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STUDY REPORT

NOA 409045

Amended Report[1]

STUDY TITLE

Adsorption / Desorption of NOA 409045 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 other requirements see page 4

AUTHOR

Dr. 5.1.2.e Wob

STUDY COMPLETED ON

November 25, 1998

TESTING FACILITY

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

STUDY NUMBER

98RF01

SPONSOR

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

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[1] according to Amendment No. 2 to Report on Study 98RF01 (November 25, 1998).

STATEMENT OF COMPLIANCE WITH GOOD LABORATORY PRACTICE

Study Number	98RF01
Test Substance	NOA 409045
Study Director	Dr. 5.1.2.e Woo
Study Title	Adsorption / Desorption of NOA 409045 in various Soils

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 Swiss Federal Department of Interior and the Intercantonal Office for the Control of Medicaments, Switzerland. These procedures are based on the OECD Principles of GLP adopted on May 12, 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

November 25, 1998
Date

5.1.2.e Woo

Study Director
Novartis Crop Protection AG
Environmental Safety / Ecochemistry
CH-4002 Basel, Switzerland

Quality Assurance Statement

Novartis Crop Protection AG, GLP Quality Assurance, Prod. Safety Services, 4002 Basel
(Successor in business of Ciba-Geigy Ltd. and Sandoz Ltd.)

Study	**98RF01**
Test substance	**NOA 409045**
Study Title	**Adsorption / Desorption of NOA 409045 in various Soils**
Study Director	**Dr.** 5.1.2.e Woo
QA Inspector	5.1.2.e Woo

I hereby certify that the following Quality Assurance activities were performed:

Activity	**Performed**	**Reported**
Facility Based Inspection	October 8, 1997	October 15, 1997
Protocol Audit	January 5, 1998	January 5, 1998
Study Based Inspection	February 17, 1998	February 17, 1998
Facility Based Inspection	March 10, 1998	March 26, 1998
Final Report Audit	August 5, 1998	August 5, 1998
Amendment to Final Report, Audit	November 26, 1998	November 26, 1998

November 26, 1998

Date

Form. QSSTAT01

5.1.2.e Woo

Quality Assurance Inspector

GENERAL INFORMATION

Guidelines	The study was conducted in compliance 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: NOA 409045
Characterisation	Metabolite of fungicide CGA 329351
Study Number	98RF01
Sponsor	Novartis Crop Protection AG[2] Environmental Safety / Ecochemistry CH-4002 Basel, Switzerland
represented by:	Dr. 5.1.2.e Woo, 5.1.2.e Woo
Study Director[3]	Dr. 5.1.2.e Woo Novartis Crop Protection AG Environmental Safety / Ecochemistry CH-4002 Basel, Switzerland
Technical Personnel[3]	Mr 5.1.2.e Woo (principal co-worker)

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[2] Novartis Crop Protection AG has resulted from the merger of the companies CIBA-GEIGY Ltd. and Sandoz Ltd. and is partial successor in business from above-named companies. This applies also to all aspects concerned with the requirements of Good Laboratory Practice.

[3] The job descriptions and the professional curricula vitae for all personnel participating in this study are archived in the testing facility.

Testing Facility	Novartis Crop Protection AG Environmental Safety / Ecochemistry CH-4002 Basel, Switzerland
Supplier of ^{14}C-labelled Test Substance	Novartis Crop Protection AG Discovery Technologies and Natural Products / Chemistry Support CH-4002 Basel, Switzerland
represented by:	Dr. [redacted]
Supplier of Unlabelled Test and Reference Substances	Novartis Crop Protection AG Discovery Technologies and Natural Products / Chemistry Support CH-4002 Basel, Switzerland
represented by:	Dr. [redacted]
Study Dates	Study Initiation: December 19, 1997 Experimental Start: February 04, 1998 Experimental Termination: March 16, 1998 Study Completion: November 25, 1998
Archives	Protocols, raw data, correspondence, and the final report are archived at: Novartis Crop Protection AG Environmental Safety / Ecochemistry CH-4002 Basel / Switzerland
Quality Assurance	Novartis Crop Protection AG R & D Services / Quality Assurance GLP CH-4002 Basel, Switzerland
represented by:	Dr. [redacted] / Dr. [redacted]
Integrity of Study	There were no circumstances observed affecting the integrity of the study.
Signature for the Report	November 25, 1998 .... [redacted]
	Date Dr. Study Director

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SUMMARY

The adsorption and desorption of NOA 409045, i.e., R-2-[(2,6-dimethyl-phenyl)-(2-methoxy-acetyl)-amino]-propionic acid, a metabolite of the fungicide metalaxyl-M (CGA 329351), was studied on various soil types and compared to other pesticides.

Pre-test data showed, that adsorption reached approximate equilibrium within less than two hours of exposure. Adsorption ranged for a soil-to-solution ratio of 15 g soil and 30 ml 0.01 M $CaCl_2$ and for an initial concentration in the aqueouse phase of 3.8 to 4.6 µg/ml from 6.9 % (soil Staffort, sandy loam) to 15.3 % (soil Vetroz, silt loam) of the radioactivity applied. Desorption reached approximate steady state conditions after less than two hours. Desorption accounted for 2.9 and 6.9 % of the radioactivity applied to the Staffort and Vetroz soil system, respectively. Adsorption to glass walls was negligible.

Based on these findings, samples of the final adsorption / desorption experiment were exposed for two hours only at initial concentrations in the aqueous phases from 0.2 to 4.3 µg/ml.

The Freundlich adsorption coefficients k_{ads} varied between 0.1 ml/g (soil Staffort, sandy loam) and 0.4 ml/g (soil Vetroz, silt loam).

When related to the organic carbon content of the soils a significant difference in K_{oc}-values between neutral soils and the slightly acidic soil was observed:

- K_{OC} (neutral soils, Vetroz and Gartenacker): 8.9 to 9.9 ml/g;
- K_{OC} (acidic soil, Stafford): 15.4 ml/g.

The corresponding values related to organic matter content were:

- K_{OM} (neutral soils): 5.2 to 5.8 ml/g;
- K_{OM} (acidic soil): 8.9 ml/g.

The slopes 1/n for the adsorption isotherms ranged from 0.93 to 0.96.

The Freundlich desorption coefficients k_{des} for both desorption steps ranged from 0.3 ml/g (soil Gartenacker, loam - silt loam) to 1.5 ml/g (soil Staffort, sandy loam).

Based on these findings the following desorption constants related to the organic carbon content were determined:

- K_{OC} (neutral soils) desorption 1: 12.2 to 12.9 ml/g, desorption 2: 16.9 to 18.6 ml/g;
- K_{OC} (acidic soil) desorption 1: 53.9 ml/g, desorption 2: 198.4 ml/g.

These data clearly demonstrate that the desorption constants ($K_{oc\text{-}des2}$) were more than 2 and 10 times higher than the adsorption data (K_{oc}) for neutral and acidic soils (hysteresis), respectively. The significantly higher values are mainly due to a concentration and/or ageing effect. In a supplementary study [1] it was proven that at least for the acidic soil adsorption of NOA 409045 strongly depended on the concentration of the solute in the aqueous phase, i.e. adsorption was much higher for concentrations in the range of 0.05 to 0.2 µg/ml than for concentrations in the range of 0.8 to 1.8 µg/ml.

Finally, it must be pointed out that the above given lower concentration range represents a realistic scenario for NOA 409045. Based on findings in the laboratory the highest amount of NOA 409045 which might be expected from the degradation of CGA 329351 in soil is about 20 to 40 % of the dose applied [2]. Assuming the highest recommended field rate per application of 250 g/ha for CGA 329351, 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 0.05 to 0.1 μg/g of soil.

Furthermore, desorption represents as an approximation to a large extent (ageing effects excluded) an equilibrium of the test compound between adsorbent and its aqueous phase at a lower concentration range. For reasons discussed above desorption constants are considered to reflect more realistically the adsorptivity of the test compound, i.e. they classify NOA 409045 on slightly acidic soils as a strongly adsorbed compound (little mobile) and on neutral soils as a mobile compound.

In all experiments comprising adsorption and both desorption steps, the recoveries were in the range of 97.7 - 112.4 % of the radioactivity applied; the overall mean recovery was 100.8±2.7 %.

For samples extracted with organic solvents after the adsorption step, the recoveries ranged from 106.1±0.9 % (Staffort) to 116.8±0.1 % (Vetroz). The mean amount of radioactivity found in the aqueous phase after adsorption accounted for 89.7±0.7 % (Staffort), 88.3±1.4 % (Gartenacker), and 82.3±0.7 % (Vetroz). Extractable radioactivity amounted to 15.9 ± 0.3 % (Staffort), 22.5 ± 0.4 % (Gartenacker), and 25.7±0.8 % (Vetroz) of the dose applied. The non-extractable radioactivity accounted for 0.4±0.1 % (Staffort), 3.6±0.1 % (Gartenacker), and 8.8±0.1 % (Vetroz) of the dose applied. HPLC analysis of the aqueous adsorption solutions and extractable phases of all soils demonstrated no degradation of NOA 409045 during the study.

1 Introduction

Soil Adsorption / Desorption data are necessary for the evaluation of the migratory 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

As reference material unlabelled NOA 409045 was used[4]. As NOA 409045 is the R-enantiomer of the enantiomer mixture of CGA 62826 and the physico-chemical data are not available at present, the corresponding data of CGA 62826 are presented. The data were taken from Ciba-Geigy report: "Physico-chemical Properties of CGA 62826", (Dr. H. Widmer, February 22, 1994).

Company Code	CGA 62826
Proposed Use	Metabolite of fungicide metalaxyl (CGA 48988)
Chemical Name (IUPAC)	R,S-2-[(2,6-dimethyl-phenyl)-(2-methoxy-acetyl)-amino]-propionic acid
Empirical Formula	$C_{14}H_{19}NO_4$
Molecular Weight	265.31 g / mole
Physical State at 20°C	solid
Vapour Pressure	$1.0 \cdot 10^{-5}$ Pa at 20°C
Partition Coefficient (n-octanol / water)	log P_{ow} = -1.29 at pH 6.88
Dissociation Constant	pK_a = 4.04 (acid)
Water Solubility	water 7320 mg/l at pH 3.06 (buffer sol.) 20990 mg/l at pH 4.39 (buffer sol.) 265 g/l at pH 7.27 (neutralised with NaOH)

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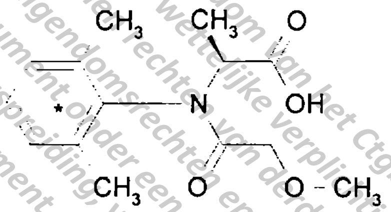
[4] Metalaxyl (CGA 48988) is a mixture of two enantiomers (R-enantiomer (CGA 329351) and S-enantiomer). The acidic metabolite of metalaxyl, CGA 62826, also consists of two enantiomers. The R-enantiomer of CGA 62826 is NOA 409045, a metabolite of CGA 329351 (metalaxyl-M).

Batch Number	RV-3057/3 (NOA 409045)
Purity	92.00 %
Expiration Date	December 1999
Amount Received	10 mg
Storage Conditions	< 10 °C (refrigerator, in the dark)
Precautions	routine hygiene procedures

2.1.2 ^{14}C-labelled Test Substance

Code	^{14}C-NOA 409045
Structure / Label *(* = Position of Labelling)*	
Chemical Name (IUPAC)	R-2-[(2,6-dimethyl-phenyl)-(2-methoxy-acetyl)-amino]-propionic acid
Batch Number	ILS-182.1
Label	Phenyl-(U)^{14}C
Specific Radioactivity	1.76 MBq / mg (= 47.57 µCi / mg)
Radiochemical Purity	99.2 % (Data Sheet)
Amount Received	4.00 mg corresponding to 7.04 MBq
Stability in Vehicle	The stability of the test substance was determined by TLC using an aliquot of the application solution of the test substance before and after treatment.
Storage Conditions	Short term: 0 - 5 °C in the dark Long term: ca. ≤ -18 °C in the dark
Precautions	Routine hygienic procedures. Additional safety precautions according to Standard Operating Procedures based on Swiss regulation on radiation protection.

2.2 Test System (Soils)

Types	Three 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 320 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, as it was impossible to use the estimated ratio (see 2.5.2) calculated with the given log P_{ow} of CGA 62826.
Amount of Soil	Pre-test: 15 g for all soils (dry weight basis) Main test: 10 g for all soils (dry weight basis).
Aqueous Phase	Pre-test: 30 ml of 0.01 M $CaCl_2$ solution Main test: 20 ml of 0.01 M $CaCl_2$ solution.
Concentrations	The test substance was applied at 5 concentrations ranging between about 0.3125 and 5.0 µg/ml. In addition, untreated control samples (vehicle only) were set up. Except for the highest concentration all samples were prepared in duplicate. For the highest concentration four samples were prepared.
Equilibration Time	The time required to reach the adsorption and desorption equilibria 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 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 3).

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 (8 tubes, two for each soil and two tubes only containing 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 Table 3) centrifuged, duplicate sub-samples were removed from the clear aqueous phase and the radioactivity 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 exposed in duplicate per soil (total 10 per soil). Furthermore, two untreated samples per soil were set up as background samples. 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 where aqueous phases and soil 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

Prior to the preparation of the treatment solutions, the total amount of ^{14}C-labelled NOA 409045 (about 4 mg) was dissolved in 5 ml acetone. The accurate amount of radioactive material present was determined by LSC to be 4.177 mg. This stock solution was used for the preparation of the treatment dilutions. For this purpose, a series of aqueous pre-dilutions with 0.01 M $CaCl_2$ solution was prepared (see Table below). The amount of radioactivity of the various dilutions was determined by LSC. For more details see Tables 5 - 7.

Sample	Amount of Solution	Final Volume of Treatment Solution made up with 0.01 M $CaCl_2$	Concentration of NOA 409045 in Treatment Solution
	(ml)	(ml)	(µg/ml = ppm)
E	3.0 ml from stock solution	500	5.309
F	1.5 ml from stock solution	500	2.654
G	250 ml from solution F	500	1.327
H	250 ml from solution G	500	0.664
I	250 ml from solution H	500	0.332

2.3.4 Pre-Test

The equilibration time was determined in a preliminary test with all soils at an initial test concentration of 5.309 µg/ml.

For the test, an amount of 15 g air-dry soil was weighed into a tarred centrifuge tube and suspended with 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 about 30 ml of treated aqueous phase (5.309 µg/ml) was added (for more details see Table 2) and the mixture shaken (320 rpm). After various time intervals (see Figure 1) the mixture was centrifuged for 10 min. at 3000 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.

In addition, treated aqueous samples (30 ml) without soil were exposed for 24 hours and analysed by LSC at the same time intervals (adsorption only).

All aqueous phases from adsorption and desorption were analysed by HPLC for amount of parent molecule and degradates.

2.3.5 Adsorption / Desorption Experiments

Into tarred centrifuge tubes an amount of 10.0±0.1 g (dry weight) of each soil was weighed and suspended with about 20 ml 0.01 M $CaCl_2$-solution (without a.i.). After an equilibration time of 24 hours the samples were centrifuged and the $CaCl_2$-solution was decanted. Then the corresponding treated aqueous 0.01 M $CaCl_2$ phases (20 ml) with initial test concentrations between 0 (blank) and about 5 µg/ml were added (Tables 5 - 7). All additions of soil and solutions were controlled by weighing the test vessel.

The centrifuge tubes were shaken with about 320 rpm at 20°C for 2 hours. The soils and solutions were then separated by centrifugation at 2000 rpm for 10 min. Directly from the clear supernatant three aliquots of 0.5 ml each were taken, mixed with 15 ml of scintillation solution (IrgaSafe Plus™[5]) and submitted to liquid scintillation counting to determine the equilibrium concentration in the aqueous phase (C_e).

Then the remaining supernatants were cautiously removed and the centrifuge tubes still containing the wet soil were weighed again. Thereafter, fresh 0.01 M $CaCl_2$-solution (without a.i., 20 ml) was added to the wet soil containing the adsorbed a.i., the weight was determined and the test tubes were shaken again for 2 hours at 20°C (first desorption step).

After the first desorption step the solutions and soils were separated by centrifugation. Thereafter, desorption was repeated once.

