Study Report

CGA 329351

Study Title

Adsorption / Desorption of CGA 329351 in various Soils

Data Requirement

Commission Directive 95/36/EC amending Council Directive 91/414/EEC; Annex II; Fate and Behaviour in the Environment; 7.1 Fate and behaviour in soil, 7.1.2 Adsorption and Desorption, 1995
For further guidelines see section 'General Information'.

Author

Dr. [redacted]

Study Completed on

August 25, 1999

Testing Facility

Novartis Crop Protection AG
Environmental Safety/Ecochemistry
4002 Basel, Switzerland

Study Number

98RP05

Sponsor

Novartis Crop Protection AG
Environmental Safety/Ecochemistry
4002 Basel, Switzerland

Total Number of Pages 100

STATEMENT OF COMPLIANCE WITH GOOD LABORATORY PRACTICE

This study was performed in compliance with Good Laboratory Practice (GLP) in Switzerland, Procedures and Principles, March 1986 [Verfahren und Grundsätze der Guten Laborpraxis (GLP) in der Schweiz, März 1986] issued by the Federal Department of the Interior and the Intercantonal Office for the Control of Medicaments, Switzerland. These procedures are based on OECD Principles of GLP adopted on 12 May 1981 by Decision of the OECD Council concerning Mutual Acceptance of Data in the Assessment of Chemicals [C(81)30 (Final)].

Exception:
Soil characterisation was performed by AGROLAB AG, Ebikon / Root, Switzerland.

This exception does not affect the scientific validity of the study.

5.1.2.e Woo

August 25, 1999
Date

Dr. 5.1.2.e Woo
Study Director
Novartis Crop Protection AG
Environmental Safety /
Ecochemistry
4002 Basel, Switzerland

Quality Assurance Statement

Novartis Crop Protection AG, GLP Quality Assurance, Prod. Safety Services, 4002 Basel

Study	**98RP05**
Test Item	**CGA 329351**
Study Title	**Adsorption / Desorption of CGA 329351 in various Soils**
Study Director	**Dr.** 5.1.2.e Woo
QA Inspector	5.1.2.e Woo

It is herewith confirmed that the following Quality Assurance activities were performed:

Activity	Performed	Reported
Facility Based Inspection	March 10, 1998	March 26, 1998
Study Plan Check	July 8, 1998	July 8, 1998
Study Based Inspection	July 14, 1998	July 14, 1998
Facility Based Inspection	October 13, 1998	October 27, 1998
Facility Based Inspection	March 11, 1999	March 15, 1999
Final Report Inspection	June 16, 1999	June 16, 1999

September 13, 1999
Date

5.1.2.e Woo
Quality Assurance Inspector

Form QSSTAT01

GENERAL INFORMATION

Guidelines	The study was conducted in accordance with: Commission Directive 95/36/EC amending Council Directive 91/414/EEC; Annex II; Fate and Behaviour in the Environment; 7.1 Fate and behaviour in soil, 7.1.2 Adsorption and Desorption, 1995 OECD Guideline For Testing of Chemicals, No. 106, Adsorption / Desorption, adopted May 12,1981 Environmental Chemistry and Fate, Guidelines for Registration of Pesticides in Canada, July 15, 1987 and under consideration of Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 163 - 1: Leaching and Adsorption / Desorption Studies, October 18, 1982.
Test Substance	Company Code: CGA 329351
Proposed Use	Fungicide
Study Number	98RP05
Head of Testing Facility[1]	*Dr.* 5.1.2.e Woo Novartis Crop Protection AG Environmental Safety/Ecochemistry 4002 Basel, Switzerland
Study Director	*Dr.* 5.1.2.e Woo
Technical Personnel	*Mr.* [redacted] (principal co-worker)
Testing Facility	Novartis Crop Protection AG Environmental Safety/Ecochemistry 4002 Basel, Switzerland

[1] Head of testing facility is representing the sponsor of Novartis Crop Protection AG.

Supplier of ^{14}C- Labelled Test Substance	Novartis Crop Protection AG Research Support Isotope Laboratory 4002 Basel, Switzerland *Represented by: Dr.* 5.1.2.e Woo
Supplier of Unlabelled Test and Reference Materials	Novartis Crop Protection AG Research Support / Chemistry Support Metabolite Laboratory 4002 Basel, Switzerland *Represented by: Dr.* 5.1.2.e Woo
Study Dates	Study Initiation (issue of protocol): July 7, 1998 Experimental Start: July 10, 1998 Experimental Termination: January 26, 1998 Study Termination: August 25, 1999
GLP - Guidelines	See: Statement of compliance
Quality Assurance	Novartis Crop Protection AG Product Safety Services / Quality Assurance (GLP) 4002 Basel, Switzerland Represented by: *Dr.* 5.1.2.e Woo
Archives	Protocol, raw data, correspondence, and the final report are archived in the testing facilities at Novartis Crop Protection AG Environmental Safety/Ecochemistry, Basel / Switzerland
Integrity of the Study	No circumstances affecting the study were observed

Signature for the Report August 25, 1999

Date Dr. 5.1.2.e Woo

TABLE OF CONTENTS

STATEMENT OF COMPLIANCE WITH GOOD LABORATORY PRACTICE 2
QUALITY ASSURANCE STATEMENT 3
GENERAL INFORMATION 4
SUMMARY 10
1 Introduction 12
2 Materials and Methods 12
2.1 Chemicals 12
2.1.1 Unlabelled Test Substance 12
2.1.2 ^{14}C-Labelled Test Substance 13
2.2 Test System (Soils) 14
2.3 Study Conduct 14
2.3.1 Experimental Conditions 14
2.3.2 Study Procedures and Rationale 15
2.3.3 Preparation of the Radioactive Test Substance Solutions 16
2.3.4 Pre-Test 16
2.3.5 Adsorption / Desorption Experiments 17
2.3.6 Mass-Balance 18
2.4 Analytical Methods 18
2.4.1 Liquid Scintillation Counting (LSC) of Radioactivity 18
2.4.2 High - Performance Liquid Chromatography (HPLC) 19
2.4.3 Thin - Layer Chromatography (TLC) 20
2.5 Calculations 20
2.5.1 Region of Interest (ROI) 20
2.5.2 Calculation of Soil-to-Solution Ratio 20
2.5.3 Adsorption / Desorption Coefficients 21
3 Results and Discussion 23
3.1 Radiochemical Purity and Stability of the Test Substance 23
3.2 Pre-Test (Equilibration Test) 23
3.3 Recovery, Distribution and Analysis of Radioactivity 23
3.3.1 Recovery 24

3.3.2 Analysis of Radioactivity (Mass Balance Samples) 24
3.4 Adsorption and Desorption Isotherms 24
4 Conclusion 25
5 References 25

LIST OF TABLES

Table 1: Soil Characteristics 26
Table 2: Pre Test Adsorption 27
Table 3: Pre Test Desorption 28
Table 4: Balance of Radioactivity for Soil Borstel after Adsorption and Desorption 29
Table 5: Balance of Radioactivity for Soil Pappelacker after Adsorption and Desorption 30
Table 6: Balance of Radioactivity for Soil Gartenacker after Adsorption and Desorption 31
Table 7: Balance of Radioactivity for Soil Vetroz after Adsorption and Desorption 32
Table 8: Balance of Radioactivity for Soil Illarsaz after Adsorption and Desorption 33
Table 9: Concentration of CGA 329351 in Aqueous Phases and in Soil Borstel after Adsorption and Desorption 34
Table 10: Concentration of CGA 329351 in Aqueous Phases and in Soil Pappelacker after Adsorption and Desorption 35
Table 11: Concentration of CGA 329351 in Aqueous Phases and in Soil Gartenacker after Adsorption and Desorption 36
Table 12: Concentration of CGA 329351 in Aqueous Phases and in Soil Vetroz after Adsorption and Desorption 37
Table 13: Concentration of CGA 329351 in Aqueous Phases and in Soil Illarsaz after Adsorption and Desorption 38
Table 14: Adsorption- and Desorption Coefficients of CGA 329351 for various Soils 39
Table 15: Relative Mobility Factors (RMF), Sorption Coefficients and Mobility-Adsorption Classes for a Variety of Pesticides. 40

LIST OF FIGURES

Figure 1: Rate of Adsorption of CGA329351 in various Soils (Pre-Test). 41
Figure 2: Rate of Desorption of CGA 329351 in various Soils (Pre-Test). 42

Figure 3: Purity of CGA329351 (HPLC) 43
Figure 4: Purity of CGA329351 (TLC) 44
Figure 5: Stability of CGA 329351 45
Figure 6: HPLC of Aqueous Phase after 24 h of Adsorption (Pre-Test Borstel) 46
Figure 7: HPLC of Aqueous Phase after 24 h of Adsorption (Pre-Test Pappelacker) 47
Figure 8: HPLC of Aqueous Phase after 24 h of Adsorption (Pre-Test Gartenacker) 48
Figure 9: HPLC of Aqueous Phase after 24 h of Adsorption (Pre-Test Vetroz) 49
Figure 10: HPLC of Aqueous Phase after 24 h of Adsorption (Pre-Test Illarsaz) 50
Figure 11: HPLC of Aqueous Phase after Adsorption Step with Soil Borstel (Sample BO_5_3) 51
Figure 12: TLC of Aqueous Phase after Adsorption Step with Soil Borstel (Sample BO_5_3) 52
Figure 13: HPLC of the Extract after Adsorption Step with Soil Borstel (Sample BO_5_3) 53
Figure 14: TLC of the Extract after Adsorption Step with Soil Borstel (Sample BO_5_3) 54
Figure 15: HPLC of Aqueous Phase after Adsorption Step with Soil Pappelacker (Sample PA_5_3) 55
Figure 16: HPLC of the Soil Extract after Adsorption Step with Soil Pappelacker (Sample PA_5_3) 56
Figure 17: HPLC of Aqueous Phase after Adsorption Step with Soil Gartenacker (Sample GA_5_3) 57
Figure 18: HPLC of the Soil Extract after Adsorption Step with Soil Gartenacker (Sample GA_5_3) 58
Figure 19: HPLC of Aqueous Phase after Adsorption Step with Soil Vetroz (Sample VE_5_3) 59
Figure 20: HPLC of the Soil Extract after Adsorption Step with Soil Vetroz (Sample VE_5_3) 60
Figure 21: HPLC of Aqueous Phase after Adsorption Step with Soil Illarsaz (Sample IL_5_3) 61
Figure 22: TLC of Aqueous Phase after Adsorption Step with Soil Illarsaz (Sample IL_5_3) 62
Figure 23: HPLC of the Soil Extract after Adsorption Step with Soil Illarsaz (Sample IL_5_3) 63

Figure 24: TLC of the Soil Extract after Adsorption Step with Soil Illarsaz (Sample IL_5_3) ... 64
Figure 25: Freundlich Plots (log-log) for Adsorption and Desorption of CGA 329351 for Soil Borstel Sandy Loam ... 65
Figure 26: Freundlich Plots (lin-lin) for Adsorption and Desorption of CGA 329351 for Soil Borstel Sandy Loam ... 66
Figure 27: Freundlich Plots (log-log) for Adsorption and Desorption of CGA 329351 for Soil Pappelacker Sandy Loam ... 67
Figure 28: Freundlich Plots (lin-lin) for Adsorption and Desorption of CGA 329351 for Soil Pappelacker Sandy Loam ... 68
Figure 29: Freundlich Plots (log-log) for Adsorption and Desorption of CGA 329351 for Soil Gartenacker Sandy Loam ... 69
Figure 30: Freundlich Plots (lin-lin) for Adsorption and Desorption of CGA 329351 for Soil Gartenacker Sandy Loam ... 70
Figure 31: Freundlich Plots (log-log) for Adsorption and Desorption of CGA 329351 for Soil Vetroz Sandy Loam ... 71
Figure 32: Freundlich Plots (lin-lin) for Adsorption and Desorption of CGA 329351 for Soil Vetroz Sandy Loam ... 72
Figure 33: Freundlich Plots (log-log) for Adsorption and Desorption of CGA 329351 for Soil Illarsaz Sandy Loam ... 73
Figure 34: Freundlich Plots (lin-lin) for Adsorption and Desorption of CGA 329351 for Soil Illarsaz Sandy Loam ... 74
Figure 35: Plots of k - Values vs. Organic Carbon Content and vs. Clay Content ... 75

LIST OF APPENDICES

Appendix A: Representative Data ... 76
Appendix B: Validation of Analytical Methods ... 92
Appendix C : Limits of Detection ... 98

SUMMARY

The adsorption and desorption of the fungicide CGA 329351, i.e., (R)-2-[N-(2,6-dimethyl-phenyl)-methoxyacetylamino]-propionic acid methyl ester was studied on various soil types and compared to other compounds.

Pre-test data showed, that adsorption and desorption had reached apparent equilibrium after about two to 24 hours of exposure. Adsorption after 24 h ranged from 11.2 % (soil Pappelacker, loamy sand) to 59.9 % (soil Illarsaz, silt loam) of the amount applied. Desorption ranged from 24.2 % to 55.7 %, of the amount adsorbed. Adsorption to glass walls was negligible. No degradation of CGA 329351 was observed during the experiment.

For the final adsorption / desorption experiment, soil samples were exposed for 24 hours at a substance concentration range in the aqueous phase from 4.71 to 0.23 µg / ml. The soil-to-solution ratio was set to 10 g soil per 20 ml aqueous phase (5 g soil per 20 ml aqueous phase for soil Illarsaz).

The Freundlich adsorption coefficients k_{ads} were in the range of 0.3 ml/g of soil Pappelacker (loamy sand) and 7.9 ml/g of soil Illarsaz (silt loam).

When related to the organic carbon content K_{OC} - values of 40.0, 28.9, 31.0, 35.5 and 39.8 ml/g were calculated for soils Borstel, Pappelacker, Gartenacker, Vetroz and Illarsaz, respectively, with a mean value of 35 ml/g. This indicated a good correlation of the adsorptivity of CGA 329351 with the soil organic carbon content. The corresponding values related to the organic matter content were 23.2, 16.8, 18.0, 20.6 and 23.1 ml/g. Except for the peaty soil Illarsaz a correlation beween clay content and adsorption was observed.

The Freundlich desorption coefficients k_{des} for both desorption steps were in the range of 0.5 ml/g of soil Pappelacker (loamy sand) and 10.4 ml/g of soil Illarsaz (silt loam). For the first desorption step the following desorption constants related to organic carbon content were determined: 55.7, 44.1, 38.8, 42.0 and 47.0 ml/g for soils Borstel, Pappelacker, Gartenacker, Vetroz and Illarsaz, respectively (mean: 46 ml/g). The corresponding values for the second desorption step were 77.7, 72.4, 52.9, 48.0 and 52.8 ml/g (mean: 61 ml/g)

The slopes 1/n for the adsorption isotherms were 0.92, 0.90, 0.91, 0.93 and 0.93 for Borstel, Pappelacker, Gartenacker, Vetroz and Illarsaz, respectively. The difference from unity indicated a distinct correlation between adsorptivity and concentration of the test substance in the aqueous phase. The shape of the adsorption/desorption isotherms (linear scale) indicated significant adsorption and low mobility towards lower concentrations. This effect was more pronounced in the in the sandy soils for the desorption isotherms.

The differences in K_{OC}-values between adsorption and both desorption steps showed that adsorption onto soil particles became stronger with time (ageing) and at lower

concentrations. The present adsorption isotherms were established at rather high concentrations (roughly in the range of 5 to 0.2 mg/l) which were far away from the expected field concentrations. Therefore, the desorption K_{OC}-values (39-78 ml/g) are considered to better reflect the adsorptivity of the compound in the field situation.

In all experiments comprising adsorption and both desorption steps, the recoveries were in the range of 99.3 - 108.1 % of the radioactivity applied.

HPLC analysis of the aqueous solutions and of the soil extracts after the adsorption step demonstrated stability of CGA 329351 during the study.The non-extractable radioactivity accounted for at highest 0.6 % of the dose applied for all soils.

In conclusion, CGA 329351 can be classified as moderately mobile (mobility class III).

1 Introduction

Soil Adsorption / Desorption data are necessary for the evaluation of the migration tendency of chemicals within the environment. They are needed to estimate, for example, the leaching behaviour through the soil, the evaporation from soil surfaces, etc. The availability of the test substance in the soil-water-air environment and finally its degradability are significantly influenced by its adsorption / desorption characteristics.

2 Materials and Methods

2.1 Chemicals

2.1.1 Unlabelled Test Substance

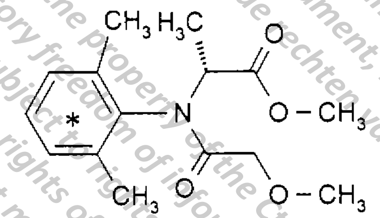
Data were taken from Ciba-Geigy "Status Report" of CGA 329351, (Dr. 5.1.2.e Woo May 9, 1994) and from Novartis "Data Sheet: Physico-Chemical Properties" of CGA 329351, (June 19, 1995)

Chemical Name (IUPAC)	(R)-2-[N-(2,6-dimethyl-phenyl)-methoxyacetylamino]-propionic acid methyl ester	
Company Code	CGA 329351	
Product category	fungicide	
Max. Rec. Field Rate	75 - 150 g/ha per Application, 300 - 600 g/ha per season	
Batch	AMS 758/101	
Molar mass	279.34 g/mol	
Empirical formula	$C_{15}H_{21}NO_4$	
Vapour pressure	3.3×10^{-3} Pa at 25°C	
Purity	99.4 %	
Physical state	pale yellow, clear, viscous, liquid	
Solubility at 20°C	Water	26 g/l (OECD No. 105, EEC A.6)
	Acetone	miscible
	Ethylacetate	miscible
	Hexane	59 g/l

	Methanol	miscible
	Methylenechloride	miscible
	n-Octanol	miscible
n-Octanol / water partition coefficient	log P_{OW} = 1.71 (OECD No. 117, EEC A.8)	
pk_a-value	No pk_a in the relevant pH-range	
Stability in vehicle	See 2.1.2	
Storage	Refrigerator in the dark	
Expiration date	08/00	
Toxicity	LD_{50} >200 mg/kg (female rat)	
Precautions	Routine hygiene procedures	

2.1.2 ^{14}C-Labelled Test Substance

Structure/Position of labelling (★)



Batch	ILS-114.1
Label	Phenyl-(U)^{14}C
Specific radioactivity	1.44 MBq/mg
Radiochemical purity	96 %
Expiration date	November 30, 1998
Stability in vehicle	The stability of the test substance was determined by HPLC using an aliquot of the application solution before and after treatment.
Storage	Short term: refrigerator in the dark; long term: ≤ -18 °C in the dark.
Precautions	Routine hygiene procedures. Additional safety precautions should be followed according to the Swiss regulation on radiation protection.

2.2 Test System (Soils)

Types
Five soils differing in particle size, organic matter content, cation exchange capacity, pH and $CaCO_3$ content were used. The specifications and sources are given in Table 1.

Sources
See Table 1

Specifications
The soils were specified for the various soil parameters by AGROLAB AG Ebikon/Root Switzerland. The corresponding data are given in Table 1.

Preparation
Before use the soils were air dried at room temperature and sieved through a 2 mm sieve.

2.3 Study Conduct

2.3.1 Experimental Conditions

Apparatus
The adsorption and desorption experiments were conducted in 150 ml centrifuge tubes, which were shaken at ca. 200 strokes per minute.

Temperature
20 ± 1 °C (climatic room).

Soil-to-Solution Ratio
A soil-to-solution ratio of 1 : 2 was chosen for pre- and main test for all soils except Illarsaz (1 : 4).

Amount of Soil
Pre-test and main test: 10 g for all soils except Illarsaz (5 g).

Aqueous Phase
Pre-test and main test: 20 ml of 0.01 M $CaCl_2$ solution.

Concentrations
For the pre-test the test substance was applied at a concentration of about 4.87 µg/ml to all soils in duplicate. For the main test the test substance was applied at five concentrations ranging between about 0.23 and 4.71 µg/ml. Except for the highest concentration all samples were prepared in duplicate. For the highest concentration quadruples were prepared.

Equilibration Time
The time required to reach the adsorption and desorption equilibrium of the test substance was elaborated in a pre-test (see 2.3.4).

Adsorption onto Glass Wall

The amount of test substance adsorbed onto the glass wall was determined in duplicate. Therefore, two treated aqueous samples were prepared and shaken for 24 hours. The loss of radioactivity from the aqueous solution was measured (see pre-test 2.3.4 and Table 2).

2.3.2 Study Procedures and Rationale

The study consisted of three steps:

1. Pre-Test:

The pre-test was performed with the highest concentration to evaluate equilibration time (12 tubes, two for each soil and two tubes containing only the treated aqueous phase: pre-estimate of glass adsorption). The purpose of the study was:

- to establish a soil solution ratio for each soil so that adsorption lies between 20 and 80%;
- to establish the time for each soil needed to reach equilibrium in the adsorption / desorption test;
- to assure that the test compound is stable during the selected exposure time;
- to estimate the influence of glass adsorption.

For this purpose the tubes were shaken and after various times (see Tables 2 and 3) centrifuged. Duplicate sub-samples were removed from the clear aqueous phase and the radioactivity was determined by LSC (Liquid Scintillation Counting). Based on these data the dissipation of radioactivity from the aqueous phase into the solid phase was followed and the percentage of adsorption was calculated. Finally, the aqueous samples were submitted to HPLC analysis and the stability of the test compound confirmed. No balance was established since this was not the purpose of the pre-test.

2. Adsorption / desorption study part:

In the adsorption / desorption study part five concentrations of the test substance were investigated in duplicate per soil (total 10 samples per soil). After each exposure step (adsorption or desorption steps) the radioactivity in the clear aqueous phase was determined by LSC. Based on these measurements the adsorption or desorption (concentration of test substance in soil) was calculated by difference in concentration (initial 'C_i' versus exposed 'C_e' etc.). After the second desorption step the remaining soil was submitted to combustion and the exposure tubes were washed and a full balance was established for each sample. Data obtained were used to establish adsorption or desorption isotherms and adsorption coefficients.

3. Balance study:

The balance study was performed with the highest concentration. Aqueous phases and soils were worked up and analysed for parent molecule and degradates directly after the adsorption step (two tubes per soil, set up simultaneously with adsorption-desorption samples). The purpose of this step was:

- to directly determine the nature of radioactivity adsorbed onto the soil particles by extraction, analysis and combustion of residual soil radioactivity;
- in addition to the above samples (step 2) to analyse the aqueous phase for amount of parent molecule and possible degradates and
- to determine the amount of non-extractable residues to establish a material balance comprising aqueous phase, extractables and non-extractables.

2.3.3 Preparation of the Radioactive Test Substance Solutions

For preparation of the highest concentration the total amount of ^{14}C-labelled CGA 329351 (about 5 mg) was dissolved in 1000 ml 0.01 M $CaCl_2$ solution. The accurate amount of radioactive material present was determined by LSC to be 4.87 mg. This stock solution was used for the preparation of the dilutions (see Table below). The amount of radioactivity of the various dilutions was determined by LSC.

Sample	Amount of Solution	Final Volume of Treatment Solution made up with 0.01 M $CaCl_2$	Concentration of CGA 329351 in Treatment Solution (corrected for purity)
[ppm]	[ml of stock solution]	[ml]	[ppm]
5	1000	1000	4.71
2.5	125	250	2.33
1	50	250	0.95
0.5	25	250	0.46
0.25	12.5	250	0.23

2.3.4 Pre-Test

The equilibration time was determined in a preliminary test with all soils at an initial test concentration of 4.87 µg/ml.

For the test, an amount of 10 g air-dry soil (Illarsaz: 5 g) was weighed into a tared centrifuge tube and suspended with ca. 20 ml 0.01 M $CaCl_2$-solution (without a.i.) and the slurry left at room temperature for 24 hours. Prior to treatment the mixture was centrifuged and the supernatant aqueous phase decanted. To the wet soil 20 ml

of treated aqueous phase (4.87 µg/ml) was added and the mixture shaken (ca. 200 rpm). After various time intervals (see Table 2 and Figure 1) the mixture was centrifuged for 5 min. at 2000 rpm and duplicates of 1 ml each of the clear aqueous phase removed for LSC.

After adsorption, the desorption of radioactivity from soil was followed for another 24 hours. For this purpose, the treated aqueous layer was removed after centrifugation and replaced by untreated $CaCl_2$-solution (same volume) and shaken as described above. After various time intervals the mixture was centrifuged and aliquots (1 ml) of the clear aqueous phase submitted to LSC and the desorption calculated (see Table 3 and Figure 2).

In addition, treated aqueous samples (20 ml) without soil were exposed for 24 hours and analysed by LSC at the same time intervals.

All aqueous phases from adsorption and desorption were analysed by HPLC for amount of parent molecule and degradates (see Figures 6 to 10).

2.3.5 Adsorption / Desorption Experiments

An amount of 10.0 ± 0.1 g of each soil was weighed into tarred centrifuge tubes and suspended with about 20 ml 0.01 M $CaCl_2$-solution (without a.i.). After an equilibration time of ca. 40 hours (weekend) the samples were centrifuged and the $CaCl_2$-solution was decanted. Then the treated aqueous 0.01 M $CaCl_2$ phases (20 ml) with initial test concentrations between 0.23 and 4.71 µg/ml were added (Tables 9 - 13). All additions of soil and solutions were controlled by weighing the test vessel.

The centrifuge tubes were shaken with about 200 rpm at 20°C for 24 hours. The soils and solutions were then separated by centrifugation at 2000 rpm for 5 min. Directly from the clear supernatant two aliquots of 1 ml each were taken, mixed with 15 ml of scintillation solution (IrgaSafe Plus™) and submitted to liquid scintillation counting to determine the equilibrium concentration in the aqueous phase (C_e).

Then the remaining supernatants were cautiously decanted and the centrifuge tubes still containing the wet soil were weighed again. Thereafter, 20 ml of fresh 0.01 M $CaCl_2$-solution (without a.i.) were added to the wet soil containing the adsorbed a.i., the weight was determined and the test tubes were shaken again for 24 hours at 20°C (first desorption step).

After the first desorption step solutions and soils were treated as after the adsorption step. Thereafter, desorption was repeated once.

After completion of the adsorption- and desorption steps, the radioactivity in the aqueous phases was determined by LSC. The amounts adsorbed onto soil (x/m) for each step were calculated from the initial amount of active ingredient and the amounts found in the aqueous phases. The residual radioactivity in soil after the second desorption was determined by combustion. The radioactivity remaining

adsorbed to the centrifuge tube was dissolved in about 10 ml acetonitrile and determined by LSC. Thereafter, a balance was established comprising the radioactivity found in adsorption and desorption solutions, in soil by combustion and in the washings of the test tubes (radioactivity adsorbed to the glass-walls).

Results were expressed in percentage of the radioactivity initially applied (see Tables 4 to 8).

2.3.6 Mass-Balance

Mass-balance samples were worked-up directly after the adsorption step. The soil was extracted three times with about 20 ml acetonitrile : water (80 : 20; v : v) and as a last step with methanol in a Soxhlet extractor.

The radioactivity in all extracts was determined by LSC. The aqueous phases and the extracts were analysed by HPLC for possible degradates (see Figures 11 to 24). Finally, the not extracted radioactivity in the soil was determined by combustion and the test tubes were carefully washed with acetonitrile (radioactivity adsorbed to glass walls).

A balance was given comprising the radioactivity found in soil (extractables and non-extractables), in the aqueous phase and in the washings of test tubes. Values are given in percentage of the radioactivity initially applied (see Tables 4 - 8).

2.4 Analytical Methods

Samples from the adsorption- and extraction steps were directly analysed.

