Anexo 1.H – Potencial de Bioacumulação

REPORT

Study Title

CALCULATION OF THE PARTITION CONSTANT (N-OCTANOL/WATER) OF NPARC13+

Author

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Study completion date

07 February 2007

Test Facility

NOTOX B.V.
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The Netherlands

Laboratory Project Identification

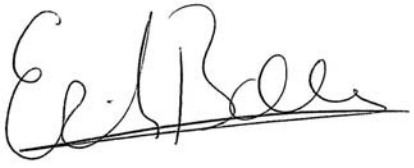
NOTOX Project 484581
NOTOX Substance 166599

1. CONTENTS

2. REPORT APPROVAL

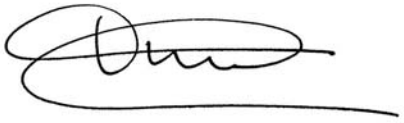
The study described in this report has been correctly reported and was conducted according to the study plan.

Dr. Ir. E. Baltussen
Study Director



Date: February 08, 2007

Dr. Ir. T.H.M. Noij
Head of Chemistry



Date: February 08, 2007

3. INTRODUCTION

3.1. Preface

Sponsor	PETROBRAS/CENPES/PDEDS/AMA Gerência de Avaliação e Monitoramento Ambiental Avenida Jequitibá, 950 - Cidade Universitária Ilha do Fundão - Rio de Janeiro, RJ CEP: 21.941- 598 - Brasil
Study Monitor	Leticia Falcão Veiga
Test Facility	NOTOX B.V. Hambakenwetering 7 5231 DD 's-Hertogenbosch The Netherlands
Study Director	Dr. Ir. E. Baltussen
Study Plan	Start : 02 February 2007 Completion : 02 February 2007

3.2. Aim of the study

The aim of the study was to calculate the partition constant (n-octanol/water) of NPARC13+.

3.3. Storage and retention of records and materials

Records and materials pertaining to the study including protocol, raw data, specimens (except specimens requiring refrigeration or freezing) and the final report are retained in the NOTOX archives for a period of at least 10 years after finalization of the report. After this period, the sponsor will be contacted to determine whether raw data and specimens should be returned to them, retained or destroyed on their behalf.

Those specimens requiring refrigeration or freezing will be retained by NOTOX for as long as the quality of the specimens permits evaluation but no longer than three months after finalization of the report.

NOTOX will retain a test substance sample until the expiry date, but no longer than 10 years after finalization of the report. After this period the sample will be destroyed.

4. MATERIALS

4.1. Test substance information

Identification	NPARC13+	
Composition	n-C7	<0.01%
	n-C8	<0.01%
	n-C9	0.03%
	n-C10	0.13%
	n-C11	0.18%
	n-C12	0.17%
	n-C13	2.13%
	n-C14	63.67%
	n-C15	24.30%
	n-C16	5.80%
	n-C17	1.33%
	n-C18	0.27%
	n-C19	0.07%
	n-C20	0.02%
	n-C21	<0.01%
	n-C22	<0.01%
	n-C23	<0.01%

4.2. Guidelines

Organization for Economic Co-operation and Development (OECD), OECD Guideline for Testing of Chemicals no. 117: "Partition Coefficient (n-Octanol/Water) High Performance Liquid Chromatography (HPLC) Method", Adopted April 13, 2004.

European Economic Community (EEC), EEC directive 92/69 EEC, Part A, Methods for the Determination of Physico-Chemical Properties A.8: "Partition Coefficient", EEC Publication no. L383, December 1992.

5. PERFORMANCE OF THE STUDY

Four methods are available for the determination of the P_{ow}. The principle of each method is described below:

1. Flask-shaking method
Test substance is partitioned in a two-phase system of n-octanol and water. After phase separation, the concentration of the test substance in both phases is determined by a suitable analytical method.

2. HPLC-method
A solution of the test substance is injected onto a reversed-phase HPLC-column. The log P_{ow} value is calculated from the retention time of the test substance.

3. Estimation method
The solubility of the test substance in n-octanol and in water is determined. The quotient of the n-octanol solubility and the water solubility is an estimation of the P_{ow}.

4. Calculation method
The calculation method is based on the theoretical fragmentation of the molecule into suitable substructures for which reliable log P_{ow} increments are known. The log P_{ow} is obtained by summing the fragment values and the correction terms for intramolecular interactions. Lists of fragment constants and correction terms are available.

For this test substance a high log P_{ow} (> 6.5) was expected based on its composition. Therefore methods 1-3 cannot be used. Consequently method 4, the calculation method, was used for a calculation of the log P_{ow} values of the 2 main components of the test substance.

Calculation was performed using the Rekker calculation method (PrologP 6.0, module in Pallas 3.0, CompuDrug International, San Francisco, CA, USA).

The test substance is a mixture of normal alkanes. The partition constant was calculated for the two most abundant alkanes in the mixture, i.e. tetradecane (n-C14) and Pentadecane (n-C15).

6. RESULTS

An overview of the structures/fragments used for the calculation is shown in appendix I.

The partition constant of tetradecane (n-C14) was calculated to be 7.63.

The partition constant of pentadecane (n-C15) was calculated to be 8.15.

These results confirm that for this test substance, the calculation method is the only possible method for an exact determination of the log P_{ow}.

APPENDIX I CALCULATION RESULTS

log*P* prediction of TETRADECANE

Database: database\compdb.cdb

$\log P_{CDR}$ = 7.63

PREDICTION DETAILS

Fragment database CDR

Occ.	Name of contributor	Value
12	-CH2-	0.52
2	-CH3	0.70

$\log P_{CDR}$ = 7.63

PALLAS CompuDrug

log*P* prediction of **PENTADECANE**

Database: database\compdb.cdb

$\log P_{CDR}$ = 8.15

PREDICTION DETAILS

Fragment database CDR

Occ.	Name of contributor	Value
13	-CH2-	0.52
2	-CH3	0.70

$\log P_{CDR}$ = 8.15

PALLAS CompuDrug