After completion of the adsorption and desorption steps, the radioactivity in the aqueous phases was determined by LSC and the amount adsorbed onto soil (x/m) calculated from the amount dissipating from the aqueous phase. The residual radioactivity in soil after desorption was determined by combustion. The radioactivity remaining adsorbed to the centrifuge tube was dissolved in about 20 ml acetone and determined by LSC. Thereafter, a balance was established (samples 3 - 12) comprising the radioactivity found in adsorption and desorption solutions, in soil after combustion and in washings of the test tubes (radioactivity adsorbed to glass-walls). Results were expressed in percentage of the radioactivity initially applied. Samples 1 and 2 served as background control and were worked-up after the adsorption step. The background radioactivity in the aqueous and solid phase (soil) was determined by LSC and combustion and LSC, respectively.

2.3.6 Mass Balance

Samples 13 / 14 (Tables 5 - 7) were worked-up directly after the adsorption step. The soil was extracted twice with about 50 - 80 ml acetone : water (80 : 20; v : v) and a third time with acetone.

The radioactivity in all extracts was determined by LSC and thereafter the extracts were combined for further analysis. Finally, the not extracted radioactivity in the soil was determined by combustion and the test tubes were carefully washed with acetone (radioactivity adsorbed to glass walls).

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[5] Packard Instruments Company Inc., One State Street, Meriden, CT 06450, US

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. Aqueous phase and organic extracts were further analysed as described below.

2.3.7 Sample Preparation for Analysis

2.3.7.1 Supernatant Aqueous Phases after Adsorption

An aliquot of 5 ml of the aqueous phases (samples 13 and 14) was evaporated to almost dryness using a vacuum rotary evaporator (35°C; 20 mbar). The residual radioactivity was dissolved in acetonitrile : water (1 : 1), made up to 1 ml and then submitted to HPLC analysis.

2.3.7.2 Organic Soil Extracts

An aliquot of the combined extracts of 50 ml was taken and concentrated at 35 °C to 2 - 3 ml using a vacuum rotary evaporator. Thereafter, the solution was made up to 5 ml with acetonitrile and submitted to HPLC analysis.

2.3.7.3 Non-Extractables

The extracted soils were air-dried, homogenised, and their residual radioactivity determined by combustion and LSC of triplicate samples.

2.4 Analytical Methods

2.4.1 Measurement of Radioactivity

All measurements were performed at minimum in duplicate using a model 2500 TR Liquid Scintillation Spectrometer (Packard Instruments Company Inc., One State Street, Meriden, CT 06450, US). The measurements were corrected for background and counting efficiency (a quench curve was established using Packard quenched standards). Based on the double background the limit of detection was determined to be 0.028 % of the radioactivity applied corresponding to 0.003 ppm (see Appendix B).
The following scintillation cocktails were used:

Scintillator I:	IrgaSafe Plus™
Scintillator II:	Oxysolve C-400®[6]

2.4.1.1 Measurement of Organic Samples

Organic samples up to 1.0 were mixed with 15 ml Scintillator I and submitted to liquid scintillation counting.

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[6] Zinsser Analytik, Frankfurt, FRG

2.4.1.2 Measurement of Non-Extractable Radioactivity

Residual radioactivity in aliquots of soil samples of up to approximately 1.55 g was determined by combustion in an oxygen stream at about 800 °C with copper oxide as catalyst using a Robox II sample oxidiser[7]. $^{14}CO_2$ liberated from soil was absorbed in a vial, containing 15 ml of Scintillator II. Radioactivity present in the absorption solution was measured by liquid scintillation counting. Based on the double background the limit of detection was determined to be 0.003 % of the radioactivity applied corresponding to 0.0003 ppm (Appendix B).

2.4.2 High Performance Liquid Chromatography (HPLC)

The identification and quantification of NOA 409045 and degradation products was performed with a Spectra Physics[8] Liquid Chromatograph equipped with a Spectra-Chrom UV/VIS-detector and a Berthold radioactivity monitoring system. Based on the double background of the chromatogram the limit of detection was determined to be 1.8 % of the radioactivity applied corresponding to 0.194 ppm (see Appendix B).

Instruments:

HPLC-System:	Pump:	SP 8800
	Autosampler:	SP 8880
	Integrator:	SP 4400
	Oven:	SP 8792
	Data System:	Spectra Physics Chromstation/IBM P/S 2
Detectors:	UV/VIS:	SpectraChrom 200
	RAM:	Berthold LB 506 C-1 equipped with a 150 µl solid flow cell (YG 150) and the Berthold "Winflow" data system[9]. Radioactive fractions were quantified using the Berthold evaluation software.

Operating conditions:

Column:	NU5C18, length: 25 cm, inner diameter: 4.6 mm, particle size: 5 µm. The column was equipped with a Nucleosil 100 / 5 µm / C 18 Guardcartridge (Bischoff, Leonberg, FRG).	
Oven:	Ambient temperature	
Mobile phases:	A:	0.0125 % trifluoroacetic acid (TFA) : acetonitrile 90 : 10 (v : v)
	B:	acetonitrile
	Flow:	1 ml/min.

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[7] Zinsser Analytik, Frankfurt, FRG

[8] Thermo Separation Products, CH-4123 Allschwil, Switzerland

[9] Berthold AG, CH-8105 Regensdorf, Switzerland

Gradient Program:

Time (min)	Mobile Phases	
	A	B
0 - 25	90 → 60	10 → 40
25 - 32	60 → 90	40 → 10
32 - 35	90	10

Injector: Injection volume: 100 - 300 µl
Detectors: UV/VIS: Wavelength (nm) 230
RAM: Cell volume: 150 µl

The following retention time was observed on HPLC:
NOA 409045 (Parent): 20.5 (min)

The retention time may vary depending on column properties or on properties of samples.

2.4.3 Thin Layer Chromatography (TLC)

Two dimensional TLC:
Pre-coated glass-backed silica gel 60F 254 plates with a layer thickness of 0.25 mm (20 x 20 cm, E. Merck AG, Darmstadt, Germany) were used.
The following solvent systems were used:
SS 1: chloroform : methanol : ammonium hydroxide : water, (80:30:4:2, v:v:v:v).
SS 2: chloroform : methanol : formic acid : water, (70:25:4:2, v:v:v:v).
After development the position of the radiolabelled compounds was determined by a Digital Autoradiograph (Dr. Berthold, Wildbad, Germany), equipped with a Compaq Deskpro 66M PC system.
The following Rf-values of the compound were observed in the different solvent systems:

Compound	Rf	
	SS 1	SS 2
NOA 409045	0.29 - 0.31	0.65 - 0.66

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

Based on the below given correlation[10] the Freundlich adsorption coefficient (k) of a given soil can be estimated:

$$\log (K_{oc}) = 0.60338 \cdot \log (P_{ow}) + 0.81826 \rightarrow k = \frac{K_{oc} \cdot \%\ OC}{100}$$

The soil-to-solution ratio can now be calculated using the following formula:

1. Estimation of k-value of CGA 62826 (instead of NOA 409045 see 2.1.1):

Example for soil Vetroz:

Soil OC (%)	4.39			
	$\log (P_{ow})$	$\log (K_{oc})$	K_{oc}	$k = \frac{K_{oc} \cdot \%\ OC}{100}$
Compound	-1.29	0.0399	1.096	0.048

2. Estimation of Soil-to-Solution Ratio (R):

Equation: $$R = \frac{1}{k \cdot (\frac{1}{A} - 1)}$$

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

Example: (derived from equation given in Annex 5 OECD Guideline 106; updating proposal September 1996)

Adsorption (%)	20.00
Adsorption ratio = (% ads / 100) = A =	0.20
k =	0.048
R =	5.19

$$R = \frac{M_{soil}}{V_{water}} \rightarrow V_{water} = \frac{M_{soil}}{R}$$

e.g. for 1 g soil a water volume of 0.2 ml is needed to achieve 20% adsorption.
Therefore, a soil-to-solution ratio of 1 : 2 was chosen for pre- and main test, as it was impossible to use the estimated ratio calculated with the given log P_{ow} of CGA 62826.

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[10] Novartis internal data

2.5.3 Adsorption / Desorption Coefficients

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

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

X/m: amount of the test substance adsorbed per unit mass of adsorbent (µg/g),

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

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) and the organic matter content (OM) of the various soils using the following equations[11]:

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

and

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

2.5.4 Limits of Detection / Quantitation

Limits of detection and quantitation were calculated for the various methods applied. The results are presented in Appendix B.

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[11] 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.

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

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

3 Results and Discussion

3.1 Purity and Stability of the Test Substance

Purity:

TLC-analysis of NOA 409045 in the application solution before treatment showed a purity of 100 % (Figure 3).

Stability:

The radiochemical purity of the radiolabelled test compound after the treatment procedures was found to be 100 % (TLC, Figure 4). Thus, the test substance proved to be stable in the vehicle.

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 3.8 to 4.6 µg/ml test solution (Table 2).

Already after about two hours of shaking at 20°C the concentration of a.i. reached approximate steady state conditions in the supernatant water phase for all samples (Table 3, Figure 1). Adsorption ranged from 5.86 (2 h) to 6.92 % (24 h) for soil Staffort and from 13.26 (2 h) to 15.29 % (24 h) for soil Vetroz. The amount adsorbed by soil Gartenacker was with 7.85 % (2 h) and 8.49 % (24 h) in between the two others.

The glass walls adsorbed only the low amount of 3.01% of the radioactivity applied.

The desorption reached approximate steady state conditions after 2 hours (Table 4, Figure 2). After 24 h desorption accounted for 2.93 and 6.90 % of the radioactivity applied to the Staffort and Vetroz soil system, respectively. These figures corresponded to a relative desorption of 46.4 and 48.9 % of the radioactivity adsorbed by the corresponding soils after 2 hours.

During the study no degradation of NOA 409045 was observed in the aqueous adsorption solutions (Figure 5 and 6).

Based on these findings, samples of the final adsorption / desorption experiment were exposed for two hours only at initial concentrations in the aqueous phases from 0.2 to 4.3 µg/ml.

3.3 Recovery, Distribution and Analysis of Radioactivity

Adsorption / desorption isotherms were established for all soils. For this purpose a series of aqueous concentrations (0.3 to 5 µg / ml) was equilibrated over 2 hours with the corresponding soils. The soil-to-solution ratio was set to 10 g soil per 20 ml aqueous phase, as it was impossible to use the estimated ratio (see 2.5.2) calculated with the given log P_{ow} of CGA 62826.

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 8 - 11.

3.3.1 Recovery

The recoveries of all samples are reported in Tables 8 - 10.

Samples 3 - 12 of all soils (adsorption / desorption samples):

The recoveries were in the range of 97.66 - 112.38 % of the radioactivity applied; the overall mean recovery was 100.78±2.65 %.

The total amount of radioactivity still adsorbed to the soil after the last desorption step ranged from 2.12±4.22 (Staffort) to 5.86±0.15 % (Vetroz). In the aqueous phases, the radioactivity decreased from 94.76±1.04 % (Staffort) to 86.33±0.65 % (Vetroz) for the adsorption step, from 2.02±1.01 % (Staffort) to 6.73±039 % (Vetroz) for the first desorption step and from 0.62 ± 0.16 % (Staffort) to 2.77±0.14 % (Vetroz) for the second desorption step.

Samples 13 - 14 of all soils (balance and analysis samples):

The mean amount of radioactivity found in the aqueous phase after adsorption accounted for 89.74±0.66 % (Staffort), 88.33±1.40 % (Gartenacker), and 82.31±0.74 % (Vetroz). Extractable radioactivity amounted to 15.94±0.29 % (Staffort), 22.46±0.42 % (Gartenacker), and 25.71±0.80 % (Vetroz) of the dose applied.

The non-extractable radioactivity accounted for 0.38±0.02 % (Staffort), 3.64±0.03 % (Gartenacker), and 8.78±0.02 % (Vetroz) of the dose applied. Total recoveries of these samples worked-up after the adsorption step ranged from 106.06±0.93 % (Staffort) to 116.81±0.08 % (Vetroz).

3.3.2 Analysis of Radioactivity

After adsorption the supernatant aqueous solution and the extractable radioactivity of samples 13/14 were analysed by HPLC (for examples see Figures 7 - 12). Results are summarised in Table 11.

Analysis of the aqueous adsorption solutions and extractable phases of all soils showed, that only NOA 409045 was present.

3.4 Adsorption and Desorption Isotherms

The results are summarised in Table 12 and in Figures 13 - 15. The individual concentrations of the test compound in aqueous phases and in soil after adsorption and desorption are given in Tables 13 to 15.

The Freundlich adsorption coefficients k_{ads} varied in the range of 0.1 ml/g of soil Staffort (sandy loam) and 0.4 ml/g of soil Vetroz (silt loam).

When related to the organic carbon content of the soils a significant difference in K_{oc}-values between neutral soils and the slightly acidic soil was observed (Table 12):

- K_{OC} (neutral soils, Vetroz and Gartenacker): 8.9 to 9.9 ml/g;
- K_{OC} (acidic soil, Stafford): 15.4 ml/g.

The corresponding values related to organic matter content were:

- K_{OM} (neutral soils): 5.2 to 5.8 ml/g;
- K_{OM} (acidic soil): 8.9 ml/g.

The slopes 1/n for the adsorption isotherms ranged from 0.93 to 0.96 (Table 12). The Freundlich desorption coefficients k_{des} for both desorption steps ranged from 0.3 ml/g (soil Gartenacker, loam - silt loam) to 1.5 ml/g (soil Staffort, sandy loam). Based on these findings the following desorption constants related to the organic carbon content were determined:

- K_{OC} (neutral soils) desorption 1: 12.2 to 12.9 ml/g, desorption 2: 16.9 to 18.6 ml/g;
- K_{OC} (acidic soil) desorption 1: 53.9 ml/g, desorption 2: 198.4 ml/g.

These data clearly demonstrate that the desorption constants ($K_{oc\text{-}des2}$) were more than 2 and 10 times higher than the adsorption data (K_{oc}) for neutral and acidic soils (hysteresis), respectively. The significantly higher values are mainly due to a concentration and/or ageing effect. In a supplementary study [1] it was proven that at least for the acidic soil adsorption of NOA 409045 strongly depended on the concentration of the solute in the aqueous phase, i.e. adsorption was much higher for concentrations in the range of 0.05 to 0.2 µg/ml than for concentrations in the range of 0.8 to 1.8 µg/ml.

Finally, it must be pointed out that the above given lower concentration range represents a realistic scenario for NOA 409045. Based on findings in the laboratory the highest amount of NOA 409045 which might be expected from the degradation of CGA 329351 in soil is about 20 to 40 % of the dose applied [2]. Assuming the highest recommended field rate per application of 250 g/ha for CGA 329351, 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 0.05 to 0.1 µg/g of soil.

Furthermore, desorption represents as an approximation to a large extent (ageing effects excluded) an equilibrium of the test compound between adsorbent and its aqueous phase at a lower concentration range. For reasons discussed above desorption constants are considered to reflect more realistic the adsorptivity of the test compound, i.e. they classify NOA 409045 on slightly acidic soils as a strongly adsorbed compound (little mobile) and on neutral soils as a mobile compound (Table 16).

In addition, the Freundlich adsorption coefficients k_{ads} were correlated to the organic carbon content of the tested soils showing a linear relationship between the corresponding parameters (Figure 16).

4 Conclusion

The adsorption / desorption behaviour of ^{14}C-NOA 409045 has been studied in three different soil types. According to the results obtained, in neutral soils NOA 409045 has to be classified as a low adsorbing compound and is hence considered to be mobile. In slightly acidic soils NOA 409045 has to be classified as a strongly adsorbed compound and is hence considered to be little mobile.

5 References

[1] 5.1.2.e Woo Adsorption of ^{14}C-NOA 409045 onto two Soils (Supplementary Data), Novartis Crop Protection AG Project Report 98EH06, November 24, 1998

[2] 5.1.2.e Woo Influence of Biomass on Rate of Degradation of CGA 329351 and CGA 48988 at 20°C and a Dose Rate of 0.2 kg/ha. Rate of Degradation of CGA 329351 at 30°C and a Dose Rate of 1 kg/ha, Novartis Crop Protection AG Project Report 97EH02, May 15, 1998.

6 Acknowledgements

The skilled technical assistance of Mr 5.1.2.e Woo is gratefully acknowledged.

Table 1: Soil Types and their Characteristics.

