Competent Authority Report

DOCUMENT III-A

Study Summaries Active Substance

Alkyl (C12-16) dimethylbenzyl ammonium chloride
(C_{12-16}-BKC, CAS no. 68424-85-1)

Product types 3-4
(Veterinary hygiene; Food and feed area)

eCA: Italy

February 2021

Section A7.2.1	*Biodegradation in soil*	For official use only
	1 REFERENCE	
1.1 Reference	[ring-U-14C]Benzalkonium chloride Aerobic Transformation in Soil Author [redacted] [redacted]	
1.2 Data protection	Yes	
1.2.1 Data owner	Sponsors ADBAC Issue Steering Committee (ISC) c/o The Household & Consumer Products Association (HCPA) 1667 K Street NW Suite 300 20006 Washington DC United States of America Representing: LONZA Inc, with offices at 90 Boroline Road Allendale New Jersey 07401, United States; STEPAN COMPANY, whose registered office is at 22 W. Frontage Road, Northfield, IL, 60093, United States; MASON CHEMICAL COMPANY, with its registered office located at 723 B West Alonquin Road, Arlington Heights, IL 60005, United States AND European Quat Consortium (EQC) pIa Akzo Nobel Chemicals nv Velperweg 76 P.O. Box 9300 6800 SB Arnhem The Netherlands Representing: AKZO NOBEL SURFACE CHEMISTRY AB; trading under the trade name Nouryon, with its registered office at Stenunge Allé 3, SE-444 85 Stenungsund, Sweden; THOR ESPECIALIDADES SA, with its registered office at Polígon Industrial el Pla, Avinguda de la Industria 1, 08297, Castellgalí, Barcelona, Spain, INNOSPEC UK Ltd., with its registered office at Innospec Manufacturing Park, Oil Sites Road, Ellesmere Port, United Kingdom;	

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1.2.2	Criteria for data protection	*Data submitted to the MS after 13 May 2000 on existing [a.s. / b.p.] for the purpose of its [entry into Annex I/IA / authorisation]*	
		2 GUIDELINES AND QUALITY ASSURANCE	
2.1	**Guideline study**	OECD Guideline 307 for Testing of Chemicals (April 2002)	
2.2	**GLP**	yes	
2.3	**Deviations**	Deviations from the study plan none Deviation from GLP The 14C-labelled test item was not retained due to its radioactivity and small sample amount.	
		3 MATERIALS AND METHODS	
3.1	**Test material**	[redacted]	
3.1.1	Lot/Batch number	[redacted]	
3.1.2	Specification	*Representative for the 2 major alkylchain length of* [redacted]	
3.1.3	Purity	[redacted]	
3.1.4	Further relevant properties	[redacted]	
3.1.5	TS inhibitory to microorganisms	na	
3.1.6	Specific chemical analysis	[redacted]	
3.2	**Reference substance**	According to the guideline no reference item is recommended for this test.	
3.2.1	Initial concentration of reference substance	na	

Section A7.2.1	*Biodegradation in soil*	For official use only
3.3 Testing procedure	[redacted] **Test vessels** [redacted] **Replicates** [redacted]	
3.3.1 Inoculum / test species	na	
3.3.2 Test system	[redacted]	
3.3.3 Test conditions	**Incubation** All replicates were incubated at 20 ± 2 °C in the dark. Aerobic conditions (exchange of air) were maintained by diffusion from the headspace and ambient atmosphere. **Soil moisture content** At application the soils were adjusted to 42 – 50 % of the maximum water holding capacity. All replicates were checked at least in two weeks intervals for losses by evaporation	

Section A7.2.1		*Biodegradation in soil*	For official use only
3.3.4	Method of preparation of test solution	[redacted]	
3.3.5	Initial TS concentration	[redacted]	
3.3.6	Duration of test	Soil 2.2: 122 days Soil 2.3: 120 days Soil 2.4: 128 days Soil 5M: 120 days	

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3.3.7 Analytical parameter	**Extraction of the Soils** [redacted] **Method of Accelerated Solvent Extraction** [redacted] **Analytical Evaluation by LSC** [redacted] **Analytical Evaluation by LC – FSA (radio-HPLC)** [redacted] **Additional Analytical Evaluation by LC-FSA (radio-HPLC)** [redacted]	

3.3.8 Sampling

[redacted]

Sampling Times

Soil	Number of Samplings	Sampling Times
2.2	10	0, 1, 2, 3, 4, 7, 10, 21, 74, 122 days
2.3	10	0, 1, 2, 3, 4, 8, 22, 46, 80, 120 days
2.4	10	0, 2, 3, 6, 8, 13, 20, 56, 87, 128 days
5M	10	0, 1, 3, 7, 11, 21, 36, 60, 94, 120 days

