111 (9-23-99)

DATA EVALUATION RECORD
DER 6

SHAUGHNESSY No.061402
COMMON NAME: Acibenzolar
CHEMICAL NAME: Benzo(1,2,3)thiadiazole-7carbothioic acid-S-methyl ester (IUPAC)
FORMULATION: Active Ingredient
DATA REQUIREMENT: (162-4) Aerobic Aquatic Metabolism

MRID No:44537038
D Adam. December 18, 1995. Degradation and Metabolism of ^{14}C-CGA-245704. Performed by Novartis Crop Protection AG (Formerly Ciba-Geigy Ltd. Crop Protection Division). Submitted by Novartis Crop Protection, Inc. (Formerly Ciba Crop Protection, Inc.) 410 Swing Road Greensboro, NC 27409. Project Number 94DA01, Novartis Number 487-94.

REVIEWED BY: Kevin L. Poff/Chemist FMB/EFED Signature: Kevin L. Poff
Date: 9/23/99

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CONCLUSIONS:

1. Study MRID #44537038 is currently considered supplemental but may be upgraded to acceptable to satisfy the aerobic aquatic metabolism (162-4) data requirement if the following information is submitted:

a) The Rhine river sediment was not adequately compared to those sediments in the continental United States.

2. In the river sediment:water system [U-phenyl-^{14}C]CGA-245704, Benzo(1,2,3)thiadiazole-7carbothioic acid-S-methyl ester; radiochemical purity >96%, specific activity 2.08 MBq/mg degraded with a registrant calculated first order half-life (DT_{50}) of 0.82 days (combined total residues from sediment and water). The half-life calculated from acibenzolar concentrations in water only was 1.18 days and in sediment only 0.36 days. The calculated DT_{90} (ln 10/k) was 2.73 days (total residues, water and sediment). In contrast, acibenzolar degraded in the pond sediment:water system with a first order half-life of 0.63 days. The half-life calculated from acibenzolar concentrations in water only was 0.57 days and in sediment only, 0.67 days. A DT_{90} in the pond system of 2.10 days was calculated using total residues and 1.88 days for the water phase and 2.23 days for the sediment phase.

METHODOLOGY:

Samples (265 g wet, 94.55 g dry weight) of Rhine river sediment (Rhine Mohlin, ((AG, CH) 8.2% sand, 67.2% silt, 24.6% clay, 4% OC, 23.1 CEC mmol/z/100B) of wet sediment was filled into 1-liter flasks at 2.5 cm; 500 ml of river water (characterization Table 2) were added to a height of 6 cm layer. The river water was filtered through a 0.2 mm sieve and the sediment through a 2 mm sieve. The sediment;water systems were equilibrated at 20 ± 1C in the dark under moistened air flow (60-100 ml/min) for a five week period before inoculation of the treatment solution. The water layer was stirred without disturbing the sediment layer with a magnetic stirrer. Ethylene glycol (50 ml) and 2N NaOH traps were connected to collect volatiles. During the five week equilibration dissolved oxygen, pH and redox potential was measured once or twice a week. Following the five week incubation, [U-phenyl-^{14}C]CGA-245704, Benzo(1,2,3)thiadiazole-7carbothioic acid-S-methyl ester; radiochemical purity >96%, specific activity 2.08 MBq/mg, (source unknown) dissolved in acetonitrile was added to the Rhine River system at 973 ppm. The concentration of acetonitrile was ≤ 0.1% of the amount of water that was present. Duplicate sediment:water and volatiles were collected at day 0, 1, 3, 7, 14, 28, 59, 91, 181, and 363. At each sampling interval pH, redoxpotential and oxygen concentration were measured from the water phase. The redoxpotential was determined in the sediment as well.

A duplicate system under identical conditions as those above were treated with soil samples (250 g wet, 111.03 g dry) of pond water and sediment (Judenteich, Rheinfelden CH) 39.5% sand, 32.8 silt, 27.7 clay, 3.1% OC, 25.2 mmol/z/100B). With an initial added concentration of 1035 ppm of acibenzolar. The sampling schedule differed from the above; samples were collected at day 0, 1, 3, 7, 14, 28, 59, 91, 181, and 350.