Parameter Type[12]	Soil		
	1	2	3
Name	Staffort	Gartenacker	Vetroz
Origin	F	CH	CH
Batch-No	30.09.97*	10 / 93	2 / 75
Classification	Sandy loam	Loam - silt loam	Silt loam
pH	5.2	7.2	7.1
$CaCO_3$ (%)	< 0.3	7.8	55.7
Organic carbon (%)	0.77	2.4	4.39
CEC (meq / 100 g soil)	6.35	15.5	30.70
Particle size:			
Clay (%)	8.78	11.3	24.8
Silt (%)	15.08	49.9	56.8
Sand (%)	76.14	38.8	18.4

* date of analysis

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[12] Soil properties were determined by the AGROLAB AG, Labor für Landwirtschaft und Umwelt, CH-6030 Ebikon, CH-6037 Root, Switzerland.

Table 2: Preparation of the Treatment Solution and Initial Concentrations of NOA 409045 in 0.01 M $CaCl_2$-Solution for Pre-Test.

Sample No.	Soil	Conc. a.i. Stock sol. (µg/ml)	Volume Stock sol. (ml)	Volume added $CaCl_2$ (ml)	Final Volume (added + rest*) (ml)	Amount NOA 409045 (µg)	Conc. a.i.** (µg/ml)
1	Staffort	5.309	500	29.89	34.27	158.68	4.630
2		5.309	500	29.93	34.23	158.89	4.642
3	Gartenacker	5.309	500	29.86	38.69	158.52	4.097
4		5.309	500	29.88	38.98	158.62	4.069
5	Vetroz	5.309	500	29.89	41.55	158.68	3.819
6		5.309	500	29.89	41.57	158.68	3.817

* rest = $CaCl_2$ solution from pre-wetting the soil.

** concentration based on the total volume of $CaCl_2$ solution.

Table 3: Rate of Adsorption of NOA 409045 in various Soils (Pre-Test).

Sample	Adsorption Time	Staffort	Gartenacker	Vetroz	Glass
	h	% adsorbed	% adsorbed	% adsorbed	% adsorbed
0.1	0	0.00	0.00	0.00	0.00
0.2	0	0.00	0.00	0.00	0.00
Mean	0	0.00	0.00	0.00	0.00
1.1	1	6.09	10.95	12.42	2.44
1.2	1	6.76	9.82	12.28	2.80
Mean	1	6.43	10.38	12.35	2.62
2.1	2	5.38	7.15	13.36	2.44
2.2	2	6.35	8.56	13.16	3.06
Mean	2	5.86	7.85	13.26	2.75
4.1	4	6.19	7.66	12.70	4.26
4.2	4	6.78	7.72	13.79	3.62
Mean	4	6.48	7.69	13.25	3.94
6.1	6	7.20	7.23	14.39	3.29
6.2	6	6.75	8.82	14.18	2.61
Mean	6	6.98	8.02	14.28	2.95
8.1	8	7.33	7.71	13.74	3.62
8.2	8	6.92	8.54	14.06	2.47
Mean	8	7.12	8.13	13.90	3.05
24.1	24	6.72	8.13	14.96	2.60
24.2	24	7.13	8.84	15.61	2.88
Mean	24	6.92	8.49	15.29	2.74

Mean of adsorption to glass: 3.01 %.

Table 4: Rate of Desorption of NOA 409045 in various Soils (Pre-Test).

Sample	Desorption Time	Staffort	Gartenacker	Vetroz
	h	% desorbed	% desorbed	% desorbed
0.1	0	0.00	0.00	0.00
0.2	0	0.00	0.00	0.00
Mean	0	0.00	0.00	0.00
1.1	1	2.64	2.87	6.19
1.2	1	2.79	3.38	6.28
Mean	1	2.72	3.13	6.23
2.1	2	2.65	3.15	6.41
2.2	2	2.79	3.58	6.58
Mean	2	2.72	3.37	6.49
4.1	4	2.66	3.33	6.54
4.2	4	2.83	3.48	6.68
Mean	4	2.75	3.40	6.61
6.1	6	2.76	3.35	6.77
6.2	6	2.90	3.51	6.83
Mean	6	2.83	3.43	6.80
8.1	8	2.79	3.07	6.75
8.2	8	2.95	3.94	6.66
Mean	8	2.87	3.51	6.70
24.1	24	2.84	3.34	6.73
24.2	24	3.02	3.63	7.08
Mean	24	2.93	3.49	6.90

Table 5: Preparation of the Treatment Solution and Initial Concentrations of NOA 409045 in 0.01 M $CaCl_2$-Solution for Adsorption Study with Soil Staffort.

Sample	Volume of Solution (ml)	Final Volume of Treatment Solution (0.01 M $CaCl_2$) (ml)	Conc. of NOA 409045 in Treatment Sol. (µg/ml = ppm)
E	3.0 ml from stock solution	500	5.309
F	1.5 ml from stock solution	500	2.654
G	250 ml from solution F	500	1.327
H	250 ml from solution G	500	0.664
I	250 ml from solution H	500	0.332

Sample No.	Conc. a.i. Treatment Sol. (µg/ml)	Volume applied (ml)	Final Volume* (ml)	Conc. a.i. in $CaCl_2$** (µg/ml)	Conc. a.i. in $CaCl_2$*** (µg/ml)
1	0	20.14	23.55	0.000	0.000
2	0	19.99	23.17	0.000	0.000
3	0.332	20.03	23.39	0.332	0.266
4	0.332	20.05	23.56	0.332	0.264
5	0.664	20.02	23.52	0.663	0.537
6	0.664	20.02	23.67	0.664	0.532
7	1.327	20.04	23.35	1.327	1.077
8	1.327	20.01	23.38	1.325	1.107
9	2.654	20.04	23.48	2.599	2.144
10	2.654	20.00	23.48	2.653	2.139
11	5.309	19.99	23.32	5.308	4.309
12	5.309	20.01	23.29	5.308	4.314
13	5.309	20.04	23.43	5.309	4.309
14	5.309	20.00	23.56	5.309	4.314

* Volume of treatment solution plus volume of residual 0.01 M $CaCl_2$ remaining in the soil after centrifugation.

** Conc. a.i. corrected for radioactivity found in tube washings = C_i.

*** Conc. a.i. calculated with the final volume of 0.01 M $CaCl_2$ solution.

Table 6: Preparation of the Treatment Solution and Initial Concentrations of NOA 409045 in 0.01 M $CaCl_2$-Solution for Adsorption Study with Soil Gartenacker.

Sample	Volume of Solution	Final Volume of Treatment Solution (0.01 M $CaCl_2$)	Conc. of NOA 409045 in Treatment Sol.
	(ml)	(ml)	(µg/ml = ppm)
E	3.0 ml from stock solution	500	5.309
F	1.5 ml from stock solution	500	2.654
G	250 ml from solution F	500	1.327
H	250 ml from solution G	500	0.664
I	250 ml from solution H	500	0.332

Sample No.	Conc. a.i. Treatment Sol. (µg/ml)	Volume applied (ml)	Final Volume* (ml)	Conc. a.i. in $CaCl_2$** (µg/ml)	Conc. a.i. in $CaCl_2$*** (µg/ml)
1	0	20.01	26.03	0.000	0.000
2	0	20.02	26.14	0.000	0.000
3	0.332	19.99	26.34	0.332	0.232
4	0.332	20.01	26.43	0.332	0.230
5	0.664	20.00	26.25	0.663	0.467
6	0.664	20.06	26.75	0.663	0.460
7	1.327	20.03	26.18	1.327	0.941
8	1.327	19.98	26.20	1.327	0.932
9	2.654	20.03	26.30	2.653	1.875
10	2.654	19.98	26.48	2.654	1.854
11	5.309	19.98	26.30	5.308	3.743
12	5.309	20.01	26.36	5.307	3.731
13	5.309	20.02	26.77	5.308	3.681
14	5.309	20.03	26.47	5.308	3.735

* Volume of treatment solution plus volume of residual 0.01 M $CaCl_2$ remaining in the soil after centrifugation.

** Conc. a.i. corrected for radioactivity found in tube washings = C_i.

*** Conc. a.i. calculated with the final volume of 0.01 M $CaCl_2$ solution.

Table 7: Preparation of the Treatment Solution and Initial Concentrations of NOA 409045 in 0.01 M $CaCl_2$-Solution for Adsorption Study with Soil Vetroz.

Sample	Volume of Solution	Final Volume of Treatment Solution (0.01 M $CaCl_2$)	Conc. of NOA 409045 in Treatment Sol.
	(ml)	(ml)	(µg/ml = ppm)
E	3.0 ml from stock solution	500	5.309
F	1.5 ml from stock solution	500	2.654
G	250 ml from solution F	500	1.327
H	250 ml from solution G	500	0.664
I	250 ml from solution H	500	0.332

Sample No.	Conc. a.i. Treatment Sol. (µg/ml)	Volume applied (ml)	Final Volume* (ml)	Conc. a.i. in $CaCl_2$** (µg/ml)	Conc. a.i. in $CaCl_2$*** (µg/ml)
1	0	20.03	27.90	0.000	0.000
2	0	20.03	28.00	0.000	0.000
3	0.332	20.03	28.01	0.332	0.202
4	0.332	20.05	28.33	0.332	0.202
5	0.664	20.03	28.23	0.663	0.403
6	0.664	19.99	28.29	0.663	0.404
7	1.327	19.99	27.89	1.327	0.820
8	1.327	20.03	28.08	1.327	0.820
9	2.654	20.04	28.24	2.654	1.640
10	2.654	20.01	28.35	2.654	1.634
11	5.309	20.03	28.18	5.308	3.260
12	5.309	20.01	28.14	5.308	3.281
13	5.309	20.02	27.92	5.308	3.303
14	5.309	20.04	28.25	5.309	3.296

* Volume of treatment solution plus volume of residual 0.01 M $CaCl_2$ remaining in the soil after centrifugation.

** Conc. a.i. corrected for radioactivity found in tube washings = C_i.

*** Conc. a.i. calculated with the final volume of 0.01 M $CaCl_2$ solution.

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

(Values given in % of the radioactivity applied)

Sample		Aqueous Phase ($CaCl_2$-Solution)				Soil			Recovery
No.	ppm	Adsorption	Desorption 1	Desorption 2	Washings	Total*	Extractable	Non-extractable	
3	0.33	93.67	3.11	0.64	0.01	0.78			98.21
4	0.33	93.62	2.48	0.62	0.02	0.92			97.66
5	0.66	95.07	2.33	0.49	0.02	0.69			98.59
6	0.66	94.71	1.84	0.46	0.01	0.75			97.77
7	1.33	94.55	2.82	0.64	0.01	0.77			98.79
8	1.33	97.42	0.04	0.63	0.15	14.14			112.38
9	2.65	94.63	0.43	1.05	2.07	1.10			99.29
10	2.65	94.63	2.61	0.60	0.03	0.82			98.68
11	5.31	94.70	2.01	0.49	0.01	0.65			97.86
12	5.31	94.59	2.49	0.61	0.01	0.62			98.31
Mean		94.76±1.04	2.02±1.01	0.62±0.16	0.23±0.65	2.12±4.22			99.75±4.47
13	5.31	89.27					15.73	0.40	105.40
14	5.31	90.21					16.14	0.37	106.72
Mean		89.74±0.66					15.94±0.29	0.38±0.02	106.06±0.93

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

Table 9: Balance of Radioactivity for Soil Gartenacker after Adsorption and Desorption.

(Values given in % of the radioactivity applied)

Sample		Aqueous Phase ($CaCl_2$-Solution)				Soil			Recovery
No.	ppm	Adsorption	Desorption 1	Desorption 2	Washings	Total*	Extractable	Non-extractable	
3	0.33	92.15	4.33	1.60	0.02	2.86			100.97
4	0.33	91.52	4.61	1.70	0.02	2.79			100.64
5	0.66	92.32	4.44	1.55	0.03	2.87			101.22
6	0.66	92.50	3.31	1.20	0.02	2.74			99.77
7	1.33	92.71	4.33	1.39	0.02	2.39			100.85
8	1.33	92.12	4.57	1.56	0.03	2.88			101.16
9	2.65	92.73	4.51	1.65	0.03	2.81			101.73
10	2.65	92.59	4.03	1.47	0.03	2.59			100.71
11	5.31	92.82	4.56	1.54	0.02	2.47			101.40
12	5.31	92.58	3.84	1.40	0.02	2.45			100.28
Mean		92.40±0.39	4.25±0.42	1.51±0.14	0.02±0.01	2.68±0.19			100.87±0.57
13	5.31	87.34					22.16	3.61	113.12
14	5.31	89.33					22.76	3.66	115.76
Mean		88.33±1.40					22.46±0.42	3.64±0.03	114.44±1.86

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

Table 10: Balance of Radioactivity for Soil Vetroz after Adsorption and Desorption.

(Values given in % of the radioactivity applied)

Sample		Aqueous Phase ($CaCl_2$-Solution)				Soil			Recovery
No.	ppm	Adsorption	Desorption 1	Desorption 2	Washings	Total*	Extractable	Non-extractable	
3	0.33	85.28	7.00	3.09	0.02	6.06			101.45
4	0.33	85.88	7.14	2.68	0.01	5.95			101.66
5	0.66	85.52	7.01	2.81	0.02	6.08			101.45
6	0.66	86.18	5.83	2.77	0.02	5.86			100.64
7	1.33	86.21	6.96	2.95	0.02	5.83			101.98
8	1.33	86.57	7.03	2.68	0.01	5.81			102.09
9	2.65	87.07	6.72	2.70	0.01	5.87			102.37
10	2.65	87.23	6.45	2.65	0.02	5.90			102.25
11	5.31	86.39	6.53	2.73	0.02	5.57			101.23
12	5.31	86.92	6.64	2.66	0.02	5.72			101.96
Mean		86.33±0.65	6.73±0.39	2.77±0.14	0.02±0.01	5.86±0.15			101.71±0.53
13	5.31	81.79					26.28	8.79	116.86
14	5.31	82.84					25.14	8.76	116.75
Mean		82.31±0.74					25.71±0.80	8.78±0.02	116.81±0.08

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

Table 11: Distribution of ^{14}C-NOA 409045 in Soil Extractables and Aqueous Phase.

(Values given in % of the radioactivity applied)

Soil Sample		Extractable	Non- extract.	Subtotal	Aqueous Phase	Total	Relative Proportion of NOA 409045 in aqueous Phase
		M1			M1		
		Identity			Identity		Identity
		NOA 409045			NOA 409045		NOA 409045
Staffort	13	15.73	0.40	16.13	89.27	105.40	100.00
	14	16.14	0.37	16.51	90.21	106.72	100.00
Garten-acker	13	22.16	3.61	25.77	87.34	113.12	100.00
	14	22.76	3.66	26.42	89.33	115.76	100.00
Vetroz	13	26.28	8.79	35.07	81.79	116.86	100.00
	14	25.14	8.76	33.90	82.84	116.75	100.00

Table 12: Adsorption- and Desorption Coefficients of NOA 409045 for various Soils.

	Soil	Org. C	Intercept	k	Slope (1/n)	r^2	K_{oc}	K_{om}
		(%)		(ml/g)			(ml a.i./g org C)	(ml a.i./g org M)
Adsorption	Staffort	0.77	-0.926957	0.12	0.934746	0.928632	15.37	8.91
	Gartenacker	2.40	-0.671166	0.21	0.960409	0.998239	8.88	5.15
	Vetroz	4.39	-0.359931	0.44	0.955835	0.999007	9.94	5.77
Desorption 1	Staffort	0.77	-0.382126	0.41	0.989201	0.981148	53.87	31.25
	Gartenacker	2.40	-0.534244	0.29	0.925087	0.983062	12.18	7.06
	Vetroz	4.39	-0.247976	0.56	0.945413	0.992395	12.87	7.46
Desorption 2	Staffort	0.77	0.184004	1.53	0.957773	0.947256	198.39	115.07
	Gartenacker	2.40	-0.392122	0.41	0.866738	0.906092	16.89	9.80
	Vetroz	4.39	-0.087614	0.82	0.932718	0.984655	18.62	10.80

Table 13: Concentration of NOA 409045 in Aqueous Phases and in Soil Stafffort after Adsorption and Desorption.