Test item and transformation products

[redacted]

14CO2

[redacted]

Volatile organic transformation products

[redacted]

NER

[redacted]

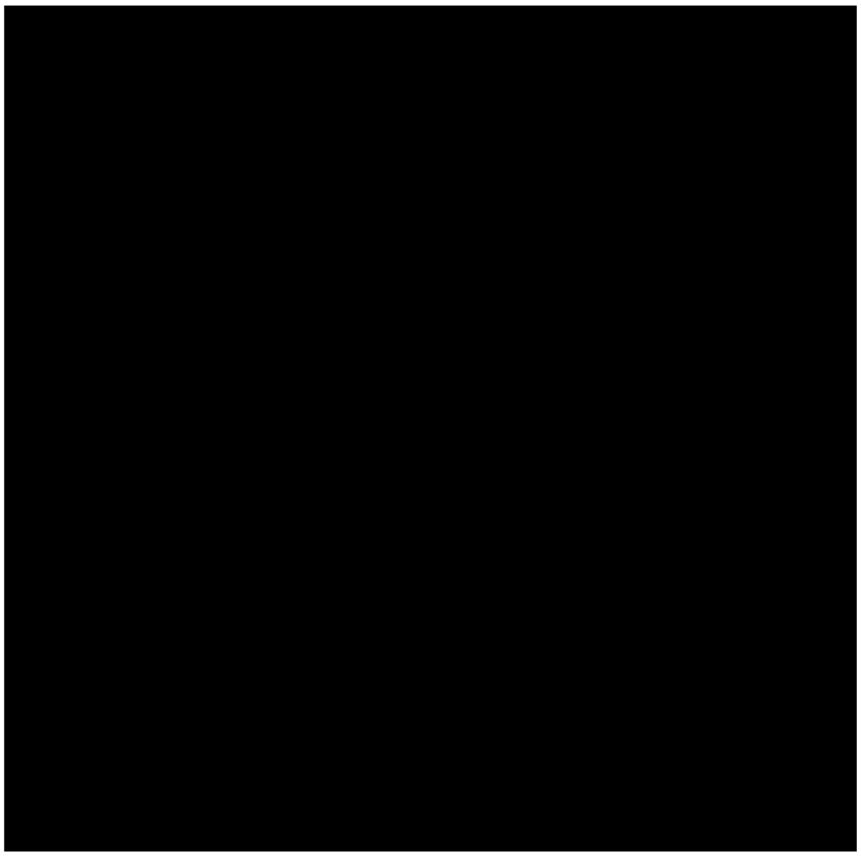
Soil moisture

[redacted]

Biomass activity

Section A7.2.1		*Biodegradation in soil*	For official use only
		[redacted]	
3.3.9	Intermediates/ degradation products	**Sampling for Metabolite Identification and Evaluation of Transformation Pathway** [redacted] **Analytical Evaluation by LC-HRMS (Metabolite Identification)** [redacted] **Analytical Evaluation by LC-MS/MS (Metabolite Confirmation)** [redacted]	
3.3.10	Nitrate/nitrite measurement	na	
3.3.11	Controls	Control soil samples were not treated with the test item and were incubated under the same aerobic conditions as the treated soil samples. These samples were used for biomass measurements at test start, during and at the end of the study.	
3.3.12	Statistics	[redacted]	
		4 RESULTS AND DISCUSSION	

Section A7.2.1	*Biodegradation in soil*	For official use only
4.1 Degradation of test substance	[redacted]	

