DATA EVALUATION RECORD

STUDY 10

CHEM 122990 Mesotrione §163-1
CAS No. 104206-82-8
FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 44505201
Diaz, D. 1996. [^{14}C]MNBA: adsorption and desorption properties in soil of a ZA1296 ***metabolite***. Laboratory Study ID: PMS 411; Report No.: RR 96-008B. Unpublished study performed by ZENECA Inc., Richmond, CA; and submitted by ZENECA Inc., Wilmington, DE.

DIRECT REVIEW TIME = 52.5 Hours

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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 MNBA*** in five soils (two U.S. and three foreign). EPA Subdivision N Guideline requirements for soil mobility (batch equilibrium) for the degradate MNBA 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 MNBA to three of the five test soils was essentially negligible within method limits.

   The mobility of uniformly benzoyl ring-labeled [^{14}C]MNBA, at nominal concentrations of 0.02, 0.2, 1.0, and 5.0 ppm, was determined in silt loam (U.S.), sandy loam (U.S.), silty clay loam (British), clay (French), and loam (French) soil:solution slurries that were equilibrated in darkness for 24 hours at **20 ± 2°C**. **Freundlich K_{ads} values** were **0.05** for the silt loam soil, **0.16** for the silty clay loam soil, and were **estimated as <0.1 for the sandy loam, clay, and loam soils**; corresponding **K_{oc} values** were **3.2 and 6.1 mL/g**, and estimated values were **less than 20, 6, and 10 mL/g**, respectively. The 1/N values for adsorption were 0.61 for the silt loam, and 0.32 for the silty clay loam soil; 1/N values were not available for the remaining three soils. Freundlich K_{des} values determined following a 24-hour equilibration period were 0.21 for the silt loam soil, 0.41 for the silty clay loam soil, and were estimated as <0.1 for the sandy loam, clay, and loam soils; corresponding K_{oc} values were 13.3 and 15.6 mL/g, and were estimated as <20 mL/g for the remaining three soils. The 1/N values for desorption were 0.70 for the silt loam soil, and 0.38 for the silty clay loam soil; 1/N values were not available for the remaining three soils. *This study essentially demonstrates that, within method limits, MNBA was essentially unretained by these five soils with sorption coefficients approaching zero.*

METHODOLOGY

Based on the results of a preliminary study of the adsorption of the mesotrione degradate uniformly benzoyl ring-labeled [^{14}C]MNBA (4-(methylsulfonyl)-2-nitrobenzoic acid; radiochemical purity >98%, specific activity 37.1 mCi/mmol; p. 13) to silt loam (from Wisconsin), sandy loam (from Visalia, California), British silty clay loam, French clay, and French loam soils, an adsorption equilibration period of 24 hours was chosen for all soils; for desorption, a 24-hour equilibration period was chosen for all soils (p. 25). In a preliminary study, degradation of the test compound in the soil:solution slurries was not observed at the high treatment rate (p. 19). In a preliminary study, adsorption of the test compound to the Teflon centrifuge tubes was not observed (p. 24).

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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 (4.0 g) of air-dried, sieved (2 mm) silt loam, sandy loam, silty clay loam, clay, and loam soils (soil properties in Table I, p. 29) and the samples were pre-equilibrated on a shaker (p. 18). The soil:solution slurries were treated with uniformly benzoyl-ring labeled [^{14}C]MNBA, 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 (pp. 13-14, 16). Duplicate tubes were prepared for each soil type/treatment rate combination (Table II, p. 30). The soil:solution slurries (1:2.5, w:v) were equilibrated by shaking in darkness for 24 hours at 20 ± 2°C. Following the adsorption equilibration period, soil:solution slurries were centrifuged and the supernatants were decanted. Duplicate aliquots of the supernatants were analyzed for total radioactivity by LSC (p. 19); the limit of detection was twice background (Appendix A, p. 49).

For the desorption phase of the definitive study, an aliquot of pesticide-free 0.01 M $CaCl_2$ solution equivalent to the volume of solution removed following adsorption was added to the soil from the adsorption phase of the study (pp. 18, 19). The soil:solution slurries were equilibrated by shaking in darkness for 24 hours at 20 ± 2°C. Following equilibration, the soil:solution slurries were centrifuged and the supernatants decanted. Duplicate aliquots of the desorbates 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 C-18 column) using a mobile phase gradient of water:acetonitrile (0.1% H_3PO_4; 95:5 to 50:50, v:v; pp. 21, 22) with radioactive flow detection (p. 19). 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. Samples were analyzed immediately or stored frozen until analysis.

