US EPA ARCHIVE DOCUMENT

(9-23-99)

DATA EVALUATION RECORD
DER 5

SHAUGHNESSY No.061402
COMMON NAME: Acibenzolar
CHEMICAL NAME: Benzo(1,2,3)thiadiazole-7carbothioic acid-S-methyl ester (IUPAC)
FORMULATION: Active Ingredient
DATA REQUIREMENT: (162-3) Anaerobic Aquatic Metabolism

MRID No:44537037
Barbara Schwartz. March 12, 1998. Anaerobic Aquatic Metabolism of [U-phenyl-^{14}C]CGA-245704. Performed by Environmental Safety Department Novartis Crop Protection, Inc. Greensboro, North Carolina. ABR-97122, Novartis Number 219-96. Sponsored by Novartis Crop Protection, Inc. Post Office Box 18300 Greensboro, NC 27419.

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CONCLUSIONS:

1. Study MRID #44537037 is acceptable and satisfies the anaerobic aquatic metabolism (162-3) data requirement for acibenzolar.

2. [U-phenyl-^{14}C]CGA-245704, Benzo(1,2,3)thiadiazole-7carbothioic acid-S-methyl ester, radiochemical purity 98.2% degraded with a two phase half-life of 3.98 days and 95.47 days. This half-life reflects the sum of [U-phenyl-^{14}C]CGA-245704 total recovered in the water fractions and soil extracts. A half-life was calculated for the total recovered [U-phenyl-^{14}C]CGA-245704 in the water fraction only, the two phase half-life was 2.68 days and 50.71 days. The half-life calculations were determined by fitting an exponential decay curve to the data. The major degradate (only one to exceed 10% of the total dose at any sampling interval) was CGA-210007 (the acid derivative) that reached a maximum average sum of 90.89% of the total dose after one year of incubation in the kinetic set. Unextracted [^{14}C]residues accounted for an average of 4.65% of total dose on Day 0 and averaged 5.11% of total dose during the twelve months of incubation. [^{14}C]volatiles (uncharacterized, from KOH, foam plug and foam plug rinsate) were found at a maximum of 1.36% of applied by day 130. [^{14}C]Residues associated with the water fraction of the sediment:water systems was comprised mainly of the degradate CGA-210007 and was at a maximum of 70.87% of applied by day 272 and was at 70.05% of

applied at day 360.

METHODOLOGY:

Samples (50 grams dry weight) of sieved (2 mm) sandy loam soil, Horizon A (78% sand, 10% silt, 12% clay, 0.8% OM, pH 6.3) were placed in 250 ml amber flasks. 200 mg of alfalfa was added to the soil to enhance microbial growth. The soils were flooded with 100 ml of purchased nitrogen sparged water (pH 6.9, conductivity = 0.06 mmhos, total dissolved solids 42 ppm, calcium 0.5 mg/L, Magnesium 0.1 mg/L, Sodium 0.2 mg/L, Hardness mg equivalent CaCO3/L = 2.0 mg/L) was used to flood the soils and the headspace was purged with nitrogen. The flasks were monitored for dissolved oxygen and oxidation/reduction potential as well as pH. They were placed in an incubator for a three week period at 25 ± 1C to establish anaerobic conditions. Following the three week incubation, [U-phenyl-^{14}C]CGA-245704, Benzo(1,2,3)thiadiazole-7carbothioic acid-S-methyl ester; radiochemical purity 98.2%, specific activity 83.2 uCi/mg, Novartis] dissolved in acetonitrile was added to each soil:water system at 0.407 ppm for the kinetic system and 4.07 ppm for a larger bulk set system (prepared by placing 100 grams dry weight soil into 500 ml amber bottles. The headspace was purged with nitrogen gas prior to capping the bottles with a Teflon lined septum seal and incubated at 25 ± 1°C. Three glass scintillation vial traps were connected in series with thin Teflon tubing sealed with a Teflon septum. The first trap contained two foam plugs, the next two contained 10% aqueous potassium hydroxide solution, a flow of nitrogen (7 ml/min) was maintained through the headspace of the traps. Duplicate flasks were collected at 0, 3, 7, 14, 28, 62, 130, 187, 272, and 360. The bulk sampling set days were: 0, 62, 130, 187 and 360. At each sampling interval volatiles were collected, weight measurements, anaerobicity measurements (dissolved oxygen (DO), pH and Eh), and separation of the water fraction from the soil and initiation of extraction procedures.