4.1.1 Graph	[redacted]  	

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

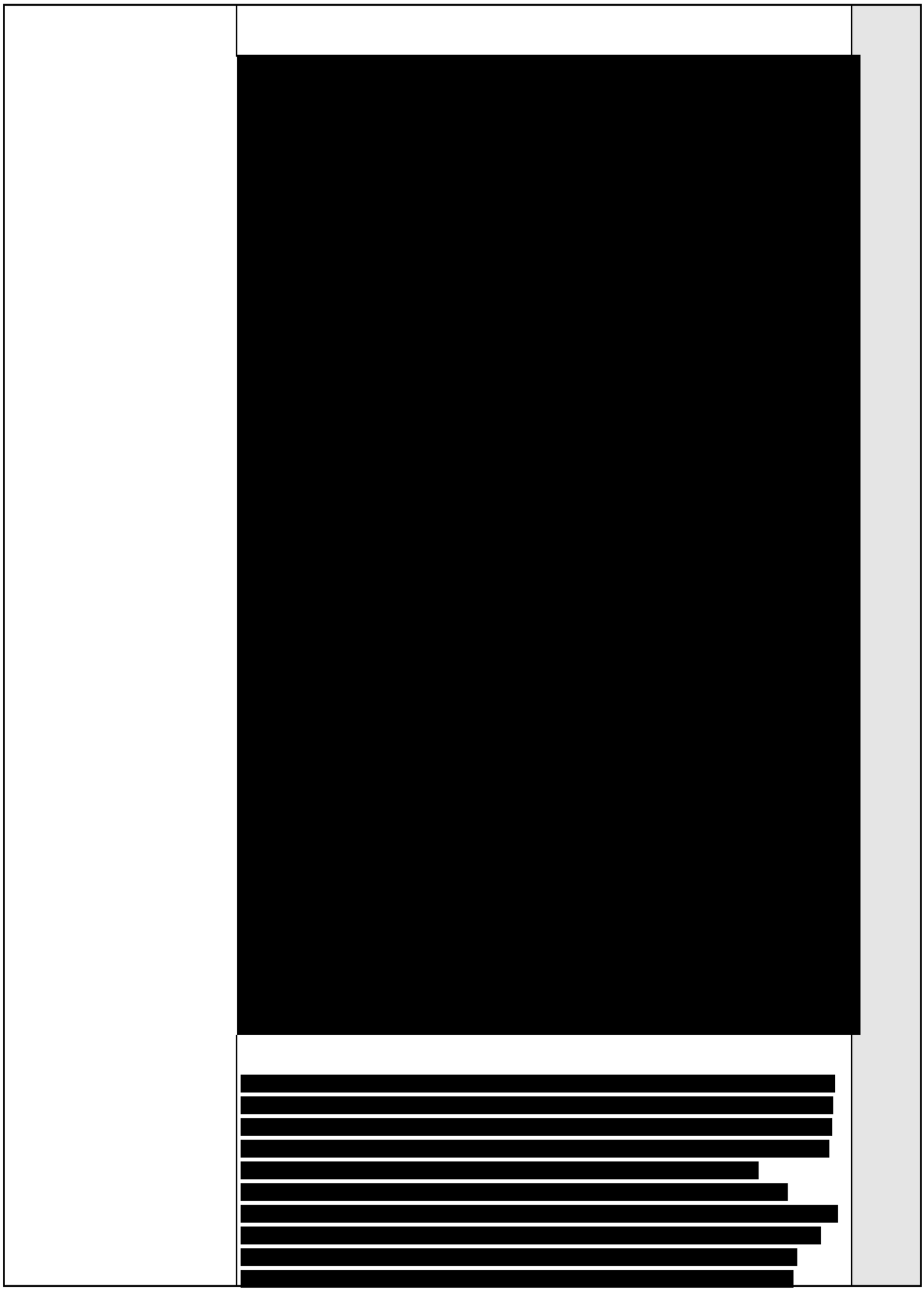
Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
4.1.2 Degradation	**Kinetic Analysis** [redacted]	

Section A7.2.1		*Biodegradation in soil*	For official use only
4.1.3	Other observations	**Microbial Biomass** [redacted] **Mass Balance** [redacted] **Characterization of Non-Extractable Residues (NER)** [redacted]	
4.1.4	Degradation of TS in abiotic control	na	
4.1.5	Degradation of reference substance	na	

4.1.6	Intermediates/ degradation products	**Formation of Metabolites and Transformation Pathway** [redacted] **Metabolite Identification** [redacted] **Results and Data Assessment – LC-HRMS Analysis** [redacted]	



[redacted]

Confirmatory – LC-MS/MS Analysis

[redacted]

[redacted]

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
	5 APPLICANT'S SUMMARY AND CONCLUSION	
5.1 Materials and methods	[redacted] **Principle of the Study** [redacted]	

5.2 Results and discussion	**Transformation of [ring-U-14C]Benzalkonium chloride** [redacted] **Characterization of Non-Extractable Residues (NER)** [redacted] **Mass Balance** [redacted]	

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted] **Formation of Metabolites and Evaluation of Transformation Pathway** [redacted] **DTx Values** [redacted]	

