

## Release of substances from joint grouts based on various binder types and their ecotoxic effects

Ute Schoknecht<sup>1\*</sup>, Ute Kalbe<sup>1</sup>, Ines Heisterkamp<sup>2</sup>, Martina Kretzschmar<sup>2</sup>, Stefan Gartiser<sup>2</sup>, Oliver Happel<sup>3</sup>, Outi Ilvonen<sup>4</sup>

<sup>1</sup>BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87 12205 Berlin, Germany

<sup>2</sup>Hydrotox GmbH, Freiburg, Germany

<sup>3</sup>TZW: DVGW-Technologiezentrum Wasser (German Water Center), Karlsruhe, Germany

<sup>4</sup> German Environment Agency, Dessau, Germany

\* Corresponding author: ute.schoknecht@bam.de, phone: +49 (0)30 / 8104 1413

### Supporting Information

#### SI 1: Limits of quantification (LOQs) for anions and cations

##### LOQs for anions

Anion	LOQ for experiments 1 and 2a in mg L <sup>-1</sup>	LOQ for experiments 2b, 3a and 3b in mg L <sup>-1</sup>
F <sup>-</sup>	0.014	0.27
Cl <sup>-</sup>	0.54	0.095
Br <sup>-</sup>	0.010	0.076
NO <sub>2</sub> <sup>-</sup>	0.015	0.10
NO <sub>3</sub> <sup>-</sup>	0.11	0.27
PO <sub>4</sub> <sup>3-</sup>	0.032	0.27
SO <sub>4</sub> <sup>2-</sup>	0.81	0.19

##### LOQs for elements

Cation	LOQ ICP-OES Experiments 1 and 2a in µg L <sup>-1</sup>	LOQ ICP-OES Experiments 2b, 3a and 3b in µg L <sup>-1</sup>	LOQ ICP-MS Experiments 1 and 2a in µg L <sup>-1</sup>	LOQ ICP-MS Experiments 2b, 3a and 3b in µg L <sup>-1</sup>
As			0.03	1.50
Ba	2.0	0.36		0.05
Cd	2.5		0.026	
Cr	3.5	0.77	0.031	
Cu			0.77	2.54

Cation	LOQ ICP-OES Experiments 1 and 2a in $\mu\text{g L}^{-1}$	LOQ ICP-OES Experiments 2b, 3a and 3b in $\mu\text{g L}^{-1}$	LOQ ICP-MS Experiments 1 and 2a in $\mu\text{g L}^{-1}$	LOQ ICP-MS Experiments 2b, 3a and 3b in $\mu\text{g L}^{-1}$
Hg			0.050	0.34
Mn	2.4	0.30		0.05
Mo	2.0	0.49	0.12	
Ni			0.15	
Pb			0.050	
Sb			0.034	7.7
Sn	4.1	1.0		0.020
Sr	2.3	0.3		
V	1.4	1.4		
Zn			0.022	
Co	2.5		0.019	
Al	470	34		
Ca	80	67		
Fe	62	86		
K	77	170		
Mg	95	51		
Na	170	4100		0.46
B	93	11		
P	19	13		
S	23	13		0.014
Se			0.18	1.50
Si	250	4900		0.05
Ti	8400	2500		
Tl			0.022	

## SI 2: Analytical methods on organic substances applied at BAM

### Sample preparation for quantitative analysis and GC-MS screening of eluates at BAM

100 ml of the sample were transferred to a separating funnel of 250 ml capacity. Extraction was performed first under acidic conditions and then repeated under alkaline conditions. The pH of the samples was adjusted to pH 2 by 1 ml HCl (1 mol L<sup>-1</sup>) and controlled by means of pH paper. Subsequently, the samples were extracted twice for 3 min using 30 ml dichlormethane for each step. The dichlormethane extracts were dried on sodium sulfate and transferred to a 100 ml pear shaped flask and combined. The remaining aqueous samples were adjusted to pH 10 by addition of 4 ml NaOH (1 mol L<sup>-1</sup>). Again, the pH was controlled by means of pH paper. The procedure was continued as described for extraction under acidic conditions. The combined extracts were reduced to a volume of 1 ml using a rotary evaporator, completely transferred to 2 ml vials and analyzed.

### GC-MS methods

GC-MS-System:	Agilent 6890N GC-System equipped with an Agilent 7683B autosampler
Detector:	Agilent 5973Network Mass Selective Detector
Column:	HP-5MS, 30 m x 0.25 mm ID, 0.25 µm
Carrier gas:	Helium
Flow rate:	He, 1.0 ml min <sup>-1</sup>
Split-Mode:	Pulsed splitless
Injection volume:	1.0 µl
Injector temperature:	280 °C
Oven program:	60 °C (2 min), 30 ° min <sup>-1</sup> to 120°C, 5 ° min <sup>-1</sup> to 320 °C (5 min)

### MS-Parameters for Screening

Mode:	EI-SCAN
Tune:	Autotune (Atune)
Transfer line temperature:	280 °C
MS Source temperature:	230 °C
MS Quad temperature:	150 °C
Ionization Energy:	70 eV
Scan Mass Range:	m/z 30 to m/z 650

### MS-Parameters for quantitative analysis of benzyl alcohol, 4-tert-butylphenol, 1,3-benzenedimethanamine, N,N-dimethyl-1-dodecanamine, 2-ethylhexanoic acid

Mode:	EI-SIM
Tune:	Autotune (Atune)
Transfer line temperature:	280 °C
MS Source temperature:	230 °C
MS Quad temperature:	150 °C
Ionization Energy:	70 eV

### Calibration standards

Substance	CAS	Supplier	Purity in %
Benzyl alcohol	100-51-6	Chemsolut	99.8
2-Ethylhexanoic acid	149-57-5	Sigma-Aldrich	>99.0
4-tert-Butylphenol	98-54-4	HPC Standards GmbH	99.9
1,3-Benzenedimethanamine	1477-55-0	Sigma-Aldrich	99.0
<i>N,N</i> -Dimethyl-1-dodecanamine	112-18-5	HPC Standards GmbH	98.3

### Signals for quantification by external calibration

Substance	CAS	Signal	Retention time	Calibration range
		In m/z	In min	In mg l <sup>-1</sup>
Benzyl alcohol	100-51-6	108	5.13	1 - 20
2-Ethylhexanoic acid	149-57-5	88	5.89	1 - 20
4-tert-Butylphenol	98-54-4	135	8.14	1 - 20
1,3-Benzenedimethanamine	1477-55-0	106	9.45	1 - 20
<i>N,N</i> -Dimethyl-1-dodecanamine	112-18-5	58	11.75	1 - 20

### Identification of substances

Substances were tentatively identified by comparing observed mass spectra with the spectra libraries NIST 14 and RTLpest 2. Selected spectra were also compared with the spectra library NIST 17.

The structures of the quantified substances were confirmed by reference standards.

### SI 3: Analytical methods on organic substances applied at TZW

#### Sample preparation for GC-MS screening at TZW

200 ml of the sample were extracted first under acidic conditions and then repeated under alkaline conditions. Before extraction approx. 5 mg ascorbic acid and the mixture of labelled internal standards (100 µl) were added to the sample. The pH of the samples was adjusted to pH 2 by HCl (10 %). The samples were extracted twice using 50 ml dichlormethane for each step. The dichlormethane extracts were dried on sodium sulfate and transferred to a 100 ml pear shaped flask and combined. The remaining aqueous samples were adjusted to pH 10 by NaOH (0.5 mol L<sup>-1</sup>). The procedure was continued as described for extraction under acidic conditions (2x extraction by 50 mL dichlormethane and drying on sodium sulfate). The combined extracts were reduced in a first step to a volume of approx. 5 ml using a rotary evaporator (30 °C, approx. 580 mbar) and in a second step evaporated to 0.5 ml by using a TurboVap.