Sample		Adsorption		Desorption 1		Desorption 2	
No.	ppm	C_e Ads.	X/m Ads.	C_e Des. 1	X/m Des. 1	C_e Des. 2	X/m Des. 2
		(µg/ml)	(µg/g)	(µg/ml)	(µg/g)	(µg/ml)	(µg/g)
3	0.332	0.266	0.041	0.047	0.020	0.009	0.016
4	0.332	0.264	0.041	0.046	0.024	0.009	0.020
5	0.664	0.537	0.064	0.093	0.033	0.017	0.027
6	0.664	0.532	0.069	0.092	0.044	0.017	0.038
7	1.327	1.077	0.139	0.185	0.064	0.034	0.047
8	1.327	1.107	0.063	0.160	0.062	0.030	0.045
9	2.654	2.144	0.164	0.324	0.141	0.071	0.085
10	2.654	2.139	0.283	0.376	0.145	0.069	0.113
11	5.309	4.309	0.566	0.705	0.353	0.123	0.301
12	5.309	4.314	0.568	0.721	0.304	0.129	0.239
13	5.309	4.309	0.520				
14	5.309	4.314	0.452				

Table 14: Concentration of NOA 409045 in Aqueous Phases and in Soil Gartenacker after Adsorption and Desorption.

Sample		Adsorption		Desorption 1		Desorption 2	
No.	ppm	C_e Ads.	X/m Ads.	C_e Des. 1	X/m Des. 1	C_e Des. 2	X/m Des. 2
		(µg/ml)	(µg/g)	(µg/ml)	(µg/g)	(µg/ml)	(µg/g)
3	0.332	0.232	0.052	0.067	0.023	0.020	0.013
4	0.332	0.230	0.056	0.067	0.025	0.021	0.014
5	0.664	0.467	0.102	0.133	0.043	0.040	0.022
6	0.664	0.460	0.095	0.132	0.051	0.039	0.035
7	1.327	0.941	0.188	0.266	0.073	0.077	0.037
8	1.327	0.932	0.209	0.267	0.089	0.079	0.048
9	2.654	1.875	0.375	0.538	0.136	0.162	0.049
10	2.654	1.854	0.394	0.536	0.182	0.161	0.104
11	5.309	3.743	0.775	1.082	0.289	0.322	0.125
12	5.309	3.731	0.779	1.052	0.372	0.310	0.224
13	5.309	3.681	0.762				
14	5.309	3.735	0.730				

Table 15: Concentration of NOA 409045 in Aqueous Phases and in Soil Vetroz after Adsorption and Desorption.

Sample		Adsorption		Desorption 1		Desorption 2	
No.	ppm	C_e Ads.	X/m Ads.	C_e Des. 1	X/m Des. 1	C_e Des. 2	X/m Des. 2
		(µg/ml)	(µg/g)	(µg/ml)	(µg/g)	(µg/ml)	(µg/g)
3	0.332	0.202	0.097	0.074	0.050	0.029	0.030
4	0.332	0.202	0.092	0.076	0.045	0.028	0.027
5	0.664	0.403	0.190	0.150	0.097	0.057	0.059
6	0.664	0.404	0.184	0.146	0.107	0.056	0.070
7	1.327	0.820	0.367	0.298	0.182	0.112	0.104
8	1.327	0.820	0.353	0.301	0.166	0.112	0.095
9	2.654	1.640	0.676	0.603	0.319	0.226	0.175
10	2.654	1.634	0.672	0.602	0.330	0.227	0.190
11	5.309	3.260	1.430	1.188	0.736	0.446	0.446
12	5.309	3.281	1.383	1.198	0.677	0.446	0.395
13	5.309	3.303	1.397				
14	5.309	3.296	1.306				

Table 16: Relative Mobility Factors (RMF), Sorption Coefficients and Mobility-Adsorption Classes for a Variety of Pesticides[13].

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 > 500	> 0.15 < 0.8	< 1725 > 172	< 1000 >100	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), Metolachlor (0.68)	strong	II	little mobile
< 500 > 150	> 0.8 < 1.3	<172 > 86	< 100 > 50	Monuron (1.00), Atrazine (1.03), Simazine (1.04), Fluometuron (1.18)	moderate	III	moderately mobile
< 150 > 50	> 1.3 < 2.5	< 86 > 34	< 50 > 20	Prometon (1.67), Cyanazine (1.85), Bromacil (1.91), Karbutilate (1.98)	slight	IV	considerably (slightly) mobile
< 50 > 20	> 2.5 < 5	< 34 > 17	< 20 > 10	Carbofuran (3.00), Dioxacarb (4.33)	low	V	mobile
< 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
$K_{oc} = 1.724 \cdot K_{OM}$;
$K_{oc} = k_F \cdot 100$ / %-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

---

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

Figure 1: Rate of Adsorption of NOA 409045 in various Soils (Pre-Test).

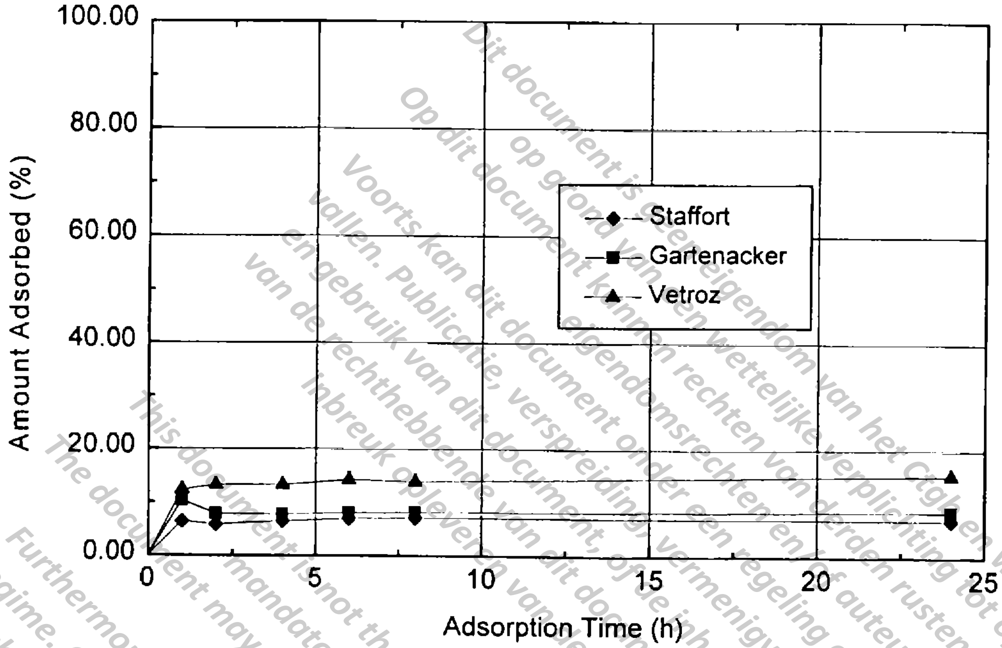


Figure 2: Rate of Desorption of NOA 409045 in various Soils (Pre-Test).

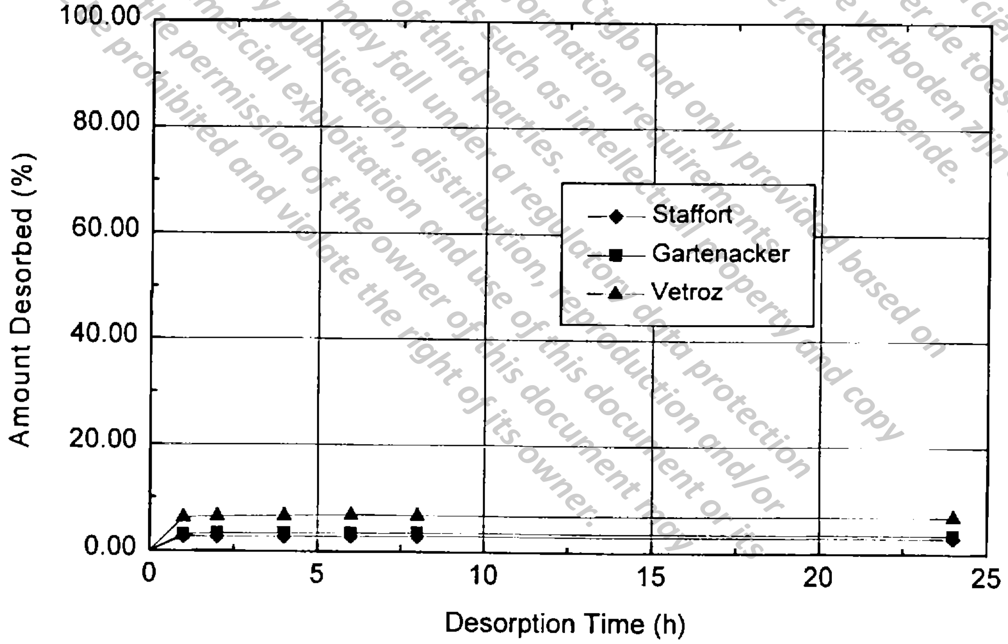
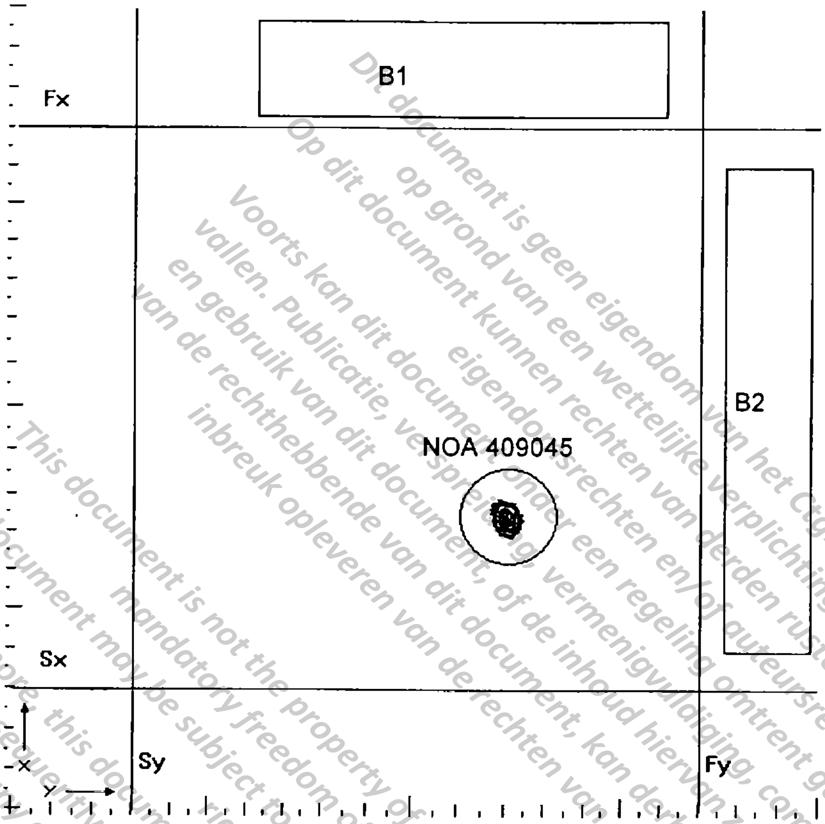


Figure 3: Purity of ^{14}C-NOA 409045.



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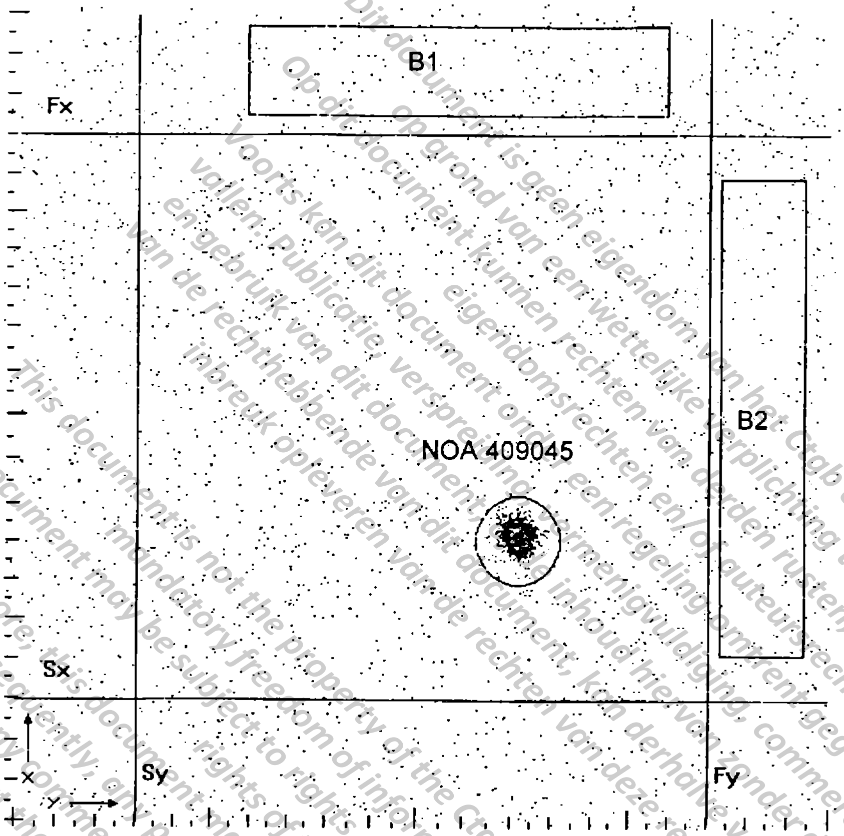
DAR Region Integration Report  EG&G Berthold
Meas date:        3 Feb 1998        15:39:16          Plate name:        purity
Run time:         01 hrs  00 min  17 sec          File name:          C:\WINDAR\NORBERT\98RF01\PURITY.DAR
Gain:             High resolution                 Z-calibration:      Relative
Start x:          3.00    Front x:   17.00        Instr backgrnd:     1.5049     cpm/cm²
Start y:          3.00    Front y:   17.00        Dead time:          0.9        sec (active)
Pk search params:       n/a
Comments:         LM1 Chloroform:Methanol:NH3:Wasser 80:30:4:2
                  LM2 Chloroform:Methanol:HCOOH:Wasser 70:25:4:2
                  Projekt 98RF01 Adsorption/Desorption Purity
Analysis of 100% region 1: AllPlate
                                      Position              Net      Net         Net          %      %       %
Rgn      Label          Rf(x)   Rf(y)   x(cm)    y(cm)     cts      cpm        cpm/cm²      SD    ROIs     All      Shape
B1                       1.11    0.57   18.48    11.04     8354     46.3        2.0          1.2   42.18    —        Rect
B2                       0.49    1.12    9.93    18.72    11450     63.5        2.6          1.2   57.82    —        Rect
Average background =   416.635 cts/cm²                                          2.31     cpm/cm²

1 NOA 409045             0.31    0.65    7.41    12.11    35349    196.1       45.5          0.6 100.00  209.3      Circ
Unresolved:                                                    0     —                                     —

                  Counts       Cpm
Total gross:      183546      1018.1
Total net:        16892         93.7
Gross in ROIs:    37144        206.0
Net in ROIs:      35349        196.1
```

Figure 4: Stability of ^{14}C-NOA 409045.

(TLC of the application solution after treatment procedures)



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DAR Region Integration Report   EG&G Berthold
Meas date:      27 Feb 1998     12:49:41              Plate name:        stability
Run time:       01 hrs  00 min  06 sec          File name:       C:\WINDAR\NORBERT\98RF01\STABIL.DAR
Gain:           High resolution                 Z-calibration:   Relative
Start x:        3.00     Front x:   17.00       Instr backgrnd:  1.5049      cpm/cm²
Start y:        3.00     Front y:   17.00       Dead time:       0.3         sec (active)
Pk search params:        n/a
Comments:       LM1 Chloroform:Methanol:NH3:Wasser 80:30:4:2
                LM2 Chloroform:Methanol:HCOOH:Wasser 70:25:4:2
                Projekt 98RF01 Adsorption/Desorption Stabilitaetsprüfung
Analysis of 100% region 1: AllPlate
                                   Position           Net      Net        Net        %     %        %
Rgn    Label          Rf(x)  Rf(y)  x(cm)    y(cm)    cts      cpm        cpm/cm²    SD    ROIs     All     Shape
B1                     1.11   0.56  18.60    10.83    2582     43.0       2.0        2.2   42.11    —       Rect
B2                     0.50   1.10   9.97    18.36    3549     59.1       2.5        2.1   57.89    —       Rect
Average background =  136.427 cts/cm²                                    2.27   cpm/cm²

1 NOA 409045           0.29   0.66   7.03    12.19    4989     83.0       23.8       1.5 100.00    <0.01   Ellps
Unresolved:                                           0        —                                  —

                 Counts      Cpm
Total gross:     53445       889.3
Total net:       —           —
Gross in ROIs:   5464        90.9
Net in ROIs:     4989        83.0
```

Figure 5: HPLC of Aqueous Phases after 24 h of Adsorption (Pre-Test).

