.3	0.2	0.3-0.9	1.2-1.7	1.0-1.2	2.3-2.9	
Nonextractable residues	0.2-0.3	0.7-0.8	0.9	1.1	1.0-1.1	1.1-1.2	1.0-1.1	1.1-1.3	1.1-1.2	1.0-1.1	1.0-1.1	1.0-1.1	
Total % recovery	95.7 ± 2.7	92.5 ± 1.3	93.5 ± 0.9	94.7 ± 0.5	93.1 ± 0.7	94.7 ± 0.5	94.0 ± 0.3	95.3 ± 2.9	93.7 ± 0.3	94.4 ± 1.6	99.7 ± 2.0	99.4 ± 0.3	

¹Standard deviations determined by the reviewer (Attachment J). Data obtained from pp. 39, 41 of the study report.

²As total radioactivity (LSC) recovered in 2% TPA in DMSO solutions (pp. 33, 34).

³Not analyzed.

⁴Summation of ¹⁴CO₂ detected in soil purge and volatiles NaOH trapping solutions; verified by barium chloride precipitation.

⁵Summation of [¹⁴C]residues detected in coconut charcoal trap and radioactivity remaining in solution following barium chloride precipitation of NaOH solutions.

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

C. TRANSFORMATION OF PARENT COMPOUND: [¹⁴C]iodomethane (as total radioactivity in 2% TPA in DMSO solutions) dissipated from the soil decreasing from 92.7-97.9% of the applied radioactivity at time 0 posttreatment to 43.1-56.4% at 2 hours, 19.9-24.9% at 4 hours, 5.5-9.8% at 8 hours, <1% at 24 hours and was not detected (<0.1%) at 168 hours (p. 41).

HALF-LIFE/DT₅₀: A half-life of 2.1 hours for the volatilization of [¹⁴C]iodomethane from the soil was determined by the reviewer using linear regression analysis based on first-order kinetics as calculated by Quattro Pro 8 (p. 41, Attachment 1). DT₅₀ and DT₉₀ values (50% and 90% dissipation times, respectively) were determined by the study author using nonlinear regression analysis based on one-phase exponential decay as calculated by GraphPad Prism version 3.00 for Windows (pp. 31, 35, 49).

Table 7: Half-life (t_{1/2})/DT₅₀ values for the volatilization of iodomethane in aerobic sandy loam soil.

Soil	First order Linear ¹			Nonlinear			
	Half-life (hrs)	Regression equation	r ²	Regression equation	r ²	DT ₅₀ (hrs)	DT ₉₀ (hrs)
Sandy loam	0- to 3-hour data: 2.1	y = -0.32464x + 4.594	0.915	y = span x exp(-0.3408x) + 0	0.9837	2.0	6.8

¹Data used for calculations obtained from p. 41 of the study report.

Nonlinear data obtained from pp. 31, 35.

TRANSFORMATION PRODUCTS: No major transformation products of [¹⁴C]iodomethane were detected in the soil. Minor products detected following the heated nitrogen purge of the soil were ¹⁴CO₂ and other unidentified volatile [¹⁴C]organics each detected at ≤0.2% of the applied radioactivity (p. 40).

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: Extractable (heated nitrogen purge) [¹⁴C]residues rapidly decreased from 92.8-98.1% of the applied radioactivity at time 0 to 0.7-0.8% at 24 hours and ≤0.1% at 96 hours, while nonextractable [¹⁴C]residues only increased from 0.2-0.3% at time 0 to 1.1-1.2% at 24 hours (maximum 1.3% at 8 hours) and were 1.0-1.1% at 288 hours (p. 39).

