# DATA EVALUATION RECORD 5

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5-cyclopropyl-4-(2-methanesulphonyl-4-trifluoromethylbenzoyl)isoxazole
§162-3

FORMULATION--00--ACTIVE INGREDIENT

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STUDY ID 43588007
Burr, C.M., M.K. Jones, and S.E. Newby. January 30, 1995. Anaerobic aquatic metabolism of RPA 201772. Rhone Poulenc Project No. P30/045. Unpublished study performed by Rhone Poulenc, Essex, England, and submitted by Rhone Poulenc, N.C.

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## CONCLUSIONS:

### Metabolism - Anaerobic Aquatic

1. The anaerobic aquatic metabolism study is acceptable and satisfies the 162-3 data requirement.

2. $^{14}$C-Isoxaflutole [5-cyclopropyl-4-(2-methanesulphonyl-4-trifluoromethylbenzoyl)isoxazole] degraded with an estimated half-life of <2 hours in anaerobic water/sediment mixtures. Isoxaflutole was not detected after 2 hours in the anaerobic water/sediment mixture, and was not detected in the sediment at any time. Total residues in water partitioned to extractable residues on sediment with time. The behavior of isoxazole residues was primarily associated with the main degradate, RPA-202248 (**isoxaflutole with the isoxazole-ring opened**). RPA-202248 partitioned from water onto sediment, and reached a steady-state concentration in both water and sediment by 28 days. RPA-202248 reached a maximum concentration of

69 % in water by 6 hours after treatment, and declined to a relatively constant 24-31 % by 28-365 days. On sediment, RPA-202248 increased to a relatively constant 52-57 % of applied by 28-365 days. The other identified degradates were RPA-205834 [2-aminomethylene-1-cyclopropyl-3-(2-methylsulphonyl-4-trifluoromethyl-phenyl)propan-1,3-dione: **cyano-hydrated RPA-202248**] and RPA-203328 [2-methanesulphonyl-4-trifluoromethyl benzoic acid, **decarboxylated RPA-202248 and RPA-205834**]. RPA-205834 reached a maximum concentration of 7.3-25 % by 1 day in water, was 7.5-9.7 % of applied at 7-56 days in sediment, and was 3.1 % by 365 days. In water and sediment, RPA-203328 [2-methanesulphonyl-4-trifluoromethyl benzoic acid, **decarboxylated RPA-202248 and RPA-205834**], was detected at <1.3 % at any sampling interval. Bound residues increased from 0.18 % at zero time to 17 % by 365 days. Volatiles never exceeded 0.08 % at any sampling interval and the material balance ranged from 96.5-103.4 % of applied in no discernable pattern.

3. Total radioactivity in water decreased from 96.8 % at zero time to 22.6 % at 365 days. In sediment, total radioactivity increased from 2.1 % at zero time to 80.6 % at 365 days. Sediment-extractable residues increased from 1.9 at zero time to 59-67 % by 28-365 days, while bound residues increased from 0.18 % at zero time to 17 % by 365 days.

## METHODOLOGY:

Solutions containing 7.6 ppm of isoxaflutole were prepared from $^{14}$C-isoxaflutole (radiochemical purity of 98.5 %, specific activity of (51.06 uCi/mg) and non-labeled isoxaflutole (purity of 97.6 %). Sandy loam sediment (9.8 % OC, CEC 39.7, pH 6.3, Table 7.1) and associated water (pH 7.0, Table 7.2) were taken from a stream near Essex, England. The sediment was then passed through a 5 mm diameter-size sieve to remove stones and plant debris. This sediment was very similar to several different sediments that are found in the Midwestern U.S., the intended use area for isoxaflutole.

Sediment was put into flasks to 3 cm of depth and the associated stream water filled about 6 cm of depth above the sediment. The flasks were then connected to a nitrogen supply, and the flasks were then covered in foil to exclude light. Following incubation at 21 °C for 30 days, anaerobic conditions were present as evidenced by a redox potential of -420mV.

Solutions of 150 ug/ml of isoxaflutole were prepared, and 250 uL of the 150 ug/ml solution was added to each treated flask to achieve a concentration of approximately 0.19 ug isoxaflutole/g sediment. Volatility traps using 30 ml of 1,2-ethanediol and 30 ml of 1 M KOH were set up for each flask. Immediately after dosing, duplicate samples were removed at 0, 2 and 6 hours, and 1, 3, 7, 14, 28, 56, 91, 183, 274, and 365 days after dosing. The trap solutions were also removed and analyzed.