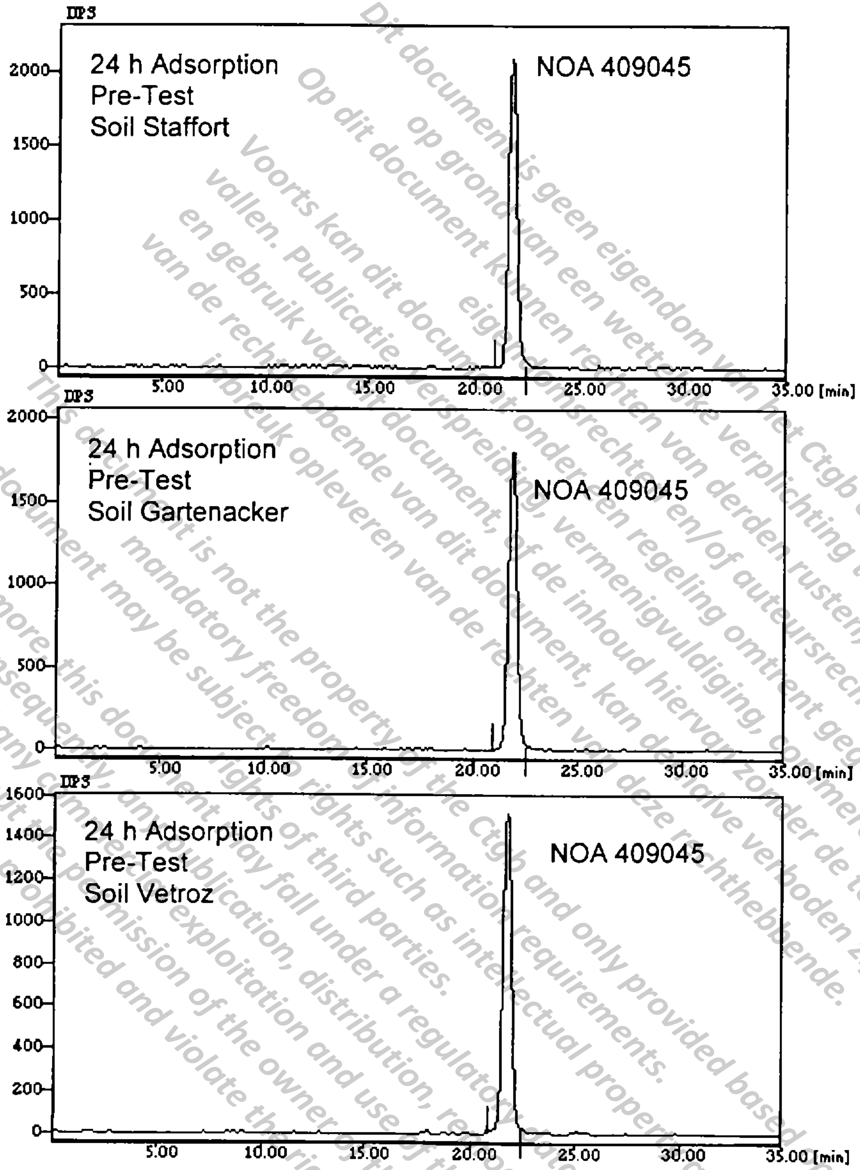


Figure 6: HPLC of Aqueous Phases after 24 h of Desorption (Pre-Test).

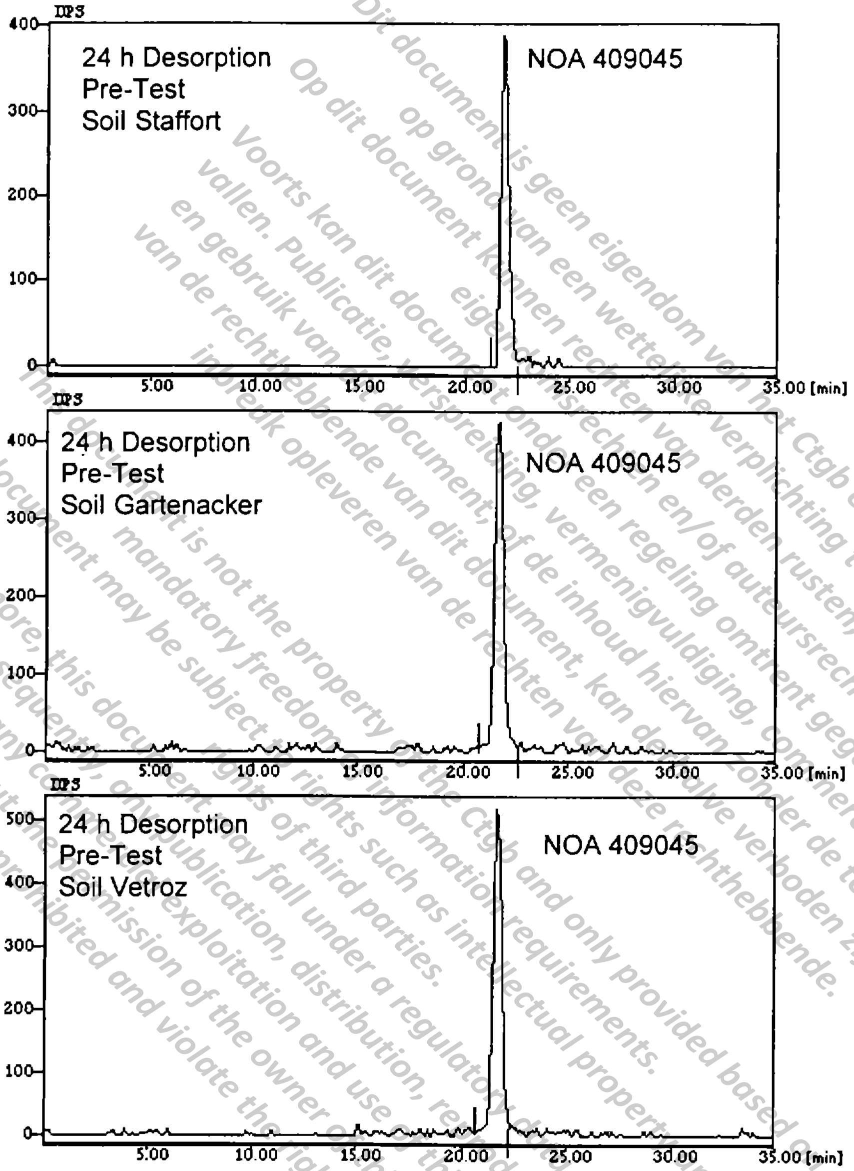
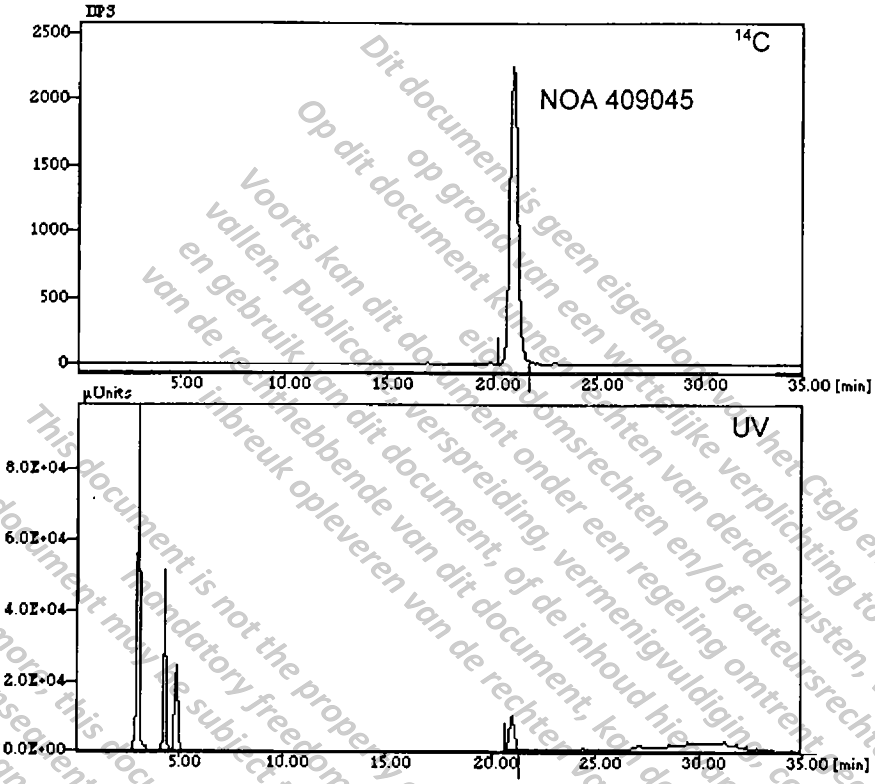


Figure 7: HPLC of Aqueous Phase after Adsorption Step with Soil Staffort (Sample 13).



File name : BAST1001.CH2 User : 98RF01
Run Length : 35.00 [min]Acqu. Date : 26-Feb-98 13:18:46
Info : Balance 5ppm Adsorption nach 2 h Staffort 1 100µl=45360 dpm
X Units : [min] Y Units : DPS
Control Method : 14C_YG
Bkg (Cpm) = 51
Efficiency % = 75

#	Name	Rt	Xstart	Xend	DPM	%Area	%Total	Quantity	Int.mode
1	NOA 409045	20.43	19.78	21.07	45899	100.00	98.20	0.000	Man

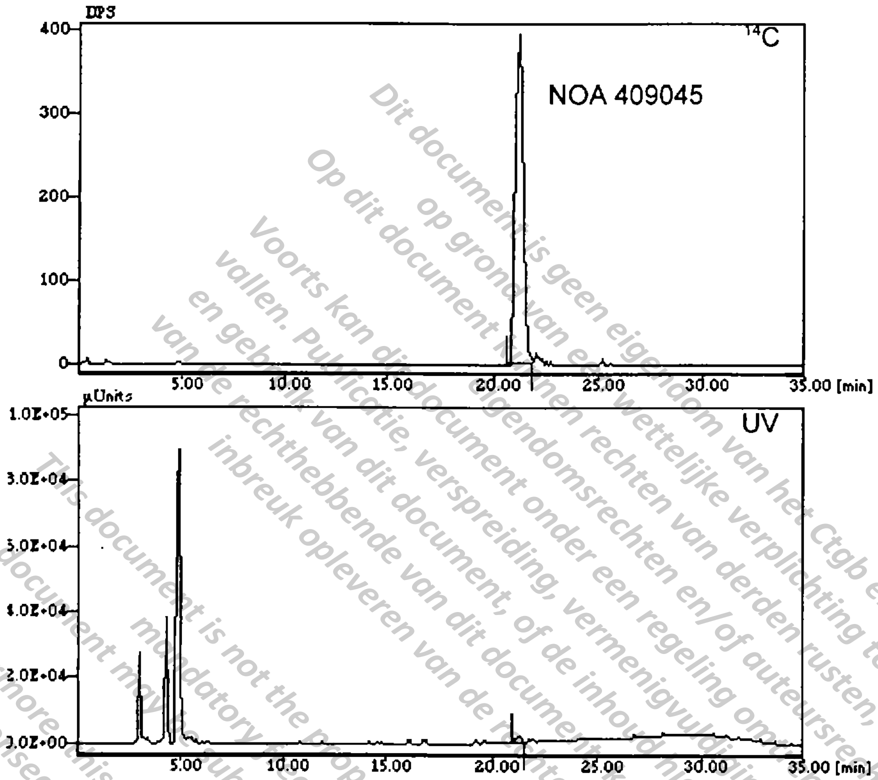
Total Area of Peak = 45898.70
Total = 46739.53
Injection Volume = 100.00 µl

File name : BAST1001.CH3 User : 98RF01
Run Length : 35.00 [min]Acqu. Date : 26-Feb-98 13:18:46
Info : Balance 5ppm Adsorption nach 2 h Staffort 1 100µl=45360 dpm
X Units : [min] Y Units : µUnits
Control Method : 14C_YG

#	Name	Rt	Xstart	Xend	µUnits	%Area	%Total	Quantity	Int.mode
1	NOA 409045	20.47	20.18	20.82	117745	100.00	8.03	0.000	Man

Total Area of Peak = 117745.00
Total = 1466127.40
Injection Volume = 100.00 µl

Figure 8: HPLC of Soil Staffort Extract (Sample 13).



File name : ST1RO001.CH2 User : 98RF01
Run Length : 35.00 [min]Acqu. Date : 26-Feb-98 20:21:06
Info : Balance 5ppm Rohextrakte 1-3 eingeengt Staffort 1 100µl=7870 dpm
X Units : [min] Y Units : DPS
Control Method : 14C_YG
Bkg (Cpm) = 44
Efficiency % = 75

#	Name	Rt	Xstart	Xend	DPM	%Area	%Total	Quantity	Int.mode
1	NOA 409045	20.70	20.15	21.33	7976	100.00	96.71	0.000	Man

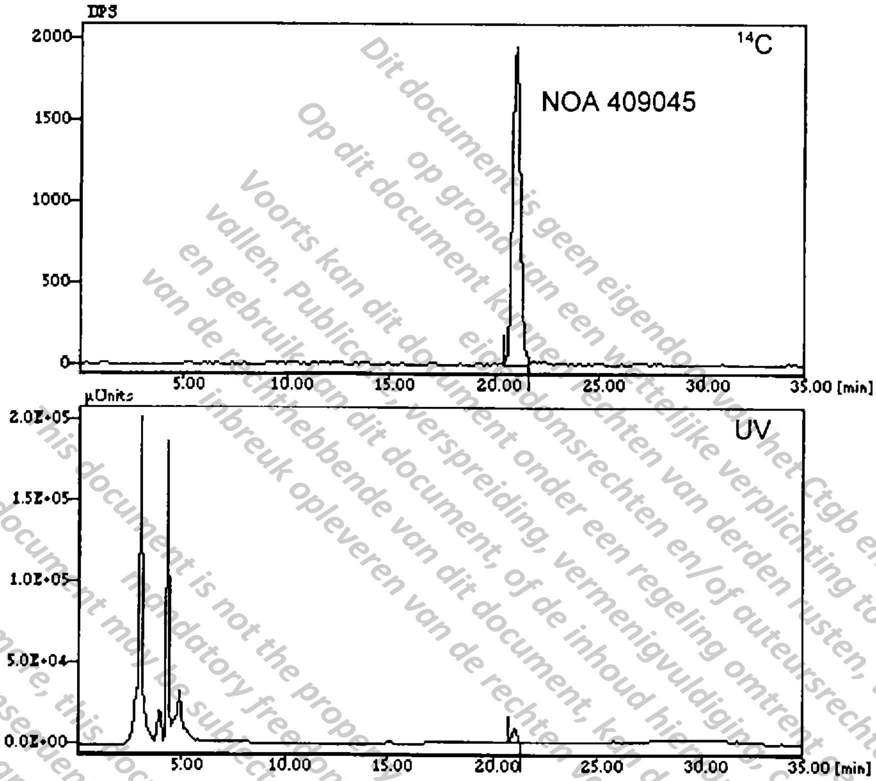
Total Area of Peak = 7975.71
Total = 8246.97
Injection Volume = 100.00 µl

File name : ST1RO001.CH3 User : 98RF01
Run Length : 35.00 [min]Acqu. Date : 26-Feb-98 20:21:06
Info : Balance 5ppm Rohextrakte 1-3 eingeengt Staffort 1 100µl=7870 dpm
X Units : [min] Y Units : DPS
Control Method : 14C_YG

#	Name	Rt	Xstart	Xend	µUnits	%Area	%Total	Quantity	Int.mode
1	NOA 409045	20.77	20.42	21.02	21697	100.00	1.10	0.000	Man

Total Area of Peak = 21696.80
Total = 1979937.60
Injection Volume = 100.00 µl

Figure 9: HPLC of Aqueous Phase after Adsorption Step with Soil Gartenacker (Sample 13).



