DATA EVALUATION RECORD

STUDY 11

CHEM 122990	Mesotrione	§163-1

CAS No. 104206-82-8
FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 44505202
Diaz, D. 1996. [^{14}C]AMBA: adsorption and desorption properties in soil of a ZA1296 **metabolite**. Laboratory Study ID: PMS 422. Unpublished study performed by ZENECA Inc., Richmond, CA; and submitted by ZENECA Inc., Wilmington, DE.

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CONCLUSIONS

Mobility - Leaching & Adsorption/Desorption

1. This study is ***acceptable*** and provides useful information on the soil mobility (batch equilibrium) of the mesotrione ***degradate/metabolite AMBA*** in five soils (two U.S. and three foreign). EPA Subdivision N Guideline requirements for soil mobility (batch equilibrium) for the degradate AMBA are ***satisfied***. However, the registrant should consider the critical elements in the Comments section of this report, as these may affect the validity and consequent acceptability of future study submissions.

2. Sorption of AMBA to the five tested soils was low.

The mobility of uniformly benzoyl ring-labeled [^{14}C]AMBA, at nominal concentrations of 0.02, 0.2, 1.0, and 5.0 ppm, was determined in silt loam (from Wisconsin), sandy loam (from California), British silty clay loam, French clay, and French loam soil:solution slurries that were equilibrated for 24 hours at **20 ± 2°C** in darkness. **Freundlich K_{ads}** values were **0.71** for the silt loam soil, **0.12** for the sandy loam soil (0.92% o.m.), **3.2** for the silty clay loam soil (4.5% o.m.), **0.91** for the clay soil, and **0.18** for the loam soil; corresponding **K_{oc} values for sorption were 44.9, 22.7, 122.1, 51.0, and 17.7 mL/g.** Respective 1/N values for adsorption were 0.85, 0.90, 0.83, 0.85, and 0.82. Freundlich K_{des} values determined following a single 24-hour equilibration period were 1.1 for the silt loam soil, 0.20 for the sandy loam soil, 4.1 for the silty clay loam soil, 2.0 for the clay soil, and 0.52 for the loam soil; corresponding **K_{oc} for values desorption were 68.9, 37.9, 155.9, 109.3, and 50.2 mL/g.** Respective 1/N values for desorption were 0.80, 0.84, 0.77, 0.78, and 0.76. The reviewer-calculated coefficients of determination for the relationships K_{ads} *vs.* organic matter, K_{ads} *vs.* soil pH, and K_{ads} *vs.* clay content were 0.84, 0.78, and 0.089, respectively.

METHODOLOGY

Based on the results of a preliminary study of the adsorption of the mesotrione degradate uniformly benzoyl ring-labeled [^{14}C]AMBA {2-amino-4-(methylsulfonyl)benzoic acid; radiochemical purity >97%, specific activity 38.9 mCi/mmol; p. 12}, an equilibration period of 24 hours was selected for both the adsorption and desorption phases of the definitive study for all five soils utilized (p. 24). In a preliminary study, adsorption of the test compound to the Teflon tubes was not observed in samples treated at the 5.0 ppm application rate (p. 23); however, some adsorption of the test compound to the tubes did occur at the 0.02 ppm application rate (see Comment #9). A preliminary stability study indicated that the test compound was stable following adsorption and desorption (p. 23).

For the adsorption phase of the definitive study, aliquots (9 mL) of 0.01 M $CaCl_2$ solution were added to Teflon centrifuge tubes containing samples (4 g) of sieved (2 mm) silt loam (from Wisconsin), sandy loam (from Visalia, California), British silty clay loam, French clay and French loam soils (Table I, p. 28) and the samples were pre-equilibrated on a shaker (p. 17). The soil:solution slurries were treated with uniformly benzoyl ring-labeled [^{14}C]AMBA, dissolved in acetonitrile and 0.01 M $CaCl_2$ (1 mL), at nominal concentrations of 0.02, 0.2, 1.0, and 5.0 ppm (p. 15). Duplicate tubes were prepared for each soil type/treatment combination. The soil:solution slurries (1:2.5, w:v) were equilibrated by shaking for 24 hours in darkness at 20 ± 2°C. Following the adsorption equilibration period, soil:solution slurries were centrifuged and the supernatants were decanted. Duplicate aliquots were analyzed for total radioactivity by LSC; the limit of detection was twice background (Appendix A, p. 53).

For the desorption phase of the definitive study, a volume of pesticide-free 0.01 M $CaCl_2$ solution equivalent to the volume that was decanted following adsorption was added to the soil pellets from the adsorption phase (pp. 17, 18). The soil:solution slurries were equilibrated by shaking at 20 ± 2°C in darkness for 24 hours. Following the equilibration period, the soil:solution slurries were centrifuged and the supernatants were decanted. Duplicate aliquots of the desorbate were analyzed for total radioactivity by LSC.

To determine the stability of the test compound in soil:solution slurries under test conditions, single aliquots of supernatant (following each sorption period) from samples treated at 5.0 ppm were analyzed by HPLC (Alltech C18 column) using a mobile phase gradient of water:acetonitrile (0.1% H_3PO_4; 90:10 to 40:60, v:v) with radioactive flow detection (p. 21). Eluent fractions were collected at one-minute intervals and analyzed by LSC. Samples were co-chromatographed with nonradiolabeled reference standards which were visualized with UV (210 and 254 nm) light.