Water was separated from sediment by decanting and the amount of ^{14}C-CO_2 was quantified (LSC) by measuring the radioactivity before and after the addition of 1 ml HCL to an aliquot of 100 ml. Aliquots of the neutral and acidified water was submitted for HPLC analysis. The acidified paddy water was passed through a 1g Chromobond HRP Cartridge. Samples were eluted, quantified by LSC and submitted for HPLC.

Sediment was extracted with acetone and twice with acetone:water 80:20, centrifuged, and extracted again with acetone in a Soxhlet apparatus. Extracts were combined, radioactivity was quantified by LSC and an aliquot was submitted for HPLC analysis. Extracts were concentrated, a portion (100ml) was acidified to pH 2.5 and partitioned with methylenechloride 3X's. Extracts were pooled and concentrated and the radioactivity was quantitated by LSC and an aliquot was submitted for HPLC and TLC analysis. A harsh extraction procedure was completed on samples 180 (River) and 181 (Pond) with 0.6N HCL/acetone (2:8) shaken at R.T. for 24 hr.,

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centrifuged, decanted then the supernatant was analyzed by HPLC and TLC. There after the soil was shaken with distilled water for 2 hr. and centrifuged. The supernatant was decanted and the radioactivity measured in LSC. The centrifuged soil was extracted under shaking with 0.6N NaOH acetone (2:8 v/v) for 24 hr., centrifuged and the supernatant was decanted and analyzed by HPLC and TLC. Soil was submitted for combustion analysis.

DATA SUMMARY:

In the river sediment:water system [U-phenyl-^{14}C]CGA-245704, Benzo(1,2,3)thiadiazole-7carbothioic acid-S-methyl ester; radiochemical purity >96%, specific activity 2.08 MBq/mg degraded with a registrant calculated first order half-life of 0.82 days (combined total residues from sediment and water). The half-life calculated from acibenzolar concentrations in water only was 1.18 days and in sediment only 0.36 days. The calculated DT_{90} (ln 10/k) was 2.73 days (total residues, water and sediment). In contrast, acibenzolar degraded in the pond sediment:water system with a first order half-life of 0.63 days. The half-life calculated from acibenzolar concentrations in water only was 0.57 days and in sediment only, 0.67 days. A DT_{90} in the pond system of 2.10 days was calculated using total residues and 1.88 days for the water phase and 2.23 days for the sediment phase.

In the river test system, CGA-245704 (Table 10) decreased from an average (2 replicates) of 71.64% of applied at day 0, to 33.85% at day 1 and then to 1.51% of applied at day 3. The degradation led to the formation of the acid derivative CGA-210007 which reached a maximum of 95.74% of applied by day 7. The acid was at 0.68% at day 0, 61.88% at day 1, 92.87% at day 3, 95.74% by day 7, 91.77% by day 14, 89.33% by day 28, 84.48% by day 59, 76.05% by day 90, 73.76% by day 181, 56.64% by day 363.

In the pond test system, CGA-245704 (Table 13) decreased from an average (2 replicates) of 88.59% of applied at day 0, to 29.7% at day 1, 2.59% at day 3 and 0.43% at day 7. The degradate CGA-210007 (acid derivative) reached a maximum of 93.39% by day 7. CGA-210007 was at 3.55% of applied at day 0, 67.05% by day 1, 93.0% at day 3, 93.39% by day 7, 92.34% at day 14, 92.14% at day 28, 82.14% at day 59, 78.37% at day 91, 64.98% at day 181, 47.99% at day 350.

A minor degradate was in river sediment, 94DA01_A, which was detected at 0.53% of applied after 363 days. During the incubation the radioactivity in the water phase decreased slowing reaching values of 33.62% on day 363 (river) and 25.03% on day 350 of the study (pond). In contrast, extractable radioactivity from sediments were lowest at day one and increased thereafter during the incubation, reaching maximum values on day 59 of 35.26% for river and 38.18% for pond water. Thereafter the extractable radioactivity decreased to values of 23.82% (river) and 22.96% (pond) after 363 and 350 days of incubation respectively. The

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amount of non-extractable radioactivity increased to 26.39% and 36.19% for river and pond water on day 363 and 350 respectively. The recovered total radioactivity averaged 93.10 ± 7.43% of the total applied radioactivity for the river system and 96.6 ± 3.03% for the pond system.

DISCUSSION:

1. Soils were not adequately compared to those soils in the continental US.

2. Duplicate samples were presented as an averaged concentration (Tables 8-13). In order to determine variability between replicates each individual analyzed sample should be presented.