For discussion of the limits of detection (LD) and limits of quantification (LQ) of the various analytical techniques see Appendix C.

2.4.1 Liquid Scintillation Counting (LSC) of Radioactivity

All measurements were performed with model Tri-Carb 2500 TR Liquid Scintillation Counters (Packard Instruments Company Inc., Meriden, CT, USA) correcting for background and for counting efficiency.

Scintillator I	Irga-Safe Plus™ (Packard Instruments) for aqueous and organic solutions.
Scintillator II	Oxysolve C-400 (Zinsser Analytics, Frankfurt, Germany) for combustions.

Measurement of Aqueous and Organic Samples

Aqueous and organic samples up to 2.0 ml were mixed with 15 ml Scintillator I and submitted to liquid scintillating counting.

Measurement of Non-extractable Radioactivity

Non - extractable radioactivity was analysed by combustion of soil subsamples in an oxygen stream at approximately 800°C with copper oxide as catalyst using a Robox II sample oxidiser (Zinsser Analytik, Frankfurt, FRG). The $^{14}CO_2$ liberated was trapped and measured in 15 ml of scintillator II.

2.4.2 High - Performance Liquid Chromatography (HPLC)

A Shimadzu HPLC System LC10A equipped with two pumps, model LC10-AD, a variable wavelength UV/VIS detector, model SPD-10A, an autosampler, model SIL-10A equipped with a 500 µl loop, a column oven CTO-10A, and a communication module CBM10A linked to a personal computer was used (Shimadzu Europa GmbH, Duisburg, Germany). The injection volume was 100 µl.

The radioactivity was measured with a HPLC-Radioactivity Monitor (RAM) Berthold LB 506 C-1 equipped with a 150 µl solid flow cell (YG 150) and a Berthold data system.
The following chromatographic conditions were applied:

Column:	NUCLEOSIL RP-C18, 10 µm (250 x 4.6 mm) (CIBA-GEIGY Ltd., Basle/CH) Temperature: Ambient		
Mobile phase:	Eluent A: Water (bidistilled) Eluent B: Acetonitrile (Lichrosolve, Merck)		
Flow:	1.0 ml/min		
UV-Detector:	wavelength 254 nm		
Ratio of Eluents:		Eluent A	Eluent B
	start	85%	15%
	4.00 min.	85%	15%
	10.00 min.	5%	95%
	14.00 min.	5%	95%
	18.00 min.	85%	15%
	20.00 min.	85%	15%
	21.00 min.	stop	

The typical retention time of CGA 329351 was 14.85 min.

2.4.3 Thin - Layer Chromatography (TLC)

For the identification and quantification of ^{14}C-CGA 329351 and of its degradation products the following TLC conditions were used:

Precoated 20 x 20 cm glass-backed silica gel plates 60F254 (E. Merck AG, Darmstadt, Germany) thickness: 0.25 mm,

The development chambers were equipped with one filter paper each (20 x 20 cm, CAMAG, Muttenz, Switzerland) and allowed to saturate for 20 min.

The following solvent systems were used:

SS1	Chloroform/Acetone	(9:1) v/v
SS2	Chloroform/Methanol/Formic Acid/Water	(75:20:4:2) v/v/v/v

The typical Rf - values for CGA 329351 were 0.53 (SS1) and 0.93 (SS2).

2.5 Calculations

2.5.1 Region of Interest (ROI)

Values given in ROI % were calculated as follows:

$$\text{ROI \% of fraction A} = \frac{\text{radioactivity of fraction A}}{\text{radioactivity of all selected fractions}} \cdot 100$$

2.5.2 Calculation of Soil-to-Solution Ratio

Knowing the water-octanol partition-coefficient log (P_{ow}) and the percentage of organic carbon (% OC) the Freundlich adsorption coefficient (k) can be estimated using the following correlation[2]

$$\log\left(K_{OC}\right) = 6.0338 * \log\left(P_{ow}\right) + 0.81826 \quad \text{and} \quad k = \frac{K_{OC} * \%\,OC}{100}$$

With the Freundlich adsorption coefficient (k) the soil-to-solution ratio can be estimated using:

$$R = \frac{1}{k * \left(\frac{1}{A} - 1\right)}$$

[2] Novartis internal data

with R = soil-to-solution ratio = $\frac{\text{Mass soil [g]}}{\text{Volume water [ml]}}$

A = adsorption ratio = $\frac{M_{soil}}{M_{initial}}$

M_{soil}: mass of test substance (µg) adsorbed on soil

$M_{initial}$: mass of test substance (µg) initially added to the test tubes

2.5.3 Adsorption / Desorption Coefficients

The results of the adsorption / desorption studies were assessed using the equation for Freundlich adsorption isotherms:

$$\frac{X}{m} = k * C_e^{\frac{1}{n}}$$

or

$$\log\left(\frac{X}{m}\right) = \log(k) + \frac{1}{n} \cdot \log(C_e)$$

with X/m = amount of the test substance adsorbed per unit mass of adsorbent [µg/g]

k = the Freundlich sorption coefficient $\left(\frac{\mu g \text{ a.i. adsorbed / g soil}}{\mu g \text{ a.i. / ml solution}} = \frac{ml}{g}\right)$

1/n = slope of the adsorption / desorption isotherm

C_e = equilibrium concentration of the test substance in the aqueous phase [µg/ml].

The equilibrium concentration C_e was determined directly by liquid scintillation counting and X/m was calculated from the difference between the initial (C_i) and final amount of the test substance in the aqueous phase at equilibrium (C_e). Variables were expressed in µg/ml (C_e) and in µg/g (X/m).

Furthermore, the initial as well as the equilibrium concentration after adsorption were corrected for the actual amount of parent molecule present in the aqueous phase.

Finally, the Freundlich adsorption and desorption coefficients (k = k_{ads} or k_{des}) were related to the organic carbon content (OC), to the organic matter content (OM), and to the clay content of the various soils using the following equations[3]:

$$K_{OC} = \frac{k \cdot 100}{\%\ OC},$$

$$K_{OM} = Q = \frac{K_{OC}}{1.724},$$

and

$$K_{Clay} = \frac{k \cdot 100}{\%\ Clay}.$$

---

[3] The Freundlich sorption coefficient $\left(k = \frac{x}{m \cdot C_e^{1/n}}\right)$ is a direct measure of the relative affinities of a compound for water and a soil surface, and % OC / 100 "normalises" this ratio for the amount of soil organic carbon present. The assumption is that substance sorption by soils is entirely due to organic matter, which is a complex mixture of carbon/hydrogen/nitrogen compounds that acts as a nonpolar film at the surface of soils.

$$K_{OC} = \frac{\mu g\ a.i.\ adsorbed\ /\ g\ soil\ /\ g\ organic\ carbon}{\mu g\ a.i.\ /\ ml\ solution\ /\ g\ soil} = \frac{\mu g\ a.i.\ adsorbed\ /\ g\ organic\ carbon}{\mu g\ a.i.\ /\ ml\ solution};$$

$$K_{OM} = \frac{K_{OC}}{1.724}.$$

3 Results and Discussion

3.1 Radiochemical Purity and Stability of the Test Substance

The radiochemical purity of ^{14}C-CGA 329351 was found to be 98.2% as determined in the testing facility on July 22, 1998. The stability during the application procedure was proven (see Figures 3 and 5).

3.2 Pre-Test (Equilibration Test)

The equilibration time was established with all test soils by measuring the decrease in radioactivity in the supernatant aqueous phase after various incubation times for up to 24 hours. The initial concentration used was 4.87 µg/ml test solution (see Table 2 and Figure 1). After about two to 24 hours of shaking at 20°C the concentration of a.i. reached almost steady state conditions in the supernatant water phase for all samples (Table 2, Figure 1). Adsorption ranged from 10.2 (2 h) to 15.0 % (4 h) for soil Pappelacker and from 54.6 (6 h) to 59.9 % (24 h) for soil Illarsaz. The amounts adsorbed by the three other soils were in between the two others (17.6 %, 21.8 % and 38.3 % for soils Borstel, Gartenacker and Vetroz after 24 h, respectively).

Only 2.3% of the radioactivity applied was adsorbed to the glass walls after 24 hours.

The apparent desorption equilibrium was also reached after about 2 to 24 hours (see Table 3 and Figure 2). After 24 h desorption accounted for 55.7 %, 47.5 %, 43.3 %, 34.5 % and 24.2 % of the amount adsorbed for soils Borstel, Pappelacker, Gartenacker, Vetroz and Illarsaz, respectively.

During the study no degradation of CGA 329351 was observed in the aqueous adsorption solutions (Figures 3 and 5).

Samples of the final adsorption / desorption experiment were exposed for 24 hours.

3.3 Recovery, Distribution and Analysis of Radioactivity

Adsorption / desorption isotherms were established for all soils. For this purpose a series of aqueous concentrations (0.23 to 4.71 µg / ml) was equilibrated over 24 hours with the corresponding soils. The soil-to-solution ratio was set to 10 g soil per 20 ml aqueous phase (5 g soil per 20 ml aqueous phase for soil Illarsaz) in accordance with the estimated ratio (see 2.5.2 and Appendix A).

The recovery and distribution pattern of ^{14}C-activity for the soil types and samples submitted to the adsorption / desorption procedure are summarised in Tables 4-8.

3.3.1 Recovery

The recoveries of all samples are reported in Tables 4 - 8.

Adsorption / Desorption Samples of all Soils:

The individual recoveries were in the range of 99.3 % (Pappelacker) and 108.1 % (Vetroz) of the radioactivity applied.

Mass Balance Samples:

The recoveries were in the range of 93.5 % (Vetroz) - 101.7 % (Pappelacker) of the radioactivity applied.

The non-extractable radioactivity accounted for at highest 0.6 % of the dose applied for all soils.

3.3.2 Analysis of Radioactivity (Mass Balance Samples)

After adsorption the supernatant aqueous solution and the extractable radioactivity of the mass balance samples were analysed by HPLC and TLC (for examples see Figures 6 - 24).

Analysis of the aqueous adsorption solutions and the extracts of all soils showed, that only CGA 329351 was present.

3.4 Adsorption and Desorption Isotherms

The results are summarised in Table 14 and in Figures 25 - 34. The individual concentrations of the test compound in aqueous phases and in soil after adsorption and desorption are given in Tables 9 to 13.

The Freundlich adsorption coefficients k_{ads} were in the range of 0.3 ml/g of soil Pappelacker (loamy sand) and 7.9 ml/g of soil Illarsaz (silt loam). For details see Table 14.

When related to the organic carbon content K_{OC} - values of 40.0, 28.9, 31.0, 35.5 and 39.8 ml/g were calculated for soils Borstel, Pappelacker, Gartenacker, Vetroz and Illarsaz respectively, with a mean value of 35 ml/g. This indicated a good correlation of the adsorptivity of CGA 329351 with the soil organic carbon content (see also Figure 35, top). The corresponding values related to the organic matter content were 23.2, 16.8, 18.0, 20.6 and 23.1 ml/g. Except for the peaty soil Illarsaz a correlation beween clay content and adsorption was observed. (see Table 14 and Figure 35, bottom).

The Freundlich desorption coefficients k_{des} for both desorption steps (Table 14) were in the range of 0.5 ml/g for soil Pappelacker (loamy sand) and 10.4 ml/g for soil Illarsaz (silt loam). For the first desorption step the following desorption constants related to organic carbon content were determined: 55.7, 44.1, 38.8, 42.0 and 47.0 ml/g for soils Borstel, Pappelacker, Gartenacker, Vetroz and Illarsaz,

respectively (mean value: 46 ml/g). The corresponding values for the second desorption step were 77.7, 72.4, 52.9, 48.0 and 52.8 ml/g (mean: 61 ml/g)

The slopes 1/n for the adsorption isotherms were 0.92, 0.90, 0.91, 0.93 and 0.93 for Borstel, Pappelacker, Gartenacker, Vetroz and Illarsaz respectively (see Table 14). The difference from unity indicated a distinct correlation between adsorptivity and concentration of the test substance in the aqueous phase.

For comparison purposes, the adsorption and desorption isotherms were plotted in a linear scale (X/m against C_e; see Figures 26, 28, 30, 32, and 34). The isotherms showed the so called L-shape (1), i.e. the isotherms were concave to the concentration axis. The L-shape was more pronounced towards lower concentration levels (second desorption step) in sandy soils indicating a higher relative affinity of the soil solid phases for the substance at low concentrations.

The differences in K_{OC}-values of adsorption and both desorption steps showed that adsorption onto soil particles became stronger with time (ageing) and at lower concentrations. The present adsorption isotherms were established at rather high concentrations (roughly in the range of 5 to 0.2 mg/l) which were far away from the expected field concentrations[4]. Therefore, the desorption K_{OC}-values (39-78 ml/g) are considered to better reflect the adsorptivity of the compound in the field situation.

4 Conclusion

In conclusion, CGA 329351 can be classified as moderately mobile (mobility class III).

5 References

(1) 5.1.2.e Woo: Adsorption of organic chemicals in soils, Environmental Health Perspectives, 88, pp 155-177, 1989.

[4] Assuming the highest recommended field rate per application of 100 g/ha (foliar application), uniform distribution in the top 10 cm of the soil and a soil density of 1.5 g/ml this figure corresponds to a concentration in the soil of < 0.1 ug/g of soil.

Table 1: Soil Characteristics

Origin (Textural class; USDA)	Borstel (loamy sand soil)	Pappelacker (loamy sand soil)	Gartenacker (silt loam soil)	Vetroz (silt loam)	Illarsaz (silt loam)
Batch No.	6/98	5/96	9/96	3/75	4/75
Analysis Date:	July 10, 1998	July 4, 1996	Nov. 7, 1996	April 8, 1994	April 8, 1994
pH (KCl)	5.0	7.6	7.3	7.2	6.7
Organic Carbon	1.2 %	1.1 %	2.1 %	4.7 %	19.8 %
Total Nitrogen	0.1 %	0.1 %	0.2 %	0.4 %	1.5 %
CEC[5]	7.5 mmol/z/100 g soil	6.5 mmol/z/100 g soil	12.3 mmol/z/100 g soil	28.1 mmol/z/100 g soil	102.8 mmol/z/100 g soil
Particle Size Distribution					
-Clay (<0.002 mm)	5.3 %	2.9 %	9.7 %	23.3 %	23.6 %
-Silt (0.002 - 0.05 mm)	17.5 %	22.7 %	51.0 %	58.5 %	55.4 %
-Sand (0.05 - 2 mm)	77.1 %	74.4 %	39.4 %	18.2 %	21.0 %
Maximum Water Holding Capacity (MWC)	28.3 g water / 100g dry soil	54.2 g water / 100g dry soil	64.2 g water / 100g dry soil	not available	not available

Characterisation of soils was performed by AGROLAB AG, Labor für Landwirtschaft und Umwelt, CH-6030 Ebikon / Root, Switzerland.
Microbial Biomass was determined in the testing facilities of Novartis Crop Protection AG,
CH-4002 Basel/Switzerland.

[5] Cation Exchange Capacity

Table 2: Pre Test Adsorption

Amount adsorbed in % of applied a.i.
Mean of two experiments

Soil	Borstel	Pappelacker	Gartenacker	Vetroz	Illarsaz	Control
Amount [g]	10.0	10.0	10.0	10.0	5.0	0.0
Time [h]	% a.i. of appl.	% a.i. of appl.	% a.i. of appl.	% a.i. of appl.	% a.i. of appl.	% a.i. of appl.
2	15.9	10.2	21.6	35.3	56.1	2.8
4	18.3	15.0	20.1	39.9	55.3	2.8
6	15.6	10.9	18.1	35.5	54.6	0.5
8	18.4	12.5	19.5	37.6	58.2	2.9
24	17.6	11.2	21.8	38.3	59.9	2.2

Table 3: Pre Test Desorption

Amount desorbed in % of a.i. adsorbed after 24 h (pretest adsorption)
Mean of two experiments

Soil	Borstel	Pappelacker	Gartenacker	Vetroz	Illarsaz	Control
Amount [g]	10.0	10.0	10.0	10.0	5.0	0.0
Time [h]	% a.i. of adsorbed	% a.i. of adsorbed	% a.i. of adsorbed	% a.i. of adsorbed	% a.i. of adsorbed	% a.i. of adsorbed
2	50.0	49.5	42.8	34.2	22.5	7.2
6	46.9	37.3	37.9	30.9	23.2	8.3
24	55.7	47.5	43.3	34.5	24.2	7.7

Table 4: Balance of Radioactivity for Soil Borstel after Adsorption and Desorption

Values given in radioactivity applied

Sample		Aqueous Phase				Soil			
No.	ppm	Adsorption	Desorption1	Desorption2	Washings	Total*	Extractable	Non-Extract.	Recovery
BO_5_1	4.71	84.6	9.1	3.2	0.0	3.5			100.6
BO_5_2	4.71	84.6	9.3	3.2	0.0	4.1			101.2
BO_2.5_1	2.33	84.1	9.5	3.4	0.0	4.3			101.3
BO_2.5_2	2.33	83.3	9.7	3.5	0.0	4.1			100.5
BO_1_1	0.95	83.0	9.8	3.6	0.1	4.4			100.9
BO_1_2	0.95	81.9	9.7	3.7	0.0	4.8			100.1
BO_0.5_1	0.46	81.2	10.6	3.6	0.0	5.0			100.5
BO_0.5_2	0.46	80.3	11.0	3.7	0.0	4.9			99.9
BO_0.25_1	0.23	81.8	10.8	4.0	0.1	5.2			101.9
BO_0.25_2	0.23	82.6	10.0	3.6	0.0	4.7			100.9
BO_5_3	4.71	70.4					28.5	0.1	99.1
BO_5_4	4.71	71.9					28.7	0.2	100.7

* Determined by combustion of soil (including capillary water) after 2nd desorption.

Table 5: Balance of Radioactivity for Soil Pappelacker after Adsorption and Desorption

Values given in radioactivity applied

Sample		Aqueous Phase				Soil			
No.	ppm	Adsorption	Desorption1	Desorption2	Washings	Total*	Extractable	Non-Extract.	Recovery
PA_5_1	4.71	90.5	5.4	2.2	0.0	2.6			100.7
PA_5_2	4.71	89.6	6.3	2.5	0.0	2.7			100.8
PA_2.5_1	2.33	88.1	6.3	2.3	0.0	2.9			99.6
PA_2.5_2	2.33	89.6	5.9	2.4	0.0	2.9			100.8
PA_1_1	0.95	87.7	6.4	2.3	0.0	2.9			99.3
PA_1_2	0.95	87.7	6.5	2.6	0.0	3.2			100.0
PA_0.5_1	0.46	87.4	6.8	2.7	0.0	3.3			100.2
PA_0.5_2	0.46	88.5	6.9	2.7	0.0	3.2			101.3
PA_0.25_1	0.23	86.7	7.0	3.0	0.0	3.3			100.0
PA_0.25_2	0.23	88.0	7.1	2.8	0.0	3.4			101.3
PA_5_3	4.71	70.6					28.7	0.2	99.5
PA_5_4	4.71	73.2					28.1	0.5	101.7

* Determined by combustion of soil (including capillary water) after 2nd desorption.

Table 6: Balance of Radioactivity for Soil Gartenacker after Adsorption and Desorption

Values given in radioactivity applied

Sample		Aqueous Phase				Soil			
No.	ppm	Adsorption	Desorption1	Desorption2	Washings	Total*	Extractable	Non-Extract.	Recovery
GA_5_1	4.71	83.1	9.5	3.6	0.0	6.1			102.2
GA_5_2	4.71	83.4	8.7	3.9	0.0	5.3			101.3
GA_2.5_1	2.33	81.3	9.3	4.1	0.0	6.6			101.3
GA_2.5_2	2.33	81.5	9.2	4.3	0.0	6.3			101.4
GA_1_1	0.95	79.5	9.4	4.6	0.0	6.7			100.2
GA_1_2	0.95	79.8	9.8	4.5	0.0	7.1			101.3
GA_0.5_1	0.46	79.1	10.0	4.9	0.0	7.6			101.6
GA_0.5_2	0.46	79.9	10.0	5.0	0.0	7.5			102.3
GA_0.25_1	0.23	78.9	10.1	4.9	0.0	7.6			101.5
GA_0.25_2	0.23	79.2	10.3	5.1	0.0	7.6			102.2
GA_5_3	4.71	62.8					37.2	0.4	100.4
GA_5_4	4.71	62.6					36.8	0.2	99.7

* Determined by combustion of soil (including capillary water) after 2nd desorption.

Table 7: Balance of Radioactivity for Soil Vetroz after Adsorption and Desorption

Values given in radioactivity applied

Sample		Aqueous Phase				Soil			
No.	ppm	Adsorption	Desorption1	Desorption2	Washings	Total*	Extractable	Non-Extract.	Recovery
VE_5_1	4.71	65.0	13.4	8.1	0.1	16.2			102.7
VE_5_2	4.71	65.4	13.4	8.0	0.0	13.0			99.7
VE_2.5_1	2.33	62.7	13.5	8.2	0.0	18.7			103.2
VE_2.5_2	2.33	63.1	13.7	8.4	0.0	19.1			104.3
VE_1_1	0.95	61.5	13.4	8.5	0.0	19.9			103.3
VE_1_2	0.95	61.2	13.9	8.6	0.0	16.9			100.6
VE_0.5_1	0.46	60.9	14.1	8.6	0.0	16.9			100.5
VE_0.5_2	0.46	61.4	14.2	8.7	0.0	19.8			104.2
VE_0.25_1	0.23	59.5	14.3	8.8	0.0	25.6			108.1
VE_0.25_2	0.23	61.0	13.9	8.8	0.0	21.2			105.0
VE_5_3	4.71	45.0					48.1	0.4	93.5
VE_5_4	4.71	45.3					48.6	0.4	94.3

* Determined by combustion of soil (including capillary water) after 2nd desorption.

Table 8: Balance of Radioactivity for Soil Illarsaz after Adsorption and Desorption

Values given in radioactivity applied

Sample		Aqueous Phase				Soil			
No.	ppm	Adsorption	Desorption1	Desorption2	Washings	Total*	Extractable	Non-Extract.	Recovery
IL_5_1	4.71	42.6	14.3	10.1	0.1	33.5			100.5
IL_5_2	4.71	42.6	14.4	10.1	0.1	33.3			100.4
IL_2.5_1	2.33	41.0	13.9	9.8	0.0	34.8			99.6
IL_2.5_2	2.33	40.9	14.0	10.0	0.1	35.0			100.0
IL_1_1	0.95	39.1	13.8	9.9	0.0	38.0			100.8
IL_1_2	0.95	38.8	14.0	10.1	0.2	36.6			99.7
IL_0.5_1	0.46	38.4	13.5	9.7	0.0	39.2			100.9
IL_0.5_2	0.46	38.6	14.0	10.1	0.1	37.9			100.7
IL_0.25_1	0.23	36.9	13.2	10.1	0.1	39.9			100.2
IL_0.25_2	0.23	38.1	13.7	10.2	0.1	38.0			100.0
IL_5_3	4.71	31.8					65.2	0.1	97.2
IL_5_4	4.71	32.3					66.7	0.6	99.6

* Determined by combustion of soil (including capillary water) after 2nd desorption.

Table 9: Concentration of CGA 329351 in Aqueous Phases and in Soil Borstel after Adsorption and Desorption

Sample		Adsorption		Desorption 1		Desorption 2	
No.	ppm	C_e Ads. [µg/ml]	X/m Ads. [µg/g]	C_e Des. 1 [µg/ml]	X/m Des. 1 [µg/g]	C_e Des. 2 [µg/ml]	X/m Des. 2 [µg/g]
BO_5_3	4.71	3.439	1.587				
BO_5_4	4.71	3.535	1.461				
BO_5_1	4.71	3.466	1.487	0.913	0.600	0.290	0.286
BO_5_2	4.71	3.512	1.498	0.934	0.596	0.291	0.284
BO_2.5_1	2.33	1.710	0.762	0.461	0.304	0.148	0.140
BO_2.5_2	2.33	1.711	0.803	0.462	0.336	0.148	0.170
BO_1_1	0.95	0.688	0.329	0.186	0.138	0.062	0.068
BO_1_2	0.95	0.679	0.353	0.187	0.163	0.062	0.092
BO_0.5_1	0.46	0.327	0.179	0.094	0.078	0.031	0.043
BO_0.5_2	0.46	0.322	0.187	0.095	0.083	0.031	0.047
BO_0.25_1	0.23	0.166	0.087	0.049	0.035	0.016	0.016
BO_0.25_2	0.23	0.164	0.084	0.046	0.036	0.015	0.018

Table 10: Concentration of CGA 329351 in Aqueous Phases and in Soil Pappelacker after Adsorption and Desorption

Sample		Adsorption		Desorption 1		Desorption 2	
No.	ppm	C_e Ads. [µg/ml]	X/m Ads. [µg/g]	C_e Des. 1 [µg/ml]	X/m Des. 1 [µg/g]	C_e Des. 2 [µg/ml]	X/m Des. 2 [µg/g]
PA_5_3	4.71	3.468	0.990				
PA_5_4	4.71	3.488	0.834				
PA_5_1	4.71	3.465	0.931	0.885	0.409	0.267	0.191
PA_5_2	4.71	3.463	1.014	0.896	0.402	0.259	0.191
PA_2.5_1	2.33	1.666	0.576	0.464	0.275	0.141	0.163
PA_2.5_2	2.33	1.668	0.503	0.464	0.218	0.138	0.104
PA_1_1	0.95	0.672	0.241	0.186	0.116	0.057	0.071
PA_1_2	0.95	0.682	0.241	0.186	0.114	0.056	0.062
PA_0.5_1	0.46	0.329	0.120	0.092	0.056	0.028	0.030
PA_0.5_2	0.46	0.335	0.110	0.092	0.044	0.028	0.019
PA_0.25_1	0.23	0.166	0.065	0.046	0.031	0.015	0.016
PA_0.25_2	0.23	0.167	0.058	0.047	0.024	0.015	0.011

Table 11: Concentration of CGA 329351 in Aqueous Phases and in Soil Gartenacker after Adsorption and Desorption

Sample		Adsorption		Desorption 1		Desorption 2	
No.	ppm	C_e Ads. [µg/ml]	X/m Ads. [µg/g]	C_e Des. 1 [µg/ml]	X/m Des. 1 [µg/g]	C_e Des. 2 [µg/ml]	X/m Des. 2 [µg/g]
GA_5_3	4.71	2.971	1.663				
GA_5_4	4.71	2.928	1.670				
GA_5_1	4.71	2.955	1.691	1.075	0.773	0.408	0.424
GA_5_2	4.71	2.932	1.658	1.064	0.820	0.416	0.444
GA_2.5_1	2.33	1.415	0.924	0.526	0.480	0.213	0.284
GA_2.5_2	2.33	1.425	0.914	0.529	0.470	0.215	0.263
GA_1_1	0.95	0.564	0.410	0.214	0.227	0.090	0.138
GA_1_2	0.95	0.566	0.403	0.217	0.212	0.092	0.123
GA_0.5_1	0.46	0.271	0.203	0.106	0.109	0.046	0.062
GA_0.5_2	0.46	0.277	0.196	0.107	0.101	0.045	0.054
GA_0.25_1	0.23	0.138	0.104	0.053	0.055	0.023	0.032
GA_0.25_2	0.23	0.141	0.102	0.054	0.053	0.023	0.028

Table 12: Concentration of CGA 329351 in Aqueous Phases and in Soil Vetroz after Adsorption and Desorption

