PFOS: Determination of the *n*-Octanol/Water Partition Coefficient by the Shake Flask Method - A Non-GLP Feasibility Study in Support of Wildlife International, Ltd.
Project Number: 454C-108

OCTANOL/WATER PARTITION COEFFICIENT

TEST SUBSTANCE

Identity: Perfluorooctanesulfonate; may also be referred to as PFOS or FC-95. (1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, potassium salt, CAS # 2795-39-3)

Remarks: The test substance is a white powder. Sample was taken from 3M lot number 217. Sample was stored under ambient conditions prior to testing. Purity determined to be 90.49% by LC/MS, ^{1}H-HMR, ^{19}F-NMR and elemental analyses techniques.

METHOD

Method: OECD 107
GLP (Y/N): See Remarks
Year completed: Study completed 1999. Report completed 2000

Remarks: A feasibility test was conducted to determine if the physical properties of the test substance were compatible with shake flask methodology proposed for use in an n-octanol/water partition coefficient determination.

Upon completion of the test procedure, a definitive partition interface was not obtained. Instead, a beige/white emulsion was observed throughout the sample.

RESULTS

Log P_{ow}: Not determined.

Remarks: The observation of an inseparable emulsion in the preliminary test precluded conduct of a definitive test, as indicated in the protocol (No 454/120298/107F/SUB454, 3M Lab Request U2723). Therefore, a study cancellation report was generated by the laboratory conducting the testing after consultation with 3M.

CONCLUSIONS

The study substance exhibits physical/chemical characteristics that make determination of the n-octanol/water partition coefficient infeasible by the Shake Flask Method.

Submitter: 3M Company, Environmental Laboratory, P.O. Box 33331, St. Paul, Minnesota, 55133

DATA QUALITY

Reliability: Klimisch ranking NA. Study not feasible.

REFERENCES

Study conducted at the request of 3M Company by Wildlife International, Ltd. of Easton, Maryland.

OTHER

Last changed: 5/3/00

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Introduction

A feasibility test was conducted with Perfluorooctane Sulfonic Acid Potassium Salt (PFOS) to determine if the physical properties of the material were compatible with shake flask methodology [1,2] proposed for use in an *n*-octanol/water partition coefficient determination. The test was conducted by Wildlife International, Ltd. for 3M Incorporated at the Wildlife International, Ltd. analytical chemistry facility in Easton, Maryland. The test was conducted on March 01, 1999. Raw data generated by Wildlife International, Ltd. and a copy of the letter report are filed under Project Number 454C-108 in archives located on the Wildlife International, Ltd. site.

Materials and Methods

A 100 mg/L stock solution of PFOS (Wildlife International, Ltd No. 4675) was prepared by dissolving 50.0 mg of the test substance in 500 mL of NANOpure® water. An analytical balance (ID: R-LAB-05) and a Class A glass volumetric flask were used for the preparation. The solution was sonicated (ID: SPUB-06) for approximately 20 minutes to ensure dissolution. The resulting stock concentration was not corrected for purity.

A 10-mL aliquot of the stock solution was transferred into a 40-mL glass centrifuge tube. A 10-mL aliquot of *n*-octanol (Sigma-Aldrich, Lot# 05949MN) was transferred into the 40-mL centrifuge tube. The sample was hand shaken and then centrifuged (IEC Model K, S/N 07570) for approximately 5 minutes at approximately 1500 rpm. A definitive partition interface was not obtained. Instead, a beige/white emulsion was observed throughout the sample.

Results and Discussion

The observation of an inseparable emulsion in the preliminary test precluded conduct of a definitive test, as indicated in the protocol (No 454/120298/107F/SUB454, 3M LabRequest U2723). Therefore, a study cancellation report was generated after consultation with the Sponsor.

References

1. **Organisation for Economic Cooperation and Development.** 1981. Guideline for Testing of Chemicals, 107: *Partition Coefficient (N-Octanol/water): Shake Flask Method.*

2. **U.S. Environmental Protection Agency.** 1996. Product Properties Test Guidelines, OPPTS 830.7550, *Partition Coefficient (n-Octanol/Water), Shake Flask Method.*

Report Approval:

STUDY DIRECTOR

2-11-00
DATE