DATA EVALUATION RECORD 2

5-cyclopropyl-4-(2-methanesulphonyl-4-trifluoromethylbenzoyl)isoxazole
§161-2

FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 43588004
Corgier, M.M. and A.P. Plewa. January 13, 1995. ^{14}C-RPA 201772: Photodegradation in Water. Study No. 94-11. Unpublished study performed by Rhone Poulenc, Lyon France, and submited by Rhone Poulenc, N.C.

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CONCLUSIONS:

Degradation - Photodegradation in Water

1. The aqueous photolysis study is acceptable and satisfies the 161-2 data requirement.

2. Benzyl-labeled ^{14}C-isoxaflutole [5-cyclopropyl-4-(2-methanesulphonyl-4-trifluoromethylbenzoyl)isoxazole] photolyzed in pH 5 buffer solutions with a calculated half-life of 40 hours under the xenon lamp, estimated to be 6.7 days for Florida sunlight when irradiated with Xenon light at wavelengths of >290 nm. Parent isoxaflutole declined to 39.3 % by the end of the study (54 hours of xenon light). There were only two significant degradates in the study. These were **Metabolite 20**, a photolytic rearrangement of parent isoxaflutole with both the cyclopropyl and isoxazole rings opened and the same molecular weight as parent isoxaflutole, and **Metabolite 14** (hydrated

Metabolite 20). Metabolite 20 reached up to 16.8 % by the end of the study, but could not be definitively identified since it was destroyed in preparation for HPLC/MS and NMR. The other main degradate, Metabolite 14 (hydrated Metabolite 20), reached a maximum concentration of 9.3 % by the end of the study. The registrant proposed structures for these metabolites on Page 32 of the study. The other degradates in the study (RPA-202248, RPA-205834, and RPA-203328), which were observed in metabolism studies, did not exceed 2.8 % of the applied dose at any sampling interval. There was very little volatility in the study, and only 11 % degradation in the dark controls. This is consistent with the hydrolysis study where the half-life was 11 days in pH 5 buffered solutions. The material balances ranged from 97-100 %.

METHODOLOGY:

Benzyl-labeled ^{14}C-5-cyclopropyl-4-(2-methanesulphonyl-4-trifluoromethylbenzoyl)isoxazole (RPA 201772; radiochemical purity 98%, specific activity 679 MBQ/mmol (18.35 mCi/mMol, Rhone Poulenc), was made into an acetonitrile solution containing 300 ug/ml of RPA-201772. Following sterilization of the pH 5 buffer solution (0.02 M monohydrate citric acid) and the glassware by autoclaving, duplicate one (1) ml aliquots of the acetonitrile solution were transferred to the separate photoreactors (100-ml borosilicate glass bottles connected to volatility traps), and diluted with 99 ml of the pH 5 buffer solutions. The nominal concentration of the study samples was 3 ug/ml. Duplicate test solutions were incubated in darkness in an environmental chamber and in irradiated conditions (Suntest apparatus, wavelengths >290 nm) at 25 $\pm$ 1 °C for 0, 16, 30, 40, and 54 hours, respectively. One hour of Suntest xenon lamp irradiation was estimated to be equivalent to approximately 6 hours of summer sunlight at 20-50°, meaning that the average light intensity was 612 W/m^2. Therefore, the estimated exposure times for "natural sunlight" were 0, 4, 7.5, 10, and 13 days. LSC, TLC, and HPLC were used to quantify and characterize the radioactivity from the samples. HPLC/NMR was used to confirm the identities of the residues. More details about the analytical procedure may be seen in the attachments to this DER.

DATA SUMMARY:

Benzyl-labeled ^{14}C-isoxaflutole [5-cyclopropyl-4-(2-methanesulphonyl-4-trifluoromethylbenzoyl)isoxazole] photolyzed in pH 5 buffer solutions with a calculated half-life of 40 hours under the xenon lamp, estimated to be 6.7 days for Florida sunlight when irradiated with Xenon light at wavelengths of >290 nm. Parent isoxaflutole declined to 39.3 % by the end of the study (54 hours of xenon light). There were only two significant degradates in the study. These were **Metabolite 20**, a photolytic rearrangement of parent isoxaflutole with both the cyclopropyl and isoxazole rings opened and the same molecular weight as parent isoxaflutole, and **Metabolite 14** (hydrated Metabolite 20). Metabolite 20 reached up to 16.8 % by the end of the

study, but could not be definitively identified since it was destroyed in preparation for HPLC/MS and NMR. The other main degradate, Metabolite 14 (hydrated Metabolite 20), reached a maximum concentration of 9.3 % by the end of the study. The registrant proposed structures for these metabolites on Page 32 of the study. The other degradates in the study (RPA-202248, RPA-205834, and RPA-203328), which were observed in metabolism studies, did not exceed 2.8 % of the applied dose at any sampling interval. There was very little volatility in the study, and only 11 % degradation in the dark controls. This is consistent with the hydrolysis study where the half-life was 11 days in pH 5 buffered solutions. The material balances ranged from 97-100 %.

COMMENTS:

1. The ERCB reviewer observed that once the light was filtered to remove wavelengths below 290 nm, the only absorbance of light by parent isoxaflutole was between 290 and approximately 350 nm. Even with the limited range of absorption, very rapid degradation occurred.

2. The structure of Metabolite 20 could not be verified because it was very unstable. Therefore, Metabolite 20 is probably insignificant compared to the metabolic metabolites RPA-202248 and RPA-203328.

ISOXAFLUTOLE

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