3M
Form 6747-11-A

TECHNICAL REPORT SUMMARY

Date: 1/10/79

TO: TECHNICAL COMMUNICATIONS CENTER – 201-2CN

(Important – If report is printed on both sides of paper, send two copies to TCC.)

Division: Environmental Laboratory (EE & PC)	Dept. Number: 0535
Project: Premanufacturing Notice FC-790	Project Number: 9970012600
Report Title: Distribution Coefficient of FM 3925 in n-Octanol/Water	Report Number: 015
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Author(s): E. A. Reiner	Employee Number(s): 47816
Notebook Reference: 48838, pp. 6, 8, and 9.	No. of Pages Including Coversheet:

SECURITY ▶ ☒ Open (Company Confidential) ☐ Closed (Special Authorization)

3M CHEMICAL REGISTRY ▶ New Chemicals Reported ☐ Yes ☒ No

KEYWORDS: (Select terms from 3M Thesaurus. Suggest other applicable terms.)

Distribution Coefficient

Partition Coefficient

Bioconcentration

Fluorochemical

CURRENT OBJECTIVE:

To determine the distribution coefficient of FM 3925 between n-octanol and water.

REPORT ABSTRACT: (200-250 words) This abstract information is distributed by the Technical Communications Center to alert 3M'ers to Company R&D. It is Company confidential material.

The distribution coefficient of FM 3925, lot 505, between n-octanol and water was measured according to a modification of the Environmental Laboratory procedure. The distribution coefficient was determined to be 56,800. This result suggests that this material is likely to accumulate in aquatic organisms to levels above the ambient aquatic concentration.

Information Liaison Initials: SKW

Exhibit 2795
State of Minnesota v. 3M Co.,
Court File No. 27-CV-10-28862

3M_MN01640028

Introduction

Living organisms possess the ability to concentrate and accumulate lipophilic organic compounds either directly from their environment or from their food source, a phenomenon which is well document (1,2).

In 1975 Neely, et al (3), demonstrated that the partition coefficient can be used to estimate this bioconcentration potential. As a result, it has become a common procedure to estimate bioconcentration potential from a compound's partition or distribution coefficient.

Methods

The distribution coefficient of FM 3925, lot 505, was determined by a modification of the 3M Environmental Laboratory protocol. The modifications and unique features of this study are described below.

FM 3925, lot 505, was used in the distribution coefficient determination as it was received without any further purification. Gas chromatographic analysis of this compound shows that this compound elutes as three overlapping peaks (Figure 1). The combined area of these peaks was used in the determination of sample concentrations.

Sample analysis was performed on a Hewlet-Packard Model 5713 gas chromatograph, a ^{63}Ni electron capture detector. Separations were obtained using a 6 ft. by 1/8 in. O.D. stainless steel column containing 10% Carbowax 20M on 60/80 mesh Chromosorb W-AW. Injection port, oven and detector temperatures were set at 200°, 180°, and 300° C., respectively. The gas flow rate was 40 ml/min. of a 95% Argon 5% methane mixture.

Two 25-ml n-octanol solutions of FM 3925 were added to amber glass jars, each containing 900 ml of deionized water. These n-octanol solutions contained 1000 ppm (0.018M) and 2000 ppm (0.036M) of FM 3925. High FM 3925 concentrations were used because earlier attempts at determining the distribution coefficient with concentrations below 0.01M were unsuccessful since our analytical procedures were not sufficiently sensitive to detect the FM 3925 re-extracted from the water phase into ethyl acetate.

The jars used in the distribution coefficient determination were shaken ∿16 hours at room temperature (∿22° C.). The octanol phase was drawn off and the water phase was placed in 250-ml polycarbonate centrifuge tubes and centrifuged at 10,000 rpm (13,700 x G) for 15 minutes. Following centrifugation, 600 ml of the water phase was transferred by pipet to a separatory funnel where it was, in turn, drawn off into a second separatory funnel to ensure the removal of octanol contamination transferred by the pipetting procedure.