To determine the stability of the test compound in the slurries, a single replicate (for each soil) of the post-desorption soil samples treated at the highest concentration (5.0 ppm) was extracted three times with ethyl acetate (p. 19). Supernatants were decanted and analyzed by LSC and HPLC as described previously. The silty clay loam and clay soils (5.0 ppm) were further extracted three times with 1 M ammonium acetate (pH 5) followed by three extractions with 0.5 *N* NaOH and three extractions with 1 *N* HCl. Aliquots of the NaOH extracts were acidified to pH 1 (HCl) and partitioned three times with ethyl acetate prior to HPLC analysis as previously described.

Following extraction, soil samples were air dried and analyzed for total radioactivity by LSC following combustion (p. 20); the reviewer could not confirm that data were corrected for combustion efficiency.

DATA SUMMARY

The mobility of uniformly benzoyl ring-labeled [^{14}C]AMBA (radiochemical purity >97%), at nominal concentrations of 0.02, 0.2, 1.0, and 5.0 ppm, was determined in silt loam (from Wisconsin), sandy loam (from California), British silty clay loam, French clay, and French loam soil:solution slurries that were equilibrated for 24 hours at 20 ± 2°C in darkness. Freundlich K_{ads} values were 0.71 for the silt loam soil, 0.12 for the sandy loam soil (0.92% o.m.), 3.2 for the silty clay loam soil (4.5% o.m.), 0.91 for the clay soil, and 0.18 for the loam soil; corresponding K_{oc} values were 44.9, 22.7, 122.1, 51.0, and 17.7 mL/g (Table XV, p. 42). Respective 1/N values for adsorption were 0.85, 0.90, 0.83, 0.85, and 0.82 (Table XIV, p. 41). The reviewer-calculated coefficients of determination for the relationships K_{ads} *vs.* organic matter, K_{ads} *vs.* soil pH, and K_{ads} *vs.* clay content were 0.84, 0.78, and 0.089, respectively. Freundlich K_{des} values determined following a single 24-hour equilibration period were 1.1 for the silt loam soil, 0.20 for the sandy loam soil, 4.1 for the silty clay loam soil, 2.0 for the clay soil, and 0.52 for the loam soil; corresponding K_{oc} values were 68.9, 37.9, 155.9, 109.3, and 50.2 mL/g. Respective 1/N values for desorption were 0.80, 0.84, 0.77, 0.78, and 0.76.

Data indicating the percentages of the applied radioactivity adsorbed to and desorbed from the five soils (across all application rates) were not provided. Total radioactivity data (dpm) for adsorption of the test compound to the soil, desorption of the test compound from the soil, and nonextractable radioactivity were provided, along with the initial radioactivity in the samples, for each soil type/treatment rate combination (Tables III-VII, pp. 30-34); concentration data for adsorption and desorption of the test compound to and from the soils were also provided (Tables IX-XIII, pp. 36-40).

The stability of benzoyl ring-labeled [^{14}C]AMBA under test conditions (5.0 ppm treatment rate) was confirmed by analysis of adsorption and desorption supernatants, and the ethyl acetate extracts by HPLC. The test compound was present at 96.5-99.1% of the applied radioactivity for adsorption and desorption supernatants, and was 91.9-99.5% of the applied radioactivity for ethyl acetate extracts (Table VIII, p. 35).

Material balances (for individual replicates across all application rates) were 97.3-103.6% for the silt loam soil, 96.1-105.1% for the sandy loam soil, 94.2-104.8% for the silty clay loam soil, 91.7-96.5% for the clay soil, and 93.6-103.0% for the loam soil (Tables III-VII, pp. 30-34).

COMMENTS

1. The stability of the test compound in the soil:solution slurries treated at 0.02, 0.2, and 1.0 ppm could not be determined; only samples treated at 5.0 ppm were characterized by HPLC analysis.

2. Method detection limits were not reported for LSC or HPLC analyses. Method detection and quantitation limits should be reported to allow the reviewer to evaluate the adequacy of the method for determination of the test compound.

3. The solubility of AMBA in water or in the test solution was not reported.

4. The reviewer confirmed that one of the soils (silt loam soil from Wisconsin) utilized in this study was the same type of soil used in two aerobic soil metabolism studies (MRIDs 44505130 and 44373531).

5. The soil series names was not reported for the domestic (U.S.) soils. Instead, the soils were referred to by their geographical locations (Table I, p. 28).

6. The study was conducted with two domestic (U.S.) and three foreign (one from the U.K. and two from France) soils. The EPA strongly prefers the use of domestic soils in mobility studies. However, EPA will accept foreign soils for two of the four soils required if the soils are characterized according to the USDA system. All soils were characterized according to the USDA system (Table I, p. 27).

7. The reviewer notes that the sandy loam soil had a pH of 8.2 and that this was the only soil with <1% organic matter (Table I, p. 28). Subdivision N Guidelines require the use of soils with a pH between 4 and 8 and at least one soil with an organic matter content of less than 1% for mobility studies.

8. Data indicating the percentages of the applied radioactivity adsorbed to and desorbed from the five soils (across all application rates) were not provided. Generally, batch equilibrium studies include the percentages of the applied radioactivity data for adsorption, desorption, and nonextractables.

9. The study author stated that in the preliminary study there was an indication that AMBA slightly adhered to the tube walls at the lowest (0.02 ppm) treatment rate; however, the mass balances for the definitive study indicated that AMBA preferentially adsorbed to the soil instead of the tube walls (p. 23).

10. The study author stated that Freundlich constants for both adsorption and desorption were calculated without correction for the slight decomposition of AMBA in the supernatants or extracts over the course of the experiment (p. 24).

11. The study author stated that the radiolabeled test substance was enriched with ^{13}C in the exocyclic carbonyl group to aid in the mass spectral characterization of metabolites (p. 12); however, mass spectral analysis was not conducted in this study.

MRID# 44505202

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