#### Internal standards for semiquantitative measurements (in acetone)

d21-BHT 80 ng µL<sup>-1</sup>  
d5-Chlorbenzol 20 ng µL<sup>-1</sup>  
d34-Hexadecan 10 ng µL<sup>-1</sup>  
d8-Naphthalin 10 ng µL<sup>-1</sup>  
d10-Phenanthren 20 ng µL<sup>-1</sup>  
d5-Phenol 80 ng µL<sup>-1</sup>  
d62-Squalan 80 ng µL<sup>-1</sup>

#### GC-MS method

GC-MS-System: Agilent GC/MS-system 6890N  
Detector: Agilent MSD 5973 Network Mass Selective Detector  
Column: Rtx-5MS, 60 m x 0.25 mm ID, 0.25 µm  
Carrier gas: Helium  
Flow rate: He, 1.5 ml He min<sup>-1</sup>  
Split-Mode: Splitless  
Injection volume: 1.0 µl  
Injector temperature: 280 °C  
Oven program: 38 °C (7 min), 8 ° min<sup>-1</sup> to 200°C, (4 min), 10 ° min<sup>-1</sup> to 280 °C (16 min)  
runtime approx. 55 min

#### MS-Parameters for Screening

Mode: EI-SCAN  
Tune: Autotune (Atune)  
Transfer line temperature: 280 °C  
MS Source temperature: 200 °C  
MS Quad temperature: 150 °C  
Ionization Energy: 70 eV  
Scan Mass Range: m/z 30 to m/z 650

The working range is approx. 1 µg L<sup>-1</sup> to 500 µg L<sup>-1</sup>. In contrast to DIN EN 15768, the measurement must be made at a starting temperature of 38 °C instead of 30 °C, as the measurement instrument reaches the low value only very slowly at normal ambient temperature. For the measurement it is necessary to carry a laboratory blank value. Signals that clearly differ from the laboratory blank value

are evaluated. The NIST spectrum database is used to search for matches. The evaluation and integration of the areas of internal standards and signals in the sample is done via the TIC.

#### LC-ESI-QTOF method

LC system                    Agilent 1200 Series  
 Column                      Zorbax Eclipse Plus C18 (150 mm x 2.1 mm, 3 µm, Agilent)  
 Injection volume          100 µL (direct injection)  
 Flow                          0.30 mL min<sup>-1</sup>  
 Temperature                30 °C  
 Mobile phase A            0.1% formic acid in water  
 Mobile phase B            0.1% formic acid in acetonitrile

#### Elution profile

time		mobile phase A	mobile phase B
1	min	98 %	2 %
2	min	80 %	20 %
16.5	min	0 %	100 %
22	min	0 %	100 %
22.1	min	98%	2 %
30	min	98 %	2 %

#### Detection

ESI-QTOF                    TripleTOF 6600, Sciex  
 Ionization                  positive and negative (ESI+ and ESI-)  
 Mass Range                m/z 100 to m/z 1200

#### Data evaluation

The LC screening was matched with a list of potential substances from roofing films and lack as [M+H]<sup>+</sup> or [M-H]<sup>-</sup> and with MS2 spectra from the manufacturer Sciex. In addition, a screening for signals with clearly positive hits (significant spectra, not just a fragment) was carried out at the MS2 spectra database (Sciex) (list: LC(NIST)).

Conditions for a positive hit:

- The difference of the measured mass from the exact mass is < 5 ppm (calculated from sum formula).
- The signal-to-noise (S/N) > 10 and the signal in the blank is 10 times lower to the measured signal.
- The MS2 spectrum match and a reference spectrum are present (dot in the LC(NIST) column). In addition, a score of > 70 was found.

#### LC-DAD method

LC system                    Agilent 1100 Series  
 Column                      Nucleodur C18 Gravity  
                                     (150 mm x 2 mm, 3 µm, Macherey Nagel)  
 Injection volume          20 µl (direct injection)  
 Flow                          0.45 ml/min  
 Temperature                30 °C  
 Mobile phase A            phosphoric acid in water (10 mmol L<sup>-1</sup>)

Mobile phase B          phosphoric acid in acetonitrile (10 mmol L<sup>-1</sup>)

Elution profile

time		mobile phase A	mobile phase B
0	min	90 %	10 %
1	min	90 %	10 %
10	min	0 %	100 %
15	min	0 %	100 %
15,5	min	90 %	10 %
22	min	90 %	10 %

**Detection**

diode array detector    Agilent 1100er series (G1315B)

range                      200 nm to 360 nm

**SI 4: Data on test assemblies**

1\*: percolation test, all other experiments: DSLT

DSLT: Total water volume from two eluation periods: 4.8 L, percolation test: Water volume at L/S 2: 4.8 L

28\*\*: test specimens were covered by cling film during storage

Code	Experiment	Duration of storage	Mass of test specimen or test material at the beginning of the test in g	Mass of test specimen or test material at the beginning of the test in g	Total water uptake in g	Water uptake in %
MOE1	1	12	532	589	57	11
MOE1	1*	46	2400	not determined		
MOE1	3a	7	589	667	78	13
MOE1	3a	14	550	620	70	13
MOE1	3b	28	462	530	68	15
MOE1	3b	28**	508	578	70	14
MOE2	2a	8	658	727	69	10
MOE2	2b	7	540	550	10	2
MOE3	2a	8	806	874	68	8
MOE3	2b	7	654	737	83	13
MOE4	2a	7	777	858	81	10
MOE4	2b	7	624	696	72	12
MOE5	2a	10	612	627	15	2
MOE5	2b	7	546	551	5	1
MOE6	2a	11	577	676	99	17
MOE6	2b	7	536	558	22	4
MOE7	2a	7	596	637	41	7
MOE7	3a	7	555	600	45	8
MOE7	3a	14	517	557	40	8
MOE7	3b	28	472	492	20	4
MOE7	3b	28**	479	503	23	5
MOE8	2a	12	683	697	14	2
MOE8	2b	7	550	558	8	1

Comment: formation of foam in eluate samples of MOE1, MOE2, MOE6, MOE7



### SI 5: Results for TOC, TN, pH, conductivity and turbidity of eluates

Eluates 1 + 2 originate from DSLT, L/S 2 fraction originates from percolation tests

28\*: test specimens were covered by cling film during storage

Experiment	Code	Storage in d	Sample	TOC in mg L <sup>-1</sup>	TN in mg L <sup>-1</sup>	pH	Conductivity in μS cm <sup>-1</sup>	Turbidity in FNU
1	Blank	-	Eluate 1 + 2	0.24	< 0.05	7.3	3.5	n.d.
1	MOE1	12	Eluate 1 + 2	427	81.0	9.1	240	n.d.
1	MOE1	46	L/S 2 fraction	1280	270	9.0	600	7.03
3a	Blank	-	Eluate 1 + 2	0.27	< 0.05	7.1	2.8	n.d.
3b	Blank	-	Eluate 1 + 2	1.33	< 0.05	6.9	1.7	n.d.
3a	MOE1	7	Eluate 1 + 2	401	70.1	9.1	236	n.d.
3a	MOE1	14	Eluate 1 + 2	410	77.2	9.2	262	n.d.
3b	MOE1	28	Eluate 1 + 2	324	63.5	9.2	240	n.d.
3b	MOE1	28*	Eluate 1 + 2	379	74.7	9.3	238	n.d.
2a	Blank	-	Eluate 1 + 2	0.9	< 0.05	7.0	2.0	n.d.
2b	Blank	-	Eluate 1 + 2	0.14	< 0.05	7.1	1.8	n.d.
2a	MOE2	8	Eluate 1 + 2	72.8	< 0.05	3.9	64	n.d.
2b	MOE2	7	Eluate 1 + 2	43.1	< 0.05	4.0	55	n.d.
2a	MOE3	8	Eluate 1 + 2	59.2	0.22	11.8	2310	n.d.
2b	MOE3	7	Eluate 1 + 2	105	0.50	12.0	3050	n.d.
2a	MOE4	7	Eluate 1 + 2	5.53	< 0.05	11.5	1170	n.d.
2b	MOE4	7	Eluate 1 + 2	1.50	< 0.05	11.9	1780	n.d.
2a	MOE5	10	Eluate 1 + 2	1.16	< 0.05	8.3	3.3	n.d.
2b	MOE5	7	Eluate 1 + 2	0.59	< 0.05	8.0	3.5	n.d.
2a	MOE6	11	Eluate 1 + 2	556	36.2	9.5	103	n.d.
2b	MOE6	7	Eluate 1 + 2	355	29.9	9.5	133	n.d.
2a	MOE7	7	Eluate 1 + 2	42.8	< 0.05	4.1	43.6	n.d.
3a	MOE7	7	Eluate 1 + 2	36.4	0.13	4.1	54.2	n.d.
3a	MOE7	14	Eluate 1 + 2	36.4	0.25	4.4	36.7	n.d.
3b	MOE7	28	Eluate 1 + 2	38.6	0.40	4.4	45.0	n.d.
3b	MOE7	28*	Eluate 1 + 2	44.0	0.31	4.0	63.4	n.d.
2a	MOE8	12	Eluate 1 + 2	4.55	0.19	8.8	7.1	4.55
2b	MOE8	7	Eluate 1 + 2	3.48	0.21	7.4	9.0	3.48

### SI 6: Concentration of anions in eluates from DSLT and percolation test

Eluates 1 + 2 originate from DSLT, L/S 2 fraction originates from percolation test, 28\*: test specimens were covered by cling film during storage