Sample		Adsorption		Desorption 1		Desorption 2	
No.	ppm	C_e Ads. [µg/ml]	X/m Ads. [µg/g]	C_e Des. 1 [µg/ml]	X/m Des. 1 [µg/g]	C_e Des. 2 [µg/ml]	X/m Des. 2 [µg/g]
VE_5_3	4.71	2.209	3.421				
VE_5_4	4.71	2.210	3.369				
VE_5_1	4.71	2.203	3.446	1.126	2.149	0.611	1.367
VE_5_2	4.71	2.209	3.405	1.134	2.110	0.613	1.340
VE_2.5_1	2.33	1.045	1.819	0.547	1.171	0.303	0.777
VE_2.5_2	2.33	1.058	1.799	0.551	1.143	0.307	0.742
VE_1_1	0.95	0.418	0.760	0.219	0.500	0.124	0.335
VE_1_2	0.95	0.414	0.767	0.222	0.496	0.126	0.328
VE_0.5_1	0.46	0.200	0.375	0.108	0.242	0.061	0.161
VE_0.5_2	0.46	0.201	0.371	0.109	0.236	0.062	0.154
VE_0.25_1	0.23	0.099	0.197	0.054	0.129	0.031	0.087
VE_0.25_2	0.23	0.101	0.190	0.055	0.123	0.031	0.081

Table 13: Concentration of CGA 329351 in Aqueous Phases and in Soil Illarsaz after Adsorption and Desorption

Sample		Adsorption		Desorption 1		Desorption 2	
No.	ppm	C_e Ads. [µg/ml]	X/m Ads. [µg/g]	C_e Des. 1 [µg/ml]	X/m Des. 1 [µg/g]	C_e Des. 2 [µg/ml]	X/m Des. 2 [µg/g]
IL_5_3	4.71	1.454	11.094				
IL_5_4	4.71	1.492	10.993				
IL_5_1	4.71	1.459	11.143	0.908	8.345	0.607	6.374
IL_5_2	4.71	1.468	11.145	0.909	8.339	0.607	6.366
IL_2.5_1	2.33	0.685	5.677	0.430	4.333	0.290	3.381
IL_2.5_2	2.33	0.684	5.689	0.436	4.331	0.296	3.363
IL_1_1	0.95	0.267	2.375	0.171	1.833	0.117	1.445
IL_1_2	0.95	0.270	2.383	0.174	1.834	0.120	1.436
IL_0.5_1	0.46	0.127	1.168	0.082	0.911	0.056	0.726
IL_0.5_2	0.46	0.131	1.166	0.085	0.898	0.058	0.704
IL_0.25_1	0.23	0.063	0.606	0.041	0.478	0.029	0.381
IL_0.25_2	0.23	0.065	0.596	0.042	0.463	0.029	0.365

Table 14: Adsorption- and Desorption Coefficients of CGA 329351 for various Soils

Soil	Process	pH	Org. C [%]	Clay [%]	Interce pt	k- value [ml/g]	Slope 1/n	r^2	K_{OC} [ml/g]	K_{OM} [ml/g]	K_{clay} [ml/g]
Borstel	Adsorption	5.0	1.2	5.3	-0.319	0.480	0.923	0.997	40.0	23.2	9.1
	Desorption 1				-0.175	0.668	0.931	0.993	55.7	32.3	12.6
	Desorption 2				-0.031	0.932	0.919	0.975	77.7	45.1	17.6
Pappelacker	Adsorption	7.6	1.1	2.9	-0.497	0.318	0.900	0.994	28.9	16.8	11.0
	Desorption 1				-0.314	0.485	0.932	0.985	44.1	25.6	16.7
	Desorption 2				-0.099	0.796	0.955	0.949	72.4	42.0	27.4
Gartenacker	Adsorption	7.3	2.08	9.7	-0.191	0.644	0.908	0.998	31.0	18.0	6.6
	Desorption 1				-0.093	0.808	0.907	0.995	38.8	22.5	8.3
	Desorption 2				0.042	1.100	0.942	0.990	52.9	30.7	11.3
Vetroz	Adsorption	7.2	4.7	23.3	0.222	1.668	0.928	0.999	35.5	20.6	7.2
	Desorption 1				0.295	1.973	0.940	0.999	42.0	24.3	8.5
	Desorption 2				0.353	2.255	0.947	0.998	48.0	27.8	9.7
Illarsaz	Adsorption	6.7	19.8	23.6	0.896	7.878	0.929	1.000	39.8	23.1	33.4
	Desorption 1				0.969	9.315	0.936	1.000	47.0	27.3	39.5
	Desorption 2				1.019	10.448	0.939	0.999	52.8	30.6	44.3

Table 15: Relative Mobility Factors (RMF), Sorption Coefficients and Mobility-Adsorption Classes for a Variety of Pesticides[6].

Range				Compound	Adsorption	Class	Mobility
P_{ow}	RMF	K_{oc}	K_{om} (Q-value)				
> 10000	< 0.15	> 1725	> 1000	Fluorodifen (0.15), Parathion (< 0.15)	very strong	I	immobile
< 10000	> 0.15	< 1725	< 1000	Profenophos (0.18), Propiconazole (0.23), Diazinon (0.28), Diuron (0.38), Terbuthylazine (0.52), Methidathion (0.56), Prometryn (0.59), Propazine (0.64), Alachlor (0.66),	strong	II	little mobile
> 500	< 0.8	> 172	>100	Metolachlor (0.68)			
< 500	> 0.8	<172	< 100	Monuron (1.00), Atrazine (1.03),	moderate	III	moderately
> 150	< 1.3	> 86	> 50	Simazine (1.04), Fluometuron (1.18)			mobile
< 150	> 1.3	< 86	< 50	Prometon (1.67), Cyanazine (1.85), Bromacil (1.91),	slight	IV	considerably (slightly)
> 50	< 2.5	> 34	> 20	Karbutilate (1.98)			mobile
< 50	> 2.5	< 34	< 20	Carbofuran (3.00),	low	V	mobile
> 20	< 5	> 17	> 10	Dioxacarb (4.33)			
< 20	> 5	< 17	< 10	Monocrotophos (> 5), Dicrotophos (> 5)	very low	VI	very mobile

P_{ow}: Octanol-Water Partition Coefficient

K_{oc}: Adsorption coefficient related to µg active ingredient (a.i.) adsorbed to 1 g organic carbon at equilibrium concentration C_e = 1 µg a.i./ml

K_{OM}: Adsorption coefficient related to µg active ingredient (a.i.) adsorbed to 1 g organic matter at equilibrium concentration C_e = 1 µg a.i./ml

$K_{oc} = 1.724 \cdot K_{OM}$;

$K_{oc} = k_F \cdot 100 / \%\text{-OC}$; k_F: Freundlich adsorption coefficient

k_F: Adsorption coefficient related to µg active ingredient (a.i.) adsorbed to 1 g soil at equilibrium concentration C_e = 1 µg a.i./ml

6 Data taken from: 5.1.2.e Woo "Adsorption / Desorption", International Symposium, Canterbury, 1 - 3 July 1985.

Figure 1: Rate of Adsorption of CGA329351 in various Soils (Pre-Test).

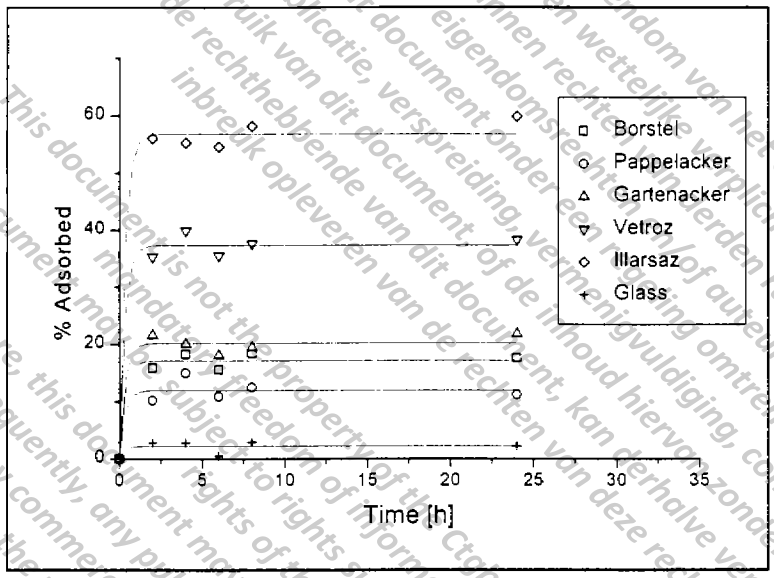


Figure 2: Rate of Desorption of CGA 329351 in various Soils (Pre-Test).

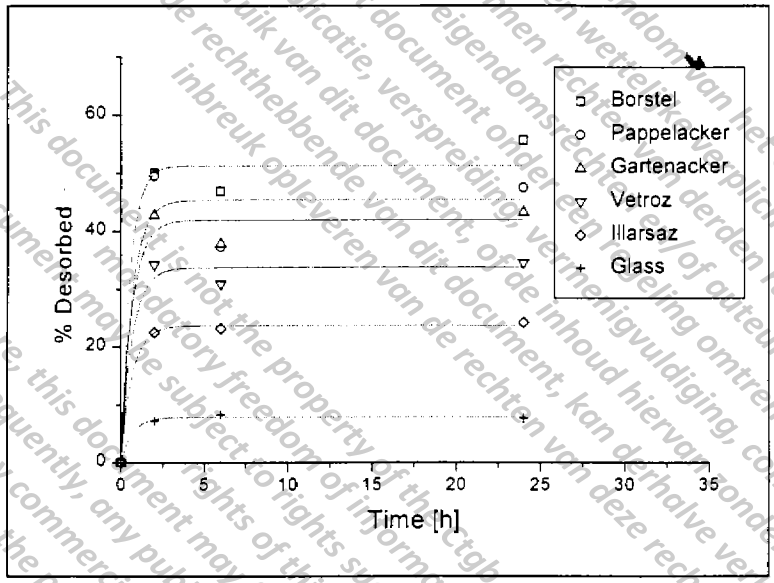
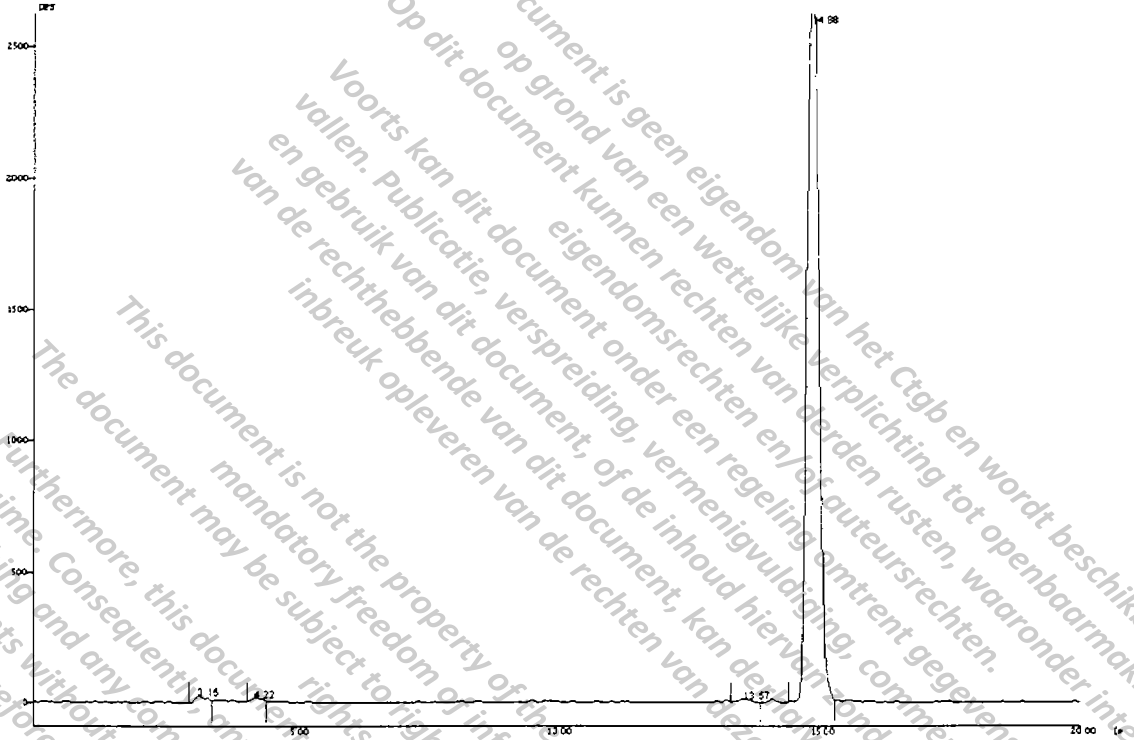


Figure 3: Purity of CGA329351 (HPLC)

HPLC of stock solution



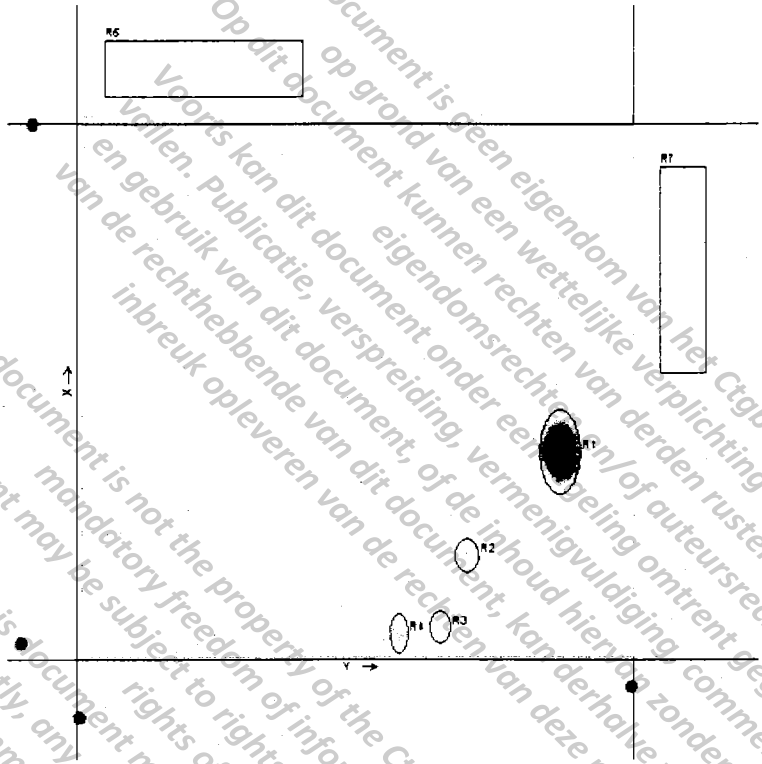
File name : 80722001.CH2 User : ROX Curr. Date : 11-Dec-98 13:15:40
Run Length : 20.00 [min]Acqu. Date : 22-Jul-98 13:57:50
Info :
Stammlösung zur Validierung
42087 dpm/100ul
Vial # = 1 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 17
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	Unknown	3.15	301	0.75	2.97	3.40	0.73	Auto
2	Unknown	4.22	229	0.57	4.07	4.45	0.55	Auto
3	Unknown	13.57	187	0.47	13.30	13.88	0.45	Auto
4	CGA329351	14.88	39315	98.21	14.42	15.30	95.35	Auto

Total Area of Peak = 40031.97
Total = 41230.66
Injection Volume = 100.00 µl

Figure 4: Purity of CGA329351 (TLC)

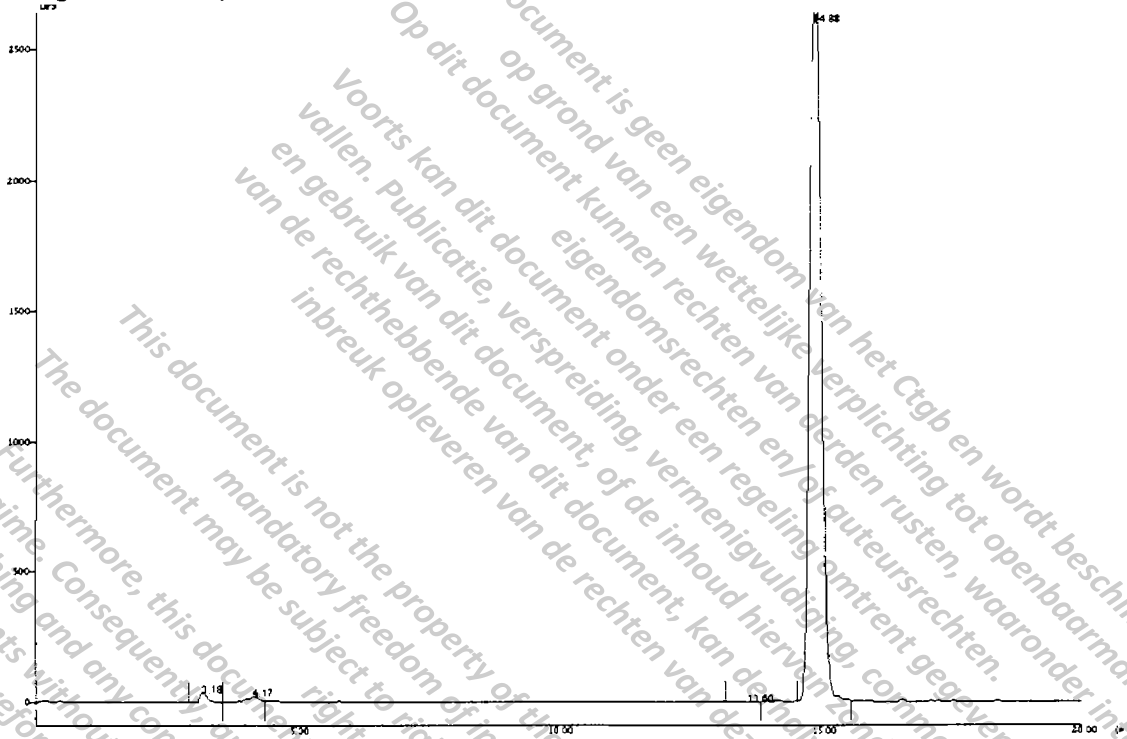
TLC of stock solution (100 µl, 42087 dpm)



Nr	Grp	Name	Typ	Fläche [mm²]	RF-X	RF-Y	PSL	PSL/mm²	PSL-Bkg	%(PSL-Bkg)
1	1	CGA 329351		210.56	0.39	0.87	44278.79	210.29	44254.78	99.45
2	1			51.68	0.19	0.7	83.54	1.62	77.65	0.17
3	1			43.68	0.06	0.66	49.4	1.13	44.42	0.1
4	1			45.04	0.05	0.58	126.78	2.81	121.64	0.27
5	1		Ges	21627.52	0.5	0.5	47909.62	2.22	45443.46	102.12
6	0		Bkg	820.8	--	0.23	89.47	0.11	0	--
7	0		Bkg	689.44	0.73	--	82.74	0.12	0	--
-	1		Sum	350.96	--	--	44538.51	126.9	44498.49	100.00 *
-	1		Rest	21276.56	--	--	3371.1	0.16	944.96	2.12

Figure 5: Stability of CGA 329351

HPLC of glass adsorption solution after 24 h of incubation

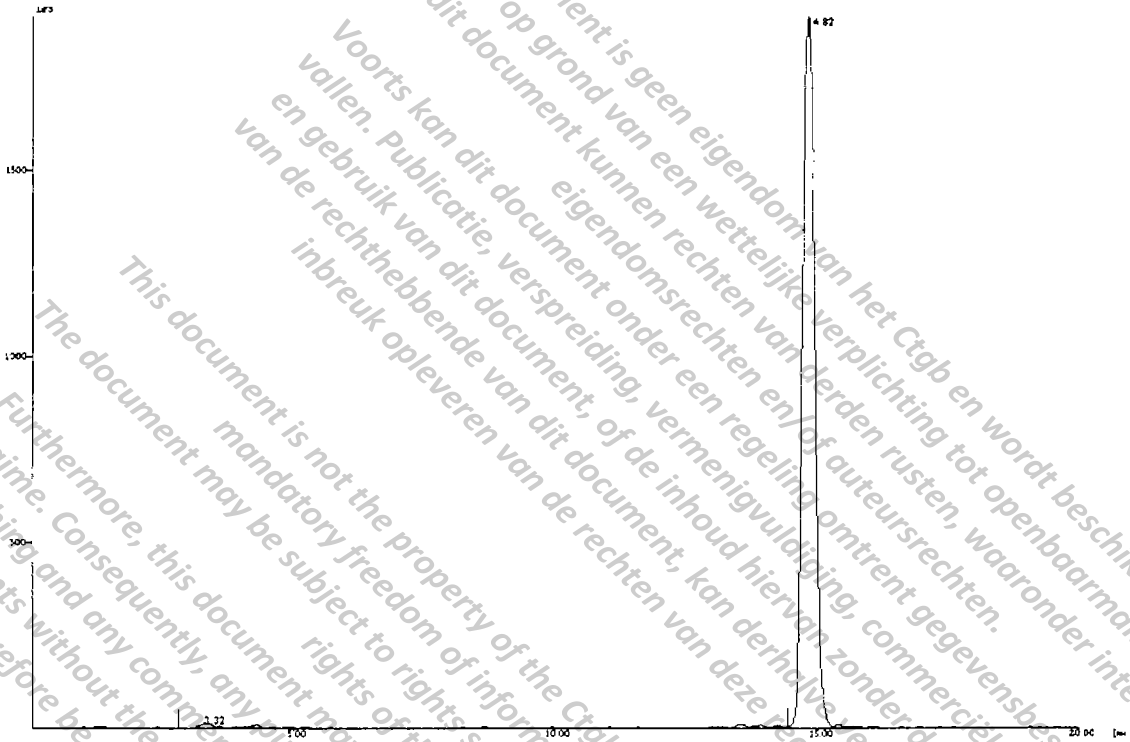


File name : 80717012.CH2 User : ROX Curr. Date : 11-Dec-98 13:31:44
Run Length : 20.00 [min]Acqu. Date : 20-Jul-98 17:01:36
Info :
Glasads1, 40413 dpm
Vial # = 0 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 22
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	Unknown	3.18	292	0.74	2.93	3.57	0.73	Auto
2	Unknown	4.17	299	0.76	3.57	4.40	0.75	Auto
3	Unknown	13.60	2	0.00	13.18	13.85	0.00	Auto
4	CGA329351	14.88	38765	98.49	14.57	15.58	97.63	Auto

Total Area of Peak = 39357.65
Total = 39706.19
Injection Volume = 100.00 µl

Figure 6: HPLC of Aqueous Phase after 24 h of Adsorption (Pre-Test Borstel)

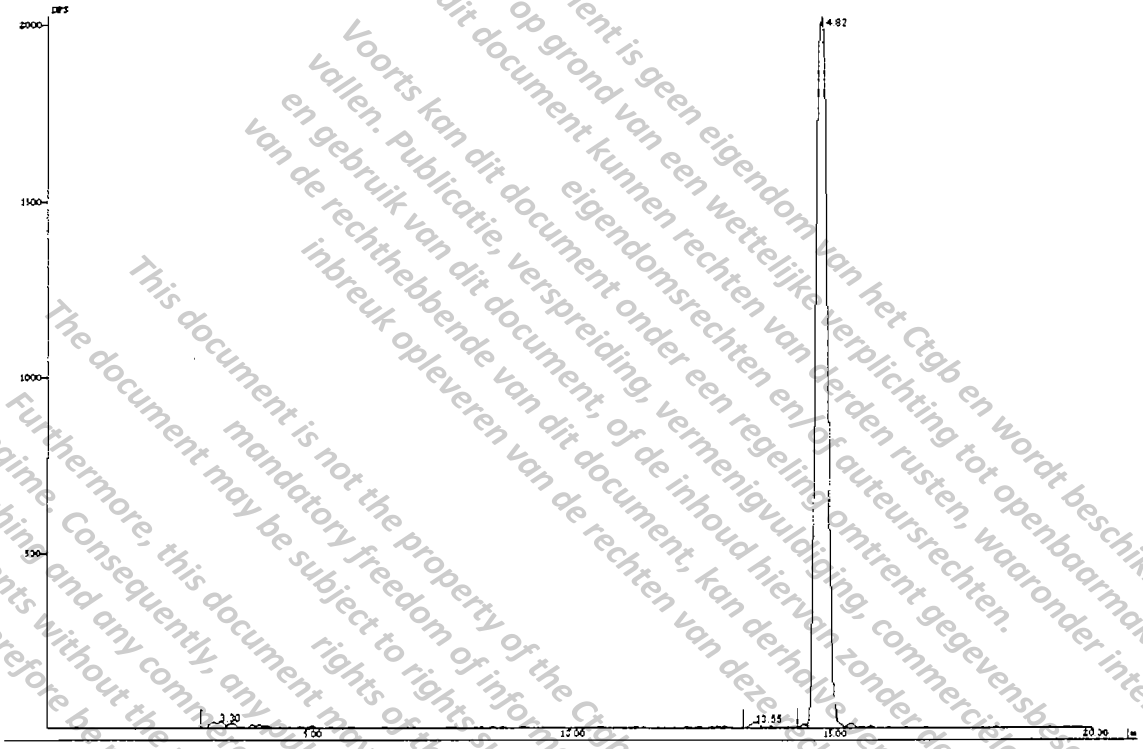


File name : 80717001.CH2 User : ROX Curr. Date : 11-Dec-98 13:36:32
Run Length : 20.00 [min]Acqu. Date : 17-Jul-98 13:44:14
Info : Borstel1, 24h , 29592 ppm
Vial # = 0 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 16
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	Unknown	3.32	238	0.83	2.80	3.70	0.80	Auto
2	CGA329351	14.82	28261	99.17	14.45	15.27	95.58	Auto

Total Area of Peak = 28499.08
Total = 29568.53
Injection Volume = 100.00 µl

Figure 7: HPLC of Aqueous Phase after 24 h of Adsorption (Pre-Test Pappelacker)

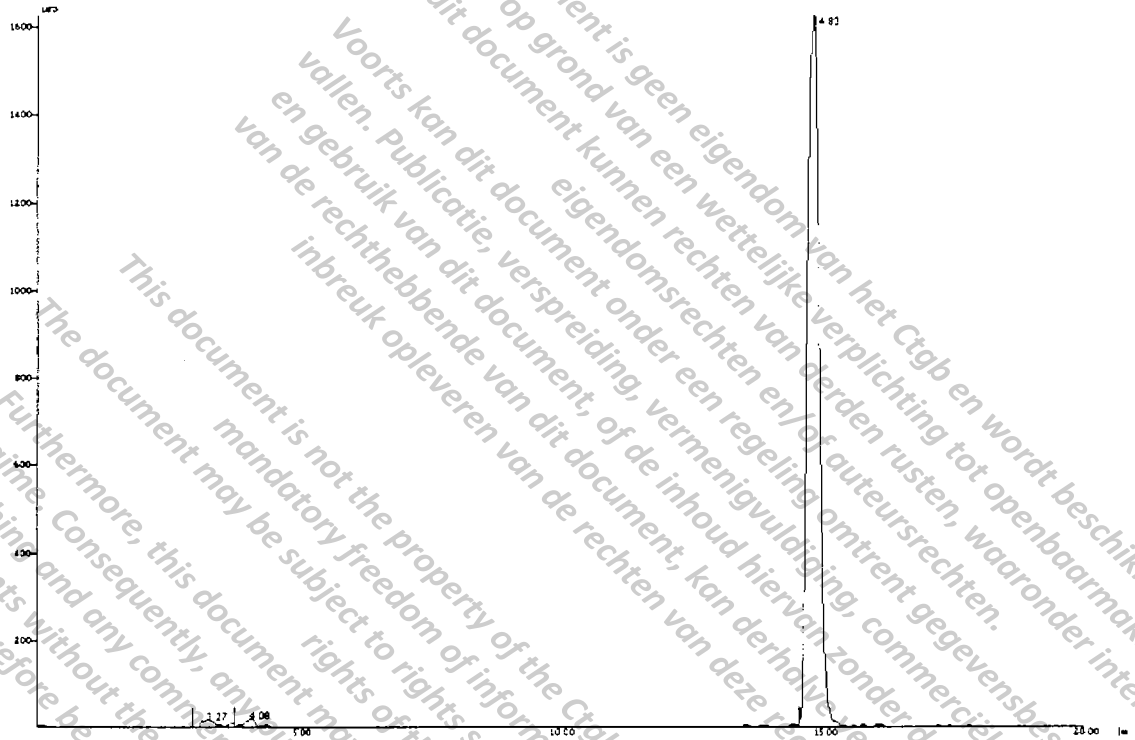


File name : 80717003.CH2 User : ROX Curr. Date : 11-Dec-98 13:38:20
Run Length : 20.00 [min]Acqu. Date : 17-Jul-98 15:20:10
Info : Pappelacker 1, 24h, 30188 dpm
Vial # = 0 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 17
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	Unknown	3.30	275	0.94	2.95	3.40	0.90	Auto
2	Unknown	13.55	179	0.61	13.30	13.67	0.59	Auto
3	CGA 329351	14.82	28850	98.45	14.35	15.23	94.61	Auto

