DATA EVALUATION RECORD

STUDY 3

CHEM 129016	XRD-498	§161-3

STUDY ID 41931730
Wolt, J.; Shepler, K.; and Yung, V. PHOTODEGRADATION OF [^{14}C-ANILINE] XRD-498 ON SOIL BY NATURAL SUNLIGHT. Performed by Pharmacology and Toxicology Research Laboratory, Richmond, CA under PTRL Report No. 258W; Submitted by DowElanco; Midland, MI under Dow Protocol No. 90096; Study completed on 16 May 1991; Received by EPA 19 June 1991.

DIRECT REVIEW TIME = 1.0 day

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CONCLUSIONS:

The photodegradation on soil study alone is not acceptable to meet Subdivision N Data Requirement. However, in combination with MRID's 41931728 and 41931729) the photodegradation on soil data requirement is fulfilled. No further photodegradation on soil data for XRD-498 is required at this time.

This soil photodegradation study of XRD-498 (the [^{14}C-aniline]XRD-498 portion of the material) appears to exhibit limited degradation in both light exposed and dark control samples. The reported extrapolated half-lives were 80 days and 127 days for light exposed and dark control data, respectively. The photodegradates were CO_2 (not >1.7% of applied) and numerous unidentified degradates which were formed in insignificant amounts (none >5% of applied radioactivity)(See Table II). The material balance averaged 101.0 ± 5.3% for the testing period. The photodegradation of the ^{14}C-pyrimidine portion of XRD-498 is discussed in DER-Study 2 and 3 of this review. Very similar results were reported.

MATERIALS AND METHODS:

Test Material: [^{14}C-aniline]XRD-498 was used which was reported to have a specific activity of 28.0 mCi/mmol and radio chemical purity of 98.0%.

An unlabeled standard was obtained from DowElanco for analytical purposes. The purity of this standard was 99.7% which was confirmed by TLC analysis.

Stock Solution: Stock solution was prepared by adding an acetone solution of [^{14}C-aniline]XRD-498 (1.35 mg in 463 µL, 2.55 x 10^8 dpm) to acetone (5537 µL). The solution was mixed prior to use.

See Table I for soil characterization.

Sampling: 0, day 5, day 10, day 17, day 24, and day 31

Test System: See Figure 4.

The irradiation source was natural sunlight. The test was conducted in Richmond, CA at 37.45°N latitude and 122.26°W longitude.

METHODOLOGY:

Silt loam soil from Wayside, MS was passed through a 2 mm sieve. Aliquots of silt loam soil (3.1 gm) were weighed onto 50 mm Petri dishes. Distilled water (3 mL) was added to each dish and the slurries allowed to air dry, forming a thin soil layer (≈0.5mm) on the bottom surface of each petri dish. 588 µL of water was added to each dish prior to application of test material to achieve 75% field capacity.

Aliquots (200 µL) of the [^{14}C-aniline]XRD-498 stock solution were transferred onto each dish as evenly as possible in a circular pattern. After treating the petri dishes with the proposed application rate of 14.6 ppm, the plates were then placed in a quartz covered stainless steel temperature controlled chamber in natural sunlight. The temperature was continuously monitored and recorded at 20 minute intervals throughout the study (See Table IV). The mean temperature for the light exposed and dark control samples was 25.9 ± 0.7°C and 24.8 ± 0.2°C, respectively.

Ethylene glycol, 10% H_2SO_4, and 10% NaOH were used to trap volatile organic compounds and CO_2, respectively. Ambient air was drawn through sterilized bacterial filters into both light and dark sample chambers into separate sets (light and dark) of the three traps. Gas dispersion tubes were used to maximize the trapping efficiency. Trapping efficiency for $^{14}CO_2$ was determined, using the identical system, by introducing a measured amount of ^{14}C-sodium bicarbonate as an aqueous solution into a petri dish and adding an excess of glacial acetic acid while air was being drawn through the system.

Sunlight intensity and cumulative sunlight energy were measured (250-700 nm integration range) and recorded at 10 minute intervals throughout the study using an International Light Photodetector equipped with a Model SED 400 probe oriented at a 30 degree angle with respect to the vertical and located approximately four feet above and six feet behind the soil chambers. The photodetector was calibrated by the manufacturer. All soil chambers were oriented in the same manner such that the chambers were perpendicular to the sun's path. Cloud cover data was provided by the City of Richmond Public Works Department. Experiments were carried out in Richmond, CA at latitude 37.45N longitude 122.26W for a period of 30 days.

Duplicate light exposed and dark control samples were removed from their respective soil chambers at the following times - Day 0, 5, 10, 17, 24, and 31. The samples were extracted immediately with acetone/water/acetic acid, 90:5:5 (v/v/v) and the extracts analyzed. Aliquots of the extracts were subjected to LSC (3 x 0.5 mL) and then analyzed by HPLC. Selected samples were analyzed by 2-dimensional TLC.

Total volumes in each gas dispersion trap were measured and aliquoted (3 x 0.5 mL) for radioassay (LSC) on each sampling day. Recovered radiocarbon from each trap was divided proportionately among the contributing samples.

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DATA SUMMARY:

The half-life for [^{14}C-aniline]XRD-498 when applied to silt loam soil and exposed to natural light was extrapolated to be 80 days from a first-order plot. The half-life of [^{14}C-aniline]XRD-498 in the dark controls was 127 days. These values were considered by the author to overestimate the reactivity of XRD-498 since unextracted radiocarbon (Tables VI) may consist largely of unreacted parent material based on soil properties.

There was decreased extractability of XRD-498 with aging in soil which was well documented prior to initiation of the study. Soils for sampling time of day 31 exhibited >10% non-extractable ^{14}C. However, these were subjected to additional extraction in an attempt to desorb additional radiocarbon. Exhaustive extraction released levels of radiocarbon not extracted initially. TLC analysis of selected additional extracts shows a single band with the same Rf as XRD-498 in both light and dark samples.

The material balance was determined by summing the radiocarbon remaining in soil, the soil extracts, and radiocarbon volatilized. Radiocarbon recoveries averaged 101.0 ± 5.3% based on nominal applied radioactivity.

[^{14}C-aniline]XRD-498 does appear to photodegrade slowly when applied to silt loam soil, producing carbon dioxide and numerous low yield (none >3.0% of applied) unidentified degradates. The data obtained in this study was consistent with other photodegradation data for XRD-498.

COMMENTS:

1. The experiments were carried out in Richmond, CA at latitude 37.45N longitude 122.26W for a period of 30 days (19 October to 19 November) using natural sunlight. The intensity of sunlight in late fall is less than the intensity of sunlight during the summer growing season. Therefore, this study did not reflect the greatest intensity of sunlight and perhaps the greatest amount of photodegradation that will occur in the environment. No comparison of sunlight intensity was given for the two seasons of year.

2. No ultraviolet spectrum of XRD-498 in water was provided from 290nm to 750nm.

3. Due to the widely varying radiocarbon recoveries obtained in the study, the half-life was calculated using the percent [^{14}C-aniline]XRD-498 detected in soil extracts by HPLC expressed as a percent of recovered radiocarbon for each sample.

4. The correlation coefficient for the calculated half-lives were 0.51 and 0.57 for the light exposed samples and the dark samples, respectively. The authors stated these reflected the relative small amount of degradation that occurred over the 30 day testing period. Based on the limited degradation of XRD-498, EFGWB believes additional data is not needed to understand its photodegradation.

TABLE 1

% sand	36%
% silt	52%
% clay	12%
% organic material	0.5%
% pH	7.4%
CEC	8.8 meq/100g

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