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File name : BAGA1001.CH2 User : 98RF01
Run Length : 35.00 [min]Acqu. Date :  26-Feb-98  9:22:52
Info : Balance 5ppm Adsorption nach 2 h Gartenacker 1 100µl=38870 dpm
X Units : [min] Y Units : DPS
Control Method :  14C_YG
Bkg (Cpm) = 38
Efficiency % = 75
# Name          Rt     Xstart   Xend    DPM     %Area   %Total   Quantity   Int.mode
 1 NOA 409045 20.50    19.98    21.15   38973   100.00   92.21    0.000      Man
Total Area of Peak =  38973.04
Total =  42266.99
Injection Volume = 100.00 µl
```

```
File name : BAGA1001.CH3 User : 98RF01
Run Length : 35.00 [min]Acqu. Date :  26-Feb-98  9:22:52
Info : Balance 5ppm Adsorption nach 2 h Gartenacker 1 100µl=38870 dpm
X Units : [min] Y Units : µUnits
Control Method :  14C_YG
# Name          Rt     Xstart   Xend    µUnits   %Area   %Total   Quantity   Int.mode
 1 NOA 409045 20.53    20.26    20.86   109249   100.00    2.18    0.000      Man
Total Area of Peak = 109249.00
Total = 5008154.20
Injection Volume = 100.00 µl
```

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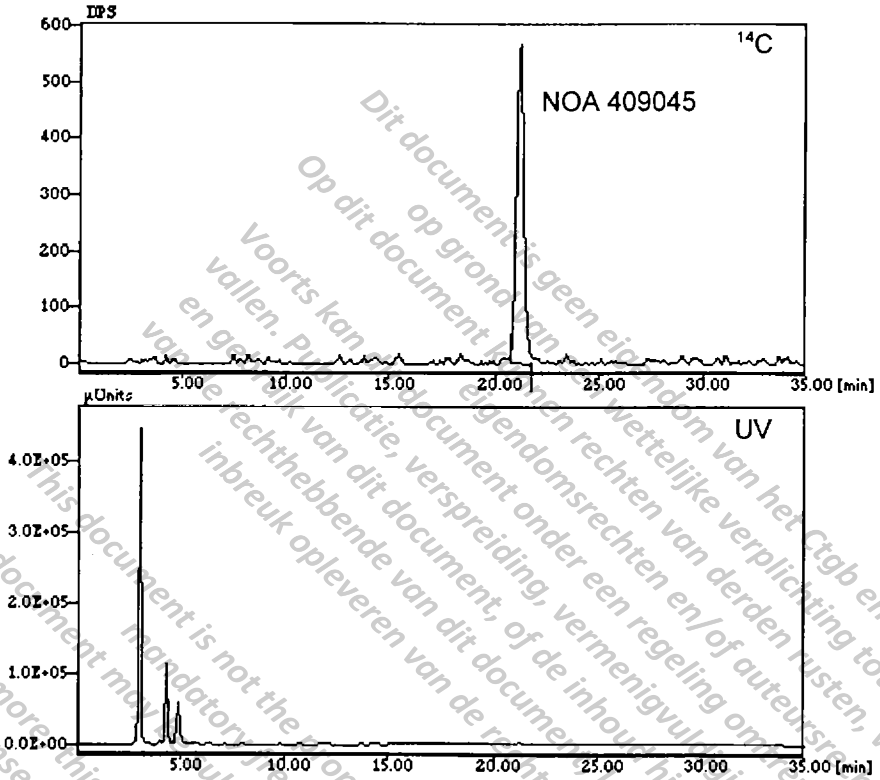
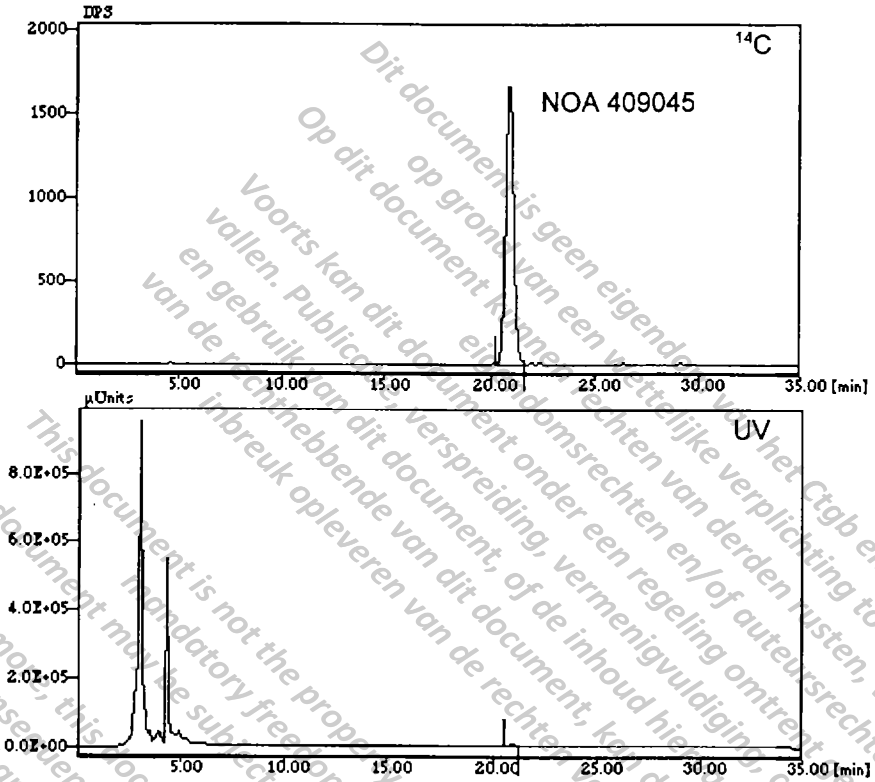
Figure 10: HPLC of Soil Gartenacker Extract (Sample 13).



```
File name : GA1RO001.CH2 User : 98RF01
Run Length : 35.00 [min]Acqu. Date :  26-Feb-98  16:19:28
Info : Balance 5ppm Rohextrakte 1-3 eingeengt Gartenacker 1 100µl=10330 dpm
X Units : [min] Y Units : DPS
Control Method :  14C_YG
Bkg (Cpm) = 36
Efficiency % = 75
# Name            Rt      Xstart    Xend     DPM     %Area    %Total    Quantity    Int.mode
 1 NOA 409045 20.67      20.23    21.22    10009    100.00    74.37     0.000        Man
Total Area of Peak =  10008.90
Total =  13457.41
Injection Volume = 100.00 µl

File name : GA1RO001.CH3 User : 98RF01
Run Length : 35.00 [min]Acqu. Date :  26-Feb-98  16:19:28
Info : Balance 5ppm Rohextrakte 1-3 eingeengt Gartenacker 1 100µl=10330 dpm
X Units : [min] Y Units : DPS
Control Method :  14C_YG
Peak Detection Not Available
```

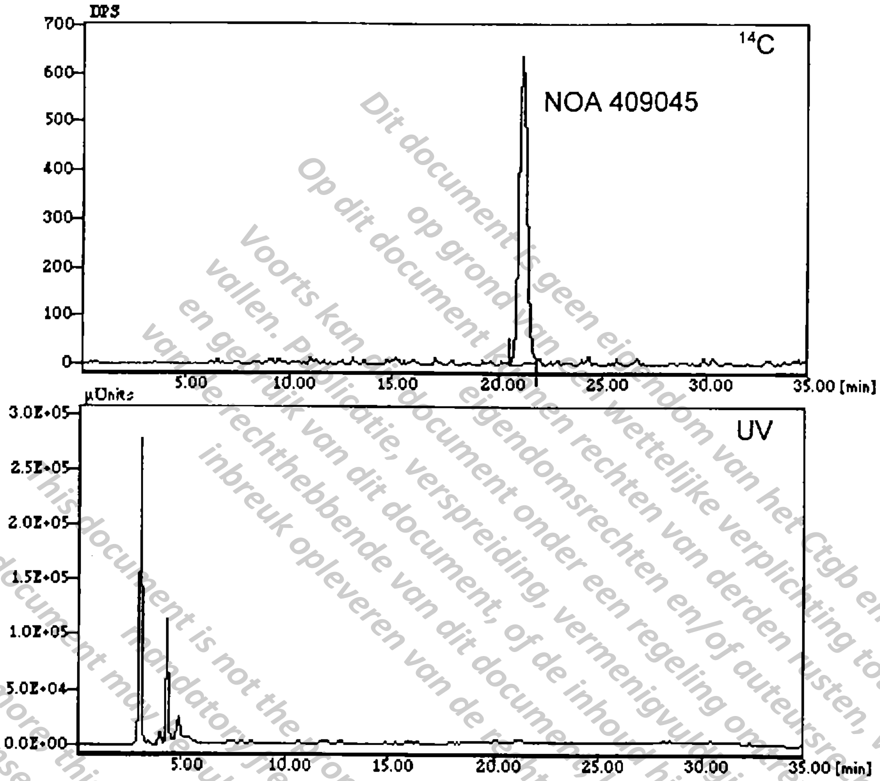
Figure 11: HPLC of Aqueous Phase after Adsorption Step with Soil Vetroz (Sample 13).



```
File name : BAVE1001.CH2 User : 98RF01
Run Length : 35.00 [min]Acqu. Date :  26-Feb-98  11:20:46
Info : Balance 5ppm Adsorption nach 2 h Vetroz 1 100µl=34880 dpm
X Units : [min] Y Units : DPS
Control Method :  14C_YG
Bkg (Cpm) = 37
Efficiency % = 75
# Name           Rt      Xstart    Xend     DPM      %Area    %Total    Quantity    Int.mode
 1 NOA 409045 20.35      19.78    21.10    34922    100.00    92.58     0.000        Man
Total Area of Peak =  34922.44
Total =  37719.57
Injection Volume = 100.00 µl
```