Experiment	Code	Storage period in d	Sample	F <sup>-</sup> in mg L <sup>-1</sup>	Cl <sup>-</sup> in mg L <sup>-1</sup>	Br <sup>-</sup> in mg L <sup>-1</sup>	NO <sub>2</sub> <sup>-</sup> in mg L <sup>-1</sup>	NO <sub>3</sub> <sup>-</sup> in mg L <sup>-1</sup>	PO <sub>4</sub> <sup>3-</sup> in mg L <sup>-1</sup>	SO <sub>4</sub> <sup>2-</sup> in mg L <sup>-1</sup>
1	Blank	-	Eluate 1 + 2	0.02	< 0.54	0.08	< 0.015	0.37	0.55	0.90
1	MOE1	12	Eluate 1 + 2	0.87	2.99	0.61	0.45	0.39	0.48	1.76
1	Blank	-	Blind column	0.05	< 0.54	0.08	0.29	0.39	0.47	0.42
1	MOE1	46	L/S 2 fraction	0.11	9.83	1.38	0.70	0.47	0.60	5.38
3a	Blank	-	Eluate 1 + 2	<0.267	<0.095	<0.105	<0.076	<0.271	<0.266	0.37
3b	Blank	-	Eluate 1 + 2	<0.267	<0.095	<0.105	<0.076	<0.271	0.847	<0.19
3a	MOE1	7	Eluate 1 + 2	<0.267	3.27	0.241	<0.076	0.31	0.89	59.5
3a	MOE1	14	Eluate 1 + 2	<0.267	3.27	0.239	0.087	0.30	0.89	57.4
3b	MOE1	28	Eluate 1 + 2	<0.267	2.70	0.189	0.15	<0.271	0.87	45.8
3b	MOE1	28*	Eluate 1 + 2	<0.267	3.17	0.216	<0.076	<0.271	0.88	52.7
2a	Blank	-	Eluate 1 + 2	0.021	0.025	<0.017	<0.016	<0.078	1.52	<0.28
2b	Blank	-	Eluate 1 + 2	<0.267	0.14	<0.105	<0.076	<0.271	<0.266	0.27
2a	MOE2	8	Eluate 1 + 2	0.33	0.11	<0.017	0.035	<0.078	1.43	0.326
2b	MOE2	7	Eluate 1 + 2	<0.267	0.10	<0.105	0.084	<0.271	<0.266	0.283
2a	MOE3	8	Eluate 1 + 2	0.066	0.06	<0.017	0.15	<0.078	2.99	0.354

Experiment	Code	Storage period in d	Sample	F <sup>-</sup> in mg L <sup>-1</sup>	Cl <sup>-</sup> in mg L <sup>-1</sup>	Br <sup>-</sup> in mg L <sup>-1</sup>	NO <sub>2</sub> <sup>-</sup> in mg L <sup>-1</sup>	NO <sub>3</sub> <sup>-</sup> in mg L <sup>-1</sup>	PO <sub>4</sub> <sup>3-</sup> in mg L <sup>-1</sup>	SO <sub>4</sub> <sup>2-</sup> in mg L <sup>-1</sup>
2b	MOE3	7	Eluate 1 + 2	<0.267	0.45	<0.105	0.20	<0.271	<0.266	3.62
2a	MOE4	7	Eluate 1 + 2	0.13	3.51	<0.017	<0.016	0.093	1.45	47.6
2b	MOE4	7	Eluate 1 + 2	<0.267	3.21	<0.105	<0.076	<0.271	1.31	34.6
2a	MOE5	10	Eluate 1 + 2	0.022	0.04	<0.017	<0.016	0.092	1.54	<0.28
2b	MOE5	7	Eluate 1 + 2	<0.267	0.10	<0.105	<0.076	<0.271	<0.266	0.182
2a	MOE6	11	Eluate 1 + 2	0.048	1.68	<0.017	0.028	0.23	1.64	2.21
2b	MOE6	7	Eluate 1 + 2	<0.267	0.87	<0.105	0.11	<0.271	0.86	2.41
2a	MOE7	7	Eluate 1 + 2	0.15	0.09	<0.017	0.024	<0.078	1.46	0.369
3a	MOE7	7	Eluate 1 + 2	<0.267	<0.095	<0.105	0.15	<0.271	<0.266	0.286
3a	MOE7	14	Eluate 1 + 2	<0.267	<0.095	<0.105	0.11	<0.271	<0.266	0.310
3b	MOE7	28	Eluate 1 + 2	<0.267	<0.095	<0.105	0.13	<0.271	<0.266	<0.19
3b	MOE7	28*	Eluate 1 + 2	<0.267	<0.095	<0.105	0.12	<0.271	<0.266	<0.19
2a	MOE8	12	Eluate 1 + 2	0.02	0.05	<0.017	0.20	<0.078	1.57	<0.28
2b	MOE8	7	Eluate 1 + 2	<0.267	0.101	<0.105	<0.076	<0.271	0.861	0.309

## SI 7: Concentration of cations in eluates from DSLT and percolation test

### Results from ICP-OES analysis (part 1)

Eluates 1 + 2 originate from DSLT, Fractions L/S 2 originate from percolation tests, 28\*: test specimens were covered by cling film during storage

Experiment	Code	Storage period in d	Sample	Ba	Cd	Cr	Mn	Mo	Sn	Sr	V	Co	Al
				in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	
1	Blank	-	Eluate 1 + 2	<2.0	<2.5	<3.5	<2.4	<2.0	<4.1	<2.3	<1.4	<2.5	<474
1	MOE1	12	Eluate 1 + 2	2.01	<2.5	<3.5	3.21	<2.0	<4.1	47.1	<1.4	<2.5	<474
1	Blank	-	Blind column	<2.0	<2.5	<3.5	<2.4	<2.0	<4.1	<2.3	<1.4	<2.5	<474
1	MOE1	46	L/S 2 fraction	25.8	<2.5	<3.5	41.3	4.85	<4.1	104	2.85	2.52	1470
3a	Blank	-	Eluate 1 + 2	<0.36	<0.031	<0.77	<0.30	<0.49	<1.0	<0.32	<1.3	<0.020	<34
3b	Blank	-	Eluate 1 + 2	<0.36	<0.031	<0.77	<0.30	<0.49	<1.0	<0.32	<1.3	<0.020	<34
3a	MOE1	7	Eluate 1 + 2	1.51	<0.031	<0.77	6.89	13.6	<1.0	48.4	<1.3	0.91	<34
3a	MOE1	14	Eluate 1 + 2	1.95	<0.031	<0.77	5.76	13.4	<1.0	51.3	<1.3	0.98	<34
3b	MOE1	28	Eluate 1 + 2	2.13	<0.031	<0.77	5.76	10.9	<1.0	47.1	<1.3	0.82	<34
3b	MOE1	28*	Eluate 1 + 2	1.06	<0.031	<0.77	6.11	12.8	<1.0	53.7	<1.3	1.03	<34
2a	Blank	-	Eluate 1 + 2	<0.51	<0.84	<1.6	<0.30	<0.80	11.2	11.2	<1.6	<2.7	<21
2b	Blank	-	Eluate 1 + 2	<0.36	<0.036	<0.77	<0.30	<0.49	<0.10	<0.32	<1.3	<0.02	<34
2a	MOE2	8	Eluate 1 + 2	8.39	<0.84	<1.6	21.3	<0.80	12.0	2.07	<1.6	1600	135
2b	MOE2	7	Eluate 1 + 2	4.37	<0.031	<0.77	522	<0.49	<0.10	1.51	<1.3	1190	<34
2a	MOE3	8	Eluate 1 + 2	674	<0.84	<1.6	<0.30	<0.80	9.03	693	<1.6	<2.7	535

Experiment	Code	Storage period in d	Sample	Ba	Cd	Cr	Mn	Mo	Sn	Sr	V	Co	Al
				in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$
2b	MOE3	7	Eluate 1 + 2	1910	<0.031	1.01	<0.30	<0.49	1.02	1480	<1.3	0.56	494
2a	MOE4	7	Eluate 1 + 2	29.5	<0.84	5.47	<0.30	7.28	10.5	231	<1.6	<2.7	31900
2b	MOE4	7	Eluate 1 + 2	33.5	<0.031	3.76	<0.30	5.52	0.36	349	<1.3	0.13	16900
2a	MOE5	10	Eluate 1 + 2	1.45	<0.84	<1.6	<0.30	<0.80	976	<0.54	<1.6	<2.7	<21
2b	MOE5	7	Eluate 1 + 2	1.52	<0.031	<0.77	<0.30	<0.49	725	<0.32	<1.3	<0.02	<34
2a	MOE6	11	Eluate 1 + 2	17.8	<0.84	<1.6	0.38	<0.80	80.3	5.51	<1.6	<2.7	33.8
2b	MOE6	7	Eluate 1 + 2	11.6	<0.031	<0.77	<0.30	<0.49	31.4	2.41	<1.3	<0.02	<34
2a	MOE7	7	Eluate 1 + 2	6.74	<0.84	<0.77	1320	<0.80	10.4	1.00	<1.6	<2.7	74.9
3a	MOE7	7	Eluate 1 + 2	3.03	<0.031	<0.77	599	<0.49	<1.0	<0.32	<1.3	<1.3	45.4
3a	MOE7	14	Eluate 1 + 2	5.28	<0.031	<0.77	655	<0.49	<1.0	1.89	<1.3	<1.3	37.6
3b	MOE7	28	Eluate 1 + 2	1.59	<0.031	<0.77	722	<0.49	<1.0	<0.32	<1.3	<1.3	<34
3b	MOE7	28*	Eluate 1 + 2	1.60	<0.031	<0.77	850	<0.49	<1.0	<0.32	<1.3	<1.3	<34
2a	MOE8	12	Eluate 1 + 2	1.18	<0.84	<1.6	0.32	<0.80	18.4	2.25	<1.6	<2.7	<21
2b	MOE8	7	Eluate 1 + 2	1.62	<0.031	<0.77	<0.30	<0.49	1.20	<0.32	<1.3	<0.02	<34