5.3 Conclusion	Transformation of the [redacted] of the test item [redacted] was rapid in all four soils. The transformation of the [redacted] started after short adaptation phase but was thereafter rapid as well. Within 7 - 21 days the concentration of the [redacted] decreased from initially 67.2 – 69.6 % of AR to < 20 % of AR. The concentration of the [redacted] decreased from initially 23.8 – 24.6 % of AR to < 10 % of AR within 10 – 36 days. Formation of NER started directly after application of the test item. Further formation of NER increased in parallel to the start of increased mineralisation, indicating that a major amount of NER is comprised by radioactivity incorporated in microbial biomass. The mass balance was in the range 99.9 – 103.0 % at test start and 90.4 – 94.0 % at test end. The predominant initial degradation step was the [redacted]. [redacted] was determined as the major metabolite, the highest concentrations of [redacted] were determined until day 22, thereafter the concentrations deceased continuously until test end. [redacted] was transient and only present in traces [redacted] a suspected metabolite, was not detected. Further metabolites containing partly degraded [redacted] were all transient and were not detected or only < 0.2 % of AR (soil 2.3) at test end. Based on the visual fit and χ2 error, the transformation of [redacted] met the requirements for both models well for all four soils. The calculated DT50 values with the Single-First-Order Model (SFO) for the dissipation of [redacted] were 2.2 – 8.7 days [redacted] and 6.1 – 28.7 days [redacted] the DT90 values were 7.2 – 28.8 [redacted] days and 20.2 – 95.4 days [redacted] The calculated DT50 values with the First-Order Multi-Compartment Model (FOMC) for the dissipation of [redacted] were 1.6 – 7.2 days [redacted] and 5.5 – 23.3 days [redacted], the DT90 values were 15.0 – 48.8 days [redacted] and 35.8 – 164.3 days [redacted] [redacted] is predominantly [redacted], with low to negligible amounts of [redacted] The chain length distribution is defined as follows: [redacted] (39-76%), [redacted] (20-52%), [redacted] (0-12%). [redacted] was not included in this study because it is present in very low amounts; there are technical difficulties with having sufficient radioactivity for substances present in small amounts relative to other constituents. [redacted] would be expected to degrade by the same route but at a slower rate than its [redacted] and [redacted] counterparts, as degradation rate tends to decrease with increasing chain lengths. To account for the potential contribution of [redacted] to the overall DT50 of ADBAC, we calculated the geometric mean SFO and FOMC DT50s for [redacted] and [redacted] in the four soils (as recommended in BPR Vol IV Part B and C) and converted these to 12° using the following equation (DT50 (12°) = DT50 (20°) * $e^{(0.08*(20-12))}$. We then did a linear extrapolation, using the geometric mean DT50s for [redacted] and [redacted], to estimate the DT50 for [redacted]. See tables below: [redacted]	X

Section A7.2.1	*Biodegradation in soil*	For official use only
	[redacted] A weighted estimate of the DT50 of [redacted] at 12°C can be calculated by assuming the highest allowable concentrations of [redacted] and [redacted] and the balance of [redacted] (i.e., 12% [redacted], 52% [redacted] and 36% [redacted]), which gives the following estimated DT50s: SFO DT50 = 19.2d at 12°C FOMC DT50 = 17.1d at 12°C Due to the relatively low levels of [redacted], the overall estimated DT50s are rather insensitive to the assumed DT50 for [redacted]	
5.3.1 Reliability	*1*	
5.3.2 Deficiencies		
	Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date		
Materials and Methods		
Results and discussion		
Conclusion		
Reliability		
Acceptability		
Remarks		
	COMMENTS FROM ...	
Date		
Materials and Methods		
Results and discussion		
Conclusion		
Reliability		
Acceptability		
Remarks		