Total Area of Peak = 29303.29
Total = 30492.63
Injection Volume = 100.00 µl

Figure 8: HPLC of Aqueous Phase after 24 h of Adsorption (Pre-Test Gartenacker)

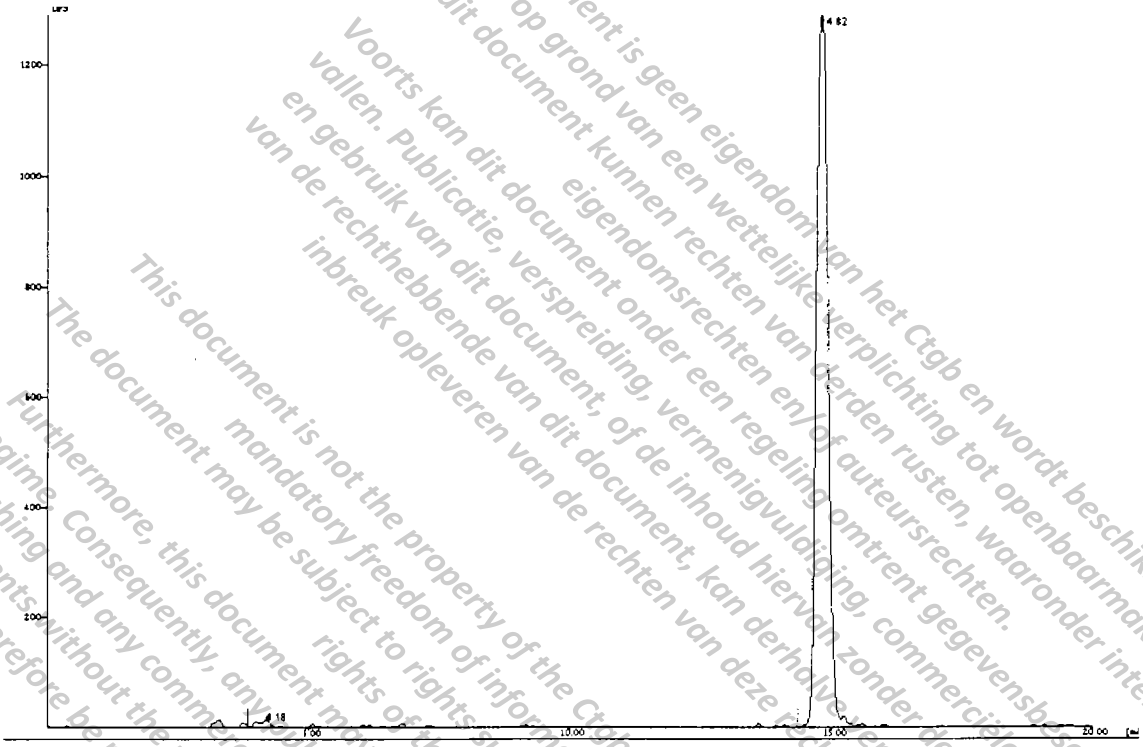


File name : 80717005.CH2 User : ROX Curr. Date : 11-Dec-98 13:39:20
Run Length : 20.00 [min]Acqu. Date : 17-Jul-98 16:20:20
Info : Gartenacker1, 24h, 24734 dpm
Vial # = 0 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 21
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	Unknown	3.27	251	1.04	2.98	3.58	1.02	Auto
2	Unknown	4.08	220	0.91	3.78	4.22	0.90	Auto
3	CGA329351	14.83	23739	98.05	14.55	15.50	96.71	Auto

Total Area of Peak = 24210.25
Total = 24546.97
Injection Volume = 100.00 µl

Figure 9: HPLC of Aqueous Phase after 24 h of Adsorption (Pre-Test Vetroz)

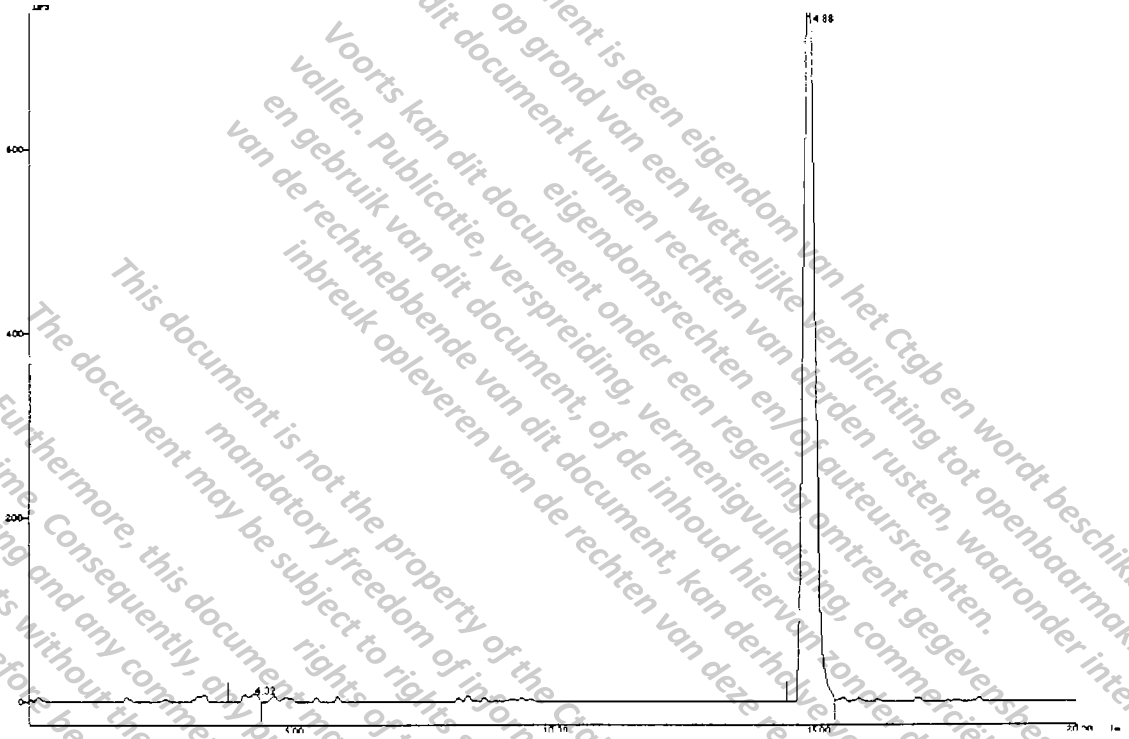


File name : 80717007.CH2 User : ROX Curr. Date : 11-Dec-98 13:40:10
Run Length : 20.00 [min]Acqu. Date : 17-Jul-98 17:20:28
Info : Vetroz1, 24 h, 18652 dpmVial # = 0 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 20
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	Unknown	4.18	197	1.06	3.85	4.37	1.03	Auto
2	CGA 329351	14.82	18432	98.94	14.35	15.43	95.83	Auto

Total Area of Peak = 18629.84
Total = 19234.95
Injection Volume = 100.00 µl

Figure 10: HPLC of Aqueous Phase after 24 h of Adsorption (Pre-Test Illarsaz)

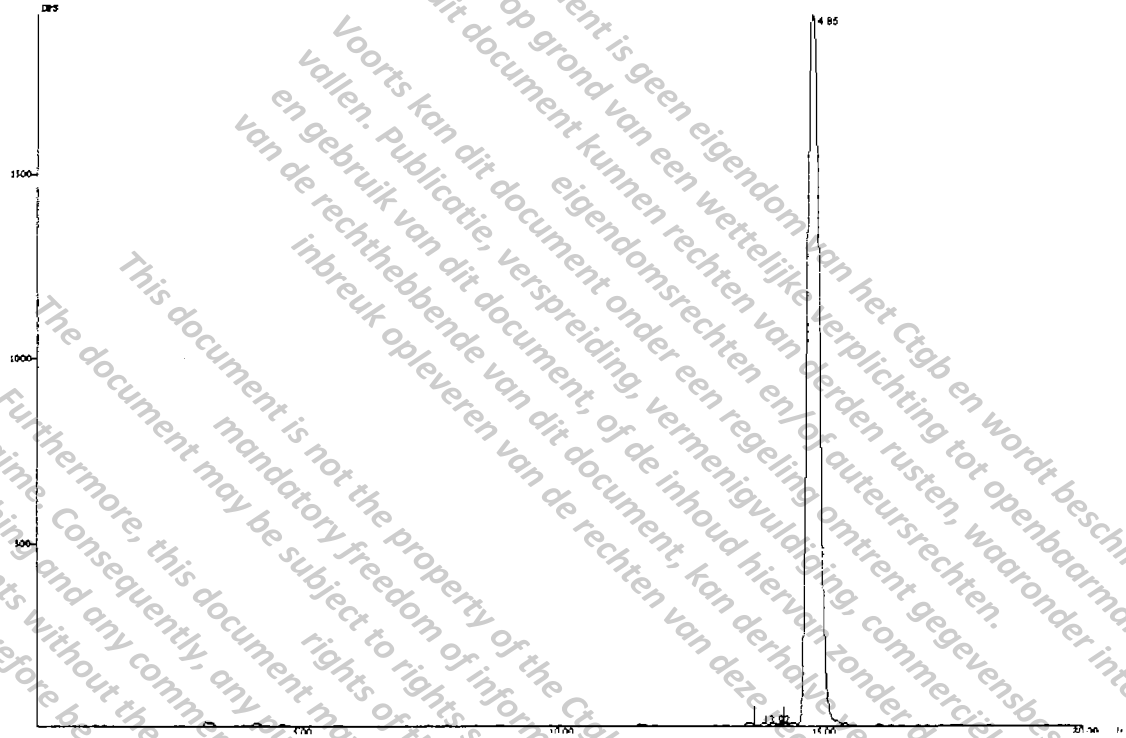


File name : 80717010 CH2 User : ROX Curr. Date : 11-Dec-98 13:42:08
Run Length : 20.00 [min]Acqu. Date : 20-Jul-98 16:16:28
Info : Illarsaz 1, 24 h, 13203 dpm
Illarsaz1
Vial # = 0 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 19
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	Unknown	4.32	134	1.18	3.80	4.45	1.13	Auto
2	CGA 329351	14.88	11182	98.82	14.47	15.37	94.41	Auto

Total Area of Peak = 11315.43
Total = 11844.25
Injection Volume = 100.00 µl

Figure 11: HPLC of Aqueous Phase after Adsorption Step with Soil Borstel (Sample BO_5_3)



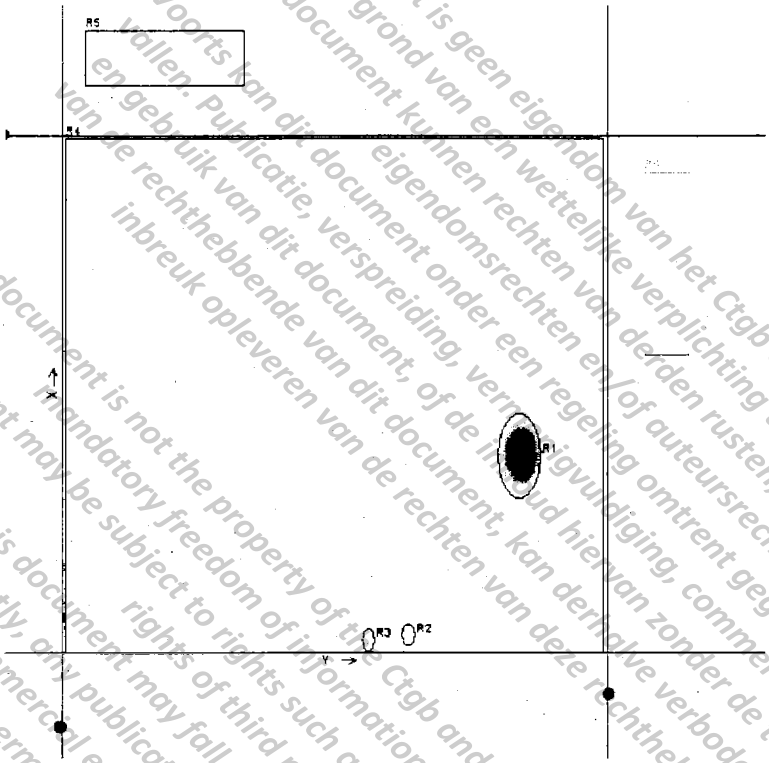
File name : 80722002.CH2 User : ROX Curr. Date : 11-Dec-98 14:00:10
Run Length : 20.00 [min]Acqu. Date : 22-Jul-98 16:26:38
Info :
BO 5_3 Validierung
29809 dpm/100ul
Vial # = 1 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 18
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	Unknown	13.92	194	0.67	13.75	14.32	0.65	Auto
2	CGA 329351	14.85	28784	99.33	14.32	15.40	96.36	Auto

Total Area of Peak = 28978.46
Total = 29871.76
Injection Volume = 100.00 µl

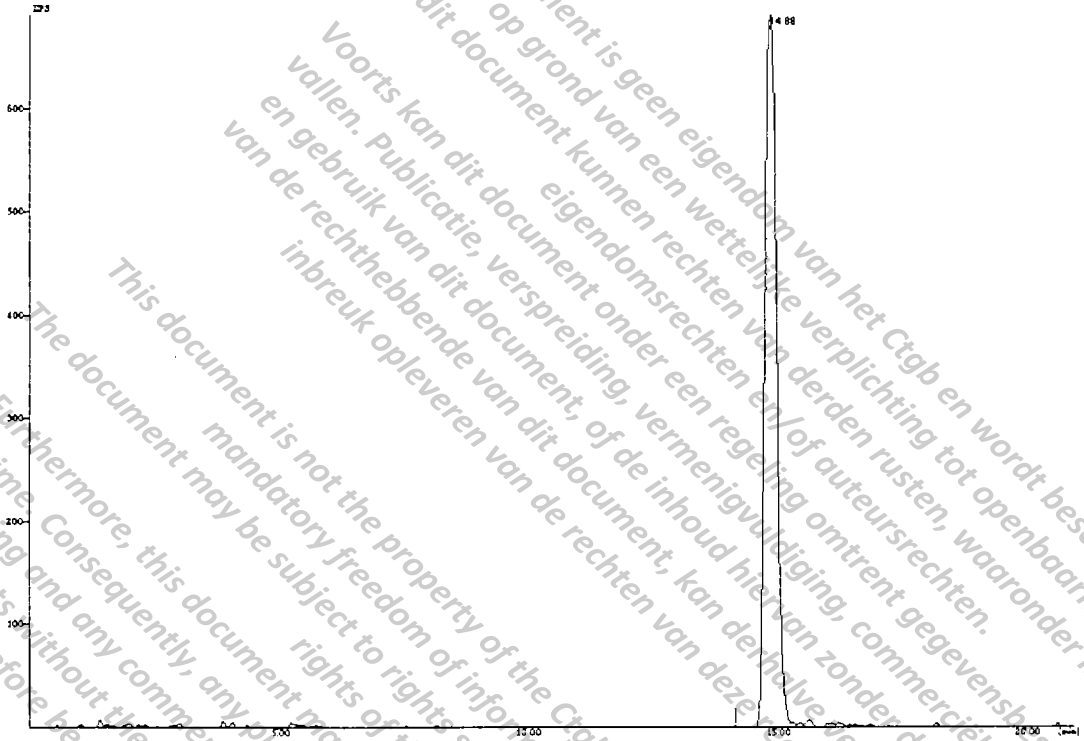
Figure 12: TLC of Aqueous Phase after Adsorption Step with Soil Borstel (Sample BO_5_3)

100 µl, 29808 dpm



Nr	Grp	Name	Typ	Fläche [mm²]	RF-X	RF-Y	PSL	PSL/mm²	PSL-Bkg	%(PSL-Bkg)
1	1			217.28	0.38	0.84	29802.04	137.16	29776.21	99.71
2	1			18.72	0.03	0.64	33.81	1.81	31.58	0.11
3	1			18.12	0.02	0.56	56.86	3.14	54.71	0.18
4	1		Ges	20157.24	0.5	0.5	32732.36	1.62	30335.83	101.59
5	0		Bkg	633.44	--	0.19	62.5	0.1	0	--
6	0		Bkg	590.4	0.75	--	83	0.14	0	--
-	1		Sum	254.12	--	--	29892.71	117.63	29862.5	100.00 *
-	1		Rest	19903.12	--	--	2839.65	0.14	473.34	1.59

Figure 13: HPLC of the Extract after Adsorption Step with Soil Borstel (Sample BO_5_3)



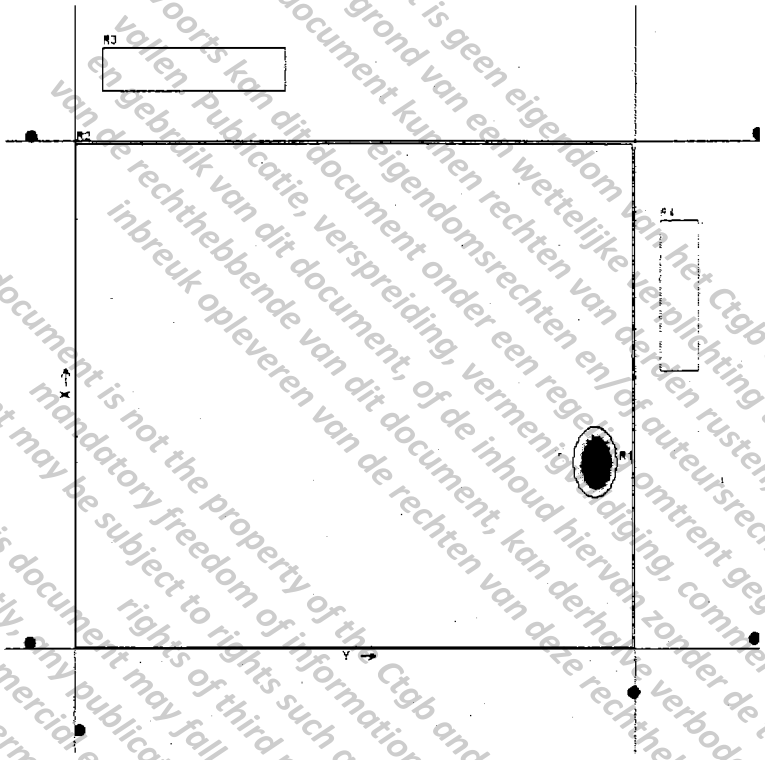
File name : 81015001.CH2 User : ROX Curr. Date : 14-Dec-98 7:55:48
Run Length : 21.00 [min]Acqu. Date : 15-Oct-98 8:36:50
Info :
BO 5_3, 10236 dpm
Vial # = 1 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 16
Efficiency % = 80

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	CGA 329351	14.88	10263	100.00	14.20	15.55	96.19	Auto

Total Area of Peak = 10262.61
Total = 10669.47
Injection Volume = 100.00 µl

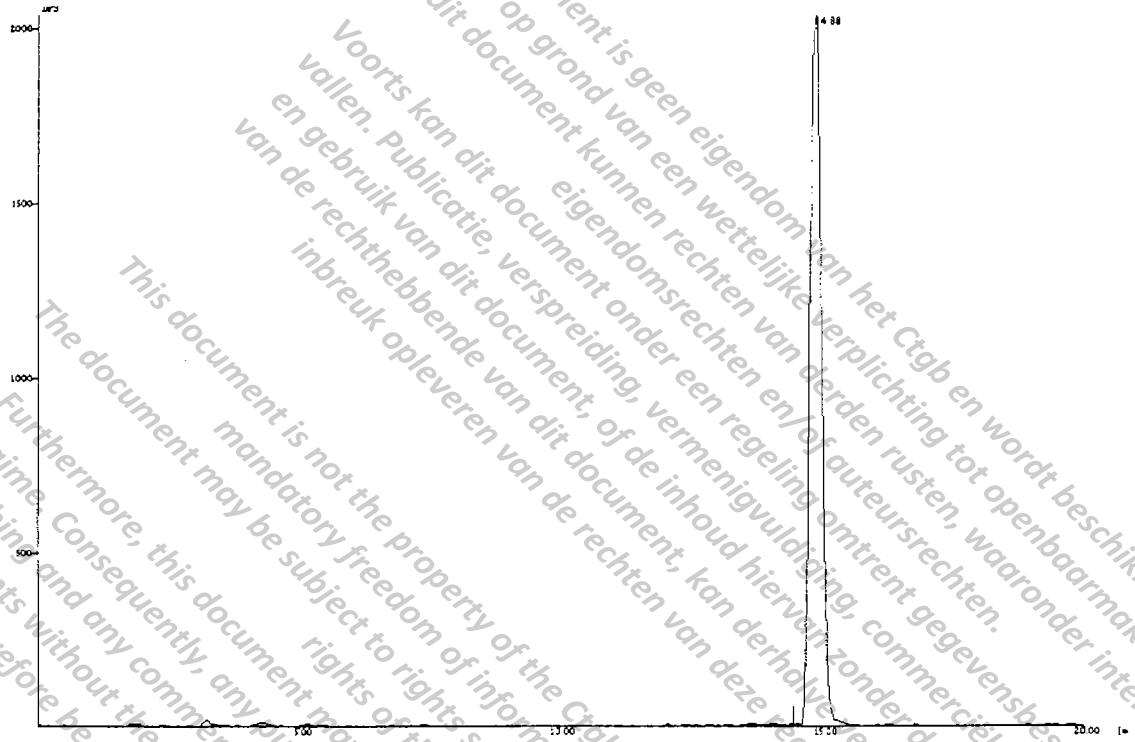
Figure 14: TLC of the Extract after Adsorption Step with Soil Borstel (Sample BO_5_3)

100 µl, 10183 dpm



Nr	Grp	Name	Typ	Fläche [mm²]	RF-X	RF-Y	PSL	PSL/mm²	PSL-Bkg	%(PSL-Bkg)
1	1			190.56	0.37	0.93	11091.02	58.2	11070.9	100
2	1		Ges	20780.24	0.5	0.5	13483.55	0.65	11289.58	101.98
3	0		Bkg	580	--	0.21	57.86	0.1	0	--
4	0		Bkg	428.48	0.7	--	48.62	0.11	0	--
-	1		Sum	190.56	--	--	11091.02	58.2	11070.9	100.00 *
-	1		Rest	20589.68	--	--	2392.52	0.12	218.68	1.98

Figure 15: HPLC of Aqueous Phase after Adsorption Step with Soil Pappelacker (Sample PA_5_3)

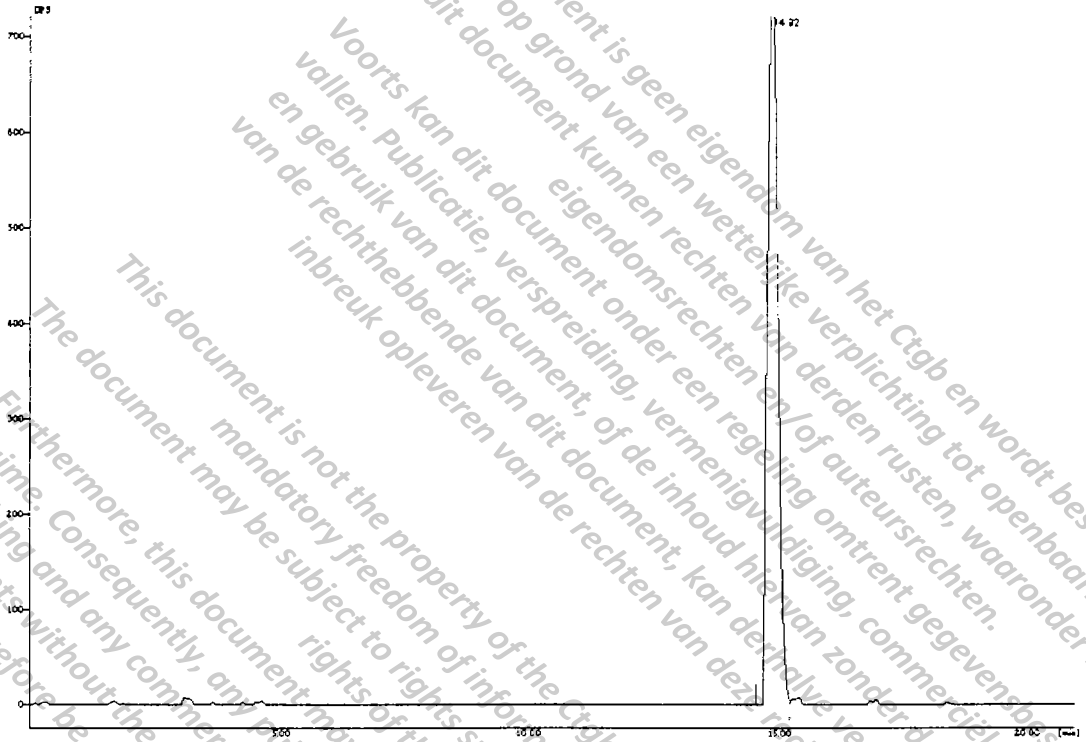


File name : 80729001.CH2 User : ROX Curr. Date : 11-Dec-98 14:02:26
Run Length : 20.00 [min]Acqu. Date : 29-Jul-98 14:09:40
Info :
PA_5_3, 100 ul, 30258 dpm
Vial # = 0 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 12
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	CGA329351	14.88	29160	100.00	14.47	15.55	95.65	Auto

Total Area of Peak = 29160.19
Total = 30486.31
Injection Volume = 100.00 µl

Figure 16: HPLC of the Soil Extract after Adsorption Step with Soil Pappelacker (Sample PA_5_3)