The sediment and water in the samples were separated and analyzed for parent compound and metabolites, total residues, and bound residues (sediment). LSC, HPLC, and HPLC/MS were used to quantity and identify residues. Further details about the analytical methodology may be seen in the attached Materials and Methods from the study. The specific chemical, physical, and microbiological properties of the soils used in this study may be seen in the Comments section.

DATA SUMMARY:

$^{14}$C-Isoxaflutole [5-cyclopropyl-4-(2-methanesulphonyl-4-trifluoromethylbenzoyl)isoxazole] degraded with an estimated half-life of <2 hours in anaerobic water/sediment mixtures. Isoxaflutole was not detected after 2 hours in the anaerobic water/sediment mixture, and was not detected in the sediment at any time. Total residues in water partitioned to extractable residues on sediment with time. The behavior of isoxazole residues was primarily associated with the main degradate, RPA-202248 (**isoxaflutole with the isoxazole-ring opened**). RPA-202248 partitioned from water onto sediment, and reached a steady-state concentration in both water and sediment by 28 days. RPA-202248 reached a maximum concentration of 69 % in water by 6 hours after treatment, and declined to a relatively constant 24-31 % by 28-365 days. On sediment, RPA-202248 increased to a relatively constant 52-57 % of applied by 28-365 days. on sediment. The other identified degradates were RPA-205834 [2-aminomethylene-1-cyclopropyl-3-(2-methylsulphonyl-4-trifluoromethyl-phenyl)propan-1,3-dione; **cyano-hydrated RPA-202248**] and RPA-203328 [2-methanesulphonyl-4-trifluoromethyl benzoic acid, **decarboxylated RPA-202248 and RPA-205834**]. RPA-205834 reached a maximum concentration of 7.3-25 % by 1 day in water, was 7.5-9.7 % of applied at 7-56 days in sediment, and was 3.1 % by 365 days. In water and sediment, RPA-203328 [2-methanesulphonyl-4-trifluoromethyl benzoic acid, **decarboxylated RPA-202248 and RPA-205834**], was detected at <1.3 % at any sampling interval. Bound residues increased from 0.18 % at zero time to 17 % by 365 days. Volatiles never exceeded 0.08 % at any sampling interval and the material balance ranged from 96.5-103.4 % of applied in no discernable pattern.

Total radioactivity in water decreased from 96.8 % at zero time to 22.6 % at 365 days. In sediment, total radioactivity increased from 2.1 % at zero time to 80.6 % at 365 days. Sediment-extractable residues increased from 1.9 at zero time to 59-67 % by 28-365 days, while bound residues increased from 0.18 % at zero time to 17 % by 365 days.

COMMENTS:

1. The pH of the water used in this study was 8.3, which is very conducive to degradation of isoxaflutole. When combined with the relatively high biomass content and very high organic carbon content of the sediment, the conditions of this study favored very rapid degradation of isoxaflutole. However, in this case, the results of

this study were extremely consistent with the hydrolysis (MRID 43573254) and aerobic soil metabolism (MRID 43588006) studies in this review. In the future, the registrant should use sediments that are more typical of U.S. sediments (e.g. lower organic carbon contents).

2. The biomass content of the soil in this study increased from 1338 to 1513 ug C/g soil (approximately 13 %). However, the ERCB failed to notice how the biomass content of the soil was determined for the study. In future studies, the registrant should either state or summarize how biomass is determined.

3. The chemical and physical characteristics of the sediment used in this study follow in the Table.

| Property | Soil |
|---|---|
| Particle Size Distribution | |
| Sand (%) | 78 |
| Silt (%) | 12 |
| Clay (%) | 10 |
| Textural Class | |
| USDA | Sandy loam |
| ADAS | Sandy loam |
| Organic Carbon | 9.8 |
| Organic Matter (% OC *1.72) | 16.8 |
| pH (water, 1 M KCl) | 7.0 |
| Cation Exchange (CEC, meq/100g) | 39.6 |
| Bulk Density | 0.7 |
| Biomass (ug/g soil) | |
| Beginning of study | 1338 |
| End of Study | 1513 |
| Soil Series | Tendering[1] |

[1] According to the registrant, these are comparable U.S. Soil Series.

Alvin (IL), Boyer (MI), Burnsville (MN), Council (WI), Eleva (WI), Dryden (MI), Elmdale (MI), Hillsdale (MI), Lamont (IA), Lapper (MI), Mecan (WI), Oshtermo (MI), Perrin (MI), Wyocena (WI).

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ISOXAFLUTOLE

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