Add tables if needed

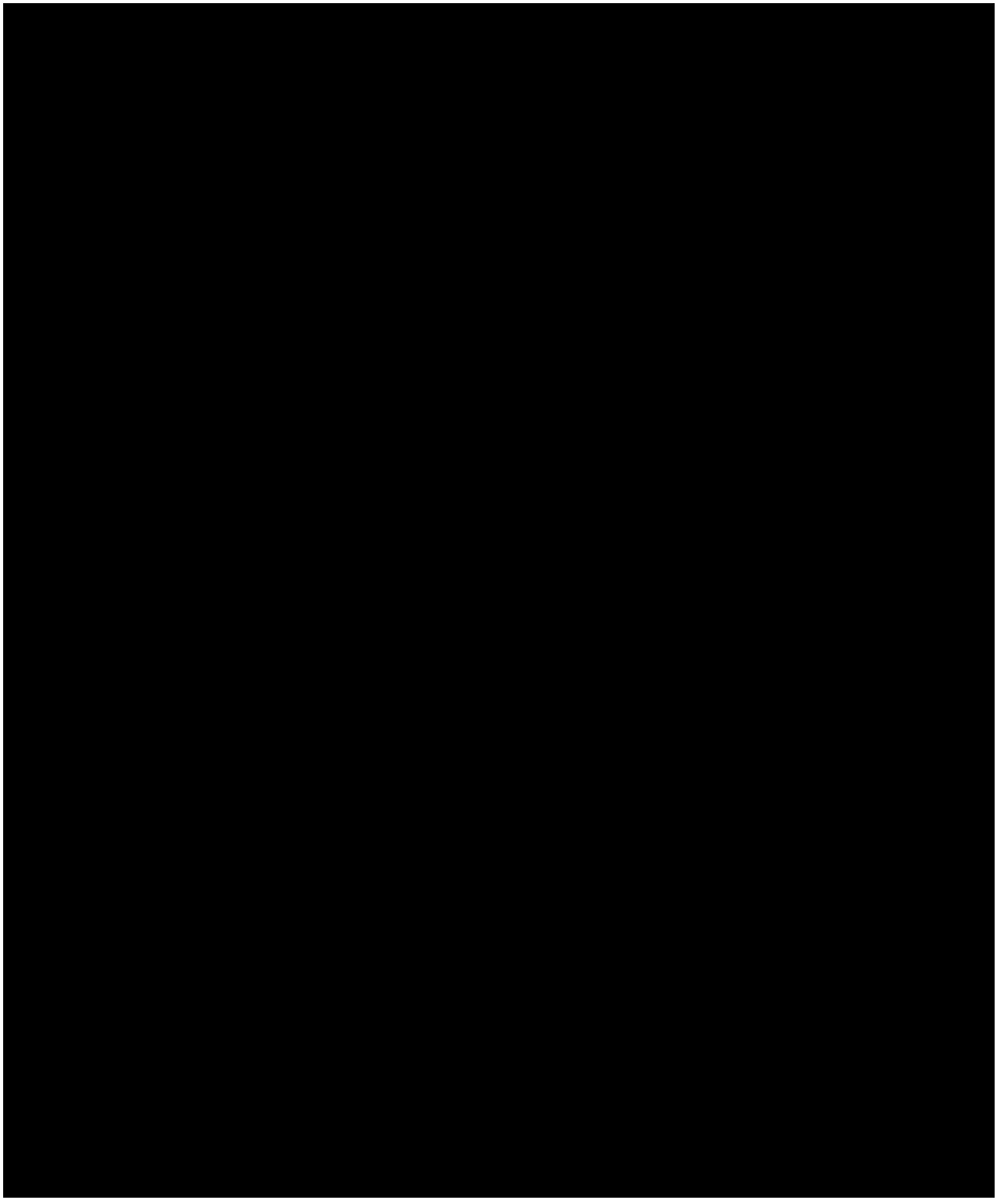
Soil Parameters

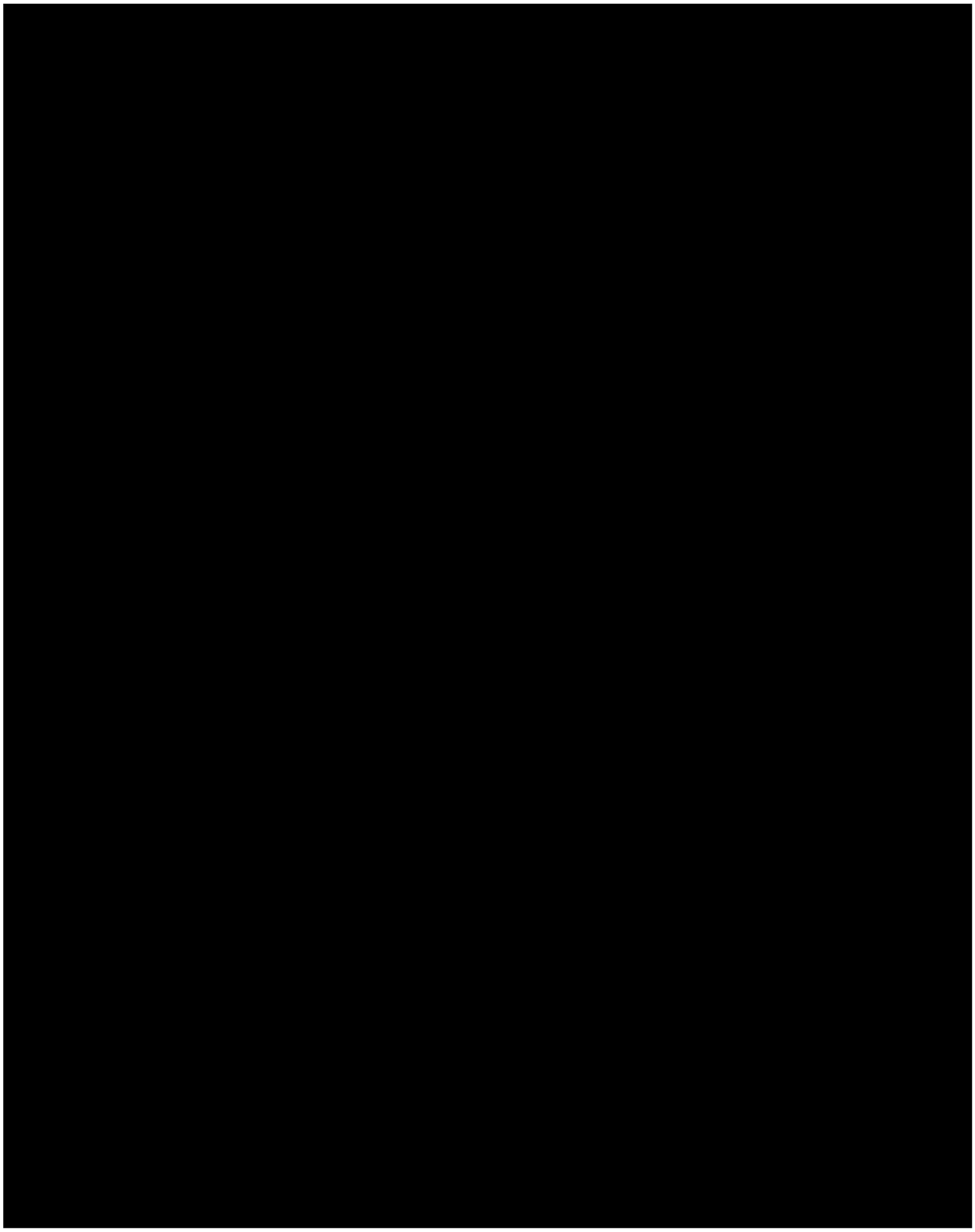
Parameter	**LUFA-soil 2.2** Batch-No. F2.2 0118	**LUFA-soil 2.2** Batch-No. F2.2 1818	**LUFA-soil 2.3** Batch-No. F2.3 4317	**LUFA-soil 2.4** Batch-No. F2.4 0118	**LUFA-soil 5M** Batch-No. F5M 4217
Sampling depth*	ca. 20 cm	ca. 20 cm	ca. 20 cm	ca. 20 cm	ca. 20 cm
pH-value*	5.6 ± 0.4	5.6 ± 0.4	5.8 ± 0.6	7.4 ± 0.1	7.3 ± 0.1
Maximum water holding capacity* [g/100 g DW]	45.8 ± 1.9	44.8 ± 2.9	35.4 ± 1.0	44.6 ± 2.2	41.6 ± 2.6
Particle size distribution#*					
Sand:					
0.63 - 2.0	0.7 ± 0.2	0.8 ± 0.2	2.8 ± 0.4	1.7 ± 0.2	1.0 ± 0.3
0.2 - 0.63	40.2 ± 1.7	41.0 ± 1.5	29.8 ± 1.0	5.9 ± 0.5	13.6 ± 1.2
0.063 - 0.2	34.8 ± 3.0	35.3 ±23.0	24.6 ± 1.0	19.7 ± 1.0	39.7 ± 1.9