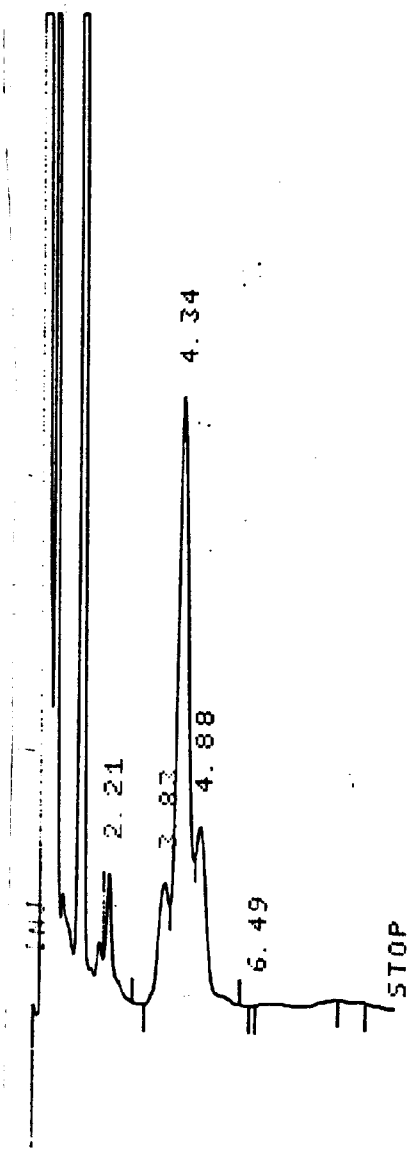

Figure 1. Gas Chromatogram of a 5 µl injection of a 1 ppm solution of FM 3925 (#081, 7/13/78). Peaks at 3.83, 4.34, and 4.88 minutes represent FM 3925. Gas chromatographic conditions are given in text.

The water phase was extracted three times with ethyl acetate, and the ethyl acetate extract was concentrated to 15 ml at room temperature under nitrogen. The FM 3925 concentration in the ethyl acetate was determined by electron capture gas chromatography. A typical gas chromatogram of the water phase is shown in Figure 2. The octanol phase from the distribution coefficient determination was not analyzed for FM 3925 content. Its FM 3925 concentration was assumed to be unchanged. This assumption was justified since measurement of the FM 3925 content from the octanol phase from previous attempts to determine the distribution coefficient had shown that the FM 3925 concentration was not detectably lowered by water extraction. A gas chromatogram showing the octanol phase after extraction is shown in Figure 3.

Results and Discussions

FM 3925 concentrations in the water phases shaken with the 1000 ppm and 2000 ppm FM 3925 n-octanol solutions were 0.0189 ppm and 0.033 ppm respectively. This data corresponds to distribution coefficients of 52,900 and 60,600. The average distribution coefficient for FM 3925 in n-octanol/water is 56,800.

Based on the method of Neely, Branson & Blair (3), this corresponds to a predicted bioconcentration factor between fish muscles and water of 500. Our laboratory findings on the structurally similar compound, FM 3422, gave values in this same range (4). Total body accumulation of FM 3422 into juvenile channel catfish indicated a bioconcentration factor of ∿500. Upon transfer to clear water, there was 50% clearance of the bioconcentrated FM 3422 within four days.

The lower distribution coefficient for FM 3925 compared to FM 3422 (56,800 vs. >100,000), and the greater water solubility of FM 3925 (0.82 mg/l vs. 0.05 mg/l) (5), suggest that FM 3925 will bioconcentrate to a lesser extent than FM 3422.

References:

(1) Burnett, R. Science 174:606, 1971.

(2) Gustafson, C. G. Env. Sci. & Tech. 4:814, 1970.

(3) Neely, W. B., D. R. Branson, and G. E. Blair, Env. Sci. & Tech. 8:1113, 1974.

(4) Welter, A. N. Evaluation of the Bioconcentration Potential of FM 3422, 3M Technical Report, August 16, 1978.

(5) Welter, A. N., E. A. Reiner, Solubility of FM 3925, 3M Technical Report, January 8, 1979.