```
File name : BAVE1001.CH3 User : 98RF01
Run Length : 35.00 [min]Acqu. Date :  26-Feb-98  11:20:46
Info : Balance 5ppm Adsorption nach 2 h Vetroz 1 100µl=34880 dpm
X Units : [min] Y Units : µUnits
Control Method :  14C_YG
# Name           Rt      Xstart    Xend     µUnits   %Area    %Total    Quantity    Int.mode
 1 NOA 409045 20.41      20.11    20.78    91355    100.00     0.51     0.000        Man
Total Area of Peak = 91354.80
Total = 17990230.40
Injection Volume = 100.00 µl
```

Figure 12: HPLC of Soil Vetroz Extract (Sample 13).



File name : VE1RO001.CH2 User : 98RF01
Run Length : 35.00 [min]Acqu. Date : 26-Feb-98 18:19:14
Info : Balance 5ppm Rohextrakte 1-3 eingeengt Vetroz 1 100µl=13410 dpm
X Units : [min] Y Units : DPS
Control Method : 14C_YG
Bkg (Cpm) = 35
Efficiency % = 75

# Name	Rt	Xstart	Xend	DPM	%Area	%Total	Quantity	Int.mode
1 NOA 409045	20.62	20.12	21.30	12522	100.00	82.09	0.000	Man

Total Area of Peak = 12522.36
Total = 15253.88
Injection Volume = 100.00 µl

File name : VE1RO001.CH3 User : 98RF01
Run Length : 35.00 [min]Acqu. Date : 26-Feb-98 18:19:14
Info : Balance 5ppm Rohextrakte 1-3 eingeengt Vetroz 1 100µl=13410 dpm
X Units : [min] Y Units : DPS
Control Method : 14C_YG
Peak Detection Not Available

Figure 13: Freundlich Plots for Adsorption and Desorption of NOA 409045 for Soil Staffort Sandy Loam.

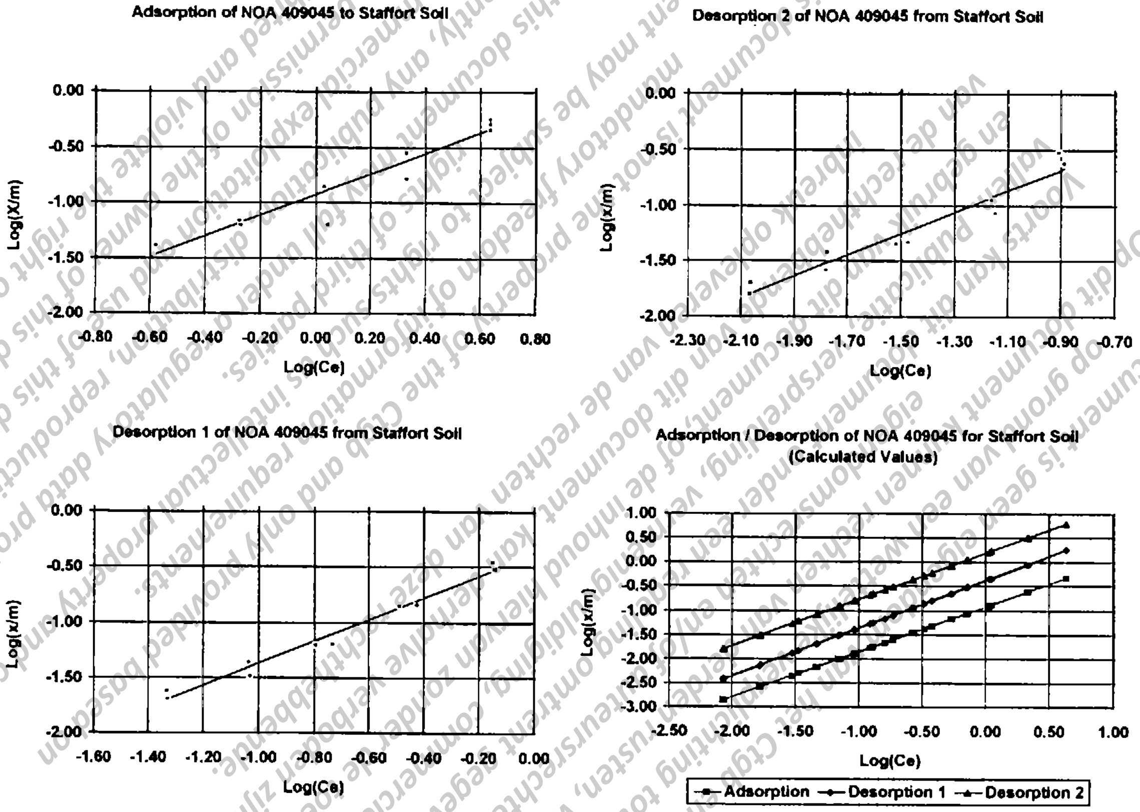


Figure 14: Freundlich Plots for Adsorption and Desorption of NOA 409045 for Soil Gartenacker Loam - Silt Loam.

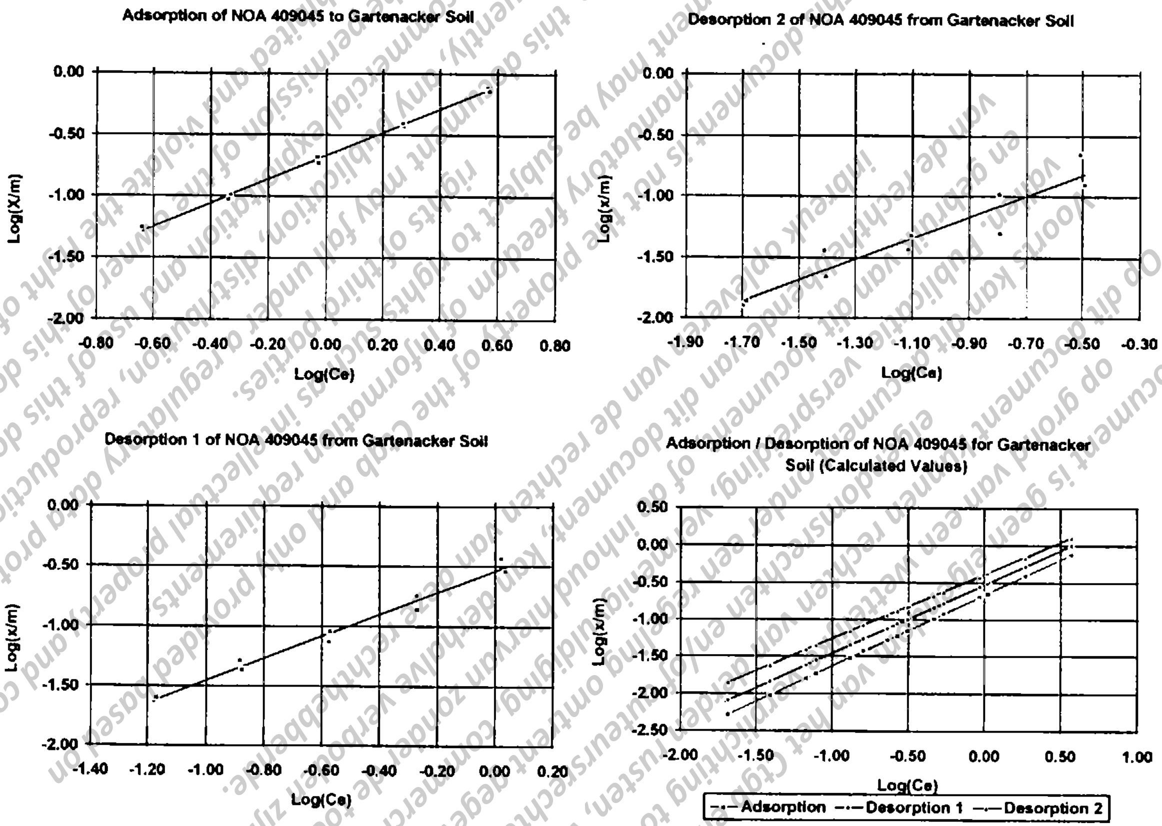


Figure 15: Freundlich Plots for Adsorption and Desorption of NOA 409045 for Soil Vetroz Silt Loam.

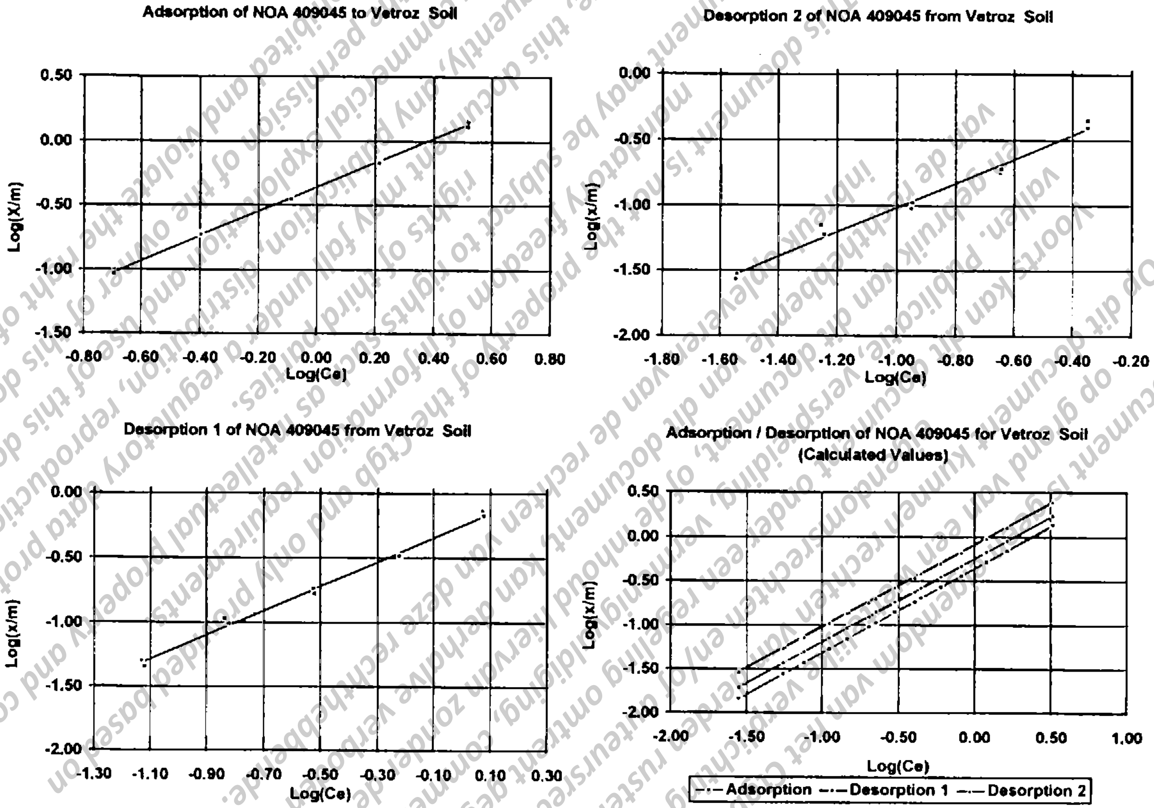
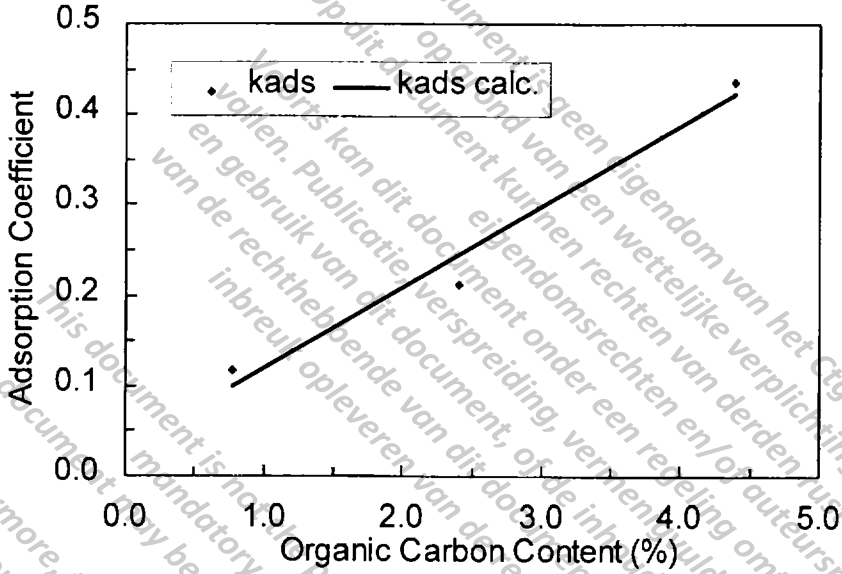


Figure 16: Relationship between Soil Organic Carbon Content and Freundlich Adsorption Coefficients.



	Org. C. cont.	kads	k calc.
Staffort	0.77	0.118	0.101
Gartenacker	2.40	0.213	0.245
Vetroz	4.39	0.437	0.422

98RF01

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.985315807
R Square	0.97084724
Adjusted R Square	0.941694479
Standard Error	0.03945493
Observations	3

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regression	1	0.051841048	0.051841048	33.30207	0.10923279
Residual	1	0.001556692	0.001556692		
Total	2	0.05339774			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	0.032257332	0.044974293	0.717239326	0.603894	-0.5391928	0.60370746	-0.539192796	0.60370746
Organic carbon content	0.088803206	0.015388385	5.770794481	0.109233	-0.1067239	0.284330335	-0.106723924	0.28433034

Appendix A: Representative Data

Analytical Data

B) Application solutions

Project: 98RF01

Soil-Type: Staffort

Applikat. solution	stock-solu. [ml]	Endvolume [ml]	conc.Parent [µg/ml]	Radioactivity [dpm/0.5ml]	Total ug prepared	Total ug used
1	0.000	500.00	0.0000	0		
2	0.000	500.00	0.0000	0		
0.3125 ppm (3)	0.199	500.00	0.3318	17519	165.89	6.64
0.3125 ppm (4)	0.199	500.00	0.3318	17519	165.89	6.64
0.625 ppm (5)	0.397	500.00	0.6636	35037	331.79	13.27
0.625 ppm (6)	0.397	500.00	0.6636	35037	331.79	13.27
1.25 ppm (7)	0.794	500.00	1.3272	70074	663.58	26.54
1.25 ppm (8)	0.794	500.00	1.3272	70074	663.58	26.54
2.5 ppm (9)	1.589	500.00	2.6543	140148	1327.16	53.09
2.5 ppm (10)	1.589	500.00	2.6543	140148	1327.16	53.09
5 ppm (11)	3.178	500.00	5.3086	280296	2654.32	106.17
5 ppm (12)	3.178	500.00	5.3086	280296	2654.32	106.17
5 ppm (13)	3.178	500.00	5.3086	280296	2654.32	106.17
5 ppm (14)	3.178	500.00	5.3086	280296	2654.32	106.17
Total					15594.12	623.76

Initialconcentrations for distribution volume CaCl2 [ml]...:

sample (Ads/Des)	Appl.-Vol. [ml]	Endvolume [ml]	concentr.(*) [µg/ml]	Radioactivity [dpm/ml]	Aktivit. tot. [dpm]	conc.** [µg/ml]
1	20.00	20.00	0.000	0	0	0.000
2	20.00	20.00	0.000	0	0	0.000
0.3125 ppm (3)	20.00	20.00	0.332	35037	700740	0.332
0.3125 ppm (4)	20.00	20.00	0.332	35037	700740	0.332
0.625 ppm (5)	20.00	20.00	0.663	70074	1401480	0.664
0.625 ppm (6)	20.00	20.00	0.664	70074	1401480	0.664
1.25 ppm (7)	20.00	20.00	1.327	140148	2802960	1.327
1.25 ppm (8)	20.00	20.00	1.325	140148	2802960	1.327
2.5 ppm (9)	20.00	20.00	2.599	280296	5605920	2.654
2.5 ppm (10)	20.00	20.00	2.653	280296	5605920	2.654
5 ppm (11)	20.00	20.00	5.308	560592	11211840	5.309
5 ppm (12)	20.00	20.00	5.308	560592	11211840	5.309
5 ppm (13)	20.00	20.00	5.309	560592	11211840	5.309
5 ppm (14)	20.00	20.00	5.309	560592	11211840	5.309

COUNTER: 7,8,9,10 **Control measurement**

sample	Radioactivity dpm in 20 ml calc	dpm in 0.5 ml aliqu. dpm	[dpm in 20 ml] mean	%
0.3125 ppm (3)	700740	17535	701400	100.1
0.3125 ppm (4)	700740	17535	701400	100.1
0.625 ppm (5)	1401480	35123	1404920	100.2
0.625 ppm (6)	1401480	35123	1404920	100.2
1.25 ppm (7)	2802960	70068	2802720	100.0
1.25 ppm (8)	2802960	70068	2802720	100.0
2.5 ppm (9)	5605920	140262	5610480	100.1
2.5 ppm (10)	5605920	140262	5610480	100.1
5 ppm (11)	11211840	280298	11211920	100.0
5 ppm (12)	11211840	280298	11211920	100.0
5 ppm (13)	11211840	280298	11211920	100.0
5 ppm (14)	11211840	280298	11211920	100.0

C)Adsorption: (2 Std.) Counter: 12

sample	tube empty [g]	tube filled [g](*) with sol.	VAds [ml]	Aliqu LSC (ml)	DPM Aliquot	DPM/ml (Ce) Bg corr.	soil dry [g]	tube with wet soil [g]
1	207.08	240.59	23.55	0.50	4	8	9.96	220.45
2	206.84	240.05	23.17	0.50	2	4	10.04	220.06
0.3125 ppm (3)	199.75	233.12	23.39	0.50	14056	28106	9.98	213.09
0.3125 ppm (4)	197.02	230.59	23.56	0.50	13961	27916	10.01	210.54
0.625 ppm (5)	208.93	242.44	23.52	0.50	28356	56706	9.99	222.42
0.625 ppm (6)	207.42	241.11	23.67	0.50	28070	56134	10.02	221.09
1.25 ppm (7)	175.01	208.42	23.35	0.50	56863	113720	10.06	188.38
1.25 ppm (8)	176.40	209.79	23.38	0.50	58427	116848	10.01	189.78
2.5 ppm (9)	183.77	217.33	23.48	0.50	113200	226394	10.08	197.29
2.5 ppm (10)	182.61	216.10	23.48	0.50	112965	225924	10.01	196.10
5 ppm (11)	209.35	242.69	23.32	0.50	227530	455054	10.02	222.70
5 ppm (12)	207.66	240.96	23.29	0.50	227797	455588	10.01	220.95
5 ppm (13)	176.55	209.99	23.43	0.50	227530	455054	10.01	189.95
5 ppm (14)	175.82	209.40	23.56	0.50	227797	455588	10.02	189.40

(*) tube+20ml Ca2Cl2-solu.+10 g dry soil

sample	DPM Total	C(e)Ads [µg/ml]	log C(e)Ads	X/m [µg/g]	log X/m	log X/mcalc	Applied CaCl2 (ml)	Rest CaCl2 solution (= Rest water)
							20.14	3.41
							19.99	3.18
0.3125 ppm (3)	657399	0.266	-0.575	0.041	-1.386	-1.464	20.03	3.36
0.3125 ppm (4)	657701	0.264	-0.578	0.041	-1.391	-1.467	20.05	3.51
0.625 ppm (5)	1333725	0.537	-0.270	0.064	-1.194	-1.179	20.02	3.50
0.625 ppm (6)	1328692	0.532	-0.274	0.069	-1.163	-1.183	20.02	3.65
1.25 ppm (7)	2655362	1.077	0.032	0.139	-0.858	-0.897	20.04	3.31
1.25 ppm (8)	2731906	1.107	0.044	0.063	-1.200	-0.886	20.01	3.37
2.5 ppm (9)	5315731	2.144	0.331	0.164	-0.786	-0.617	20.04	3.44
2.5 ppm (10)	5304696	2.139	0.330	0.283	-0.548	-0.618	20.00	3.48
5 ppm (11)	10611859	4.309	0.634	0.566	-0.247	-0.334	19.99	3.33
5 ppm (12)	10610645	4.314	0.635	0.568	-0.246	-0.333	20.01	3.28
5 ppm (13)	10661915	4.309	0.634	0.520	-0.284	-0.334	20.04	3.39
5 ppm (14)	10733653	4.314	0.635	0.452	-0.345	-0.333	20.00	3.56
							Average:	3.41

Info:
Applied CaCl2 + Rest CaCl2 solution = Vads

Output range: O64 Lineare Regress. log(X/m) [y-Wert] geg. logC(e) [x-Wert]
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.963655393
R Square	0.928631716
Adjusted R Square	0.921494888
Standard Error	0.127941755
Observations	12

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.12991793	2.12991793	130.1182632	4.69851E-07
Residual	10	0.16369093	0.01636909		
Total	11	2.29360885			

	Coefficients	*tandard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	-0.92695677	0.03847559	-24.092077	3.45424E-10	-1.012685734	-0.841227812
X Variable 1	0.934745915	0.08194537	11.4069393	4.69851E-07	0.75216021	1.11733162

K=	Koc=	Kom=
0.12	15.37	8.91

D)Desorption 1 (2 Std.) Counter: 12

sample	tube empty	tube filled	VDes1	Aliquot LSC	DPM	C(e)Des1	soil dry
	(*) [g]	[g]	[ml]	(ml)	Aliquot	[dpm/ml]	[g]
						Bg corr.	
1	220.45	240.59	23.43	0.50	3	6	9.96
2	220.06	240.05	23.19	0.50	0	0	10.04
0.3125 ppm (3)	213.09	233.09	23.36	0.50	2491	4976	9.98
0.3125 ppm (4)	210.54	230.54	23.51	0.50	2457	4908	10.01
0.625 ppm (5)	222.42	242.41	23.49	0.50	4923	9840	9.99
0.625 ppm (6)	221.09	241.12	23.68	0.50	4875	9744	10.02
1.25 ppm (7)	188.38	208.43	23.36	0.50	9757	19508	10.06
1.25 ppm (8)	189.78	209.79	23.38	0.50	8450	16894	10.01
2.5 ppm (9)	197.29	217.34	23.49	0.50	17100	34194	10.08
2.5 ppm (10)	196.10	216.12	23.50	0.50	19846	39686	10.01
5 ppm (11)	222.70	242.74	23.37	0.50	37252	74498	10.02
5 ppm (12)	220.95	240.97	23.30	0.50	38057	76108	10.01

in "DPM Aliquot"
estimated dpm
estimated dpm
otherwise negative
X/m values

(*) tube with soil and restwater

VDes1 Z21-$P21-$Q$8

sample	C(e)Des1	log C(e)Des1	X/m	log X/m	log X/m
	(µg/ml)		[µg/g] (*)		calc.
0.3125 ppm (3)	0.047	-1.327	0.020	-1.690	-1.695
0.3125 ppm (4)	0.046	-1.333	0.024	-1.617	-1.700
0.625 ppm (5)	0.093	-1.031	0.033	-1.481	-1.402
0.625 ppm (6)	0.092	-1.035	0.044	-1.354	-1.406
1.25 ppm (7)	0.185	-0.733	0.064	-1.193	-1.108
1.25 ppm (8)	0.160	-0.796	0.062	-1.208	-1.169
2.5 ppm (9)	0.324	-0.490	0.141	-0.852	-0.867
2.5 ppm (10)	0.376	-0.425	0.145	-0.839	-0.803
5 ppm (11)	0.705	-0.152	0.353	-0.452	-0.532
5 ppm (12)	0.721	-0.142	0.304	-0.517	-0.523

VDes1
[ml]
20.02
20.01
20.00
20.00
19.99
20.03
20.05
20.01
20.05
20.02
20.04
20.02

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.99052916
R Square	0.98114802
Adjusted R Square	0.97879152
Standard Error	0.06386335
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.698129366	1.69812937	416.35851	3.48007E-08
Residual	8	0.032628215	0.00407853		
Total	9	1.730757581			

	Coefficients	*tandard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	-0.382126	0.041434578	-9.2223934	1.548E-05	-0.477674353	-0.286577611
X Variable 1	0.989201	0.048478685	20.4048648	3.48E-08	0.877408884	1.100993122

K=	**Koc=**	**Kom=**
0.41	**53.87**	**31.25**

E)Desorption 2: (2 Std.) Counter: 12

sample	tube empty	tube filled	VDes2	Aliquot LSC	DPM	C(e)Des2	soil dry
	(*) [g]	[g]	[ml]	(ml)	Aliquot	[dpm/ml]	[g]
1	220.45	240.59	23.44	0.50	6	12	9.96
2	220.06	240.05	23.19	0.50	0	0	10.04
0.3125 ppm (3)	213.09	233.08	23.35	0.50	460	908	9.98
0.3125 ppm (4)	210.54	230.57	23.54	0.50	465	918	10.01
0.625 ppm (5)	222.42	242.44	23.52	0.50	884	1756	9.99
0.625 ppm (6)	221.09	241.10	23.66	0.50	894	1776	10.02
1.25 ppm (7)	188.38	208.37	23.30	0.50	1779	3546	10.06
1.25 ppm (8)	189.78	209.80	23.39	0.50	1600	3188	10.01
2.5 ppm (9)	197.29	217.32	23.47	0.50	3768	7524	10.08