Soils were extracted with acetone:water (80:20 v:v) three times. The soil solvent slurries were shaken at RT for 30 minutes on a Wrist action shaker, centrifuged, decanted and samples were taken for radioassay, the remainder was stored under frozen conditions (2 ± 1°C) as were the extracted soils. A second extraction was performed after the frozen soils were allowed to reach ambient. Soils were transferred using acetone:water to centrifuge tubes and vortexed. Soil samples were then heated at 80°C overnight, centrifuged, and decanted off. The soils were then rinsed with acetonitrile, vortexed, centrifuged and decanted off. The supernatents were combined, a portion was taken for radioassay. A third extraction was carried out using 0.5 N NaOH to characterize the distribution of radiolabel in bound residue (Humin, Humic and Fulvic acid).

DATA SUMMARY:

[U-phenyl-^{14}C]CGA-245704, Benzo(1,2,3)thiadiazole-7carbothioic acid-S-methyl ester, radiochemical purity 98.2% degraded with a two phase half-life of 3.98 days and 95.47 days. This half-life reflects the sum of [U-phenyl-^{14}C]CGA-245704 total recovered in the water fractions and soil extracts. A half-life was calculated for the total recovered [U-phenyl-^{14}C]CGA-245704 in the water fraction only, the two phase half-life was 2.68 days and 50.71 days. The half-life calculations were determined by fitting an exponential decay curve to the data. CGA-245704 decreased from an average (2 replicates, total residues, Table XXIV) of 74.04% of the applied radioactivity immediately posttreatment to 55.59% at day 3, to 19.6% by day 7, to 0.45% by day 14, to 6.24% by day 28, to 2.08% by day 62, to 0.06% by day 130, 0.63% by day 187, 0.28% by day 272 and was at 0.28% by day 360.

The degradation of CGA-245704 led to the formation of multiple degradates. The major degradate (only one to exceed 10% of the total dose at any sampling interval) was CGA-210007 (the acid) that reached a maximum average sum of 90.89% of the total dose after one year of incubation in the kinetic set. The average concentration of CGA-210007 was 89.93% on Day 14, slowly declined to 78.95% by Day 187, increasing to 89.36% after 272 days, and reached a maximum concentration of 90.89% after 360 days.

A minor degradate CGA-176315 was detected once at 0.15% of applied at day 187. A degradate labeled only as "E" detected six times, once at a maximum of 0.17% of applied. A degradate labeled only as "F" was detected once at 0.03% of applied at day 0. A degradate labeled only as "G" was detected twice, one time at a maximum of 1.08% of applied at day 187. A degradate labeled only as "I" was detected twice, one time at a maximum of 0.28% of applied. A degradate "J" was detected seven times, one time at a maximum of 0.95% of applied at day 62. "K" was detected four times, one time at a maximum of 0.20% of applied at day 62.

Unextracted [^{14}C]residues accounted for an average of 4.65% of total dose on Day 0 and averaged 5.11% of total dose during the twelve months of incubation. [^{14}C]volatiles (uncharacterized, from KOH, foam plug and foam plug rinsate) were found at a maximum of 1.36% of applied by day 130. [^{14}C]Residues associated with the water fraction of the sediment:water systems was comprised mainly of the degradate CGA-210007 and was at a maximum of 70.87% of applied by day 272 and was at 70.05% of applied at day 360. During the study, the dissolved oxygen content of the treated sediment:water systems was generally 0.0 but was recorded at a maximum of 3.0 mg/L at day 46. The pH of the treated systems ranged from 5.50 to 7.8 and was at 7.57 at day 360. The redox potential of the treated systems decreased from -196 at day 0 to -236 at day 7, then ranged from 17 to -228. Material balances ranged from 91.83 to 103.8% of applied.

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DISCUSSION:

1. The soil used in the test system was from the A horizon (0-6 inch) taken from a field in North Carolina near the town of Bunn. It is recommended that a sediment type soil that is already in a reduced state with an established anaerobic population of microbes be used.

2. The water used in the test system was purchased. It is recommended that natural waters from a pond be used to reflect a more realistic scenario.

3. It is not known how the addition of 200 mg of alfalfa to the soil affected or compromised the degradation rate of acibenzolar. Alfalfa was added prior to study initiation while the system was still in an aerobic state. The study authors state "Alfalfa was used to feed the microbes and enhance the rate at which anaerobic conditions were achieved".

4. The registrant states that the maximum use rate is 0.37 lb ai./Acre.

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