To determine the stability of the test compound in the slurries, a single sample (for each soil) from the desorption phase (5.0 ppm treatment) was extracted three times by shaking with acidified (1 *N* HCl) ethyl acetate, followed by centrifugation (p. 19). Extracts were analyzed by LSC and HPLC as previously described.

Following the desorption phase, soil samples were analyzed for total radioactivity by LSC following combustion (p. 20); it was not reported whether the data were corrected for combustion efficiency.

DATA SUMMARY

The mobility of uniformly benzoyl ring-labeled [^{14}C]MNBA (radiochemical purity >98%), 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 (1:2.5, w:v) that were equilibrated in darkness for 24 hours at 20 ± 2°C. Freundlich K_{ads} values were 0.05 for the silt loam soil (2.7% o.m.), 0.16 for the silty clay loam soil (4.5% o.m.), and were estimated as <0.1 for the sandy loam (0.92% o.m.), clay (3.1% o.m.), and loam soils (1.8% o.m.) (Table XIII, p. 41); corresponding K_{oc} values were 3.2 and 6.1 mL/g, and estimated values were less than 20, 6, and 10 mL/g, respectively. The 1/N values for adsorption were 0.61 for the silt loam and 0.32 for the silty clay loam soil (Table XI, p. 39); 1/N values were not available for the remaining three soils. Freundlich K_{des} values determined following a 24-hour equilibration period were 0.21 for the silt loam soil, 0.41 for the silty clay loam soil, and were estimated as <0.1 for the sandy loam, clay, and loam soils; corresponding K_{oc} values were 13.3 and 15.6 mL/g, and were estimated as <20 mL/g for the remaining three soils. The 1/N values for desorption were 0.70 for the silt loam soil and 0.38 for the silty clay loam soil; 1/N values were not available for the remaining three soils.

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. 31-35); concentration data for adsorption and desorption of the test compound to and from the silt loam and silty clay loam soils were also provided (Tables IX-X, p. 37-38).

The stability of benzoyl ring-labeled [^{14}C]MNBA under test conditions (5.0 ppm treatment rate; single replicates) was confirmed by analysis of adsorption and desorption supernatants, and the ethyl acetate extracts by HPLC. The test compound was present at 98.8-99.6% of the applied radioactivity for adsorption supernatants and 98.2-100% of the applied radioactivity for desorption supernatants (Table VIII, p. 36). The test compound was present at 92.3% and 93.5% of the applied radioactivity for ethyl acetate extracts of the silty clay loam and the silt loam soils, respectively; ethyl acetate extracts from the sandy loam, clay, and loam soils were not analyzed because the amount extracted was less than 5% of the total applied radioactivity.

Material balances (for individual replicates across all application rates) were 97.2-100.2% for the silt loam soil, 99.1-112.2% for the sandy loam soil, 99.4-112.6% for the silty clay loam soil, 99.1-112.0% for the clay soil, and 102.0-113.1% for the loam soil (Tables III-VII, pp. 31-35).

COMMENTS

1. The reviewer could not calculate the coefficients of determination for the relationships K_{ads} *vs.* organic matter, K_{ads} *vs.* pH, and K_{ads} *vs.* clay content (%) because Freundlich adsorption and desorption coefficients for three of the five soils studied could not be accurately determined. The study author stated that Freundlich K_{ads} values were estimated as <0.1 for the sandy loam, clay, and loam soils because the test compound did not adsorb to these soils (p. 26; Table XII, p. 40).

2. 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.

3. The method detection limit for LSC was reported as twice background (Appendix A, p. 49); however, method detection limits were not reported for HPLC and limits of quantitation were not reported for LSC or HPLC. Method detection limits and limits of quantitation should be reported to allow the reviewer to evaluate the adequacy of the method.

4. The solubility of MNBA in water or in the test solution was not reported.

5. 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).

6. The soil series names were not reported for the domestic (U.S.) soils. Instead, the soils were referred to by their geographical locations (Table I, p. 29). Subdivision N Guidelines require that the soil series names be reported for the test soils.

7. The study was conducted with two domestic (U.S.) and three foreign (one from the U.K., 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, and only if, the soils are characterized according to the USDA system. The reviewer confirmed that the soils were characterized using the USDA classification system based on information provided in Table I (p. 29).

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 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. 29). 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.

10. 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. 13). However, mass spectral analysis was not conducted in this study.

MP# 44505201

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