Silt:					
0.02 - 0.063	7.5 ± 1.6	6.9 ± 0.7	18.5 ± 1.1	23.0 ± 1.1	21.3 ± 1.5
0.006 - 0.02	5.2 ± 0.8	4.8 ± 0.4	11.4 ± 0.7	15.2 ± 1.0	9.4 ± 0.7
0.002 - 0.006	3.0 ± 1.2	2.8 ± 0.9	5.3 ± 0.7	7.9 ± 0.4	3.8 ± 1.1
Clay:					
< 0.002	8.6 ± 1.2	836 ± 0.9	7.6 ± 0.4	26.6 ± 0.6	11.2 ± 0.9
Organic carbon content [%][1]	1.70	0.939	0.55	2.47	0.88
Microbial biomass [%] of total organic carbon[2)]	2.66	2.65	3.94	3.02	3.09
Cation exchange capacity* [meq/100 g]*	9.8 ± 0.5	9.2 ± 1.4	7.5 ± 0.8	26.5 ± 15.5	15.7 ± 5.3
Weight per Volume (g/1000 mL)*	1201 ± 41	1205 ± 41	1307 ± 41	1251 ± 39	1221 ± 72
Soil texture*	loamy sand [redacted]	loamy sand [redacted]	silty sand [redacted]	clayey loam [redacted]	clayey loam [redacted]
Sampling date	2018-01-05	2018-05-02	2017-10-23	2018-01-05	2017-10-16

