

[REDACTED]

Huntingdon Life Sciences

[REDACTED]

PARTITION COEFFICIENT AND ADSORPTION/DESORPTION

Company Sanitized. Does not contain TSCA CBI

report



PARTITION COEFFICIENT AND ADSORPTION/DESORPTION

Sponsor

DuPont Specialty Chemicals
Jackson Laboratory
Chambers Works
Deepwater
NJ 08023
USA

Research Laboratory

Huntingdon Life Sciences Ltd.
Eye
Suffolk
IP23 7PX
ENGLAND

Draft: 20 August 1999
Final: 7 September 1999

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COMPLIANCE WITH GOOD LABORATORY PRACTICE STANDARDS



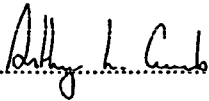
Partition Coefficient and Adsorption/Desorption

The study described in this report was conducted in compliance with the following Good Laboratory Practice standards and I consider the data generated to be valid.

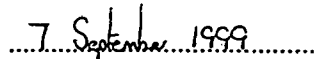
The UK Good Laboratory Practice Regulations 1997 (Statutory Instrument No 654).

EC Commission Directive 1999/11/EC of 8 March 1999 (Official Journal No L 77/8).

OECD Principles of Good Laboratory Practice (as revised in 1997), ENV/MC/CHEM(98)17.

A handwritten signature in cursive script, appearing to read 'A. L. Comb', written over a dotted line.

A. L. Comb, B.Sc., Ph.D.
Study Director
Huntingdon Life Sciences Ltd.

A handwritten date '7 September 1999' written over a dotted line.

Date

QUALITY ASSURANCE STATEMENT



Partition Coefficient and Adsorption/Desorption

The following inspections and audits have been carried out in relation to this study

Study Phase	Date of Inspection	Date of Reporting
Protocol Audit	16 August 1999	16 August 1999
Process Based Inspections Partition coefficient	4 August 1999	6 August 1999
Report Audit	6 September 1999	6 September 1999

Protocol Audit: An audit of the protocol for this study was conducted and reported to the Study Director and Company Management as indicated above.

Process based inspections: At or about the time this study was in progress inspections of routine and repetitive procedures employed on this type of study were carried out. These were conducted and reported to appropriate Company Management as indicated above.

Report Audit: This report has been audited by the Quality Assurance Department. This audit was conducted and reported to the Study Director and Company Management as indicated above.

The methods, procedures and observations were found to be accurately described and the reported results to reflect the raw data.



H. Comb, B.Sc.
Principal Auditor,
Department of Quality Assurance,
Huntingdon Life Sciences Ltd.

6 September 1999
Date

RESPONSIBLE PERSONNEL

[REDACTED]

Partition Coefficient and Adsorption/Desorption

The following staff member has reviewed this report.

T. C. Cowlyn, EurChem., C.Chem., M.R.S.C.
(Scientific Manager, Product Characterisation, Eye)

SUMMARY

A study was performed to determine the partition coefficient and adsorption/desorption coefficient of [REDACTED]

Values for the partition coefficient, P_{ow} , were calculated by a computer program (LOGKOW Version 1.63, Syracuse Research Corporation), which estimates the $\log_{10}P_{ow}$ value by reference to compound structures for which reliable partition coefficient data is available. The two components of [REDACTED] were found to have $\log_{10}P_{ow}$ values of 3.8 and 5.8 in their non-ionised state. Values for the partition coefficient in this region indicate that [REDACTED] has the potential to bioaccumulate.

Values for the adsorption/desorption coefficient, K_{oc} , were calculated through correlations with the estimated partition coefficient values. The two components of [REDACTED] were found to have $\log_{10}K_{oc}$ values of 2.3 and 3.2 in their non-ionised state. Values for the adsorption coefficient in this region indicate that [REDACTED] has medium to low mobility potential in soil.

INTRODUCTION

This study was designed to estimate the partition coefficient and adsorption/desorption coefficient of [REDACTED]. Information on such physico-chemical parameters is important in predicting the environmental fate of a test substance.

The protocol was approved by the Study Director and Huntingdon Life Sciences Management on 16 August 1999 and by the Sponsor on 18 August 1999.

The experimental phase of the study was undertaken on 17 August 1999.