VOLATILIZATION: [¹⁴C]iodomethane (as total radioactivity detected in 2% TPA in DMSO solutions) rapidly volatilized from the soil layer increasing from 12.9-15.2% of the applied at 1 hour posttreatment to 35.2-49.9% at 2 hours, 66.1-71.8% at 4 hours, 90.1-91.2% at 24 hours and was 94.5-94.7% at 288 hours (maximum 98.4% at 168 hours, p. 41). At 288 hours (study termination), volatilized ¹⁴CO₂ totaled 1.1% of the applied and other unidentified [¹⁴C]organic volatiles totaled 2.3-2.9%.

Data Evaluation Report on the aerobic biotransformation of iodomethane (TM-425) in soil

PMRA Submission Number {.....}

EPA MRID Number 45593707

TRANSFORMATION PATHWAY: The study author proposed a transformation pathway (p. 48); however, iodomethane dissipated from the soil via volatilization rather than metabolic transformation.

Table 8: Chemical names for transformation products of iodomethane in aerobic sandy loam soil.

Applicant's Code	CAS Number	Chemical Name	Chemical formula	Molecular weight (g/mol)	SMILES string
		No transformation products were identified.			

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

III. STUDY DEFICIENCIES: This study is acceptable and can be used to fulfill USEPA Subdivision N Guideline §162-1 data requirements.

IV. REVIEWER'S COMMENTS:

1. The analytical method was non-specific; however, comparative HPLC co-chromatography and MS analyses of derivatized reference standard [¹⁴C]iodomethane and suspected derivatized [¹⁴C]iodomethane recovered in 2% TPA in DMSO solutions from the treated samples indicates that only iodomethane was volatilized from the soil (pp. 29, 35, 51, 52).
2. The application rate of 31 mg a.i./kg (35 kg a.i./ha) was reported to approximate the single maximum field use rate of 235 lb a.i./A (263 kg a.i./ha) assuming a 55.9-cm (22-inch) soil layer with a bulk density of 1.5 g/cm³ (pp. 15, 58, 63). The depth of the soil layer used in this study and application to the bottom of the soil column simulated injection of iodomethane in the field to a depth of 25.4-30.5 cm (10-12 inches); under field conditions, distribution throughout the 55.9-cm range (± 27.9 cm or 11 inches from the point of injection) by diffusion is assumed.

V. REFERENCES: No references were cited in the study.

Attachment 1

Quattro Pro Graphs and Spreadsheets

Determination of means/standard deviations for applied radioactivity in trapping materials and unextractable soil [¹⁴C]residues.

Hours	Soil Purge			Unextractable [¹⁴ C]			Volatiles			Charcoal			Material Balances [†]		
	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0	92.7			0.1			NA			NA			93.0		
0	97.9	95.3	2.6	0.2	0.2	0.0	NA			NA			98.4	95.7	2.7
1	77.6			0.2			15.2			0.0			93.7		
1	77.3	77.5	0.2	0.2	0.2	0.0	12.9	14.1	1.1	0.0	0.0	0.0	91.2	92.5	1.3
2	43.1			0.1			49.9			0.2			94.3		
2	56.4	49.8	6.7	0.1	0.1	0.0	35.2	42.6	7.4	0.0	0.1	0.1	92.6	93.5	0.9
3	32.6			0.1			61.1			0.2			95.2		
3	43.2	37.9	5.3	0.1	0.1	0.0	49.7	55.4	5.7	0.1	0.0	0.1	94.2	94.7	0.5
4	24.9			0.1			66.1			0.2			92.4		
4	19.9	22.4	2.5	0.0	0.1	0.1	71.8	69.0	2.9	0.5	0.4	0.2	93.8	93.1	0.7
5	18.7			0.0			75.0			0.3			95.2		
5	14.9	16.8	1.9	0.0	0.0	0.0	77.6	76.3	1.3	0.4	0.4	0.1	94.1	94.7	0.5
6	8.5			0.0			83.9			0.5			94.2		
6	9.0	8.8	0.3	0.0	0.0	0.0	83.0	83.5	0.5	0.5	0.5	0.0	93.7	94.0	0.3
8	5.5			0.0			85.1			0.5			92.3		
8	9.8	7.7	2.2	0.0	0.0	0.0	86.6	85.9	0.8	0.4	0.5	0.1	98.2	95.2	2.9
24	0.8			0.0			91.2			0.7			94.0		
24	0.7	0.8	0.1	0.0	0.0	0.0	90.1	90.7	0.5	0.8	0.8	0.1	93.4	93.7	0.3
96	0.1			0.0			92.2			1.1			95.9		
96	0.0	0.1	0.1	0.0	0.0	0.0	89.6	90.9	1.3	1.2	1.2	0.1	92.8	94.4	1.6
168	0.0			0.0			94.5			1.3			97.6		
168	0.0	0.0	0.0	0.0	0.0	0.0	98.4	96.5	1.9	1.2	1.3	0.1	101.7	99.7	2.0
288	0.0			0.0			94.5			1.4			99.6		
288	0.0	0.0	0.0	0.0	0.0	0.0	94.7	94.6	0.1	1.3	1.4	0.0	99.1	99.4	0.3
Overall															
														95.0	2.6