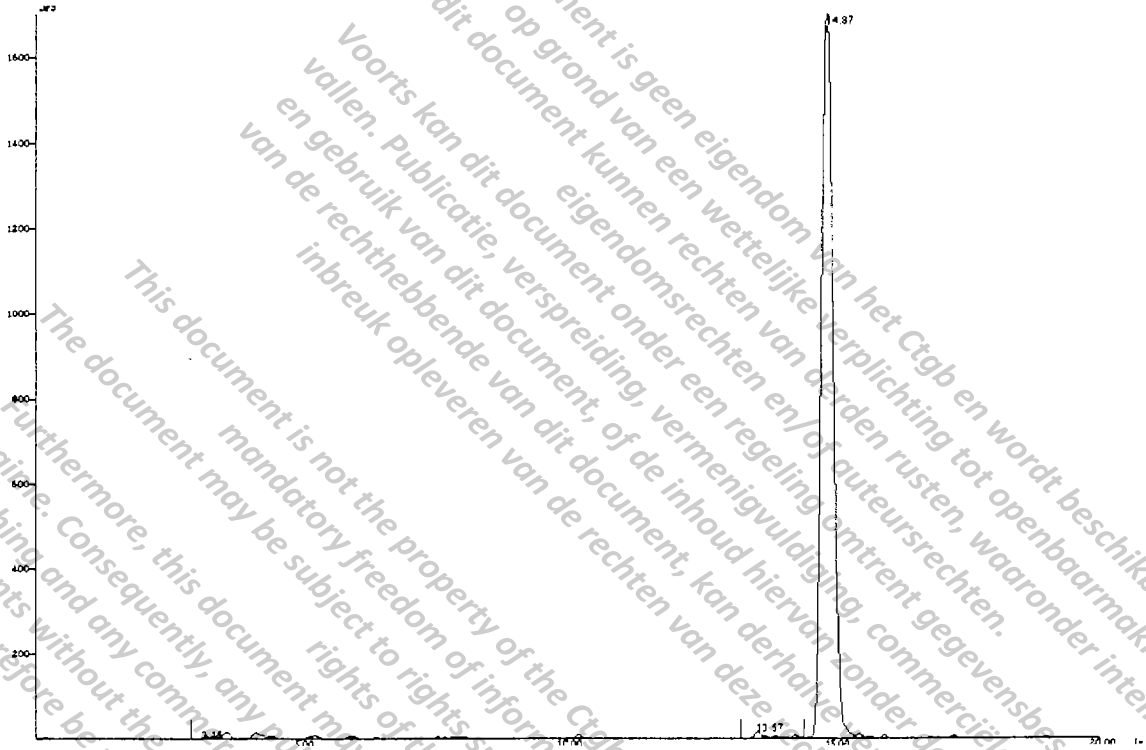


File name : 81015002.CH2 User : ROX Curr. Date : 14-Dec-98 7:58:04
Run Length : 21.00 [min]Acqu. Date : 15-Oct-98 9:03:42
Info :
PA 5_3, 10080 dpm
Vial # = 3 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 21
Efficiency % = 80

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	CGA329351	14.92	10054	100.00	14.58	15.27	97.54	Auto

Total Area of Peak = 10053.54
Total = 10307.37
Injection Volume = 100.00 µl

Figure 17: HPLC of Aqueous Phase after Adsorption Step with Soil Gartenacker (Sample GA_5_3)

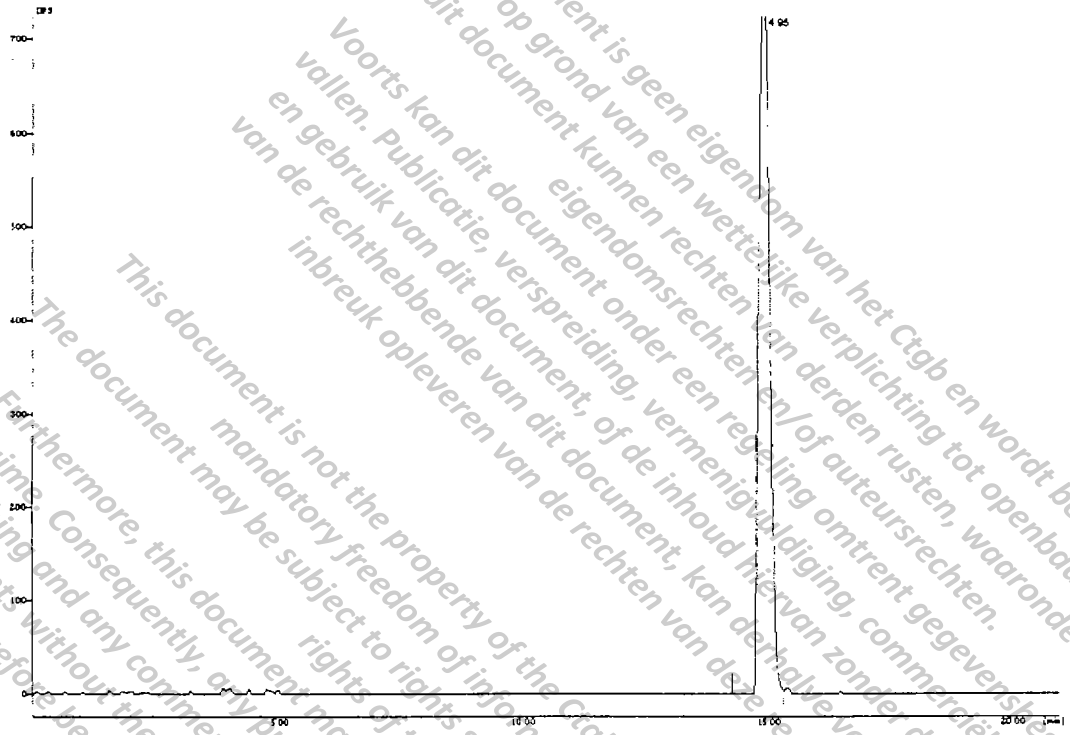


File name : 80729003.CH2 User : ROX Curr. Date : 11-Dec-98 14:03:56
Run Length : 20.00 [min]Acqu. Date : 29-Jul-98 14:58:54
Info :
GA_5_3, 100 ul, 25901 dpm
Vial # = 0 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 19
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	Unknown	3.15	72	0.30	2.93	3.43	0.29	Auto
2	Unknown	13.57	142	0.59	13.27	13.78	0.57	Auto
3	CGA 329351	14.87	23850	99.11	14.45	15.38	95.50	Auto

Total Area of Peak = 24064.14
Total = 24974.82
Injection Volume = 100.00 µl

Figure 18: HPLC of the Soil Extract after Adsorption Step with Soil Gartenacker (Sample GA_5_3)

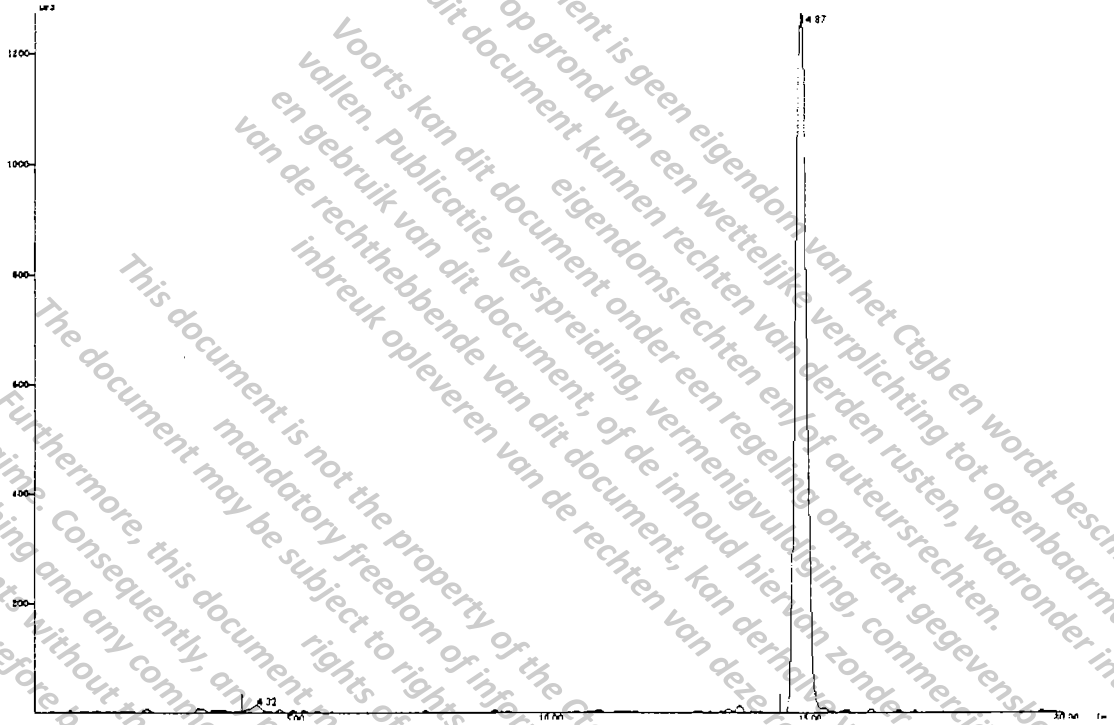


File name : 81013005.CH2 User : ROX Curr. Date : 14-Dec-98 8:17:50
Run Length : 21.00 [min]Acqu. Date : 13-Oct-98 11:46:00
Info :
Gartenacker, Kaltextrakt 5_3, 100 ul, 11918 dpm
Vial # = 0 Rack # = 1
Control Method :
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 19
Efficiency % = 80

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	CGA 329351	14.95	10742	100.00	14.32	15.35	98.15	Auto

Total Area of Peak = 10741.91
Total = 10944.57
Injection Volume = 0.00 µl

Figure 19: HPLC of Aqueous Phase after Adsorption Step with Soil Vetroz (Sample VE_5_3)

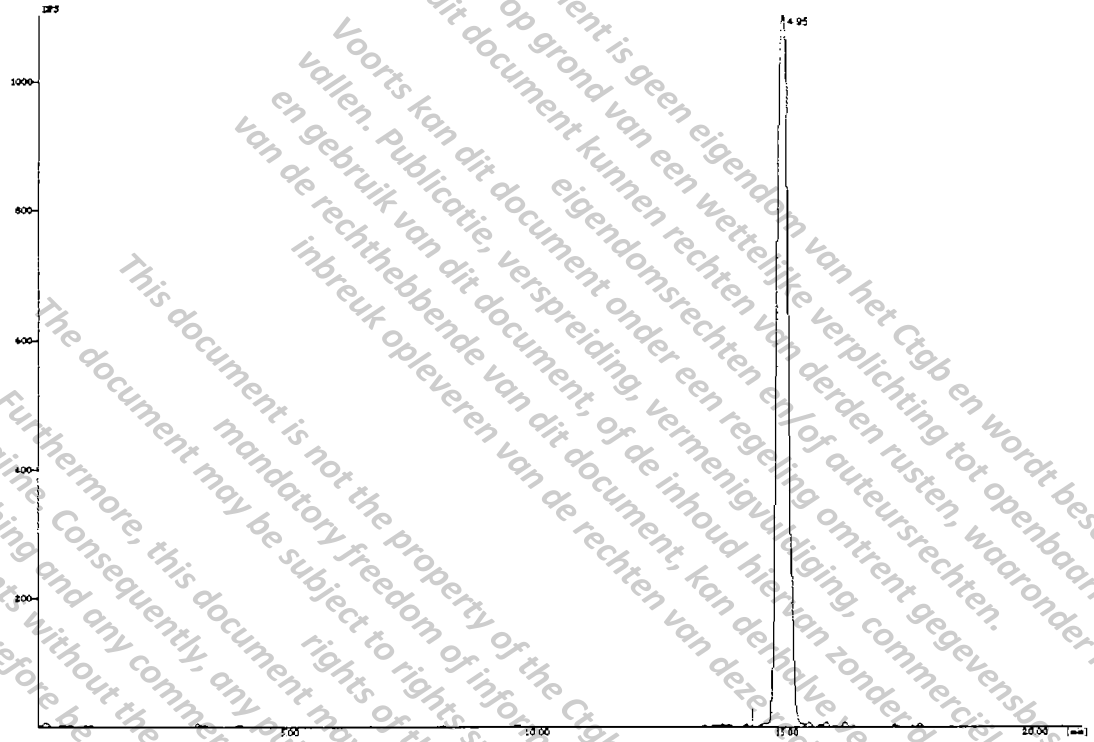


File name : 80804001.CH2 User : ROX Curr. Date : 11-Dec-98 14:05:20
Run Length : 20.00 [min]Accu. Date : 4-Aug-98 14:26:26
Info :
VE_5_3, 100 ul, 17668 dpm
Vial # = 0 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 12
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	Unknown	4.32	212	1.20	4.03	4.63	1.14	Auto
2	CGA329351	14.87	17484	98.80	14.48	15.58	93.86	Auto

Total Area of Peak = 17696.45
Total = 18628.99
Injection Volume = 100.00 µl

Figure 20: HPLC of the Soil Extract after Adsorption Step with Soil Vetroz (Sample VE_5_3)

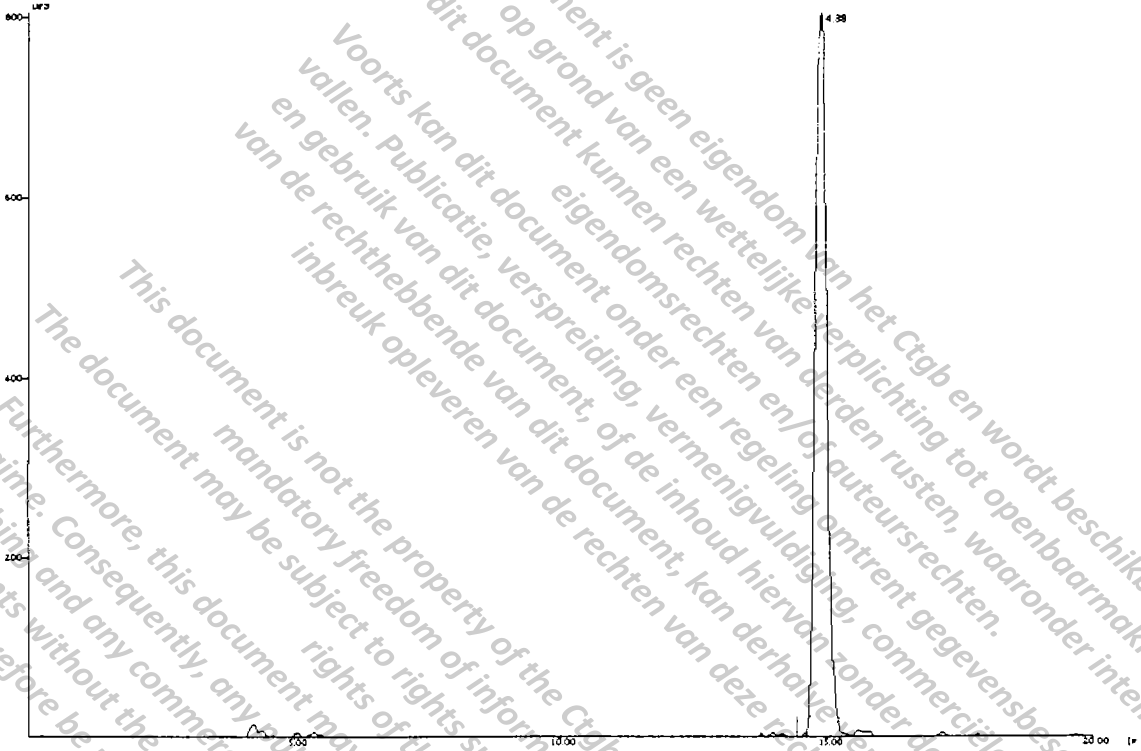


File name : 81013007.CH2 User : ROX Curr. Date : 14-Dec-98 8:19:04
Run Length : 21.00 [min]Acqu. Date : 13-Oct-98 12:31:08
Info :
Vetroz, Kaltextrakt 5_3, 100 ul, 17487 dpm
Vial # = 0 Rack # = 1
Control Method :
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 16
Efficiency % = 80

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	CGA 329351	14.95	15910	100.00	14.35	15.40	97.42	Auto

Total Area of Peak = 15909.75
Total = 16331.86
Injection Volume = 0.00 µl

Figure 21: HPLC of Aqueous Phase after Adsorption Step with Soil Illarsaz (Sample IL_5_3)



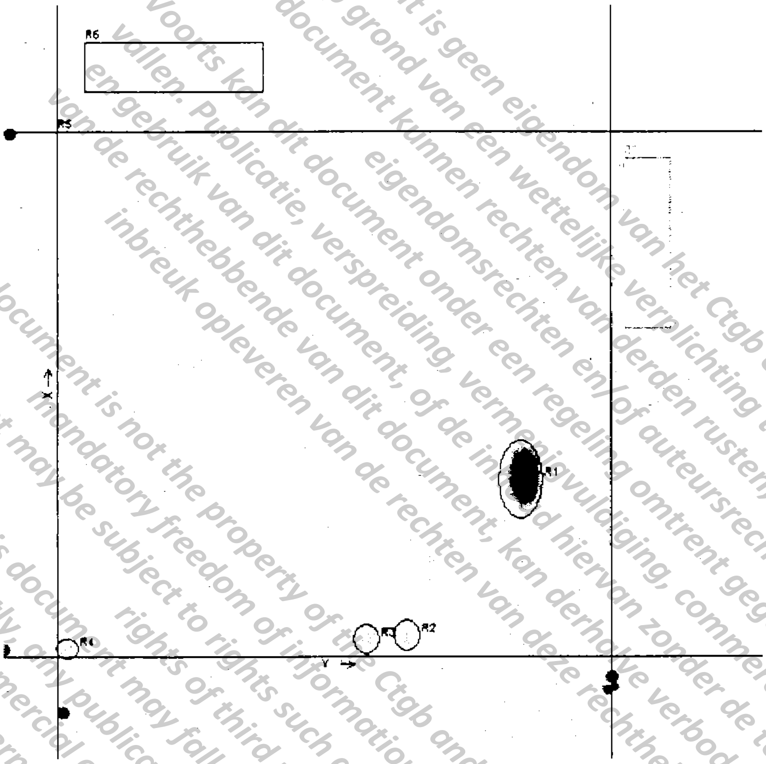
File name : 80804003.CH2 User : ROX Curr. Date : 11-Dec-98 14:06:24
Run Length : 20.00 [min]Acqu. Date : 4-Aug-98 15:14:44
Info :
IL_5_3, 100 ul, 12565 dpm
Vial # = 0 Rack # = 1
Control Method : 98RP05
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 17
Efficiency % = 85

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	CGA329351	14.88	11426	100.00	14.45	15.45	96.44	Auto

Total Area of Peak = 11425.85
Total = 11847.09
Injection Volume = 100.00 µl

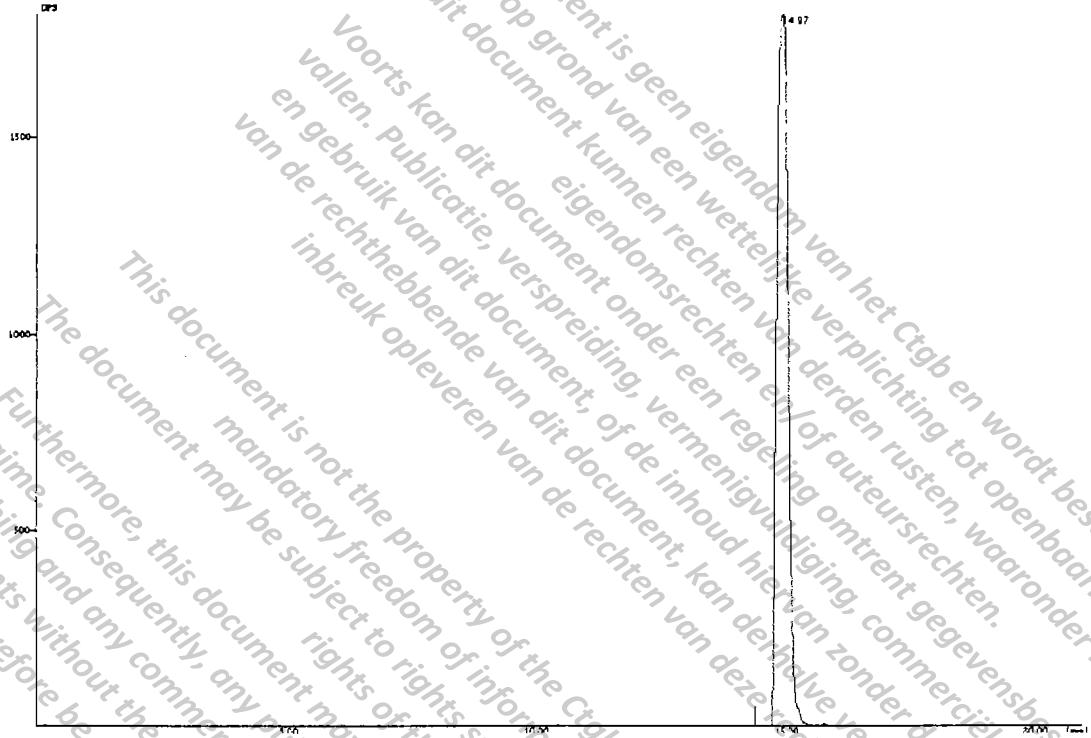
Figure 22: TLC of Aqueous Phase after Adsorption Step with Soil Illarsaz (Sample IL_5_3)

100 µl, 12565 dpm



Nr	Grp	Name	Typ	Fläche [mm²]	RF-X	RF-Y	PSL	PSL/mm²	PSL-Bkg	%(PSL-Bkg)
1	1			210.6	0.34	0.84	11855.17	56.29	11835.7	98.48
2	1			50.56	0.04	0.63	103.62	2.05	98.94	0.82
3	1			47.8	0.03	0.56	49.68	1.04	45.26	0.38
4	1			28	0.02	0.02	40.52	1.45	37.93	0.32
5	1		Ges	21304.44	0.5	0.5	14465.21	0.68	12495.13	103.97
6	0		Bkg	638.88	--	0.21	58.23	0.09	0	--
7	0		Bkg	570.4	0.79	--	53.6	0.09	0	--
-	1		Sum	336.96	--	--	12048.99	35.76	12017.83	100.00 *
-	1		Rest	20967.48	--	--	2416.22	0.12	477.3	3.97

Figure 23: HPLC of the Soil Extract after Adsorption Step with Soil Illarsaz (Sample IL_5_3)



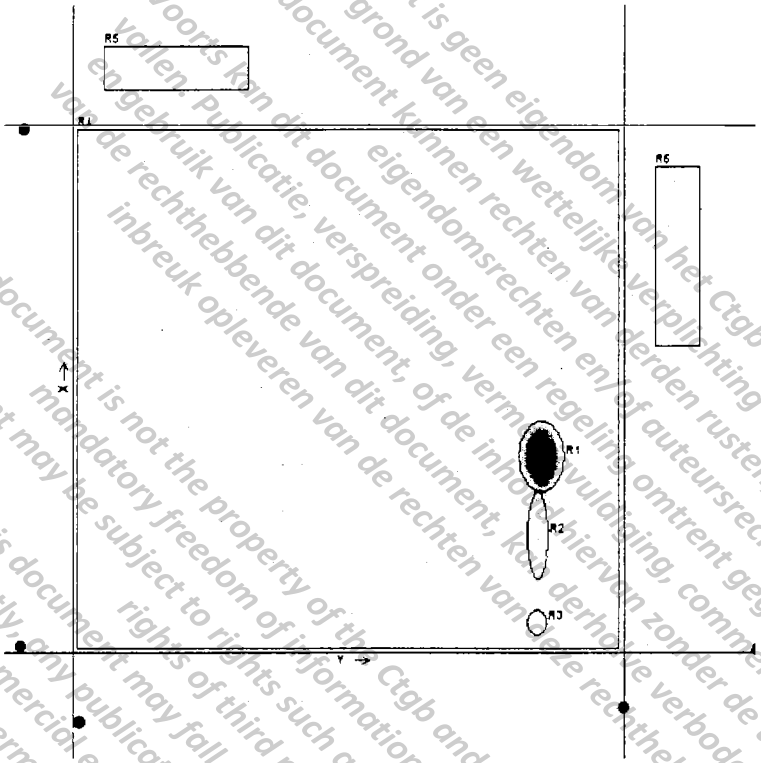
File name : 81013009.CH2 User : ROX Curr. Date : 14-Dec-98 8:20:14
Run Length : 21.00 [min]Acqu. Date : 13-Oct-98 13:16:20
Info :
Illarsaz, Kaltextrakt 5_3, 100 ul, 21077 dpm
Vial # = 0 Rack # = 1
Control Method :
Cell Size(ul) : 150.00 Flow rate (ml/min) : 1.00
Bkg (Cpm) = 22
Efficiency % = 80

#	Name	Rt	DPM	%Area	XStart	XEnd	%Total	Int.mode
1	CGA 329351	14.97	26965	100.00	14.42	15.60	99.82	Auto

Total Area of Peak = 26964.77
Total = 27012.98
Injection Volume = 0.00 µl

Figure 24: TLC of the Soil Extract after Adsorption Step with Soil Illarsaz (Sample IL_5_3)

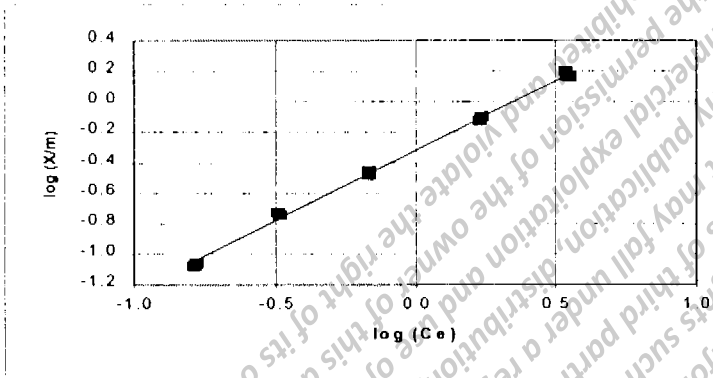
100 µl, 21077 dpm



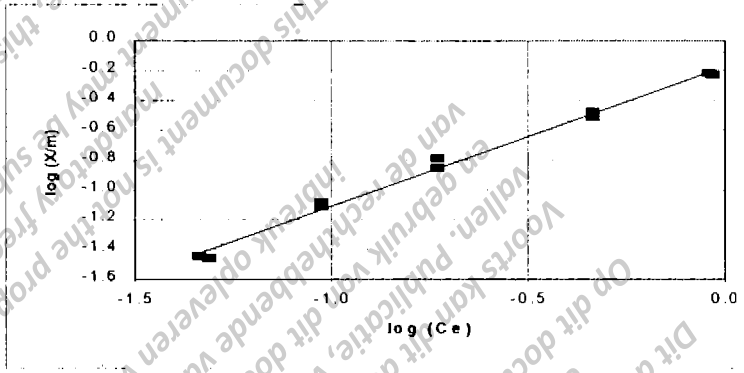
Nr	Grp	Name	Typ	Fläche [mm²]	RF-X	RF-Y	PSL	PSL/mm²	PSL-Bkg	%(PSL-Bkg)
1	1			197.36	0.37	0.85	20457.83	103.66	20440.14	98.68
2	1			112.68	0.22	0.84	217.52	1.93	207.42	1
3	1			32	0.06	0.84	67.93	2.12	65.07	0.31
4	1		Ges	20752.56	0.5	0.5	22961.96	1.11	21102.22	101.88
5	0		Bkg	459.36	--	0.19	37.5	0.08	0	--
6	0		Bkg	580.8	0.75	--	55.72	0.1	0	--
-	1		Sum	342.04	--	--	20743.27	60.65	20712.62	100.00 *
-	1		Rest	20410.52	--	--	2218.69	0.11	389.6	1.88

Figure 25: Freundlich Plots (log-log) for Adsorption and Desorption of CGA 329351 for Soil Borstel Sandy Loam

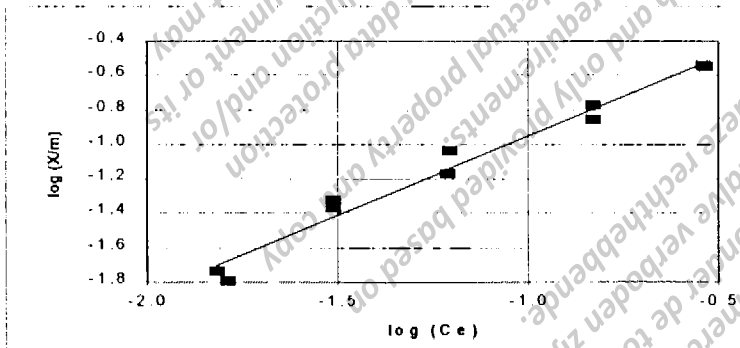
Adsorption of CGA 329351 to Borstel soil