## Results from ICP-OES analysis (part 2)

Eluates 1 + 2 originate from DSLT, Fractions L/S 2 originate from percolation tests, 28\* test specimens were covered by cling film during storage

Experiment	Code	Storage period in d	Sample	Ca in $\mu\text{g L}^{-1}$	Fe in $\mu\text{g L}^{-1}$	K in $\mu\text{g L}^{-1}$	Mg in $\mu\text{g L}^{-1}$	Na in $\mu\text{g L}^{-1}$	B in $\mu\text{g L}^{-1}$	P in $\mu\text{g L}^{-1}$	S in $\mu\text{g L}^{-1}$	Si in $\mu\text{g L}^{-1}$	Ti in $\mu\text{g L}^{-1}$
1	Blank	-	Eluate 1 + 2	<80	<62	<77	<95	<171	<93	<19	<23	<250	<8400
1	MOE1	12	Eluate 1 + 2	2190	<62	630	1190	6300	<93	<19	35900	812	<8400
1	Blank	-	Blind column	190	<62	<77	<95	650	<93	<19	43.4	366	<8400
1	MOE1	46	L/S 2 fraction	5060	<62	3080	2250	19200	<93	45.7	91800	1690	<8400
3a	Blank	-	Eluate 1 + 2	<67	<86	<167	<51	<2950	<11	<13	<13	<4930	<2460
3b	Blank	-	Eluate 1 + 2	<67	<86	<167	<51	<2950	<11	<13	24.3	<4930	<2460
3a	MOE1	7	Eluate 1 + 2	1960	<86	776	468	11100	<11	24.5	46300	<4930	<2460
3a	MOE1	14	Eluate 1 + 2	1980	<86	713	485	10200	<11	22.2	43200	<4930	<2460
3b	MOE1	28	Eluate 1 + 2	2250	<86	<167	501	9200	<11	20.0	38700	<4930	<2460
3b	MOE1	28*	Eluate 1 + 2	1749	<86	<167	301	7857	<11	30.8	44300	<4930	<2460
2a	Blank	-	Eluate 1 + 2	<31	<43	<155	<24	<4050	<14	<67	<16	<50	<3990
2b	Blank	-	Eluate 1 + 2	<67	<86	<167	<51	4120	<11	<13	<13	<4930	<2460
2a	MOE2	8	Eluate 1 + 2	624	<43	377	81.8	<3990	<14	<67	40.5	299	<3990
2b	MOE2	7	Eluate 1 + 2	618	<86	352	57.2	3974	<11	<13	22.1	<4930	<2460
2a	MOE3	8	Eluate 1 + 2	189000	<43	106000	29.8	8490	<14	<67	1310	1870	<3990
2b	MOE3	7	Eluate 1 + 2	308000	<86	106000	52.6	4820	<11	<13	1399	<4930	<2460

Experiment	Code	Storage period in d	Sample	Ca	Fe	K	Mg	Na	B	P	S	Si	Ti
				in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$	in $\mu\text{g L}^{-1}$
2a	MOE4	7	Eluate 1 + 2	45700	<43	10600	<24	25300	<14	<67	17700	823	<3990
2b	MOE4	7	Eluate 1 + 2	66700	<86	96000	<51	27700	<11	<13	12800	<4930	<2460
2a	MOE5	10	Eluate 1 + 2	170	<43	<155	<24	<3990	<14	<67	82.6	<50	<3990
2b	MOE5	7	Eluate 1 + 2	101	<86	<167	<51	4042	<11	<13	19.2	<4930	<2460
2a	MOE6	11	Eluate 1 + 2	919	<43	210	91.8	<3990	<14	<67	1082	139	<3990
2b	MOE6	7	Eluate 1 + 2	214	<86	<167	61.5	4370	<11	20	194	<4930	<2460
2a	MOE7	7	Eluate 1 + 2	282	<43	<155	60.8	<3990	<14	<67	48	92	<3990
3a	MOE7	7	Eluate 1 + 2	147	<86	<167	<51	4540	<11	30.6	28.3	<4930	<2460
3a	MOE7	14	Eluate 1 + 2	2240	<86	<167	<51	4720	<11	29.9	22.0	<4930	<2460
3b	MOE7	28	Eluate 1 + 2	163	<86	<167	<51	<2960	<11	30.7	24.2	<4930	<2460
3b	MOE7	28*	Eluate 1 + 2	133	<86	<167	<51	<2960	<11	30.0	20.6	<4930	<2460
2a	MOE8	12	Eluate 1 + 2	1520	<43	<155	<24	<3990	<14	<67	38.9	<50	<3990
2b	MOE8	7	Eluate 1 + 2	<67	<86	<167	<51	5060	<11	<13	6.98	<4930	<2460

## Results from ICP-MS analysis

Eluates 1 + 2 originate from DSLT, Fractions L/S 2 originate from percolation tests, 28\*: test specimens were covered by cling film during storage

Experiment	Code	Storage period in d	Sample	As in $\mu\text{g L}^{-1}$	Cu in $\mu\text{g L}^{-1}$	Hg in $\mu\text{g L}^{-1}$	Ni in $\mu\text{g L}^{-1}$	Pb in $\mu\text{g L}^{-1}$	Sb in $\mu\text{g L}^{-1}$	Zn in $\mu\text{g L}^{-1}$	Se in $\mu\text{g L}^{-1}$	Tl in $\mu\text{g L}^{-1}$
1	Blank	-	Eluate 1 + 2	<0.03	<0.77	0.084	64.3	0.12	0.78	10.6	<0.18	<0.022
1	MOE1	12	Eluate 1 + 2	0.148	7.89	<0.05	5.42	3.89	0.43	105	1.88	<0.022
1	Blank	-	Blind column	0.31	13.6	0.42	29.0	0.72	0.36	14.8	0.40	<0.022
1	MOE1	46	L/S 2 fraction	0.78	38.6	<0.05	8.72	6.74	0.28	236	<0.18	<0.022
3a	Blank	-	Eluate 1 + 2	<0.084	5.60	<0.048	<2.5	<0.34	<0.050	<7.7	<0.46	<0.014
3b	Blank	-	Eluate 1 + 2	<0.084	<1.56	<0.048	<2.5	<0.34	<0.050	19.0	<0.46	<0.014
3a	MOE1	7	Eluate 1 + 2	0.52	5.85	<0.048	<2.5	2.31	0.42	<7.7	<0.46	<0.014
3a	MOE1	14	Eluate 1 + 2	0.45	5.68	<0.048	<2.5	2.74	0.39	10.6	<0.46	<0.014
3b	MOE1	28	Eluate 1 + 2	0.38	11.4	<0.048	<2.5	2.86	<0.050	<7.7	<0.46	<0.014
3b	MOE1	28*	Eluate 1 + 2	0.40	9.88	<0.048	<2.5	2.84	<0.050	<7.7	<0.46	<0.014
2a	Blank	-	Eluate 1 + 2	<0.030	<0.084	<0.050	<0.15	0.01	<0.034	0.63	<0.18	<0.022
2b	Blank	-	Eluate 1 + 2	<0.084	<1.5	<0.048	<2.5	<0.34	<0.050	<7.7	<0.46	<0.014
2a	MOE2	8	Eluate 1 + 2	0.22	11.7	<0.050	1.72	1.11	<0.034	5.99	<0.18	<0.022
2b	MOE2	7	Eluate 1 + 2	0.16	39	<0.048	<2.5	54.3	0.10	60.0	<0.46	<0.014
2a	MOE3	8	Eluate 1 + 2	<0.030	3.76	<0.050	30.68	0.15	<0.034	8.76	<0.18	<0.022
2b	MOE3	7	Eluate 1 + 2	0.10	5.14	0.11	<2.5	<0.34	1.56	8.76	<0.46	<0.014