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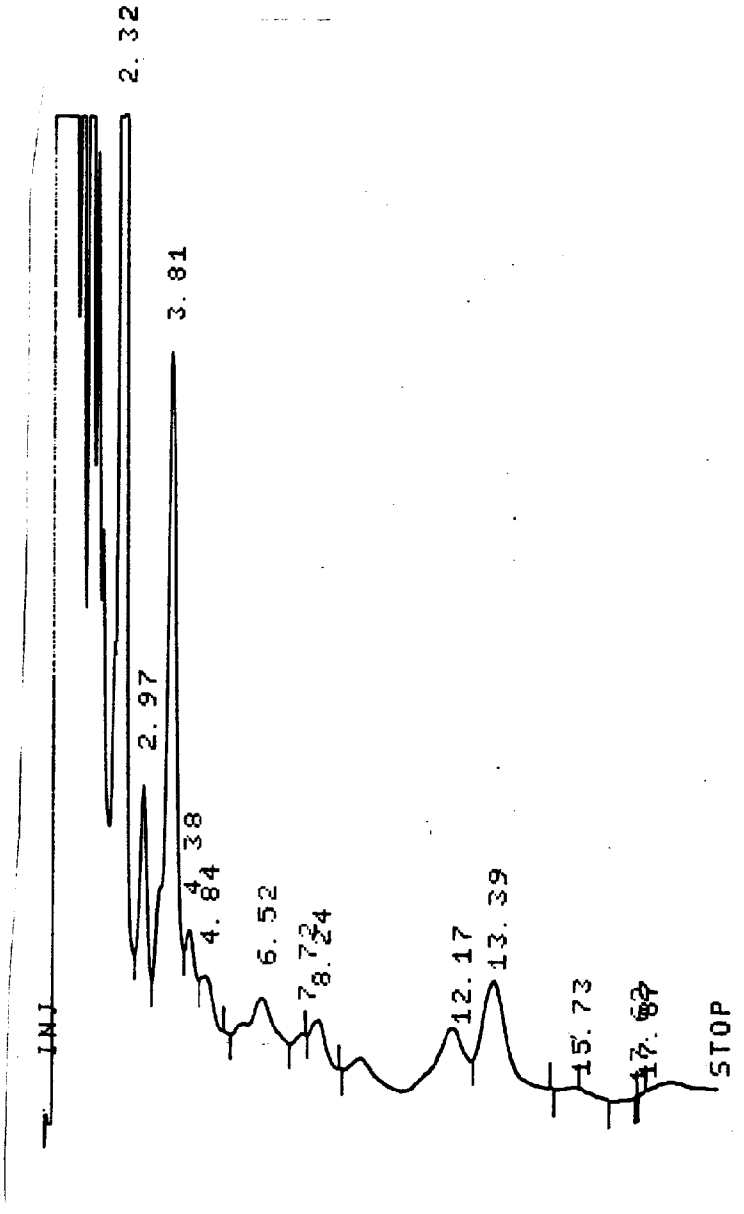

Figure 2. Gas Chromatogram of the water phase from an n-octanol/water distribution coefficient for FM 3925 (#082, 7/13/78). Peaks at 3.81, 4.38, and 4.84 minutes are taken to represent FM 3925. Gas chromatographic conditions are given in text.

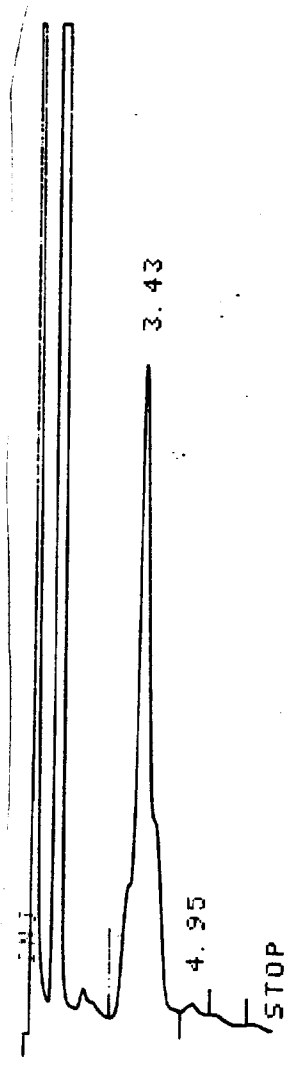

Figure 3 . Gas Chromatogram of the octanol phase from an n-octanol/water distribution coefficient determination for FM 3925 (#163, 6/20/78). The peak at 3.43 minutes and shoulders before and after this peak represent FM 3925. Gas Chromatographic conditions are given in text.