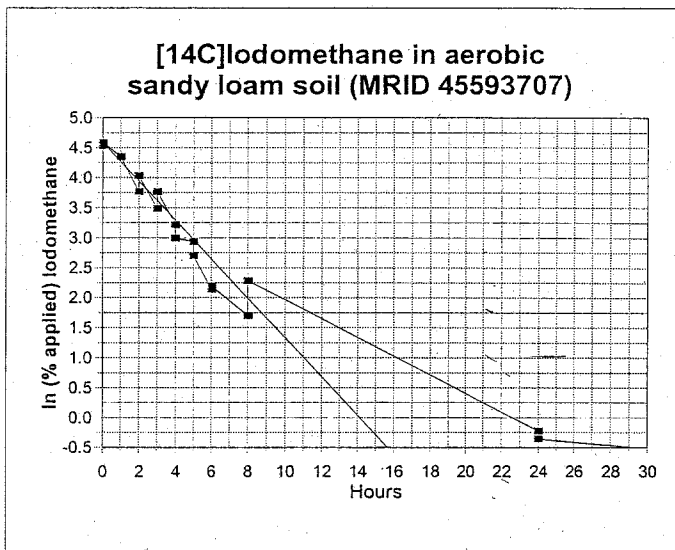
[†]Material balance = sum of soil purge, unextractable [¹⁴C] and volatiles.
 Results (% AR) from p. 39 of the study report.
 Means calculated using Corel Quattro Pro 8 program equation @avg(A1..A2).
 Standard deviations calculated using Corel Quattro Pro 8 program equation @std(A1..A2).

**Aerobic Metabolism of [¹⁴C]iodomethane in Sandy Loam Soil.
MRID 45593707**

Volatilization of [¹⁴C]iodomethane from the soil.

Half-life Determination

Iodomethane		
Day	%AR	Ln(%AR)
0	92.7	4.52937
0	97.9	4.58395
1	77.6	4.35157
1	77.3	4.34769
2	43.1	3.76352
2	56.4	4.03247
3	32.6	3.48431
3	43.2	3.76584
4	24.9	3.21487
4	19.9	2.99072
5	18.7	2.92852
5	14.9	2.70136
6	8.5	2.14007
6	9.0	2.19722
8	5.5	1.70475
8	9.8	2.28238
24	0.8	-0.22314
24	0.7	-0.35667
96	0.1	-2.30259
96	0.0	ERR
168	0.0	ERR
168	0.0	ERR
288	0.0	ERR
288	0.0	ERR



0- to 3-hour data

Regression Output:

Constant 4.594
 Std Err of Y Est 0.127
 R Squared 0.915
 No. of Observations 8
 Degrees of Freedom 6

X Coefficient(s) -0.32464
 Std Err of Coef. 0.04029

half-life 2.1 hours

*AR = Applied Radioactivity

Linear regression analysis performed using Corel Quattro Pro 8.