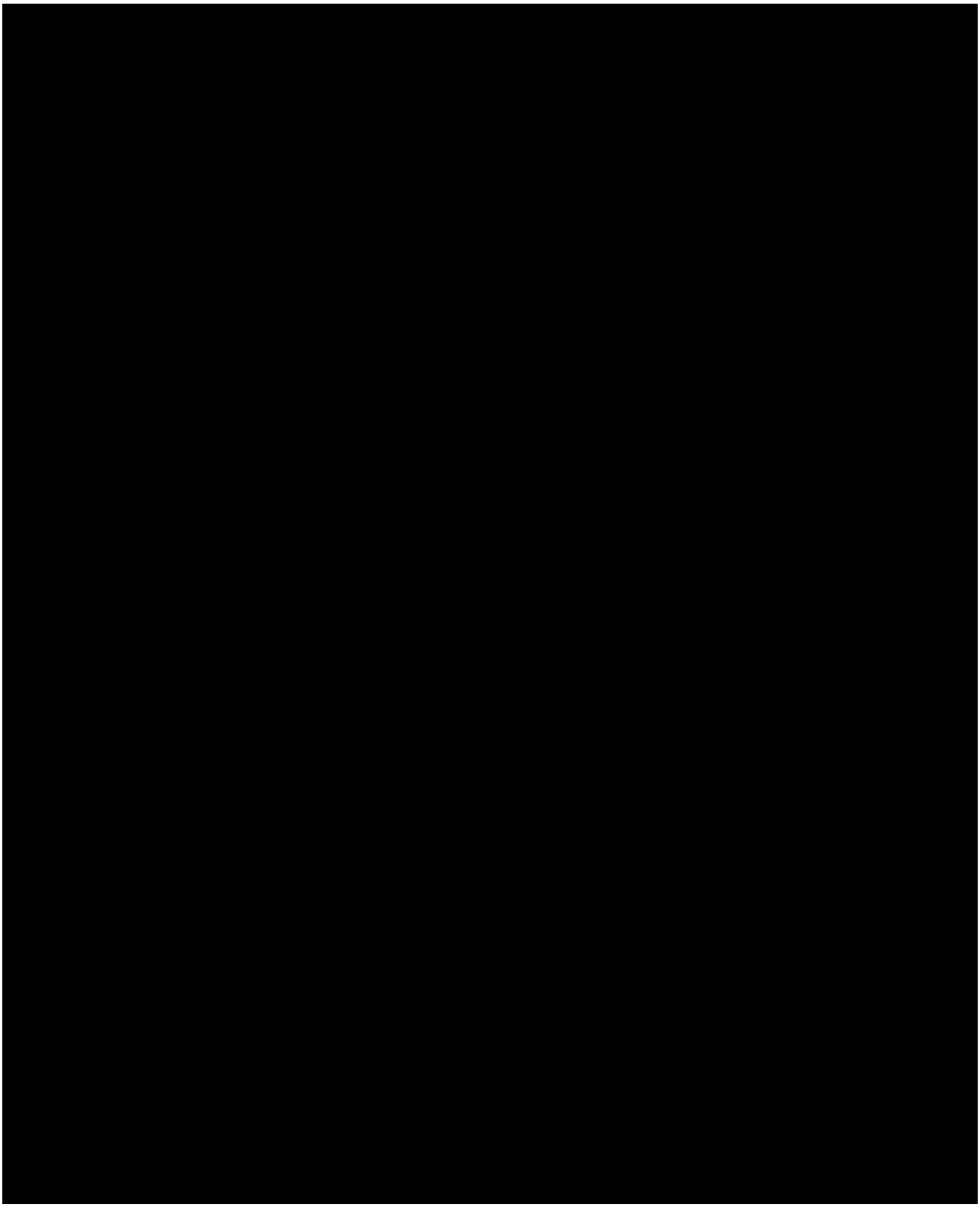
*) data provided by LUFA SPEYER [redacted]