Desorption 1 of CGA 329351 from Borstel soil



Desorption 2 of CGA 329351 from Borstel soil



Adsorption / Desorption of CGA 329351 for Borstel soil (calculated values)

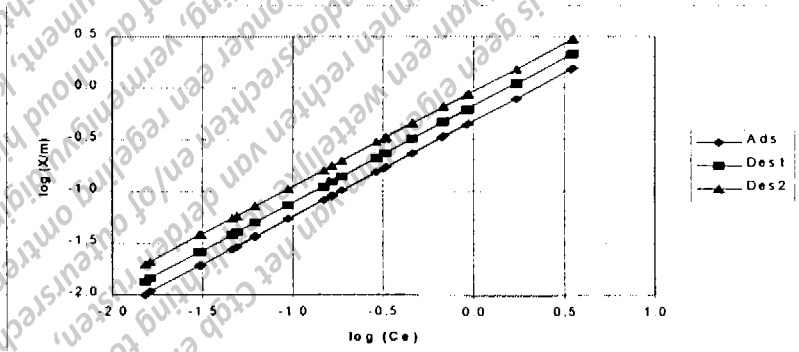
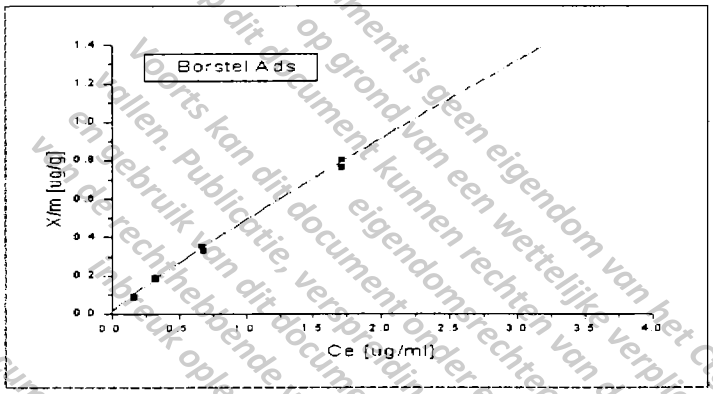
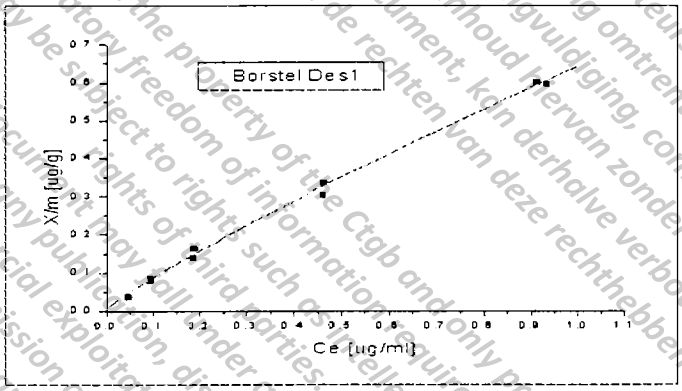


Figure 26: Freundlich Plots (lin-lin) for Adsorption and Desorption of CGA 329351 for Soil Borstel Sandy Loam

Adsorption of CGA 329351 to Borstel soil (k = 0.4834; 1/n = 0.9099)



Desorption 1 of CGA 329351 from Borstel soil (k = 0.6413; 1/n = 0.8865)



Desorption 2 of CGA 329351 from Borstel soil (k = 0.8196; 1/n = 0.8573)

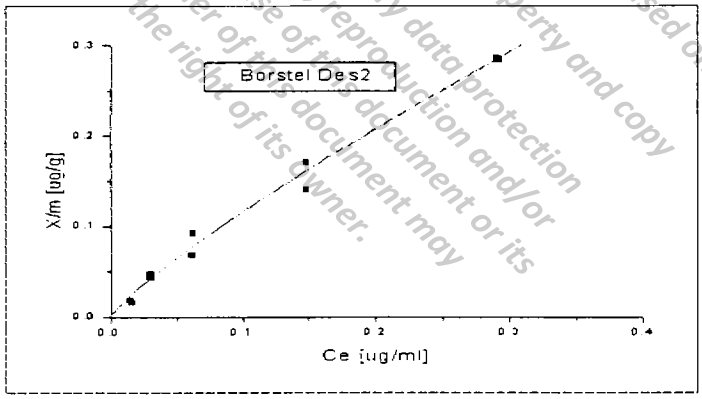
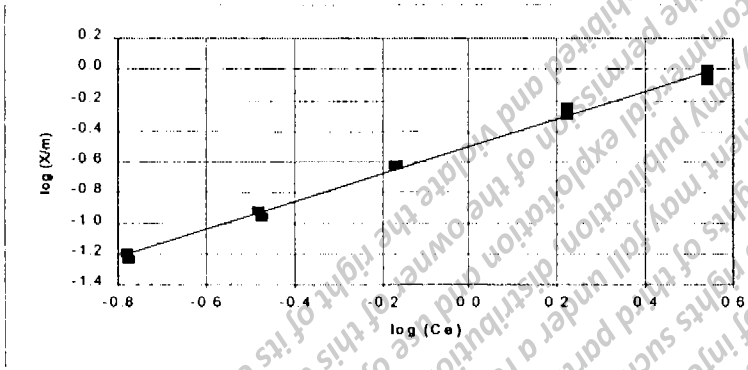
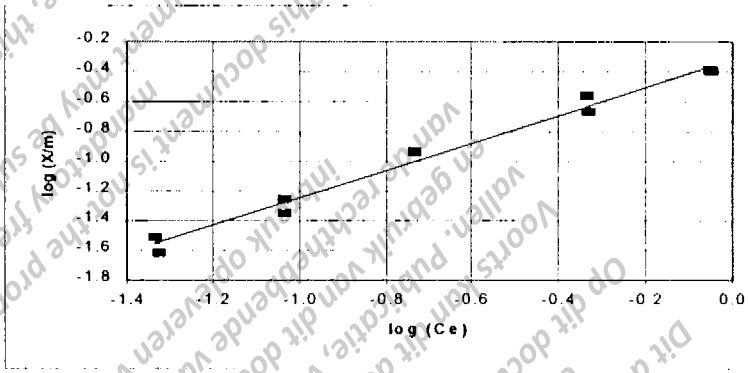


Figure 27: Freundlich Plots (log-log) for Adsorption and Desorption of CGA 329351 for Soil Pappelacker Sandy Loam

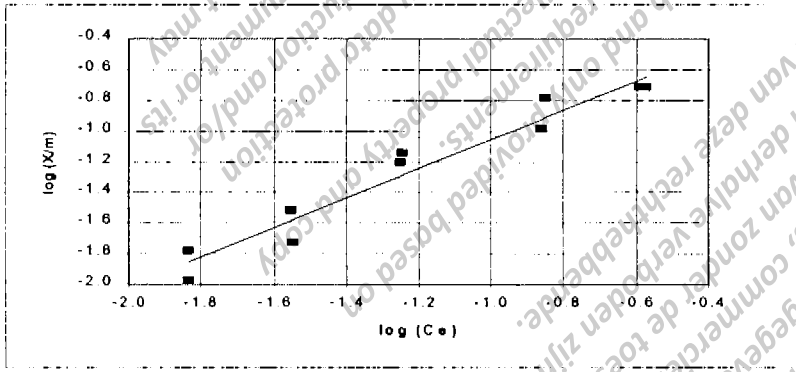
Adsorption of CGA 329351 to Pappelacker soil



Desorption 1 of CGA 329351 from Pappelacker soil



Desorption 2 of CGA 329351 from Pappelacker soil



Adsorption / Desorption of CGA 329351 for Pappelacker soil (calculated values)

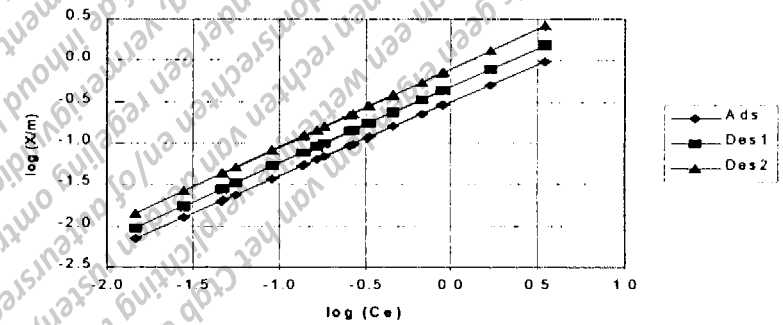
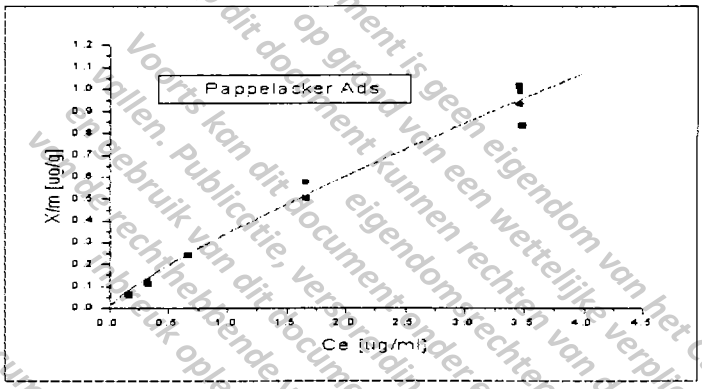
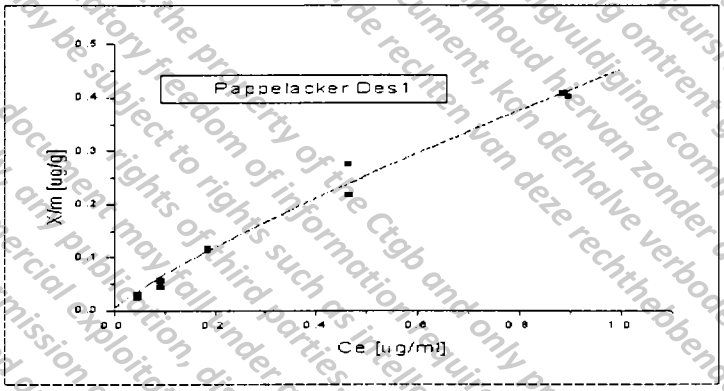


Figure 28: Freundlich Plots (lin-lin) for Adsorption and Desorption of CGA 329351 for Soil Pappelacker Sandy Loam

Adsorption of CGA 329351 to Pappelacker soil (k = 0.3358; 1/n = 0.8329)



Desorption 1 of CGA 329351 from Pappelacker soil (k = 0.4516; 1/n = 0.8389)



Desorption 2 of CGA 329351 from Pappelacker soil (k = 0.5483; 1/n = 0.7651)

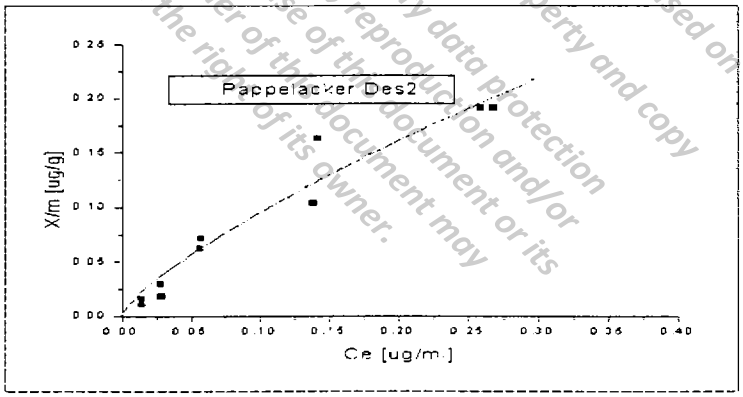
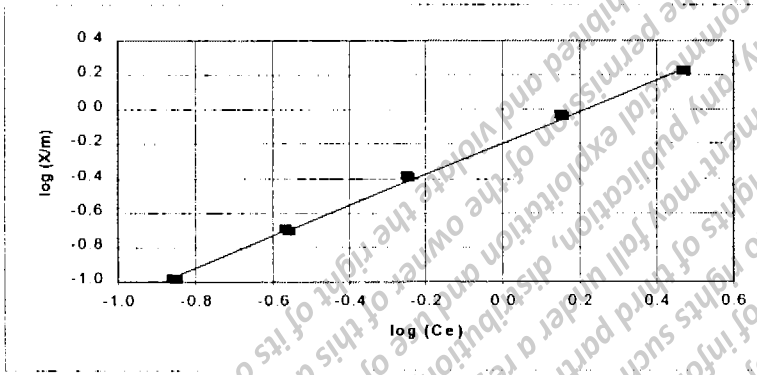
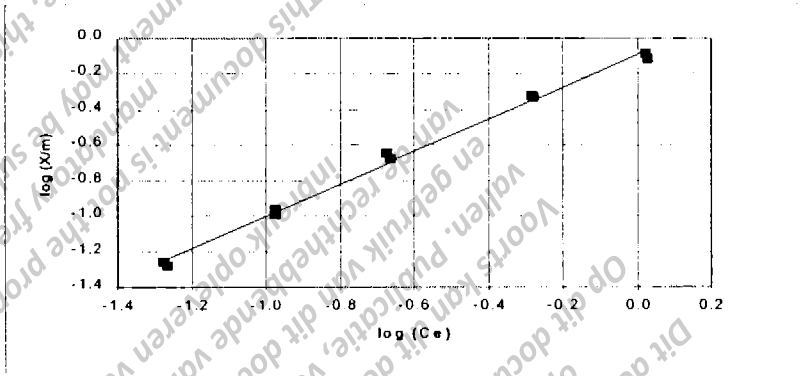


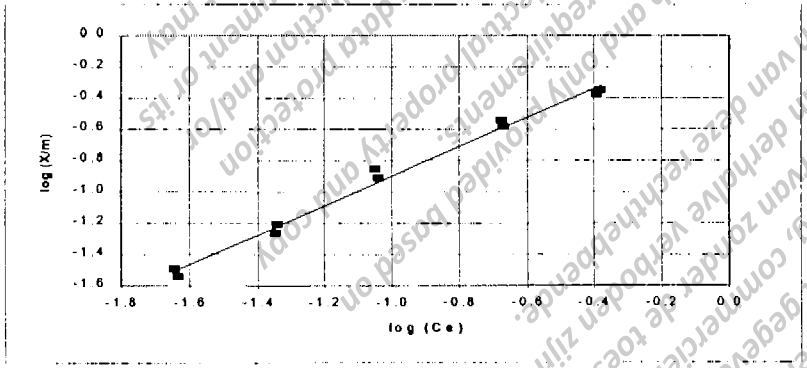
Figure 29: Freundlich Plots (log-log) for Adsorption and Desorption of CGA 329351 for Soil Gartenacker Sandy Loam

Adsorption of CGA 329351 to Gartenacker soil



Desorption 1 of CGA 329351 from Gartenacker soil





Adsorption / Desorption of CGA 329351 for Gartenacker soil (calculated values)

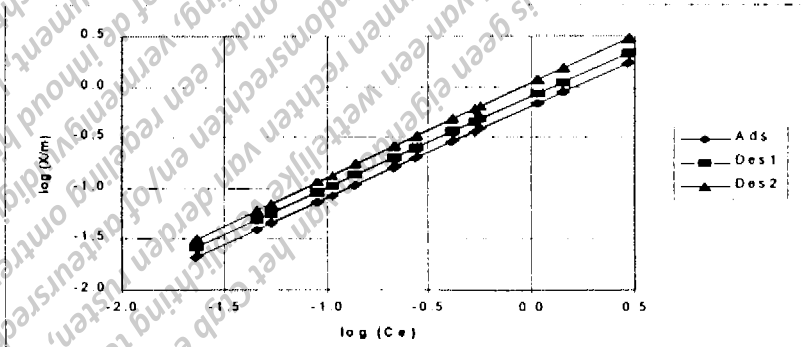
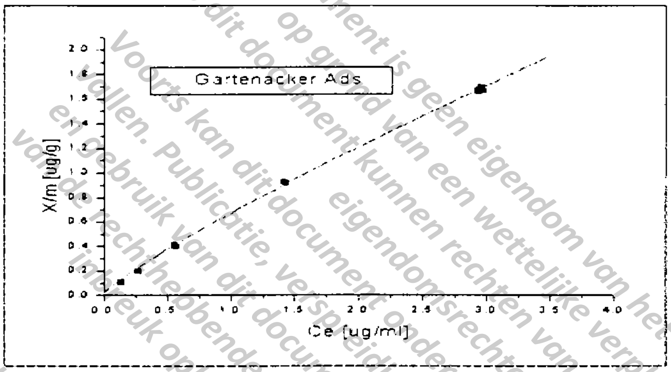
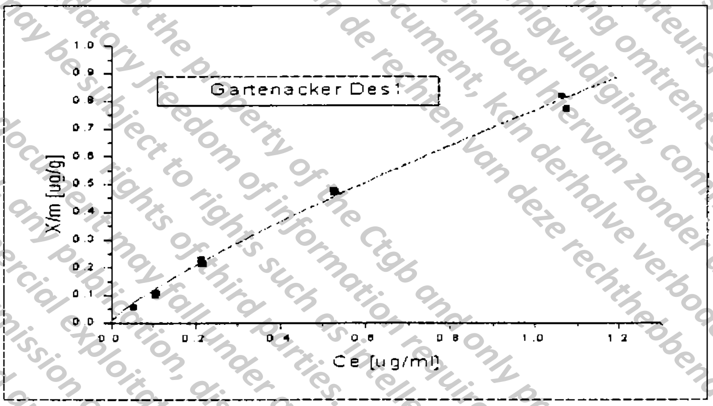


Figure 30: Freundlich Plots (lin-lin) for Adsorption and Desorption of CGA 329351 for Soil Gartenacker Sandy Loam

Adsorption of CGA 329351 to Gartenacker soil (k = 0.6621; 1/n = 0.8589)



Desorption 1 of CGA 329351 from Gartenacker soil (k = 0.7624; 1/n = 0.8177)



Desorption 2 of CGA 329351 from Gartenacker soil (k = 0.9172; 1/n = 0.8252)

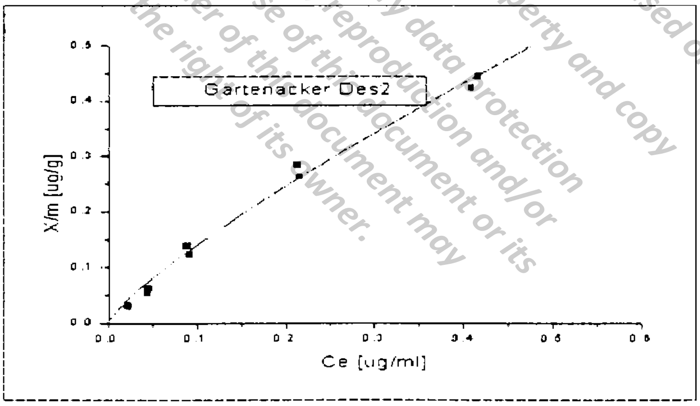
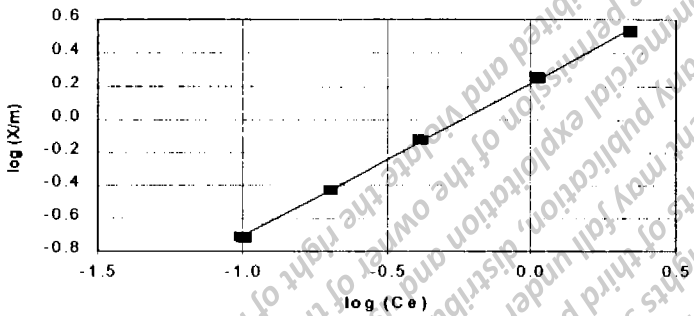
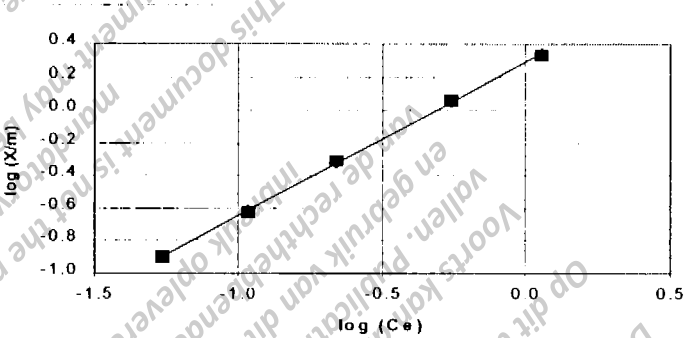


Figure 31: Freundlich Plots (log-log) for Adsorption and Desorption of CGA 329351 for Soil Vetroz Sandy Loam

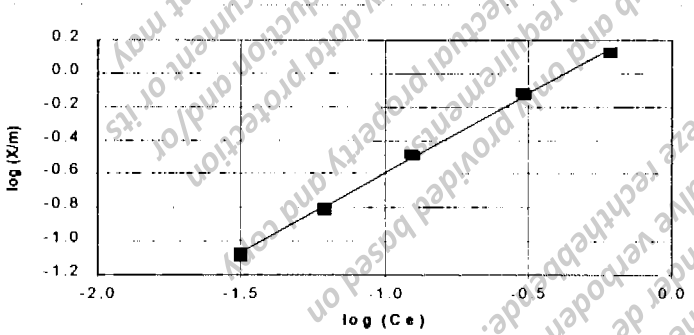
Adsorption of CGA 329351 to Vetroz soil



Desorption 1 of CGA 329351 from Vetroz soil



Desorption 2 of CGA 329351 from Vetroz soil



Adsorption / Desorption of CGA 329351 for Vetroz soil (calculated values)

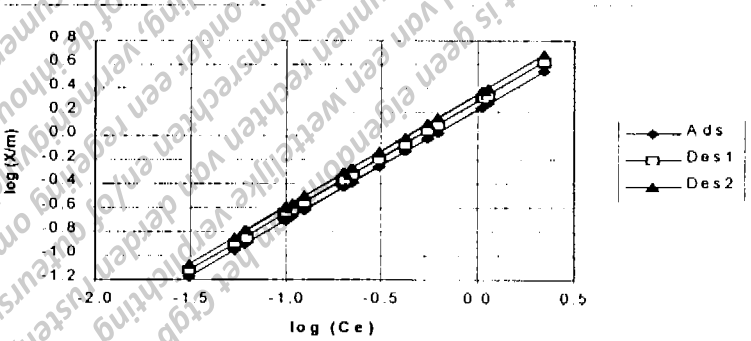
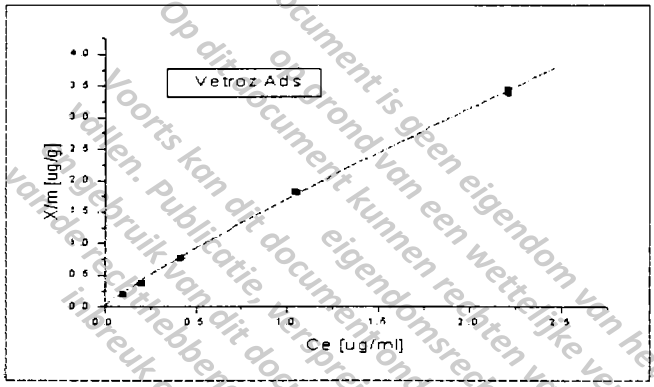
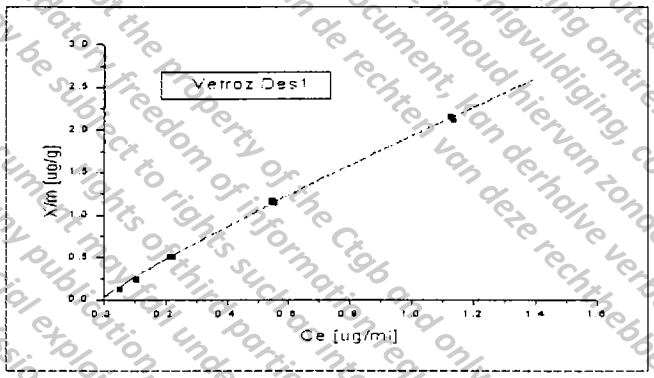


Figure 32: Freundlich Plots (lin-lin) for Adsorption and Desorption of CGA 329351 for Soil Vetroz Sandy Loam

Adsorption of CGA 329351 to Vetroz soil (k = 1.6879; 1/n = 0.8910)



Desorption 1 of CGA 329351 from Vetroz soil (k = 1.9201; 1/n = 0.8903)



Desorption 2 of CGA 329351 from Vetroz soil (k = 2.1063; 1/n = 0.8871)

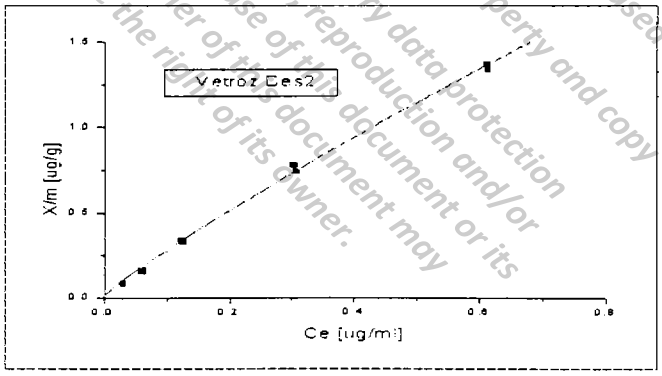
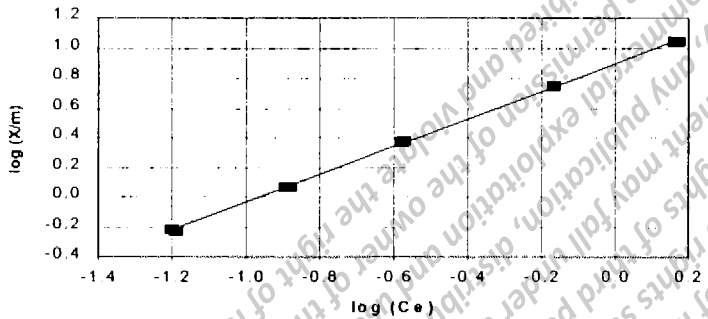
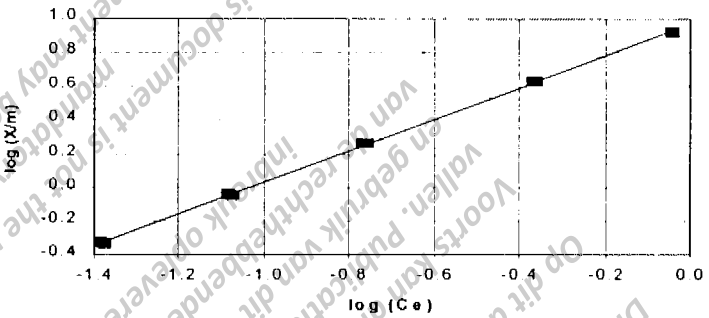


Figure 33: Freundlich Plots (log-log) for Adsorption and Desorption of CGA 329351 for Soil Illarsaz Sandy Loam