Experiment	Code	Storage period in d	Sample	As in $\mu\text{g L}^{-1}$	Cu in $\mu\text{g L}^{-1}$	Hg in $\mu\text{g L}^{-1}$	Ni in $\mu\text{g L}^{-1}$	Pb in $\mu\text{g L}^{-1}$	Sb in $\mu\text{g L}^{-1}$	Zn in $\mu\text{g L}^{-1}$	Se in $\mu\text{g L}^{-1}$	Tl in $\mu\text{g L}^{-1}$
2a	MOE4	7	Eluate 1 + 2	<0.030	2.34	<0.050	5.03	0.02	0.26	5.33	<0.18	<0.022
2b	MOE4	7	Eluate 1 + 2	<0.084	1.84	0.11	<2.5	<0.34	1.20	<7.7	<0.46	<0.014
2a	MOE5	10	Eluate 1 + 2	<0.030	1.68	<0.050	5.84	0.03	<0.034	1.71	<0.18	<0.022
2b	MOE5	7	Eluate 1 + 2	<0.084	2.62	<0.048	<2.5	1.61	0.12	<7.7	<0.46	<0.014
2a	MOE6	11	Eluate 1 + 2	0.55	16.2	<0.050	10.0	0.23	<0.034	5.90	<0.18	<0.022
2b	MOE6	7	Eluate 1 + 2	0.23	10.3	<0.048	<2.5	<0.34	<0.050	<7.7	<0.46	<0.014
2a	MOE7	7	Eluate 1 + 2	<0.030	3.77	<0.050	4.49	0.52	0.27	5.65	<0.18	<0.022
3a	MOE7	7	Eluate 1 + 2	<0.084	3.75	<0.048	<2.5	1.66	0.40	<7.7	<0.46	<0.014
3a	MOE7	14	Eluate 1 + 2	<0.084	8.81	<0.048	<2.5	1.73	0.18	<7.7	<0.46	<0.014
3b	MOE7	28	Eluate 1 + 2	0.09	15.38	<0.048	5.54	4.41	<0.050	<7.7	<0.46	<0.014
3b	MOE7	28*	Eluate 1 + 2	<0.084	<1.496	<0.048	3.25	1.81	<0.050	<7.7	<0.46	<0.014
2a	MOE8	12	Eluate 1 + 2	<0.030	4.42	<0.050	2.51	0.03	<0.034	1.16	<0.18	<0.022
2b	MOE8	7	Eluate 1 + 2	<0.084	1.80	<0.048	<2.5	<0.34	<0.050	<7.7	<0.46	<0.014

### SI 8: Comparison of emissions from MOE1 in DSLT and percolation test

Data for 5 independent DSLT experiments are summarized. The complete sets of data are given under SI 5, 6, 7 and 11.

Component	Concentration in mg L <sup>-1</sup>		Emission in mg m <sup>-2</sup>	Emission in mg kg <sup>-2</sup>	
	DSLT (mean)	Percolation	DSLT (mean)	DSLT (mean)	Percolation
TOC	390	1300	19400	3500	2600
TN	73	270	3700	670	540
Cl <sup>-</sup>	3,1	9.8	150	28	20
Br <sup>-</sup>	0,3	1.4	15	3	3
SO <sub>4</sub> <sup>2-</sup>	43	5.4	2200	400	11
4-tert-Butylphenol	6.1	22	300	56	44
1,3-Benzene- dimethanamine	27	200	1350	240	400
<i>N,N</i> -Dimethyl-1- dodecanamine	0.3	1.2	13	2	2
	Concentration in µg L <sup>-1</sup>		Emission in µg m <sup>-2</sup>	Emission in µg kg <sup>-2</sup>	
As	0.38	0.78	19	3.4	1.6
Ba	1.7	26	87	16	52
Cu	8.2	39	410	76	77
Mn	5.6	41	280	51	83
Mo	10	4.8	520	95	10
Pb	2.9	6.4	150	27	14

n = 5 for DSLT and n = 1 for percolation test

### SI 9: Results from ecotoxicity test on eluates from joint grouts

Eluates 1 + 2 originate from DSLTs, fraction L/S 2 originates from a percolation test, 28\*: test specimens were covered by cling film during storage, Comments: 1) Data from repeated tests are given in brackets. During the first experiments on MOE1 only a limited number of dilutions was tested to estimate the ranges of toxicity while the repeated tests were performed with complete sets of dilutions. This can explain differences between both tests. LIDs could be estimated more precisely from the results of the second test.

2) Ames test: can also indicate cytotoxicity

3) Algae tests for MOE2 to MOE 8 were performed using eluates from a repeated DSLT (experiments 2b and 3a) since effects on algae (LID > 6) were observed for the blank sample from experiment 2a.

Experiment	Code	Storage period in d	Sample	Algae LID <sub>A</sub>	Daphnia LID <sub>D</sub> 48 h	Fish egg LID <sub>Egg</sub>	Luminescent bacteria LID <sub>lb</sub>	Umu LID <sub>EU</sub>	Ames
1	Blank	-	Eluate 1 + 2	≤2	≤2	≤2	≤2	≤1,5	1
1	MOE1	12	Eluate 1 + 2	384 (1536)	96 (64)	12 (8)	3072 (2048)	3 (3)	1
1	Blank	-	Blind column	≤2	≤2	≤2	≤2	≤1,5	1
1	MOE1	46	L/S 2 fraction	3072 (3072)	512 (256)	32 (24)	16384 (12288)	6 (6)	1
3a	Blank	-	Eluate 1 + 2	≤2	≤2	n.d.	≤2	n.d.	n.d.
3b	Blank	-	Eluate 1 + 2	≤2	≤2	n.d.	≤2	n.d.	n.d.
3a	MOE1	7	Eluate 1 + 2	384	64	n.d.	1536	n.d.	n.d.
3a	MOE1	14	Eluate 1 + 2	384	64	n.d.	2048	n.d.	n.d.
3b	MOE1	28	Eluate 1 + 2	384	192	n.d.	2048	n.d.	n.d.
3b	MOE1	28*	Eluate 1 + 2	384	128	n.d.	2048	n.d.	n.d.
2a	Blank	-	Eluate 1 + 2	n.d.	≤2	≤2	≤2	≤1,5	1

Experiment	Code	Storage period in d	Sample	Algae LID <sub>A</sub>	Daphnia LID <sub>D</sub> 48 h	Fish egg LID <sub>Egg</sub>	Luminescent bacteria LID <sub>lb</sub>	Umu LID <sub>EU</sub>	Ames
2b	Blank	-	Eluate 1 + 2	≤2	n.d.	n.d.	n.d.	n.d.	n.d.
2a	MOE2	8	Eluate 1 + 2	n.d.	≤2	≤2	16	≤1,5	1
2b	MOE2	7	Eluate 1 + 2	32	n.d.	n.d.	n.d.	n.d.	n.d.
2a	MOE3	8	Eluate 1 + 2	n.d.	≤2	≤2	≤2	≤1,5	≥2
2b	MOE3	7	Eluate 1 + 2	3	n.d.	n.d.	n.d.	n.d.	n.d.
2a	MOE4	7	Eluate 1 + 2	n.d.	4	≤2	≤2	≤1,5	2
2b	MOE4	7	Eluate 1 + 2	inconsistent	n.d.	n.d.	n.d.	n.d.	n.d.
2a	MOE5	10	Eluate 1 + 2	n.d.	3	≤2	≤2	≤1,5	1
2b	MOE5	7	Eluate 1 + 2	4	n.d.	n.d.	n.d.	n.d.	n.d.
2a	MOE6	11	Eluate 1 + 2	n.d.	192	16	96	≤6	1
2b	MOE6	7	Eluate 1 + 2	3072	n.d.	n.d.	n.d.	n.d.	n.d.
2a	MOE7	7	Eluate 1 + 2	n.d.	3	≤2	24	≤1,5	1
3a	MOE7	7	Eluate 1 + 2	8	≤2	n.d.	24	n.d.	n.d.
3a	MOE7	14	Eluate 1 + 2	8	≤2	n.d.	24	n.d.	n.d.
3b	MOE7	28	Eluate 1 + 2	12	≤2	n.d.	24	n.d.	n.d.
3b	MOE7	28*	Eluate 1 + 2	8	≤2	n.d.	24	n.d.	n.d.

Experiment	Code	Storage period in d	Sample	Algae LID <sub>A</sub>	Daphnia LID <sub>D</sub> 48 h	Fish egg LID <sub>Egg</sub>	Luminescent bacteria LID <sub>lb</sub>	Umu LID <sub>EU</sub>	Ames
2a	MOE8	12	Eluate 1 + 2	n.d.	≤2	≤2	≤2	≤1,5	1
2b	MOE8	7	Eluate 1 + 2	≤2	n.d.	n.d.	n.d.	n.d.	n.d.