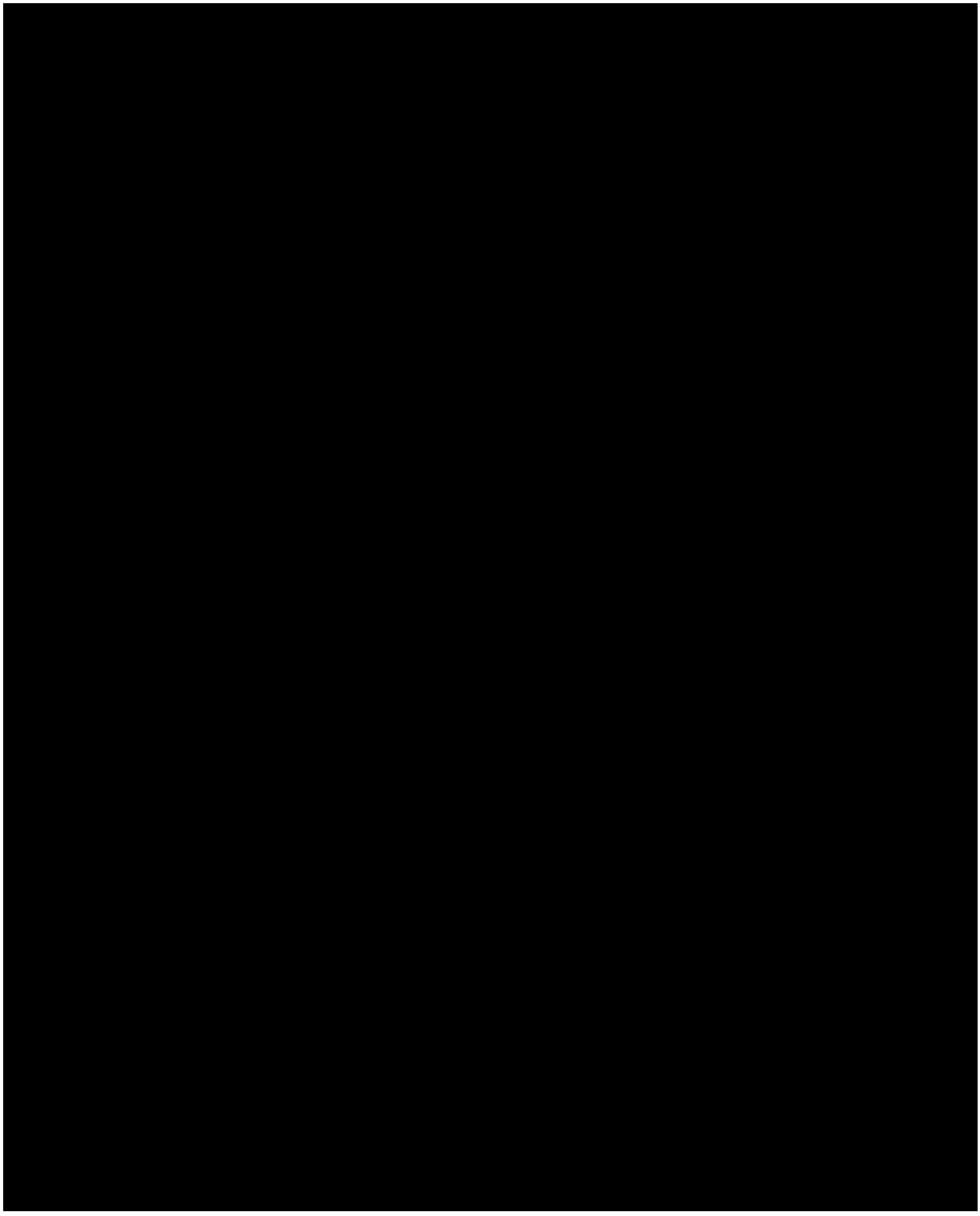
2) determined at the respective application day of the respective soil

[redacted]









Soil Organic Matter Fractionation

	Soil							
	2.2		2.3		2.4		5M	
	% of AR							
	Repl.		Repl.		Repl.		Repl.	
	1	2	1	2	1	2	1	2
Remaining NER in soil after ASE extraction	22.4	20.5	24.7	25.1	30.9	31.5	29.4	29.5
Fulvic acids Soluble fraction at low pH	13.8	14.7	13.0	13.3	14.2	15.3	14.9	15.9
Humic acids Soluble fraction at high pH	3.8	4.6	4.8	5.1	3.4	3.6	4.0	4.9
Humin Insoluble fraction	8.0	8.7	8.5	12.3	20.0	15.9	16.5	12.4
Total NER	25.6	28.0	26.3	30.7	37.6	34.8	35.4	33.2

*Total NER = % AR from Fulvic Acids Fraction + % AR from Humic Acids Fraction + % AR from Humin Fraction

[redacted]

[redacted]

[redacted]