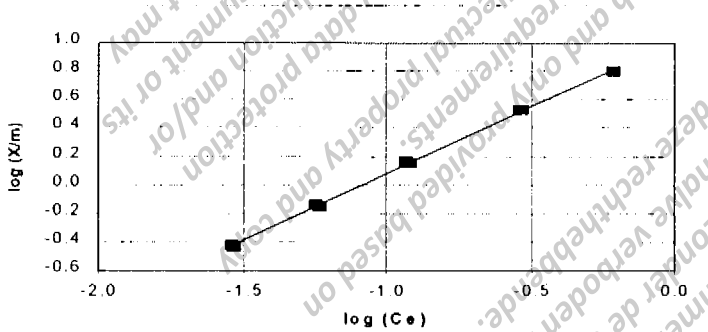
Adsorption of CGA 329351 to Illarsaz soil



Desorption 1 of CGA 329351 from Illarsaz soil



Desorption 2 of CGA 329351 from Illarsaz soil



Adsorption / Desorption of CGA 329351 for Illarsaz soil (calculated values)

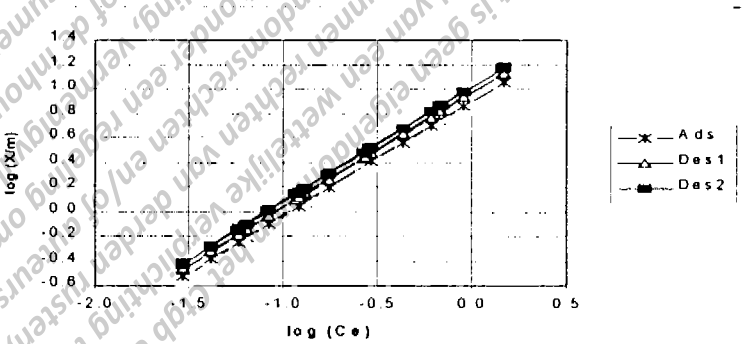
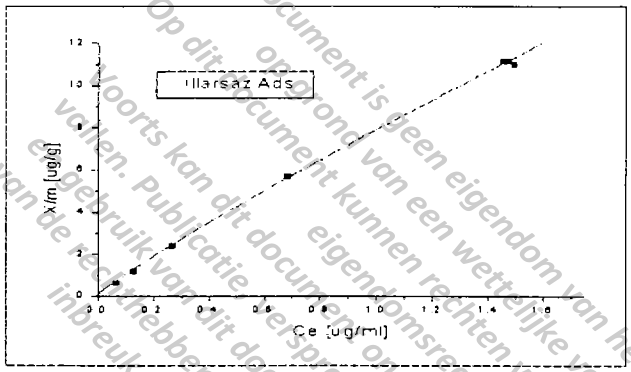
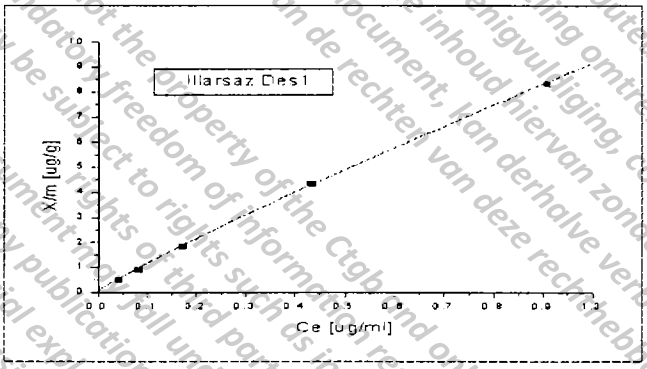


Figure 34: Freundlich Plots (lin-lin) for Adsorption and Desorption of CGA 329351 for Soil Illarsaz Sandy Loam

Adsorption of CGA 329351 to Illarsaz soil (k = 7.8586; 1/n = 0.9009)



Desorption 1 of CGA 329351 from Illarsaz soil (k = 91276; 1/n = 0.9089)



Desorption 2 of CGA 329351 from Illarsaz soil (k = 10.0433; 1/n = 0.9052)

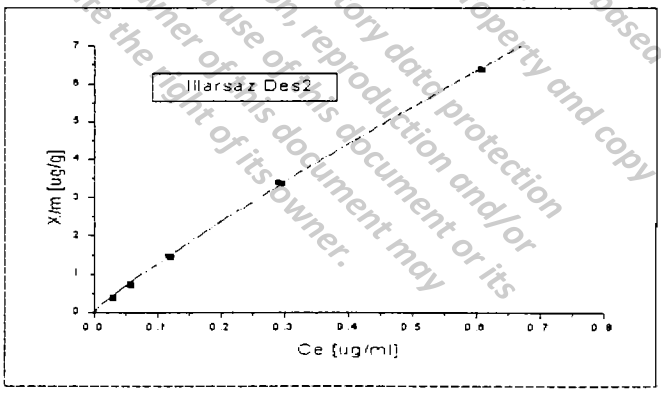
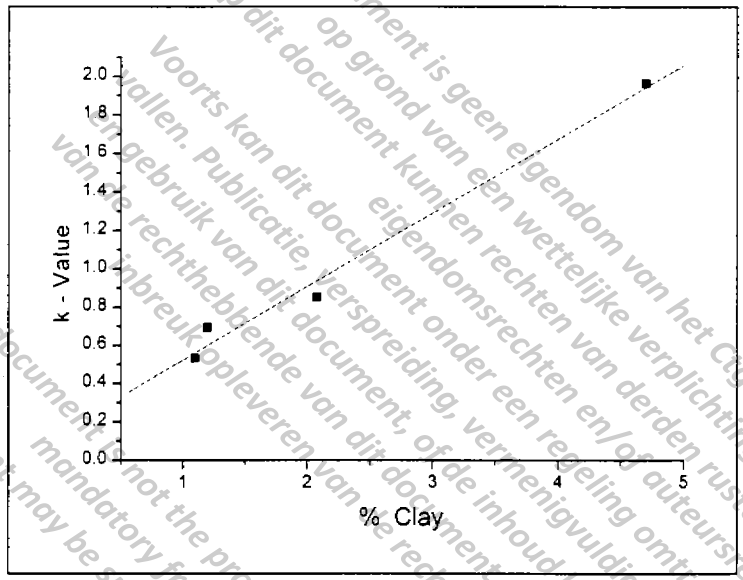
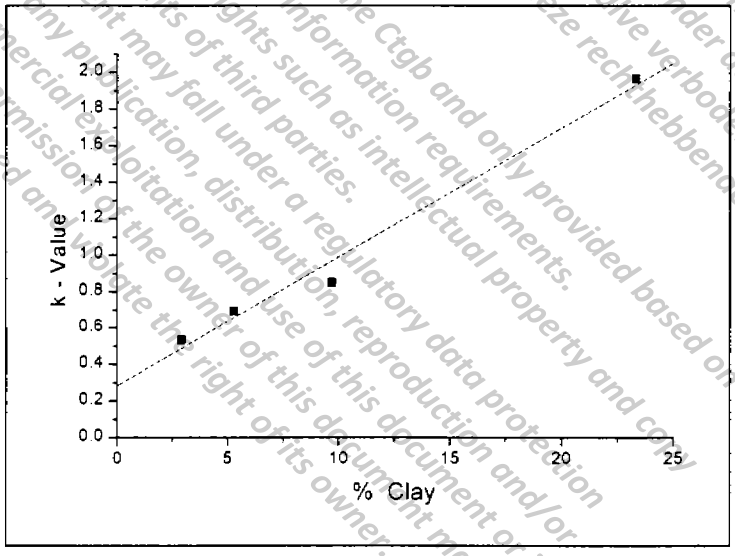


Figure 35: Plots of k - Values vs. Organic Carbon Content and vs. Clay Content

k- values vs. organic carbon content (corellation coefficient = 0.98798)



k- values vs. clay content (without peaty soil Illarsaz)



Appendix A: Representative Data

Borstel				
Calculation of Soil-to-Solution Ratio				
Soil OC (%)	1.2			
	log (Pow)	log(Koc)	Koc	k = Koc*%OC/100
Compound	1.71	1.850	70.8	0.8
Adsorption Ratio = Msoil/Minitial [ug/ug]	=			0.29
Mass soil [g]/Volume Water [ml]	=			0.49
Soil [g]	1	10		
Water [ml]	2.05	20		

Pappelacker				
Soil OC (%)	1.1			
	log (Pow)	log(Koc)	Koc	k = Koc*%OC/100
Compound	1.71	1.850	70.8	0.8
Adsorption Ratio = Msoil/Minitial [ug/ug]	=			0.28
Mass soil [g]/Volume Water [ml]	=			0.50
Soil [g]	1	10		
Water [ml]	2.00	20		

Gartenacker				
Soil OC (%)	2.08			
	log (Pow)	log(Koc)	Koc	k = Koc*%OC/100
Compound	1.71	1.850	70.8	1.5
Adsorption Ratio = Msoil/Minitial [ug/ug]	=			0.42
Mass soil [g]/Volume Water [ml]	=			0.50
Soil [g]	1	10		
Water [ml]	2.00	20		

Vetroz				
Soil OC (%)	4.7			
	log (Pow)	log(Koc)	Koc	k = Koc*%OC/100
Compound	1.71	1.850	70.8	3.328
Adsorption Ratio = Msoil/Minitial [ug/ug]	=			0.62
Mass soil [g]/Volume Water [ml]	=			0.50000
Soil [g]	1	10		
Water [ml]	2.00	20		

Illarsaz				
Soil OC (%)	19.8			
	log (Pow)	log(Koc)	Koc	k = Koc*%OC/100
Compound	1.71	1.850	70.8	14.0
Adsorption Ratio = Msoil/Minitial [ug/ug]	=			0.78
Mass soil [g]/Volume Water [ml]	=			0.25
Soil [g]	1	5.00		
Water [ml]	4.00	20		

98RP05 **Adsorption Desorption**

Pretest 1 **CGA 329351**

Projekt:		98RP05		Datum:	
Substanz:		CGA 329351		Visum	
Batch:		ILS-114 1			
Spez. Rad. (MBq/mg)		1.44			
Spez. Rad. (dpm/mg)		86400000			
Loslichkeit:	Wasser	26000 mg/l			
	Acetonitril	0			
Reinheit (%)		96			

Applikation					
Boden Vorversucht	Konz. Appl. [ug/ml]	Applik Lösg [ml]	Aktivitat [dpm]	Menge [ug]	Bodenmenge [g]
Borstel	4.87	20	8417400	93.527	10
Pappelacker	4.87	20	8417400	93.527	10
Gartenacker	4.87	20	8417400	93.527	10
Vetroz	4.87	30	12626100	140.290	10
Illarsaz	4.87	10	4208700	46.763	5
Leer*	4.87	20	8417400	93.527	

* Nur CaCl2-Lösg. ohne Boden (Glasadsorption)

Boden	BO*	PA1	GA1	VE1	IL1	Glas1
Taara	142.462	150.964	139.597	141.48	146.255	142.78
Boden	10.025	10.072	10.067	10.02	5.005	
Glas + Feuchb.	155.601	165.586	156.026	159.521	158.656	143.14
Gla + Bd + Prüfl.	175.518	185.526	175.969	179.455	178.612	163.098
Glas +Bd abd.	155.951	166.095	156.205	159.924	157.742	143.014
+ CaCl2 (des)	175.921	186.044	176.136	179.852	177.668	162.913
abd. (des)	156.313	165.704	156.322	160.033	157.957	142.997
Vol. Stammlsg.	19.92	19.94	19.94	19.93	19.96	19.96
Vol. Adslsg	23.03	24.49	26.31	27.96	27.35	20.32
konz [dpm/ml]	363965	342677	319080	300112	307066	413413

Adsorption

Dissapearance. Aliquot 0.1 ml						
Stunden	**Borstel**	**Pappelacker**	**Gartenacker**	**Vetroz**	**Illarsaz**	**Glas**
adsorbiert	dpm/0.1ml	dpm/0.1ml	dpm/0.1ml	dpm/0.1ml	dpm/0.1ml	dpm/0.1ml
0	36396	34268	31908	30011	30707	41341
2	29597	30765	24812	19662	13479	39018
4	28597	27803	24636	16720	13215	40881
6	30641	30386	25962	19469	13919	40934
8	29724	29879	25360	18548	12709	40162
24	29592	30188	24734	18652	12303	40413

Adsorption [%]						
Stunden	**Borstel**	**Pappelacker**	**Gartenacker**	**Vetroz**	**Illarsaz**	**Glas**
adsorbiert						
0	0.00	0.00	0.00	0.00	0.00	0.00
2	18.68	10.22	22.24	34.48	56.10	5.62
4	21.43	18.87	22.79	44.29	56.96	1.11
6	15.26	11.33	18.63	35.13	54.67	0.99
8	18.33	12.81	20.52	38.20	58.61	2.85
24	18.70	11.91	22.48	37.85	59.93	2.25

98RP05
Pretest 1

Adsorption Desorption
CGA 329351

Projekt:		98RP05		Datum:	
Substanz:		CGA 329351		Visum:	
Batch		ILS-114 1			
Spez. Rad. (MBq/mg)		1.44			
Spez. Rad. (dpm/mg)		86400000			
Loslichkeit	Wasser	26000 mg/l			
	Acetonitril	0			
Reinheit (%)		96			

Die zentrifugierten Muster nach 24 Std. im HPLC einspritzen.
% Eingespritzt :

Muster	Brompropylat 14.80	M2	M3	M4	HPLC
Borstel	100.00	0.00	0.00	0.00	2
Pappelacker	100.00	0.00	0.00	0.00	2
Gartenacker	100.00	0.00	0.00	0.00	2
Vetroz	100.00	0.00	0.00	0.00	2
Illarsaz	100.00	0.00	0.00	0.00	2

Appearance:	Aliquot	0.1 ml				
Stunden	**Borstel**	**Pappelacker**	**Gartenacker**	**Vetroz**	**Illarsaz**	**Glas**
desorbiert	dpm/0.1ml	dpm/0.1ml	dpm/0.1ml	dpm/0.1ml	dpm/0.1ml	dpm/0.1ml
0	0	0	0	0	0	0
2	7765	7941	9245	9584	7617	585
6	7722	7602	9193	9242	7780	611
24	7972	8207	9216	9084	7817	588
	0	0	0	0	0	0
	0	0	0	0	0	0
	0	0	0	0	0	0

Desorption [%]						
Stunden	**Borstel**	**Pappelacker**	**Gartenacker**	**Vetroz**	**Illarsaz**	**Glas**
desorbiert	%	%	%	%	%	%
0	0	0	0	0	0	0
2	50.70	45.91	43.95	36.09	24.12	12.31
6	50.06	37.42	43.23	33.04	24.97	15.03
24	53.80	52.57	43.55	31.63	25.17	12.63

98RP05 **Borstel**

Adsorption Desorption **CGA 329351**

Applikationslösung

Projekt:		98RP05		Datum:	
Substanz:		CGA 329351		Visum:	
Batch		ILS-114.1			
Spez. Rad. (MBq/mg)		1.440			
Spez. Rad. (cpm/mg)		86400000			
Loslichkeit	Wasser	26 g/l			
	Acetonitril				
Reinheit (%)		99.65			
Bodenbatch		6/98			
Organischer Kohlenstoff [%OC]		1.2			
Reinheit nach HPLC		99.67			

Applikationsstammlösung

Einwaage [mg]	5		Verschneiden der Stammlösung		
Volumen [ml]	1000				
Losungsmittel	0.01 M CaCl2		Einwaage kalt [mg]	0	Batch:
Zwischenverdünnung			Vol. Stammlosung [ml]	1	
ml Stammlösung	1		Vol. Verdunnung [ml]	1	
auf ml LM	1		Spez. Aktivität Verdunnung [MBq]	1.44	
Aliquot fur Counter [ml]	0.1		Spez. Aktivität Verdunnung [dpm]	86400000	
Anz. Aliquots	5		Zwischenverdünnung		
dpm Counter	41229		ml Lösg	1	
dpm Counter	41965		auf ml LM	1	
dpm Counter	41506		Aliquot für Counter [ml]	0.1	
dpm Counter	43346		Anz. Aliquots	1	
dpm Counter	42390		dpm Counter	42087	
Durchschnitt dpm	42087.20		dpm Counter	0	
dpm der Lösung	420872		dpm Counter	0	
mg der Lösung	0.00		dpm Counter	0	
Konzentration [ppm]	4.87		dpm Counter	0	
dpm Stammlösung	420872000		Durchschnitt dpm	42087	radioaktiv
mg Stammlösung	4.87		dpm der Lösung	420870	radioaktiv
Konz. Stammlösung (corr.) [ppm]	4.86		mg der Lösung	0.00487	radioaktiv
			Konzentration [ppm]	4.87	radioaktiv
			mg Verschnitt	0.00487	
			Konz. Verschnitt (corr.) [ppm]	4.85	

Menge Wirksubstanz						
	Geolarte Konzentrationen (ug/ml)					Total
=(ug/ml)	5	2.5	1	0.5	0.25	
Vol wassr. Phase (ml)	20	20	20	20	20	240
Anzahl Proben	4	2	2	2	2	12
Benotigte Test Substanz (mg)	0.4	0.1	0.04	0.02	0.01	0.57
Inkl. 25 % Reserve (mg)	0.5	0.125	0.05	0.025	0.0125	0.7125
Total benötigte Menge (mg) / 5 Boden		3.5625				

98RP05 **Borstel**

Adsorption Desorption **CGA 329351**

Applikation

					Datum	
Projekt:			98RP05		Visum	
Substanz:			CGA 329351			
Batch			ILS-114.1			
Spez. Rad. (MBq/mg)			1.44			
Spez. Rad. (dpm/mg)			86400000			
Löslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			

Applikationslösungen: Verdünnt mit CaCl2-Lösung						
Appl. Losung	Stammlösg. [ml]	Endvolumen [ml]	Conc Parent [ug/ml]	Aktivität [dpm/1 m]	Total ug hergestellt	Total ug gebraucht
BO_5 ppm_3	640.00	640.00	4.85	420870	3106.64	96.92
BO_5 ppm_4	640.00	640.00	4.85	420870	3106.64	96.86
BC_5 ppm_1	640.00	640.00	4.85	420870	3106.64	96.46
BO_5 ppm_2	640.00	640.00	4.85	420870	3106.64	96.78
BC_2.5 ppm_1	125.00	250.00	2.43	210435	606.77	48.23
BC_2.5 ppm_2	125.00	250.00	2.43	210435	606.77	48.30
BO_1 ppm_1	50.00	250.00	0.97	84174	242.71	19.33
BO_1 ppm_2	50.00	250.00	0.97	84174	242.71	19.34
BC_0.5 ppm_1	25.00	250.00	0.49	42087	121.35	9.67
BC_0.5 ppm_2	25.00	250.00	0.49	42087	121.35	9.67
BO_0.25 ppm_1	12.50	250.00	0.24	21044	60.68	4.84
BO_0.25 ppm_2	12.50	250.00	0.24	21044	60.68	4.85
Total	44.00				14489.58	551.25

Applikation							
Probe No (Ads/Des)	Appl.-Vol. [ml]	Gewicht vorgequollen [g]***	End Volumen [ml]	Konz.(*) [ug/ml]	Aktivität [dpm/ml]	Tot. Aktivität [dpm]	Konz.** [ug/ml]
BC_5 ppm_3	19.967	152.588	23.75	4.11	356103	8456025	4.10714
BC_5 ppm_4	19.955	156.340	23.44	4.16	360550	8450942	4.15843
BC_5 ppm_1	19.871	153.347	23.70	4.09	355079	8415368	4.09532
BO_5 ppm_2	19.938	157.569	23.46	4.15	359952	8443743	4.15152
BC_2.5 ppm_1	19.873	153.627	23.67	2.03	176201	4170150	2.03223
BC_2.5 ppm_2	19.899	154.519	23.45	2.05	178079	4175606	2.05389
BO_1 ppm_1	19.907	158.169	23.59	0.83	71786	1693289	0.82795
BO_1 ppm_2	19.923	155.655	23.58	0.83	71868	1694550	0.82890
BC_0.5 ppm_1	19.911	156.756	23.61	0.40	34909	824315	0.40263
BC_0.5 ppm_2	19.923	154.024	23.72	0.40	34770	824812	0.40102
BO_0.25 ppm_1	19.953	153.897	23.76	0.20	17646	419213	0.20352
BO_0.25 ppm_2	19.970	158.567	24.34	0.20	17236	419570	0.19879
* Concentration corrected for washings			** Concentration after dilution steps				

Konzentr (*) =(D20*B38/C38)-(D20*B38/C38*Verbr._Nachwasch!F73/100)

(*) Werte korrigiert um Glasadsorption Bilanz "Rueckwasch"

(**) Konzentration nach Zugabe der Stammloesung: Theorie

*** Glas + feuchter Boden

Aktivitatskontrolle Applikationslösungen						
Sample no	[dpm/ml]	[dpm/ml]		[ug/ml]	[ug]	[dpm]
	calc	meas	%	Conc Parent	Total	Total
BO_5 ppm_3	420870	423500	100.62	4.88	97.53	8456025
BO_5 ppm_4	420870	423500	100.62	4.88	97.47	8450942
BO_5 ppm_1	420870	423500	100.62	4.88	97.06	8415368
BO_5 ppm_2	420870	423500	100.62	4.88	97.39	8443743
BC_2.5 ppm_1	210435	209840	99.72	2.42	48.10	4170150
BC_2.5 ppm_2	210435	209840	99.72	2.42	48.16	4175606
BO_1 ppm_1	84174	85060	101.05	0.98	19.53	1693289
BO_1 ppm_2	84174	85060	101.05	0.98	19.55	1694650
BC_0.5 ppm_1	42087	41400	98.37	0.48	9.51	824315
BC_0.5 ppm_2	42087	41400	98.37	0.48	9.51	824812
BO_0.25 ppm_1	21044	21010	99.84	0.24	4.84	419213
BO_0.25 ppm_2	21044	21010	99.84	0.24	4.84	419570

98RP05 Borstel

Adsorption Desorption CGA 329351

Adsorption

Projekt:			98RP05		Datum:	
Substanz:			CGA 329351		Visum:	
Batch.			ILS-114.1			
Spez. Rad. (MBq/mg)			1.44			
Spez. Rad. (dpm/mg)			86400000			
Loslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			

Bodenmenge [g]	10	
Volumen Losung [ml]:	20	
Parent.in Ads. Sol. [%]:	99.67	(Ads.-sol. mean 3-4)

C)Adsorption: (24 Std.)

Probe-No	Gewicht leer [g]	Gewicht voll [g](*)	VAds [ml]	Aliqu.LSC (ml)	DPM Aliquot	DPM/ml (Ce)
BO_5 ppm_3	148.809	182.555	23.746	1	298086	298086
BO_5 ppm_4	142.856	176.295	23.439	1	306448	306448
BO_5 ppm_1	139.518	173.218	23.700	1	300472	300472
BC_5 ppm_2	144.049	177.507	23.458	1	304461	304461
BC_2.5 ppm_1	149.833	183.500	23.667	1	148202	148202
BC_2.5 ppm_2	150.970	184.418	23.448	1	148311	148311
BC_1 ppm_1	144.488	178.076	23.588	1	59611	59611
BO_1 ppm_2	141.998	175.578	23.580	1	58840	58840
BO_0.5 ppm_1	143.054	176.667	23.613	1	28340	28340
BO_0.5 ppm_2	140.225	173.947	23.722	1	27908	27908
BO_0.25 ppm_1	140.093	173.850	23.757	1	14433	14433
BO_0.25 ppm_2	144.194	178.537	24.343	1	14239	14239
(*) Gefäss+20ml Ca2Cl2-Loes +10 g Boden		VAds		=$C26-$B26-C15		

Sample-No	DPM Total	C(e)Ads [ug/ml]	log C(e)Ads	X/m [ug/g]	log X/m	log X/mcalc
BO_5 ppm_3	7078350.16	3.43868	0.536	1.587	0.201	0.176
BO_5 ppm_4	7182834.67	3.53515	0.548	1.461	0.165	0.187
BO_5 ppm_1	7121186.40	3.46621	0.540	1.487	0.172	0.179
BO_5 ppm_2	7142046.14	3.51223	0.546	1.498	0.175	0.185
BO_2.5 ppm_1	3507496.73	1.70964	0.233	0.762	-0.118	-0.104
BO_2.5 ppm_2	3477596.33	1.71090	0.233	0.803	-0.095	-0.104
BO_1 ppm_1	1406104.27	0.68767	-0.163	0.329	-0.482	-0.469
BO_1 ppm_2	1387447.20	0.67877	-0.168	0.353	-0.452	-0.474
BO_0.5 ppm_1	669192.42	0.32693	-0.486	0.179	-0.748	-0.767
BO_0.5 ppm_2	662033.58	0.32194	-0.492	0.187	-0.728	-0.773
BO_0.25 ppm_1	342884.78	0.16650	-0.779	0.087	-1.059	-1.038
BO_0.25 ppm_2	346619.98	0.16426	-0.784	0.084	-1.076	-1.043
			0.00			-0.319
					K graphisch	0.479748

Lineare Regress. log(X/m) [y-Wert] geg. logC(e) [x-Wert]

98RP05 **Borstel**
Adsorption 1 **CGA 329351**
Adsorption

Projekt:			98RP05		Datum:	
Substanz:			CGA 329351		Visum:	
Batch:			ILS-114.1			
Spez. Rad. (MBq/mg)			1.44			
Spez. Rad. (dpm/mg)			86400000			
Löslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			

Adsorption

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.998810237
R Square	0.997621889
Adjusted R Square	0.997384078
Standard Error	0.024828267
Observations	12

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.585988679	2.585988679	4195.017638	1.87367E-14
Residual	10	0.006164429	0.000616443		
Total	11	2.592153108			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 95.0%*	*Upper 95.0%*
Intercept	-0.31898661	0.007172751	-44.47200666	7.94683E-13	-0.334968497	-0.303004723	1.08932	1.132583
X Variable 1	0.922917385	0.014249379	64.76895582	1.87367E-14	0.891167785	0.954666985	0.838279	0.877118

Clay [%]	5.3					
K=	0.48		Koc=	39.98	Q=	23	KClay=	9.05

98RP05 Borstel
Adsorption Desorption CGA 329351
Desorption1

Projekt:			98RP05		Datum:	
Substanz:			CGA 329351		Visum:	
Batch:			ILS-114.1			
Spez. Rad. (MBq/mg)			1.44			
Spez. Rad. (dpm/mg)			86400000			
Löslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			

Bodenmenge [g]	10	
Volumen Lösung [ml]	20	
Parent in Ads. Sol. [%]	99.67	(Ads.-sol. mean 3-4)

C)Adsorption. (24 Std.)