Results from p. 41 of study report.

Attachment 2

Transformation Pathway Presented by Registrant
Illustration of Test System
Illustration of the Analytical System

Figure 7: Proposed Environmental Fate Pathway for Iodomethane in the Aerobic Soil Metabolism Study

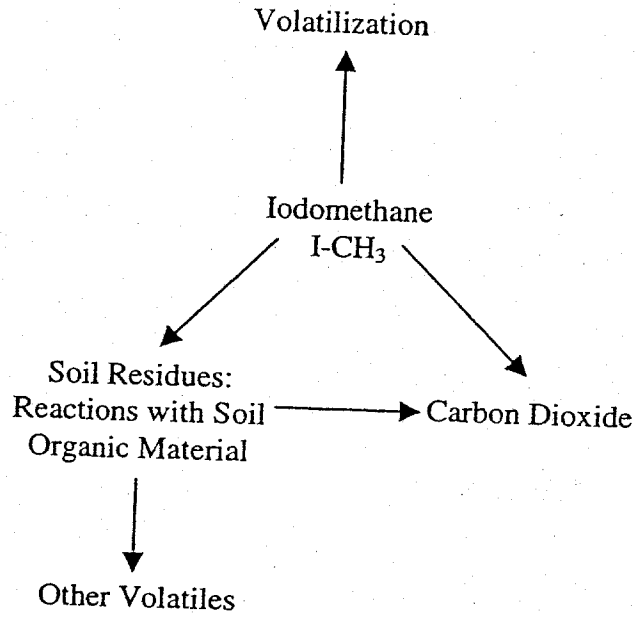


Figure 2: Volatile Sampling Assembly

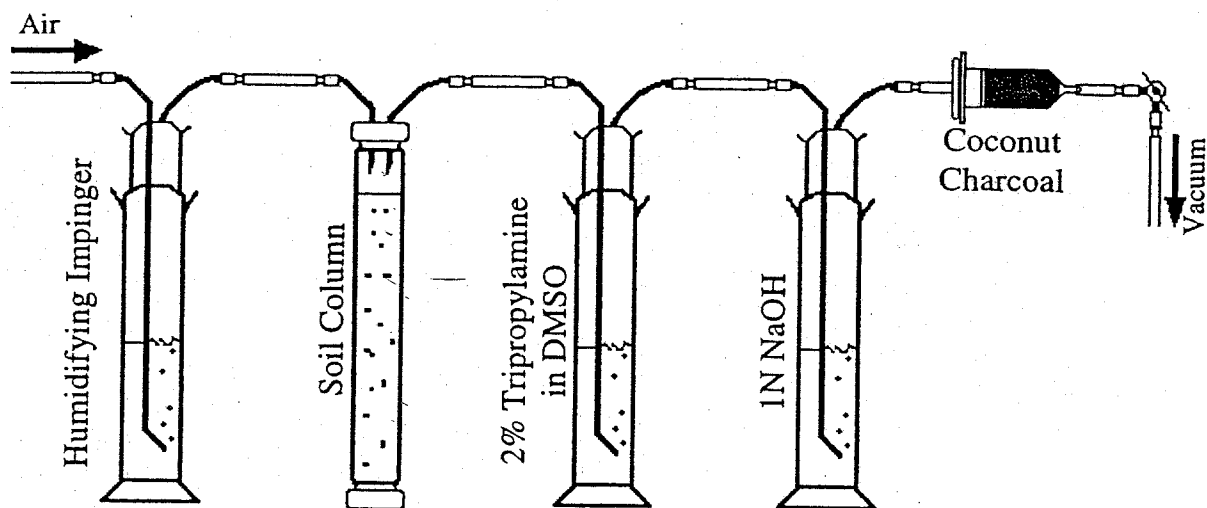


Figure 3: Heated Nitrogen Purge of Soil Column