2.5 ppm (10)	196.10	216.08	23.46	0.50	3661	7310	10.01
5 ppm (11)	222.70	242.73	23.36	0.50	6503	12994	10.02
5 ppm (12)	220.95	240.97	23.30	0.50	6836	13660	10.01

in "DPM Aliquot"
estimated dpm
otherwise negative
X/m value

(*) tube with soil and restwater

sample	C(e)Des2	log C(e)Des2	X/m	log X/m	log X/m
	(µg/ml)		[µg/g]		calc.
0.3125 ppm (3)	0.009	-2.066	0.016	-1.792	-1.794
0.3125 ppm (4)	0.009	-2.061	0.020	-1.699	-1.790
0.625 ppm (5)	0.017	-1.779	0.027	-1.576	-1.520
0.625 ppm (6)	0.017	-1.774	0.038	-1.419	-1.515
1.25 ppm (7)	0.034	-1.474	0.047	-1.326	-1.228
1.25 ppm (8)	0.030	-1.520	0.045	-1.344	-1.272
2.5 ppm (9)	0.071	-1.147	0.085	-1.069	-0.915
2.5 ppm (10)	0.069	-1.160	0.113	-0.946	-0.927
5 ppm (11)	0.123	-0.910	0.301	-0.522	-0.687
5 ppm (12)	0.129	-0.888	0.239	-0.622	-0.667

VDes2
[ml]
20.03
20.01
19.99
20.03
20.02
20.01
19.99
20.02
20.03
19.98
20.03
20.02

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.973270705
R Square	0.947255865
Adjusted R Squar	0.940662848
Standard Error	0.10559548
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.602041524	1.60204152	143.6756317	2.16237E-06
Residual	8	0.089203242	0.01115041		
Total	9	1.691244767			

	Coefficients	*tandard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	0.184004319	0.12272059	1.4993761	0.172161542	-0.098990051	0.466998689
X Variable 1	0.957773115	0.079904472	11.986477	2.16237E-06	0.773512954	1.142033276

K=	Koc=	Kom=
1.53	**198.39**	**115.07**

F soil combustion: Counter: 18,19

sample	weight		LSC (DPM)		%-applied.
	soil (g)	Aliquot	Aliquot	TOTAL	
Mean :					
0.3125 ppm (3)	9.920	1.233	689	5543	0.79
0.3125 ppm (3)	9.920	1.411	781	5491	0.78
0.3125 ppm (3)	9.920	1.286	704	5431	0.77
Mean :					0.78
0.3125 ppm/2 (4)	9.960	1.504	940	6225	0.89
0.3125 ppm/2 (4)	9.960	1.303	971	7422	1.06
0.3125 ppm/2 (4)	9.960	1.333	761	5686	0.81
Mean :					0.92
0.625 ppm (5)	9.880	1.101	1130	10140	0.72
0.625 ppm (5)	9.880	1.448	1410	9621	0.69
0.625 ppm (5)	9.880	1.264	1169	9137	0.65
Mean :					0.69
0.625 ppm/2 (6)	9.970	1.465	1418	9650	0.69
0.625 ppm/2 (6)	9.970	1.148	1267	11003	0.78
0.625 ppm/2 (6)	9.970	1.074	1153	10703	0.76
Mean :					0.75
1.25 ppm (7)	10.020	1.183	2173	18405	0.66
1.25 ppm (7)	10.020	1.466	3549	24257	0.86
1.25 ppm (7)	10.020	1.184	2660	22511	0.80
Mean :					0.77
1.25 ppm/2 (8)	9.970	1.210	54264	447117	15.94
1.25 ppm/2 (8)	9.970	1.118	43396	386993	13.80
1.25 ppm/2 (8)	9.970	1.393	49676	355542	12.68
Mean :					14.14
2.5ppm (9)	10.020	0.963	6187	64376	1.15
2.5ppm (9)	10.020	1.263	7369	58462	1.04
2.5ppm (9)	10.020	1.077	6721	62530	1.11
Mean :					1.10
2.5ppm/2 (10)	9.940	1.336	5379	40020	0.71
2.5ppm/2 (10)	9.940	1.135	5637	49367	0.88
2.5ppm/2 (10)	9.940	1.096	5257	47678	0.85
Mean :					0.82
5ppm (11)	9.930	1.230	10223	82532	0.74
5ppm (11)	9.930	1.288	8928	68832	0.61
5ppm (11)	9.930	1.224	8436	68439	0.61
Mean :					0.65
5ppm/2 (12)	9.860	1.236	8812	70296	0.63
5ppm/2 (12)	9.860	1.129	8074	70513	0.63
5ppm/2 (12)	9.860	1.189	7987	66234	0.59
Mean :					0.62
5 ppm (13)	10.010	1.198	5095	42572	0.38
5 ppm (13)	10.010	1.466	6463	44130	0.39
5 ppm (13)	10.010	1.018	4768	46884	0.42
Mean :					0.40
5 ppm/2 (14)	10.040	0.972	4338	44808	0.40
5 ppm/2 (14)	10.040	1.248	4819	38768	0.35
5 ppm/2 (14)	10.040	1.548	6082	39447	0.35
Mean :					0.37

Appendix B: Limits of Detection and Quantitation

Calculation of Limit of Detection and Quantitation.

Calculation of Limit of Detection and Quantitation

Limit of Detection and Quantitation for Liquid Scintillation Counter (LSC)

General Information		Sample Characteristics	
Project-No.:	98RF01	Soil Dry Weight (g):	10.010
NOA-No.:	409045	Batch-No. :	ILS-182.1
Sample-No.:	13	Specific Radioactivity (µCi/mg):	47.568
Soil-Type:	Staffort 1	Specific Radioactivity (Bq/mg):	1.76
		Radioactivity applied (DPM):	11234264
		Date of Storage -20C:	18.02.98
		Date of Extraction Start:	18.02.98

CaCl2 Solution (Adsorption Solution):

Sample size measured (ml)	0.50				
Volume CaCl2 Solution (ml)	23.4				
	dpm	Total dpm	%-applied	Parent equiv.	mg/l Water
				(mg)	(=ppm)
Background LSC (BG LSC) :	20	937	0.0083	0.00001	0.00038
Limit of Detection (2xBG LSC)	40	1874	0.0167	0.00002	0.00076
Limit of Quantitation (3xBG LS	60	2812	0.0250	0.00003	0.00114

Raw extracts No 1:

Sample size measured (ml)	0.50				
Volume Raw extract (ml)	39.0				
	dpm	Total dpm	%-applied	Parent equiv.	mg/kg dry sed.
				(mg)	(=ppm)
Background LSC (BG LSC) :	20	1560	0.0139	0.00001	0.00148
Limit of Detection (2xBG LSC)	40	3120	0.0278	0.00003	0.00295
Limit of Quantitation (3xBG LS	60	4680	0.0417	0.00004	0.00443

Soil combustion sample 2

Sample size measured (g)	1.198				
Total Soil weight (g)	10.0				
	dpm	Total dpm	%-applied	Parent equiv.	mg/kg dry sed.
				(mg)	(=ppm)
Background LSC (BG LSC) :	20	167	0.0015	0.00000	0.00016
Limit of Detection (2xBG LSC)	40	334	0.0030	0.00000	0.00032
Limit of Quantitation (3xBG LS	60	501	0.0045	0.00000	0.00047

DETERMINATION OF LIMIT OF DETECTION (LD) AND QUANTITATION (LQ)

FJR 20 Jun 1996

(Winflow)

Project	98RF01
Soil	Staffort 1
Sample	13 Extract
HPLC	33

1. Background (BG) of Peaks in Counts (cts)
Formula 1
BG (CPM) x Peakwidth (min.) = Peak BG (cts)

2. Background of Peaks in DPM
Formula 2

$$\frac{\text{CTS (Peak-BG)} \times \text{Flow (ml/min.)} \times 100}{\text{Efficiency (\%)} \times \text{Flow Cell Volume (ml)}} = \text{Peak BG (DPM)}$$

3. Ratio corrected peak to peak BG
Formula 3
corrected peak (dpm) devided by background dpm + 1
increase by 1 is necessary because peak is already corrected for BG

HPLC-Parameters

Flow (ml/min)	1
Efficiency (%)	75
Cell vol (ml)	0.150
BG in CPM	44

Peak data

ROI-Name	Ret. time window (min)			Peak response	Peak width	Peak BG	Peak BG	Significance of correct. Value		
	Rt	Start	End	dpm	(min)	cts	DPM	Ratio	LD and LQ	Significance
	min	min	min	corrected for BG		Formula 1	Formula 2	Formula 3		
NOA 409045	20.70	20.15	21.33	7976.00	1.18	52	462	18.282	>=LQ	name and percent-value

DETERMINATION OF LIMIT OF DETECTION (LD) AND QUANTITATION (LQ)

General data

Project	98RF01
Soil	Staffort 1
Sample	13 Extract
HPLC	33

Experimental data

Amount applied (mg)	0.10639
Amount applied (dpm)	11234264
Amount in Extractables (dpm)	1767426
Extractables (%-applied)	15.73
Amount of Soil (kg)	0.01001
Concentration in Soil (mg/kg)	10.63
Recovery (%-applied)	100.00

Limit of Detection (LD) and Quantitation (LQ)
Definitions: LD = 2 x BG; LQ = 3 x BG

ROI Name				BG
	dpm	%-ROI	%-applied	dpm
NOA 409045	7976	100.00	15.73	462
0	0	0.00	0.00	0
Total	7976	100.00	15.73	462

ROI Name	BG	LD	LQ	BG	LD	LQ	BG	LD	LQ
	%-applied			Parent equiv.		(mg)	Soil Residue		(mg/kg)
NOA 409045	0.910	1.821	2.731	0.00097	0.0019	0.0029	0.0967	0.1935	0.2902

Amendment No. 1 to Report on Study 98RF01

Test Substance: **NOA 409045**

Title: **Adsorption / Desorption of NOA 409045 in various Soils**

Modification: 3.4 Adsorption and Desorption Isotherms, Page 23, Row 12 from above

Present: These data classify NOA 409045 as a pesticide that is very low adsorbed by soil, such as monocrotophos or dicrotophos (see also Table 16).

New: These data classify NOA 409045 as a compound that is very low adsorbed by soil, such as monocrotophos or dicrotophos (see also Table 16).

Reason: NOA 409045 is not a pesticide, it is a metabolite of CGA 329351

5.1.2.e Woo

September 28, 1998
Date
Dr. 5.1.2.e Woo
Study Director

5.1.2.e Woo

September 28, 1998
Date
Dr. 5.1.2.e Woo
Sponsor

The slopes 1/n for the adsorption isotherms were close to unity (0.93 - 0.96). The linearity of the isotherms (correlation coefficients of 0.9286 - 0.9990) indicates that in the experimental concentration range the sorption potential of the soils is directly proportional to the concentration of the test substance in the aqueous phase (see also Figures 13 - 15 and Table 12).
Relating the Freundlich adsorption coefficients k_{ads} to the organic carbon contents (OC) or to the organic matter contents (OM) resulted in K_{oc}-values ranging from 8.88 to 15.37 ml/g and K_{om}-values of 5.15 to 8.91 ml/g. The mean adsorption coefficient based on the organic carbon content of all soils was determined to K_{oc} = 11.4 ml/g. With respect to the organic matter of the soils the mean adsorption coefficient was calculated to K_{om} = 6.6 ml/g.
These data classify NOA 409045 as a compound that is very low adsorbed by soil, such as monocrotophos or dicrotophos (see also Table 16).
Freundlich desorption coefficients for desorption 1 and 2 (k_{des1} and k_{des2}) were found to be similar to the corresponding adsorption coefficients and ranged from 0.29 ml/g to 0.56 ml/g for desorption step 1 and from 0.41 ml/g to 1.53 ml/g for desorption step 2, respectively (Table 12).
The average desorption coefficients based on the organic carbon content (K_{oc}) were determined to 26.31 ml/g (1st desorption) and 77.97 ml/g (2nd desorption).

4 Conclusion

The adsorption / desorption behaviour of ^{14}C-NOA 409045 has been studied in three different soil types. According to the results obtained, NOA 409045 has to be classified as a very low adsorbing compound and is hence considered to be very mobile in soil.

5 Acknowledgements

The skilled technical assistance of Mr 5.1.2.e Wob is gratefully acknowledged.

Amendment No. 2 to Report on Study 98RF01

Test Substance: **NOA 409045**

Title: **Adsorption / Desorption of NOA 409045 in various Soils**

Modifications:

Present:	Summary [page 9] 3.2 Pre-Test (Equilibration Test) [page 21] 3.4 Adsorption and Desorption Isotherms [page 22 - 23] 4 Conclusion [page 23] 5 Acknowledgements [page 23] Table 12: Adsorption- and Desorption Coefficients of NOA 409045 for various Soils. [page 35]
New:	Summary [page 9 - 10] 3.2 Pre-Test (Equilibration Test) [page 22] 3.4 Adsorption and Desorption Isotherms [page 23 - 24] 4 Conclusion [page 24] 5 References [page 25] 6 Acknowledgements [page 25] chapter number change only Table 12: Adsorption- and Desorption Coefficients of NOA 409045 for various Soils [page 37]
Reason:	Extended interpretation of data due to new results from a supplementary study (H. Ellgehausen: Adsorption of ^{14}C-NOA 409045 onto two Soils (Supplementary Data), Novartis Crop Protection AG Project Report 98EH06, November 24, 1998.)

New release of report	Due to the changes, the page numbers have changed, therefore the new report is released with the note "Amended Report".

[redacted]

November 25, 1998

Date

Dr. [redacted]

Study Director

[redacted]

November 25, 1998

Date

Dr. [redacted]

Sponsor