## SI 10: Results from GC-MS Screening at BAM

Substances that were tentatively identified in dichloromethane extracts (extracted at pH 2 and pH 10) from eluates of grouts (MOE1 and MOE6: epoxy resin-based, MOE2 and MOE7: polybutadiene-based). Selection criteria: compliance of observed and library mass at least 85 %. Only benzyl alcohol was identified in eluates of MOE3 and MOE4 (modified cement) and MOE5 and MOE8 (polyurethane-based). Substances printed in bold types were confirmed by reference substances.

\*Data from ECHA page on registered substances, <https://echa.europa.eu/de/information-on-chemicals/registered-substances>, assessed on 2022-06-21

Substance	CAS	MOE1	MOE6	MOE2	MOE7	H-phrases* Environmental hazards	H-phrases* Health hazards	Total tonnage band* in t per year
1-Methyl-3-propylcyclohexane (or structural isomer)	4291-80-9			x				no entry
Benzaldehyde	100-52-7	x	x				H302	10.000 - 100.000
1-(2-Methoxy-1-methylenethoxy)-2-propanol	20324-32-7			x				no entry
<b>Benzyl alcohol</b>	100-51-6	x	x	x	x		H302, H332	10.000 - 100.000
Methyl phenol	95-48-7	x				H412	H301, H311, H314	10.000 - 100.000
<b>2-Ethylhexanoic acid</b>	149-57-5			x	x		H361	10.000 - 100.000
2,2,4-Trimethylhexane-1,6-diamine	25513-64-8	x					H302, H314, H317	1.000 - 10.000
<b>4-tert-Butylphenol</b>	98-54-4	x				H410	H315, H318, H361	10.000 - 100.000
1,3-Cyclohexanedimethanamine	2579-20-6		x			H412	H302, H312, H314	1.000 - 10.000

Substance	CAS	MOE1	MOE6	MOE2	MOE7	H-phrases* Environmental hazards	H-phrases* Health hazards	Total tonnage band*  in t per year
3-Aminomethyl-3,5,5-trimethylcyclohexylamine	2855-13-2		x				H302, H314, H317	10.000 - 100.000
<b>1,3-Benzenedimethanamine</b>	1477-55-0	x	x			H412	H302, H332, H314, H317	10.000 - 100.000
Methyl 9-oxononanoate	1931-63-1				x			no entry
2-(2-Butoxyethoxy)-ethanol	112-34-5	x					H319	10.000 - 100.000
Nonyl-cyclopropan	74663-85-7		x					no entry
<i>N,N</i> -Dimethyl-1-dodecanamine	112-18-5	x				H410	H302, H314	100 - 1.000
<i>p</i> -Tolyl glycerol	17131-24-7	x						no entry
5-(1-Hydroxyhexyl)-tetrahydrofuran-2-one	1000131-83-9			x				no entry
Isopropyl laurate	10233-13-3			x	x			1.000 - 10.000
4-Dodecanol	10203-32-4				x			no entry
<i>N,N</i> -Dimethyl-1-tetradecanamine	112-75-4	x				H410	H302, H314	100 - 1.000
2-[(Dodecyloxy)methyl]-oxiran	2461-18-9		x					no entry

**SI 11: Results for selected organic substances in eluates of MOE1 and MOE 7 after different duration of storage of test specimens before leaching tests**

Eluates originate from DSLT (combined sample of eluate 1 and 2), 28\*: test specimens were covered by cling film during storage, the substances were not detected in the blank samples

Experiment	Code	Storage in d	Benzyl alcohol in mg l <sup>-1</sup>	4-tert-Butyl- phenol in mg l <sup>-1</sup>	1,3-Benzol- dimethanamin in mg l <sup>-1</sup>	Dodecyldimethyl- amine in mg l <sup>-1</sup>	2-Ethyl-hexanoic acid in mg l <sup>-1</sup>
1	MOE1	12	10.1	7.8	49.8	0.4	
3a	MOE1	7	15.2	3.0	27.4	0.11	
3a	MOE1	14	10.7	7.7	22.2	0.32	
3b	MOE1	28	2.9	4.4	17.4	0.19	
3b	MOE1	28*	3.8	7.4	18.2	0.28	
2a	MOE7	7	n.d.				4.2
3a	MOE7	7	7.74				7.0
3a	MOE7	14	0.06				4.5
3b	MOE7	28	0.05				2.7
3b	MOE7	28*	0.05				4.2



## SI 12: Data from TZW

**Table SI 12-1: Results for sample MOE1 in percolation test eluate (experiment 1\*, see SI 4)**

Green mark in the LC column: Identification level "probable substance". All conditions were fulfilled.

Yellow marking in LC column: Identification level "signal of a substance" means that no hit was found by MS2 spectral database comparison. Reason may be: missing reference spectrum or no measured MS2 spectrum).

#	Substance	CAS-number	Molweight in g mol <sup>-1</sup>	List	LC <sub>NIST</sub>	LC	GC
1	Benzaldehyd	100-52-7	106	GC <sub>NIST</sub>			
2	Benzylalkohol	100-51-6	108	GC <sub>NIST</sub>			
3	Methylphenol	95-48-7	108	GC <sub>NIST</sub>			
4	2-Butoxyethanol	111-76-2	118	GC <sub>NIST</sub>			
5	4-tert-Butylphenol	98-54-4	150	GC <sub>NIST</sub>			
6	<i>N,N</i> -Dibutylformamid	761-65-9	157	Lacke	•		
7	2-(Benzyloxy)propanal	53346-05-7	164	Dachfolie	•		
8	2-Phenylbutyric acid	90-27-7	164	LC <sub>NIST</sub>	•		
9	3-Phenylbutyric acid	4593-90-2	164	LC <sub>NIST</sub>	•		
10	Glycidyl-2-methylphenylether	2210-79-9	164	GC <sub>NIST</sub>			
11	2-Mercaptobenzothiazole	149-30-4	167	LC <sub>NIST</sub>	•		
12	Benzylphosphonic acid	6881-57-8	172	LC <sub>NIST</sub>	•		
13	p-Toluenesulfonic acid	104-15-4	172	LC <sub>NIST</sub>	•		
14	2-(Benzylmethylamino)ethanol N-oxide	15831-63-7	181	LC <sub>NIST</sub>	•		
15	3-(Octylamino)propionitril	29504-89-0	182	GC <sub>NIST</sub>			
16	Tripropylene glycol (PPG-3)		192	Lacke	•		
17	Tetraethylene glycol (PEG-4)	112-60-7	194	Lacke	•		
18	Sebacic acid	111-20-6	202	LC <sub>NIST</sub>	•		
19	<i>N,N</i> -Dimethyl-n-dodecylamin	112-18-5	213	GC <sub>NIST</sub>			
20	Laurylguanidine	112-65-2	227	LC <sub>NIST</sub>	•		
21	3-Ethyl-5-methylphenyl trifluoracetate		232	Dachfolie			

22	4-Amino-7-diethylamino-chromen-2-one	107995-76-6	232	Dachfolie			
23	Tetrapropylene glycol (PPG-4)		250	Lacke	•		
24	2,2,4-Trimethyl-1,3-pentandiol diisobutyrate	6846-50-0	286	Lacke	•		
25	Benzylododecyldimethylammonium cation	7281-04-1	303	LC <sub>NIST</sub>	•		
26	Clomipramine	303-49-1	314	LC <sub>NIST</sub>	•		
27	2-Ethylhexyl maleate	142-16-5	340	Lacke			
28	Bis(2-ethylhexyl)-(2E)-2-butendioat	141-02-6	340	Lacke			
29	Hexapropylene glycol (PPG-6)	74388-92-4	366	Lacke	•		
30	Heptapropylene glycol (PPG-7)	14362-16-4	424	Lacke	•		
31	Octapropylene glycol (PPG-8)	25322-69-4	482	Lacke	•		
32	Nonapropylene glycol (PPG-9)	2172326-56-4	540	Lacke	•		
33	Decapropylene glycol (PPG-10)	25322-69-4	598	Lacke	•		

**Table SI 12-2: Results for sample MOE1 in DSLT eluate (experiment 1, see SI 4)**

#	Substance	CAS-number	Molweight in g mol <sup>-1</sup>	List	LC <sub>NIST</sub>	LC	GC
1	Benzaldehyd	100-52-7	106	GC <sub>NIST</sub>			
2	Benzylalkohol	100-51-6	108	GC <sub>NIST</sub>			
3	Methylphenol	95-48-7	108	GC <sub>NIST</sub>			
4	2-Phenylacetamide	103-81-1	135	Dachfolie			
5	3-Propionylperazine	1570-48-5	135	LC <sub>NIST</sub>	•		
6	Propylphenol	644-35-9	136	GC <sub>NIST</sub>			
7	Octanic acid	124-07-2	144	Lacke	•		
8	o-Propylanisol	13629-73-7	150	GC <sub>NIST</sub>			
9	4-tert-Butylphenol	98-54-4	150	GC <sub>NIST</sub>			
10	<i>N,N</i> -Dibutylformamid	761-65-9	157	Lacke			
11	2-Phenylbutyric acid	90-27-7	164	LC <sub>NIST</sub>	•		
12	3-Phenylbutyric acid	4593-90-2	164	LC <sub>NIST</sub>	•		