Probe-No	Gewicht leer [g]	Gewicht voll [g](*)	VDes1 [ml]	Aliqu.LSC (ml)	DPM Aliquot	DPM/ml (Ce)
BO 5 ppm 3	162.575					
BO 5 ppm 4	156.472					
BO 5 ppm 1	153.174	173.131	23.61	1	79103	79103
BO 5 ppm 2	157.774	177.715	23.67	1	80933	80933
BO 2.5 ppm 1	163.534	183.493	23.66	1	39972	39972
BO 2.5 ppm 2	164.631	184.617	23.65	1	40060	40060
BO 1 ppm 1	158.072	178.017	23.53	1	16137	16137
BO 1 ppm 2	155.734	175.706	23.71	1	16215	16215
BO 0.5 ppm 1	156.766	176.735	23.68	1	8145	8145
BO 0.5 ppm 2	153.917	173.860	23.63	1	8192	8192
BO 0.25 ppm 1	153.907	173.851	23.76	1	4217	4217
BO 0.25 ppm 2	157.853	177.827	23.63	1	3970	3970

(*) Gefäss+20ml Ca2Cl2-Loes.+10 g Boden VDes1 =$C26-Adsorption.B28-$C$15

Sample-No	DPM Total	C(e)Des1 [ug/ml]	log C(e)Des1	X/m [ug/g]	log X/m	log X/mcalc
BO 5 ppm 1	1867859	0.91252	-0.040	0.600	-0.222	-0.212
BO 5 ppm 2	1915360	0.93363	-0.030	0.596	-0.225	-0.203
BO 2.5 ppm 1	945738	0.46111	-0.336	0.304	-0.517	-0.488
BO 2.5 ppm 2	947299	0.46213	-0.335	0.336	-0.473	-0.487
BO 1 ppm 1	379667	0.18615	-0.730	0.138	-0.860	-0.855
BO 1 ppm 2	384425	0.18705	-0.728	0.163	-0.787	-0.853
BO 0.5 ppm 1	192862	0.09396	-1.027	0.078	-1.111	-1.131
BO 0.5 ppm 2	193536	0.09450	-1.025	0.083	-1.082	-1.129
BO 0.25 ppm 1	100187	0.04865	-1.313	0.035	-1.453	-1.397
BO 0.25 ppm 2	93823	0.04580	-1.339	0.036	-1.446	-1.421
			0.00			-0.175
					K graphisch	0.668002

Lineare Regress. log(X/m) [y-Wert] geg. logC(e) [x-Wert]

98RP05 **Borstel**

Adsorption 1 **CGA 329351**

Desorption1

Projekt			98RP05		Datum	
Substanz			CGA 329351		Visum:	
Batch			ILS-114.1			
Spez. Rad. (MBq/mg)			1.44			
Spez. Rad. (dpm/mg)			86400000			
Löslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			

Desorption1

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.996701122
R Square	0.993413127
Adjusted R Square	0.992589768
Standard Error	0.039262075
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.859889405	1.859889405	1206.536917	5.16087E-10
Residual	8	0.012332085	0.001541511		
Total	9	1.87222149			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-0.17522241	0.02227444	-7.86652376	4.92807E-05	-0.226587394	-0.123857427	1.08932	1.132582964
X Variable 1	0.930576332	0.026790554	34.73524027	5.16087E-10	0.868797164	0.9923555	0.838279	0.877117831

Clay % 5.3

K=	0.67		Koc=	55.67	Q=	32.29	KClay= 12.60

98RP05 Borstel
Adsorption Desorption CGA 329351
Desorption2

Projekt:			98RP05		Datum	
Substanz:			CGA 329351		Visum:	
Batch:			ILS-114 1			
Spez. Rad. (MBq/mg)			1.44			
Spez. Rad. (dpm/mg)			86400000			
Löslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			

Bodenmenge [g]	10	
Volumen Lösung [ml]:	20	
Parent.in Ads. Sol. [%]:	99.67	(Ads.-sol. mean 3-4)

C)Adsorption: (24 Std.)

Probe-No	Gewicht leer [g]	Gewicht voll [g](*)	VDes1 [ml]	Aliqu.LSC (ml)	DPM Aliquot	DPM/ml (Ce)
BO_5 ppm_1	153.757	173.688	24.17	1	25128	25128
BO_5 ppm_2	158.234	178.185	24.14	1	25235	25235
BO_2.5 ppm_1	164.018	183.980	24.15	1	12808	12808
BO_2.5 ppm_2	165.091	185.054	24.08	1	12843	12843
BO_1 ppm_1	158.745	178.685	24.20	1	5348	5348
BO_1 ppm_2	156.244	176.176	24.18	1	5408	5408
BO_0.5 ppm_1	157.292	177.226	24.17	1	2660	2660
BO_0.5 ppm_2	154.222	174.153	23.93	1	2654	2654
BO_0.25 ppm_1	154.231	174.172	24.08	1	1414	1414
BO_0.25 ppm_2	158.353	178.321	24.13	1	1310	1310

(*) Gefäss+20ml Ca2Cl2-Loes.+10 g Boden VDes1 =$C26-Adsorption!B28-$C$15

Sample-No	DPM Total	C(e)Des2 [ug/ml]	log C(e)Des2	X/m [ug/g]	log X/m	log X/mcalc
BO_5 ppm_1	607343.76	0.28987	-0.538	0.2858	-0.544	-0.525
BO_5 ppm_2	609071.96	0.29111	-0.536	0.2844	-0.546	-0.523
BO_2.5 ppm_1	309274.78	0.14775	-0.830	0.1400	-0.854	-0.794
BO_2.5 ppm_2	309310.81	0.14816	-0.829	0.1701	-0.769	-0.793
BO_1 ppm_1	129405.56	0.06169	-1.210	0.0679	-1.168	-1.143
BO_1 ppm_2	130754.62	0.06239	-1.205	0.0919	-1.037	-1.138
BO_0.5 ppm_1	64297.52	0.03069	-1.513	0.0432	-1.365	-1.421
BO_0.5 ppm_2	63504.91	0.03062	-1.514	0.0473	-1.325	-1.422
BO_0.25 ppm_1	34047.71	0.01631	-1.787	0.0161	-1.794	-1.674
BO_0.25 ppm_2	31606.37	0.01511	-1.821	0.0184	-1.734	-1.704
			0.00			-0.031
					K graphisch	0.932170

Lineare Regress. log(X/m) [y-Wert] geg. logC(e) [x-Wert]

98RP05 **Borstel**
Adsorption 1 **CGA 329351**
Desorption2

Projekt:			98RP05		Datum:	
Substanz:			CGA 329351		Visum:	
Batch			ILS-114.1			
Spez. Rad. (MBq/mg)			1.44			
Spez. Rad. (dpm/mg)			86400000			
Loslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			

Desorption2

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.987659008
R Square	0.975470316
Adjusted R Square	0.972404106
Standard Error	0.074252927
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.754038989	1.754038989	318.1354695	9.99844E-08
Residual	8	0.044107977	0.005513497		
Total	9	1.798146966			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*.ower 95.0%*	*Jpper 95.0%*
Intercept	-0.030505062	0.065108131	-0.468529215	0.651907412	-0.180644779	0.119634655	-3.41242	6.149941
X Variable 1	0.919205057	0.051535484	17.83635247	9.99844E-08	0.800363941	1.038046173	-0.76563	5.489357

Clay %	5.3						
K=	0.93		Koc=	77.68	Q=	45	KClay = 17.59

98RP05 **Borstel**

Adsorption 1 **CGA 329351**

Verbrennung

Projekt:			98RP05		Datum:	
Substanz:			CGA 329351		V-sum:	
Batch:			ILS-114.1			
Spez. Rad. (MBq/mg)			1.44			
Spez. Rad. (dpm/mg)			86400000			
Löslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			

Proben Nr	Gewicht(*) leer [g]	Gewichte Sediment [g] trocken	Aliquot [g]	LSC [DPM] im Aliquot	TOTAL	%-applied	
BO_5 ppm_3		9.814	0.968	1481	15015	0.18	
BO_5 ppm_3	C	9.814	1.062	1504	13899	0.16	
BC_5 ppm_3	0	9.814	1.856	1322	699C	0.08	
Mean :							0.14
BO_5 ppm_4		9.889	0.816	1133	13731	0.16	
BO_5 ppm_4	0	9.889	0.9C1	1236	13566	0.16	
BO_5 ppm_4	0	9.889	0.863	1164	13338	0.16	
Mean :							0.16
BO_5 ppm_1		9.984	0.724	21356	294500	3.50	
BO_5 ppm_1	0	9.984	0.885	26298	296677	3.53	
BO_5 ppm_1	0	9.984	0.761	22535	295650	3.51	
Mean :							3.51
BO_5 ppm_2		10.080	0.881	29088	332812	3.94	
BO_5 ppm_2	0	9.984	0.550	20283	368192	4.36	
BO_5 ppm_2	0	10.08	0.776	26433	343356	4.07	
Mean :							4.12
BO_2.5 ppm_1		9.994	0.637	11667	183046	4.39	
BO_2.5 ppm_1	0	9.994	0.901	15889	176243	4.23	
BO_2.5 ppm_1	0	9.994	0.711	12345	173525	4.16	
Mean :							4.26
BO_2.5 ppm_2		9.972	0.922	14997	162202	3.88	
BO_2.5 ppm_2	0	9.994	0.790	13694	173238	4.15	
BO_2.5 ppm_2	0	9.972	0.803	13905	172678	4.14	
Mean							4.06
BO_1 ppm_1		9.979	0.506	3437	67782	4.00	
BO_1 ppm_1	C	9.972	0.796	6001	75178	4.44	
BO_1 ppm_1	C	9.979	0.755	5894	77902	4.60	
Mean :							4.35
BO_1 ppm_2		10.020	0.806	6664	82845	4.89	
BO_1 ppm_2	0	9.979	1.109	8978	80786	4.77	
BO_1 ppm_2	0	10.02	1.083	8586	79438	4.69	
Mean :							4.78
BO_0.5 ppm_1		10.004	0.525	2317	44151	5.36	
BO_0.5 ppm_1	0	10.02	0.755	2898	38461	4.67	
BO_0.5 ppm_1	0	10.004	0.847	3501	41351	5.02	
Mean :							5.01
BO_0.5 ppm_2		9.988	1.009	4021	39804	4.83	
BO_0.5 ppm_2	0	9.988	0.769	3272	42498	5.15	
BO_0.5 ppm_2	0	9.988	0.941	3743	39729	4.62	
Mean :							4.93
BO_0.25 ppm_1		9.990	0.927	1972	21252	5.07	
BO_0.25 ppm_1	0	9.990	0.502	1158	23045	5.50	
BO_0.25 ppm_1	0	9.99	0.9	1904	21134	5.04	
Mean :							5.20
BO_0.25 ppm_2		10.011	0.798	1572	19721	4.70	
BO_0.25 ppm_2	0	10.011	0.592	1209	20445	4.87	
BO_0.25 ppm_2	0	10.011	0.675	1287	19088	4.55	
Mean :							4.71

(*) Gefäss+10 g Boden+anhaftende Feuchtigkeit

%-appliz. =E18/Applikation!F38*100

98RP05 **Borstel**

Adsorption 1 **CGA 329351**

Rückwasch

Projekt:			98RP05		Datum:	
Substanz:			CGA 329351		Visum:	
Batch:			ILS-114.1			
Spez. Rad. (MBq/mg)			1.44			
Spez. Rad. (dpm/mg)			86400000			
Loslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			

Proben Nr.	Volumen Total (ml)	Aliquot (ml)	DPM Aliquot	Total	%-appl.
BO_5 ppm_3	0.000	2	894	0	0.00
BO_5 ppm_4	0.000	2	427	0	0.00
BO_5 ppm_1	7.496	2	894	3351	0.04
BO_5 ppm_2	8.519	2	427	1819	0.02
BO_2.5 ppm_1	9.264	2	269	1246	0.03
BO_2.5 ppm_2	10.545	2	218	1149	0.03
BO_1 ppm_1	8.680	2	287	1246	0.07
BO_1 ppm_2	10.073	2	135	680	0.04
BO_0.5 ppm_1	9.667	2	14	68	0.01
BO_0.5 ppm_2	9.738	2	72	351	0.04
BO_0.25 ppm_1	6.356	2	184	585	0.14
BO_0.25 ppm_2	9.642	2	14	67	0.02

%-appl. =E73/Applikation!F38*100

Probe	Tara Glas bzw. Soxhlethülse	Glas (bzw. Sox. Hülse) + Trockenbd	Trockenboden	Glas + Backwash	Vol. Backwash	Density [g/ml]	0.7857
BO_5 ppm_3	3.816	13.630	9.814				
BO_5 ppm_4	3.892	13.781	9.889				
BO_5 ppm_1	139.518	149.502	9.984	145.408	7.496		
BO_5 ppm_2	144.049	154.129	10.080	150.742	8.519		
BO_2.5 ppm_1	149.833	159.827	9.994	157.112	9.264		
BO_2.5 ppm_2	150.970	160.942	9.972	159.255	10.545		
BO_1 ppm_1	144.488	154.467	9.979	151.308	8.680		
BO_1 ppm_2	141.998	152.018	10.020	149.912	10.073		
BO_0.5 ppm_1	143.054	153.058	10.004	150.649	9.667		
BO_0.5 ppm_2	140.225	150.213	9.988	147.876	9.738		
BO_0.25 ppm_1	140.093	150.083	9.990	145.087	6.356		
BO_0.25 ppm_2	144.194	154.205	10.011	151.77	9.642		

98RP05
Adsorption 1
Bilanz 1

Borstel
CGA 329351

Projekt:			98RP05		Datum:	
Substanz:			CGA 329351		Visum:	
Batch:			ILS-114.1			
Spez. Rad (MBq/mg)			1.44			
Spez. Rad (dpm/mg)			86400000			
Löslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			
Appliziert			8456025			

Extrakte

Extraktionsschritt	Extraktionsmittel	Vol. [ml]	Aliquot [ml]	Aliquot dpm	Total dpm	% Appl
1	ACN	20.5	1	101829	2087494.5	24.69
2	ACN/H2O 8+2	20.5	1	13701	280870.5	3.32
3	ACN/H2O 8+2	20.5	1	2105	43152.5	0.51
4	Soxhlet	180	2	219	19710	0.23
5						
Total		241.5			2411517.5	28.52

Adsorptionslösung

	Vol. [ml]	Aliquot [ml]	Aliquot dpm	Total dpm	% Appl.
Ads. Lösg	19.98	1	298086	5955758.28	70.43
Restwasser	0	1	0	0.00	0.00
Total	19.98			5955758.28	70.43

Verbrennung

Anz. Aliquote				
Bodenmenge [g]	Aliquot [g]	Aliquot dpm	Total dpm	% Appl.
9.814	0.968	1481	15015	0.18
9.814	1.062	1504	13899	0.16
9.814	1.856	1322	6990	0.08
Mittelwert			11968	0.14

Bilanz

Kalt Extrakt.	Adsorpt. Lösung	Restwasser	Bound	Rückwasch	Recovery
28.52	70.43	0.00	0.14	0.00	99.09

98RP05 **Borstel**
Adsorption 1 **CGA 329351**
Bilanz

Projekt:			98RP05		Datum:	
Substanz:			CGA 329351		Visum:	
Batch:			ILS-114.1			
Spez. Rad. (MBq/mg)			1.44			
Spez. Rad. (dpm/mg)			86400000			
Löslichkeit	Wasser		26 g/l			
	Acetonitril		0			
Reinheit (%)			99.65			

Proben Nr	Boden	Aqu. Phases			Rückwasch	TOTAL
		Adsorp	Desorp.1 bzw. Kaltextr.	Desorp.2		
BO_5 ppm_3	0.14	70.43	28.52	0.00	0.00	99.09
BO_5 ppm_4	0.16	71.88	28.66	0.00	0.00	100.70
BO_5 ppm_1	3.51	84.62	9.14	3.23	0.04	100.55
BO_5 ppm_2	4.12	84.58	9.25	3.20	0.02	101.18
BO_2.5 ppm_1	4.26	84.11	9.53	3.40	0.03	101.33
BO_2.5 ppm_2	4.06	83.28	9.68	3.45	0.03	100.50
BO_1 ppm_1	4.35	83.04	9.81	3.59	0.07	100.85
BO_1 ppm_2	4.78	81.87	9.71	3.65	0.04	100.06
BO_0.5 ppm_1	5.01	81.18	10.64	3.61	0.01	100.45
BO_0.5 ppm_2	4.93	80.26	10.97	3.73	0.04	99.94
BO_0.25 ppm_1	5.20	81.79	10.77	3.96	0.14	101.86
BO_0.25 ppm_2	4.71	82.61	9.94	3.60	0.02	100.88

Appendix B: Validation of Analytical Methods

Validation HPLC Method

Validation with sample BO_5_3 adsorptionsolution (see Figure 11)

Validierung HPLC

Project	98RP05
Sample	BO_5_3 Adslsg.

Sample/Amount Injected

Sample	BO_5_3 Adslsg.	
Vol. injected (ml)	0.1 (automatisch)	
DPM injected	29809	
HPLC Name	80722002.ch2	

Procedure

From sample BO_5_3 : 0.1 ml will be injected into the HPLC system and radioactive fractions (peaks) and the residual eluent (remainder or background) will be collected and thereafter submitted to LSC.

Recovery

Sample		**Parent**	**Total**	**rest of run**	**Total**
		RT 14.85	**%ROI**	**BKG**	
BO_5_3 Adslsg.	Volume collected (ml)	1.00		20.00	
80722002.ch2	Volume measured (ml)	1.00		2.00	
	DPM measured	28414		86	
	Recov. (DPM)	28414	28414	860	29274
	Recov. (%)	**100.00**	100.00	**2.94**	
	Recov. (%-injected)	95.32	95.32	2.89	**98.21**
	Volume collected (ml)				
	Volume measured (ml)				
	DPM measured				
	Recov. (DPM)				
	Recov. (%)				
	Recov. (%-injected)				
Average					

	ROI Data from Berthold Winflow system		
	RT 14.85		**BKG**
80722002.ch2	**96.36**		**3.64**
Deviation %	3.78		19.31
Error %	3.64		0.7
Deviation %			
Error %			

Comment

All radioactivity injected was recovered from the sytem.
When the ROI-% values (lower table) are compared with the upper figures from LSC measurement a high agreement within the corresponding data can be stated.

Validation with sample PA_5_3 adsorptionsolution (see Figure 15)

Validierung HPLC

Project	98RP05
Sample	PA_5_3 Adslsg.

Sample/Amount Injected

Sample	PA_5_3 Adslsg.	
Vol. injected (ml)	0.1 (automatisch)	
DPM injected	30258	
HPLC Name	80729001.ch2	

Procedure

From sample PA_5_3 : 0.1 ml will be injected into the HPLC system and radioactive fractions (peaks) and the residual eluent (remainder or background) will be collected and thereafter submitted to LSC.

Recovery

Sample		Parent	Total	rest of run	Total
		RT 14.85	%ROI	BKG	
PA_5_3 Adslsg.	Volume collected (ml)	1.00		19.00	
80729001.ch2	Volume measured (ml)	1.00		2.00	
	DPM measured	28056		121	
	Recov. (DPM)	28056	28056	1150	29206
	Recov. (%)	**100.00**	100.00	**3.94**	
	Recov. (%-injected)	92.72	92.72	3.80	**96.52**
	Volume collected (ml)				
	Volume measured (ml)				
	DPM measured				
	Recov. (DPM)				
	Recov. (%)				
	Recov. (%-injected)				
Average					

	ROI Data from Berthold Winflow system		
	RT 14.85		BKG
80729001.ch2	**95.65**		**4.35**
Deviation %	4.55		9.52
Error %	4.35		0.4
Deviation %			
Error %			

Comment

All radioactivity injected was recovered from the sytem.
When the ROI-% values (lower table) are compared with the upper figures from LSC measurement a high agreement within the corresponding data can be stated.

Validation with sample GA_5_3 adsorptionsolution (see Figure 17)

Validierung HPLC

Project	98RP05
Sample	GA_5_3 Adslsg.

Sample/Amount Injected

Sample	GA_5_3 Adslsg.	
Vol. injected (ml)	0.1 (automatisch)	
DPM injected	25901	
HPLC Name	80729003.ch2	

Procedure

From sample BO_5_3 : 0.1 ml will be injected into the HPLC system and radioactive fractions (peaks) and the residual eluent (remainder or background) will be collected and thereafter submitted to LSC.

Recovery

Sample		Parent	Total	rest of run	Total
		RT 14.85	%ROI	BKG	
GA_5_3 Adslsg.	Volume collected (ml)	1.00		19.00	
80729003.ch2	Volume measured (ml)	1.00		2.00	
	DPM measured	23962		103	
	Recov. (DPM)	23962	23962	979	24941
	Recov. (%)	**100.00**	100.00	**3.92**	
	Recov. (%-injected)	92.51	92.51	3.78	**96.29**
	Volume collected (ml)				
	Volume measured (ml)				
	DPM measured				
	Recov. (DPM)				
	Recov. (%)				
	Recov. (%-injected)				
Average					

	ROI Data from Berthold Winflow system		
	RT 14.85		BKG
80729003.ch2	**99.11**		**4.50**
Deviation %	0.90		12.89
Error %	0.89		0.6
Deviation %			
Error %			

Comment

All radioactivity injected was recovered from the sytem.
When the ROI-% values (lower table) are compared with the upper figures from LSC measurement a high agreement within the corresponding data can be stated.

Validation with sample VE_5_3 adsorptionsolution (see Figure 19)

Validierung HPLC

Project	98RP05
Sample	VE_5_3 Adslsg.

Sample/Amount Injected

Sample	VE_5_3 Adslsg.	
Vol. injected (ml)	0.1 (automatisch)	
DPM injected	17668	
HPLC Name	80804001.ch2	

Procedure

From sample VE_5_3 : 0.1 ml will be injected into the HPLC system and radioactive fractions (peaks) and the residual eluent (remainder or background) will be collected and thereafter submitted to LSC.

Recovery

Sample		Parent	Total	rest of run	Total
		RT 14.85	%ROI	BKG	
VE_5_3 Adslsg.	Volume collected (ml)	1.00		19.00	
80804001.ch2	Volume measured (ml)	1.00		2.00	
	DPM measured	17451		79	
	Recov. (DPM)	17451	17451	751	18202
	Recov. (%)	**100.00**	100.00	**4.12**	
	Recov. (%-injected)	98.77	98.77	4.25	**103.02**
	Volume collected (ml)				
	Volume measured (ml)				
	DPM measured				
	Recov. (DPM)				
	Recov. (%)				
	Recov. (%-injected)				
Average					

	ROI Data from Berthold Winflow system		
	RT 14.85		BKG
80804001.ch2	**98.80**		**6.14**
Deviation %	1.21		32.90
Error %	1.20		2.0
Deviation %			
Error %			

Comment

All radioactivity injected was recovered from the sytem.
When the ROI-% values (lower table) are compared with the upper figures from LSC measurement a high agreement within the corresponding data can be stated.

Validation with sample IL_5_3 adsorptionsolution (see Figure 21)

Validierung HPLC

Project	98RP05
Sample	IL_5_3 Adslsg.

Sample/Amount Injected

Sample	IL_5_3 Adslsg.	
Vol. injected (ml)	0.1 (automatisch)	
DPM injected	12565	
HPLC Name	80804003.ch2	

Procedure

From sample BO_5_3 : 0.1 ml will be injected into the HPLC system and radioactive fractions (peaks) and the residual eluent (remainder or background) will be collected and thereafter submitted to LSC.

Recovery

Sample		Parent	Total	rest of run	Total
		RT 14.85	%ROI	BKG	
IL_5_3 Adslsg.	Volume collected (ml)	1.00		19.00	
80804003.ch2	Volume measured (ml)	1.00		2.00	
	DPM measured	11674		68	
	Recov. (DPM)	11674	11674	646	12320
	Recov. (%)	**100.00**	100.00	**5.24**	
	Recov. (%-injected)	92.91	92.91	5.14	**98.05**
	Volume collected (ml)				
	Volume measured (ml)				
	DPM measured				
	Recov. (DPM)				
	Recov. (%)				
	Recov. (%-injected)				
Average					

	ROI Data from Berthold Winflow system		
	RT 14.85		BKG
80804003.ch2	**100.00**		**3.56**
Deviation %	0.00		47.47
Error %	0.00		1.69
Deviation %			
Error %			

Comment

All radioactivity injected was recovered from the sytem.
When the ROI-% values (lower table) are compared with the upper figures from LSC measurement a high agreement within the corresponding data can be stated.

Appendix C : Limits of Detection

Liquid Scintillation Counting:

Limit of detection for liquid scintillation counting with sample BO_5_3:

Limit of Detection and Quantitation for LSC and Combustion

General Data Adsorption

Project	98RP05
Soil	Borstel
Sample	BO_5_3
	Adsorptionsisg.
Date	15.12.98
Visum	

Specific radioactivity	**(MBq/mg)**	**1.44**
	(uCi/mg)	38.919
Specific radioactivity (dpm/mg)		86400000
Amount applied (dpm)		8456025
Amount in Extract No 1(dpm)		7078350
Amount in Extract No 1 (%-applied)		83.71
Volume Extract (ml)		24
Volume aqu. Layer (ml)		
Amount soil (g)		20.00

Limit of Detection and Quantitation for Liquid Scintillation Counter

Extractables first Extract (LSC 42)

	Size	**dpm**	**Total dpm**	**%-applied**	**Parent equiv. (mg)**	**mg/kg Soil (=ppm)**
Sample size measured (ml)	1.00					
Volume extract (ml)	23.75					
Background LSC (BG LSC) :		16	379.936	0.0045	0.000004	0.00022
Limit of Detection (2x BG)		32	759.872	0.0090	0.000009	0.00044
Limit of Quantitation (3xBG)		48	1139.808	0.0135	0.000013	0.00066

HPLC Analysis:

Limits of Detection and Quantitation for HPLC Analysis calculated from a chromatogram of the adsorption solution of sample BO_5_3 (Figure 11)

Limit of Detection and Quantitation
(Sample 3C; 7 days 0.2 mg/kg; Gartenacker)

Validiert 6.2.1996
EH *fim*

Projekt	98RP05
Sample	BO5_3
	Adsorption
Date	16.10.98

Limit of Detection and Quantitation for HPLC
(Figure A)

Data from Chromatogram

Specific radioactivity (dpm/mg)	86400000	Spez.Rad.(uC/mg)	38.919
Amount applied (mg)	0.0974	Spez.Rad.(MBq/mg)	1.44
Amount applied (dpm)	8470000		
Amount in Extractables (dpm)	5929000		
Extractables (%-applied)	70.00		
Amount of Soil (kg)	0.03		
Concentration in Soil (mg/kg)	3.25		

Calculation of Percentages

Peak-No	Peak Name	Peak			Background	
	·	DPM	%-ROI	%-applied	DPM	%-applied
1	unknown	194	0.67	0.47	80	0.19
2	CGA329351	28784	99.33	69.53	152	0.37
Total		28978	100.00	70.00	233	

Limit of Detection (LD) and Limit of Quantitation (LQ)

Peak-No	Peak Name	LD	LQ	Background	LD	LQ	Background	LD
				Parent equiv.			Soil Residue	
				mg			mg/kg	
1	unknown	0.389	0.583	0.0002	0.0004	0.0006	0.0063	0.0126
2	CGA329351	0.737	1.105	0.0004	0.0007	0.0011	0.0120	0.0239

Limits of Detection and Quantitation for HPLC Analysis calculated from a chromatogram of the extracts of sample BO_5_3 (Figure 13)

Limit of Detection and Quantitation

Validiert 6.2.1996
EH *fim*

Projekt	98RP05
Sample	BO5_3 Kaltextrakt
	Adsorption
Date	16.10.98

Limit of Detection and Quantitation for HPLC
(Figure A)

Data from Chromatogram

Specific radioactivity (dpm/mg)	86400000	Spez.Rad.(uC/mg)	38.919
Amount applied (mg)	0.0940	Spez.Rad.(MBq/mg)	1.44
Amount applied (dpm)	8456025		
Amount in Extractables (dpm)	2411658		
Extractables (%-applied)	28.52		
Amount of Soil (kg)	0.02		
Concentration in Soil (mg/kg)	4.70		

Calculation of Percentages

Peak-No	Peak Name	Peak			Background	
		DPM	%-ROI	%-applied	DPM	%-applied
1	CGA329351	9935	100.00	28.52	75	0.22
Total		9935	100.00	28.52	75	

Limit of Detection (LD) and Limit of Quantitation (LQ)

Peak-No	Peak Name	LD	LQ	Background	LD	LQ	Background	LD
				Parent equiv.			Soil Residue	
				mg			mg/kg	
1	CGA329351	0.431	0.646	0.0002	0.0004	0.0006	0.0101	0.0202