Location of study : Huntingdon Life Sciences Ltd.
Eye
Suffolk
IP23 7PX
ENGLAND

Primary data from the tests performed at Huntingdon Life Sciences, and a copy of the final report, are stored in the archives of Huntingdon Life Sciences.

TEST SUBSTANCE

Identity:

[REDACTED]

Chemical name:

[REDACTED]

Intended use:

[REDACTED]

Appearance:

Pale yellow slurry

Storage conditions:

Room temperature

Lot number:

3

Expiry date:

2 years from date of receipt

Purity:

[REDACTED]

Date received:

23 June 1998

PARTITION COEFFICIENT

DEFINITION AND UNITS

The partition coefficient (P) is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of two largely immiscible solvents, in this case, n-octanol and water.

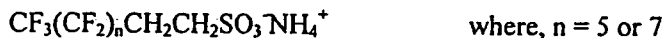
$$P_{ow} = \frac{C_{\text{octanol}}}{C_{\text{water}}}$$

The partition coefficient is usually given in the form of its logarithm to base ten ($\log_{10} P_{ow}$).

METHOD

Conventional methods for the determination of partition coefficient are not applicable to surface-active materials such as [REDACTED]. Values of $\log_{10} P_{ow}$ for [REDACTED] were thus determined by a calculation method using a LOGKOW computer program (Version 1.63, Syracuse Research Corporation). The program estimates the $\log_{10} P_{ow}$ value by reference to compound structures for which reliable $\log_{10} P_{ow}$ data is available.

[REDACTED] consists of two principle components, both of which are present in the free acid form and as the corresponding quarternary ammonium salts. The structures of the components are as follows:



The partition coefficient of a test substance is usually determined on the compound in its non-ionised form. Consequently the calculations were performed on the free acid components only.

For $n = 5$, the results were as follows:

Number	$\log_{10} P_{ow}$ Fragment description	Coefficient	Value
2	-CH ₂ - aliphatic carbon	0.4911	0.9822
6	C aliphatic carbon - no H, not tertiary	0.9723	5.8338
13	-F fluorine, aliphatic attachment	-0.0031	-0.0403
1	-SO ₂ -OH sulphonic	-3.1580	-3.1580
	equation constant		0.2290

Estimated $\log_{10} P_{ow} = 3.8467$

For $n = 7$, the results were as follows:

Number	Log ₁₀ P _{ow} Fragment description	Coefficient	Value
2	-CH ₂ - aliphatic carbon	0.4911	0.9822
8	C aliphatic carbon - no H, not tertiary	0.9723	7.7784
17	-F fluorine, aliphatic attachment	-0.0031	-0.0527
1	-SO ₂ -OH sulphonic equation constant	-3.1580	-3.1580
			0.2290

Estimated log₁₀P_{ow} = 5.7789

CONCLUSION

The two non-ionised components of [REDACTED] were estimated to have log₁₀ P_{ow} values of 3.8 and 5.8 (equivalent P_{ow} = 7100 and 600000 respectively). Values for the partition coefficient in this region indicate that [REDACTED] has the potential to bioaccumulate.

ADSORPTION/DESORPTION

DEFINITIONS

The adsorption coefficient, K_{oc} , related to the organic carbon content of the soil is a useful parameter describing the adsorption characteristics of non polar substances on a wide variety of different soils. This parameter can be estimated by correlations with the n-octanol/water partition coefficient.

METHOD

Due to the surfactant nature of the test substance, practical determination of the adsorption coefficient was not possible and thus values for $\log_{10} K_{oc}$ were estimated based on an empirical relationship* with the partition coefficient, P_{ow} , results.

Estimated K_{oc} values for [REDACTED] can be calculated as follows:

$$\log_{10} K_{oc} = 0.47 \log_{10} P_{ow} + 0.50$$

For the non-ionised components of [REDACTED] the $\log_{10} P_{ow}$ values were calculated to be 3.8 and 5.8

[REDACTED] was thus estimated to have $\log_{10} K_{oc}$ values of 2.3 and 3.2.

CONCLUSION

The two non-ionised components of [REDACTED] were calculated to have $\log_{10} K_{oc}$ values of 2.3 and 3.2 (equivalent $K_{oc} = 200$ and 1700 respectively). Values for the adsorption coefficient in this region indicate that Zonyl® FS-62 has medium to low mobility potential in soil.

**Technical Guidance Document in Support of Commission Directive 93/67/EEC on Risk Assessment of New Notified Substances*