13	2-(Benzyloxy)propanal	53346-05-7	164	Dachfolie			
14	2-Mercaptobenzothiazole	149-30-4	167	LC <sub>NIST</sub>	•		
15	Benzyolphosphonic acid	6881-57-8	172	LC <sub>NIST</sub>	•		
16	p-Toluenesulfonic acid	104-15-4	172	LC <sub>NIST</sub>	•		
17	2-(Benzylmethylamino)ethanol N-oxide	15831-63-7	181	LC <sub>NIST</sub>	•		
18	Tripropylene glycol (PPG-3)		192	Lacke	•		
19	Tetraethylene glycol (PEG-4)	112-60-7	194	Lacke	•		
20	3,4-Dihydroxymandelic acid	775-01-9	202	LC <sub>NIST</sub>	•		
21	Sebacic acid	111-20-6	202	LC <sub>NIST</sub>	•		
22	Laurylguanidine	112-65-2	227	LC <sub>NIST</sub>	•		
23	7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione	82304-66-3	276	Dachfolie			
24	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	286	Lacke	•		
25	Benzyldodecyldimethylammonium cation	7281-04-1	303	LC <sub>NIST</sub>	•		
26	Pentapropylene glycol (PPG-5)	21482-12-2	308	Lacke	•		
27	Prostaglandin A1 methyl ester	26771-94-8	310	LC <sub>NIST</sub>	•		
28	2-Ethylhexyl maleate	142-16-5	340	Lacke			
29	Bis(2-ethylhexyl)-(2E)-2-butendioat	141-02-6	340	Lacke			
30	Decamethylcyclopentasiloxane	541-02-6	370	LC <sub>NIST</sub>	•		
31	Decapropylene glycol (PPG-10)	25322-69-4	598	Lacke	•		

**Table SI 12-3: Results for inter-laboratory test sample MOE1 in percolation test (see Heisterkamp et al. 2021)**

#	Substance	CAS-number	Molweight in g mol <sup>-1</sup>	List	LC <sub>NIST</sub>	LC	GC	H-phrases	REACH	Production quantity in t per a
1	3-[N-[2-Diethylaminoethyl]-1-cyclohexenylamino]propyl nitril	959229-47-1	86	GC <sub>NIST</sub>					no	
2	Butoxyethanol	111-76-2	87	GC <sub>NIST</sub>				H302, H315, H319, H332	yes	100 000 - 1 000 000
3	Phenol	108-95-2	94	GC <sub>NIST</sub>				H301, H311, H314, H331, H341, H373, H411	yes	1 000 000 - 10 000 000
4	Benzaldehyd	100-52-7	106	GC <sub>NIST</sub>				H302, H332, H315, H319, H335, H412	yes	10 000 - 100 000

5	Benzylalkohol	100-51-6	108	GC <sub>NIST</sub>			H303, H319, H332	yes	10 000 - 100 000
6	Methylphenol	95-48-7	108	GC <sub>NIST</sub>			H301, H311, H314, H411	yes	10 000 - 100 000
7	m-Xylylendiamin	1477-55-0	117	GC <sub>NIST</sub>			H302, H332, H314, H317, H412	yes	10 000 - 100 000
8	Azabenzimidazol	273-21-2	119	GC <sub>NIST</sub>			H302	yes	1 - 10
9	Benzaldehydoxim	932-90-1	121	GC <sub>NIST</sub>				yes	1 - 10
10	Benzylchlorid	100-44-7	126	GC <sub>NIST</sub>			H302, H315, H317, H318, H331, H335, H340, H350, H373	yes	10 - 100
11	2-(2-Hydroxypropoxy)-1-propanol	106-62-7	134	Lack				no	
12	Dipropylene glycol	25265-71-8	134	Lack				yes	100 000 - 1 000 000
13	N-Methyl-N-benzyltetradecanamin	83690-72-6	134	GC <sub>NIST</sub>				no	
14	2-Phenylacetamide	103-81-1	135	Roof film	•		H302, H319	no	
15	3-Propionylperazine	1570-48-5	135	LC <sub>NIST</sub>				no	
16	2-Phenoxyethanol	122-99-6	138	Lack	•		H302, H319	yes	10000-100000
17	Isophorone	78-59-1	138	LC <sub>NIST</sub>	•		H312, H319, H335, H351, H302	yes	100 - 1 000
18	Octanoic acid	124-07-2	144	Lack	•		H412, H314	yes	10 000 - 100 000
19	Allyl o-tolyl ether	936-72-1	148	GC <sub>NIST</sub>			H302	yes	
20	4-Hydroxy-3-methoxystyrene	7786-61-0	150	Roof film				no	
21	4-Hydroxy-2-methylacetophenone	875-59-2	150	Roof film				no	
22	4-tert-Butylphenol	98-54-4	150	GC <sub>NIST</sub>			H315, H318, H361f, H410	yes	10 000 - 100 000
23	Benzylisothiazolinon	2634-33-5	151	Lack			H400, H411, H302, H315, H318, H317	yes	100 - 1 000
24	N,N-Dibutylformamide	761-65-9	157	Lack			H412	yes	10 - 100
25	Isobutyric acid anhydride	97-72-3	158	Lack			H311, H331, H314	yes	100 - 1 000
26	1-(2-Butoxyethoxy)ethanol	54446-78-5	162	Roof film, Lack				no	
27	Butyldiglycol (PEG-2 Butyl Ether)	112-34-5	162	Roof film, Lack	•			yes	10 000 - 100 000
28	2-Phenylbutyric acid	90-27-7	164	LC <sub>NIST</sub>	•		H302	yes	Intermediate use only
29	3-Phenylbutyric acid	4593-90-2	164	LC <sub>NIST</sub>	•			no	

30	2-(Benzyloxy)propanal	53346-05-7	164	Roof film					no	
31	Glycidyl-2-methylphenylether	2210-79-9	164	GC <sub>NIST</sub>				H315, H317, H341, H411	yes	1000 - 10 000
32	2-Mercaptobenzothiazole	149-30-4	167	LC <sub>NIST</sub>	•			H410, H317	yes	1 000 - 10 000
33	p-Toluenesulfonic acid	104-15-4	172	LC <sub>NIST</sub>	•				yes	100 - 1 000
34	2-(2-Butoxyethoxy)acetic acid	82941-26-2	176	LC <sub>NIST</sub>	•				no	
35	Diisopropylphenol	2934-05-6	178	GC <sub>NIST</sub>				H315, H319, H335	yes	
36	Diisopropylphenol	26886-05-5	178	GC <sub>NIST</sub>					yes	
37	3-(4-Methylphenoxy)-1,2-propandiol	17131-24-7	182	GC <sub>NIST</sub>					no	
38	3-(Octylamino)propionitril	29504-89-0	182	GC <sub>NIST</sub>					yes	1 - 10
39	Dimethyl-benzenesulfonic acid	88-61-9	186	LC <sub>NIST</sub>	•				no	
40	Decyl formate	5451-52-5	186	Lack					no	
41	1-Acetylnaphthalen-8-ol	18528-55-7	189	GC <sub>NIST</sub>					no	
42	Diethoxytetraethylenglycol	4353-28-0	190	GC <sub>NIST</sub>					yes	
43	Tripropylene glycol (PPG-3)	24800-44-0	192	Lack	•				yes	10 000 - 100 000
44	2-Isopropyl-6-tert-butylphenol	22791-95-3	192	GC <sub>NIST</sub>					no	
45	Tetraethylene glycol (PEG-4)	112-60-7	194	Lack	•				yes	100 - 1000
46	Dimethyl-4-isopropyl-naphthalen	483-78-3	198	GC <sub>NIST</sub>					yes	
47	3,4-Dihydroxymandelic acid	775-01-9	202	LC <sub>NIST</sub>	•				no	
48	Sebacic acid	111-20-6	202	LC <sub>NIST</sub>	•				yes	10 000 - 100 000
49	1-Benzyl-3-methylpiperidin-4-one	34737-89-8	203	LC <sub>NIST</sub>	•				no	
50	3-Benzoylpiperazin-2,5-dion	5037-75-2	204	GC <sub>NIST</sub>					no	
51	2-(2-(2-Methoxypropoxy)propoxy)-1-propanol		206	Lack						
52	N,N-Dimethyl-n-dodecylamin	112-18-5	213	GC <sub>NIST</sub>				H302, H314, H410	yes	1 - 10
53	Diphenylmethylphosphine oxide	2129-89-7	216	LC <sub>NIST</sub>	•				no	
54	Diethyl phthalate	84-66-2	222	LC <sub>NIST</sub>	•				yes	1 000 - 10 000
55	Laurylguanidine	112-65-2	227	LC <sub>NIST</sub>	•				no	
56	Dodecanedioic acid	693-23-2	230	LC <sub>NIST</sub>	•			H319	yes	10 000 - 100 000
57	3-Ethyl-5-methylphenyl trifluoroacetate		232	Roof film						

58	Diphenoxypropanol	622-04-8	244	GC <sub>NIST</sub>				H302, H319	yes	1 - 10
59	Tetrapropylene glycol (PPG-4)	24800-25-7	250	Lack	•				no	
60	7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione	82304-66-3	276	Roof film					no	
61	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	286	Lack	•			H412, H361	yes	1 000 - 10 000
62	Bis(phenoxyethoxy)methane	13879-32-8	288	Lack					no	
63	Benzyl dodecyl dimethyl ammonium cation	7281-04-1	303	LC <sub>NIST</sub>	•			Component of biocides	no	
64	1-(1-Pentyl-1H-indol-3-yl)-2-phenyl-ethanone		305	LC <sub>NIST</sub>	•					

**Table SI 12-4: Results for inter-laboratory test sample MOE1 in DSLT (see Heisterkamp et al. 2021)**

#	Substance	CAS-number	Molweight in g mol <sup>-1</sup>	List	LC <sub>NIST</sub>	LC	GC	H-phrases	REACH	Production quantity in t per a
1	Benzaldehyd	100-52-7	106	GC <sub>NIST</sub>				H302, H332, H315, H319, H335, H412	yes	10 000 - 100 000
2	Benzylalkohol	100-51-6	108	GC <sub>NIST</sub>				H303, H319, H332	yes	10 000 - 100 000
3	Methylphenol	95-48-7	108	GC <sub>NIST</sub>				H301, H311, H314, H411	yes	10 000 - 100 000
4	Benzylchlorid	100-44-7	126	GC <sub>NIST</sub>				H302, H315, H317, H318, H331, H335, H340, H350, H373	yes	10 - 100
5	<i>N</i> -Methyl- <i>N</i> -benzyltetradecanamin	83690-72-6	134	GC <sub>NIST</sub>					no	
6	2-Phenylacetamide	103-81-1	135	Roof film	•			H302, H319	no	
7	3-Propionylperazine	1570-48-5	135	LC <sub>NIST</sub>				H302, H312, H332, H315, H319, H335	no	
8	Octanoic acid	124-07-2	144	Lack	•			H412, H314	yes	10 000 - 100 000
9	4-tert-Butylphenol	98-54-4	150	GC <sub>NIST</sub>				H315, H318, H361f, H410	yes	10 000 - 100 000
10	<i>N,N</i> -Dibutylformamide	761-65-9	157	Lack				H412	yes	10 - 100
11	2-Phenylbutyric acid	90-27-7	164	LC <sub>NIST</sub>	•			H302	yes	
12	3-Phenylbutyric acid	4593-90-2	164	LC <sub>NIST</sub>	•				no	
13	2-(Benzyloxy)propanal	53346-05-7	164	Roof film					no	
14	Glycidyl-2-methylphenylether	2210-79-9	164	GC <sub>NIST</sub>				H315, H317, H341, H411	yes	1000 - 10 000
15	2-Mercaptobenzothiazole	149-30-4	167	LC <sub>NIST</sub>	•			H410, H317	yes	1 000 - 10 000
16	<i>p</i> -Toluenesulfonic acid	104-15-4	172	LC <sub>NIST</sub>	•				yes	100 - 1 000

17	3-(Octylamino)propionitril	29504-89-0	182	GC <sub>NIST</sub>					
18	Tripropylene glycol (PPG-3)	24800-44-0	192	Lack	•			yes	10 000 - 100 000
19	Tetraethylene glycol (PEG-4)	112-60-7	194	Lack	•			yes	100 - 1000
20	Sebacic acid	111-20-6	202	LC <sub>NIST</sub>	•			yes	10 000 - 100 000
21	<i>N,N</i> -Dimethyl- <i>n</i> -dodecylamin	112-18-5	213	GC <sub>NIST</sub>			H302, H314, H410	yes	1 - 10
22	Diphenoxypropanol	622-04-8	244	GC <sub>NIST</sub>			H302, H315, H319, H335	yes	
23	Tetrapropylene glycol (PPG-4)	24800-25-7	250	Lack	•			no	
24	Octapropylene glycol (PPG-8)	25322-69-4	482	Lack	•			yes	10 000 - 100 000

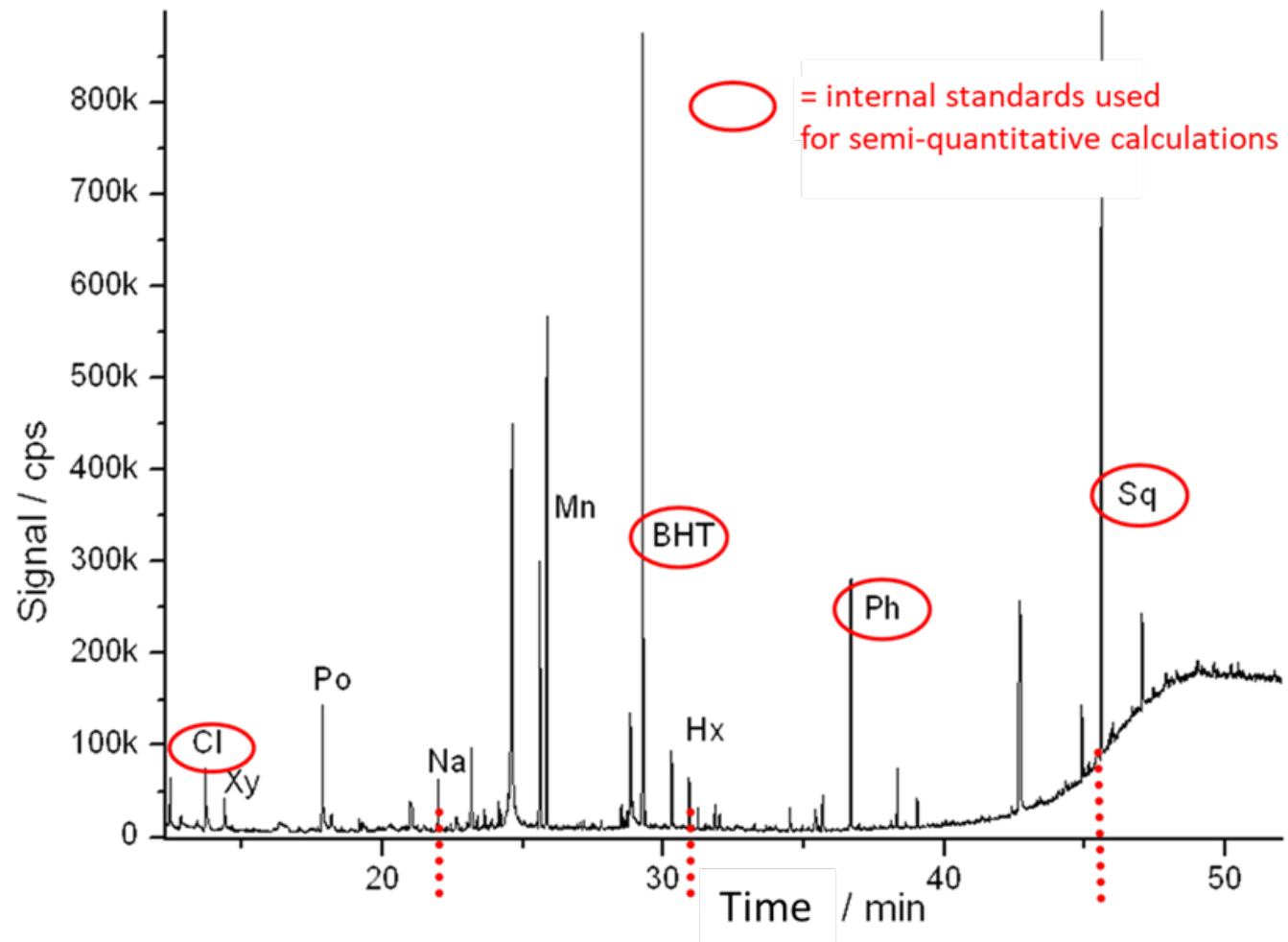


Figure SI 12-1: GC-MS chromatogram of the laboratory blank with spiked internal standards. Standards used for the evaluation of the semi-quantitative determinations are outlined in red.



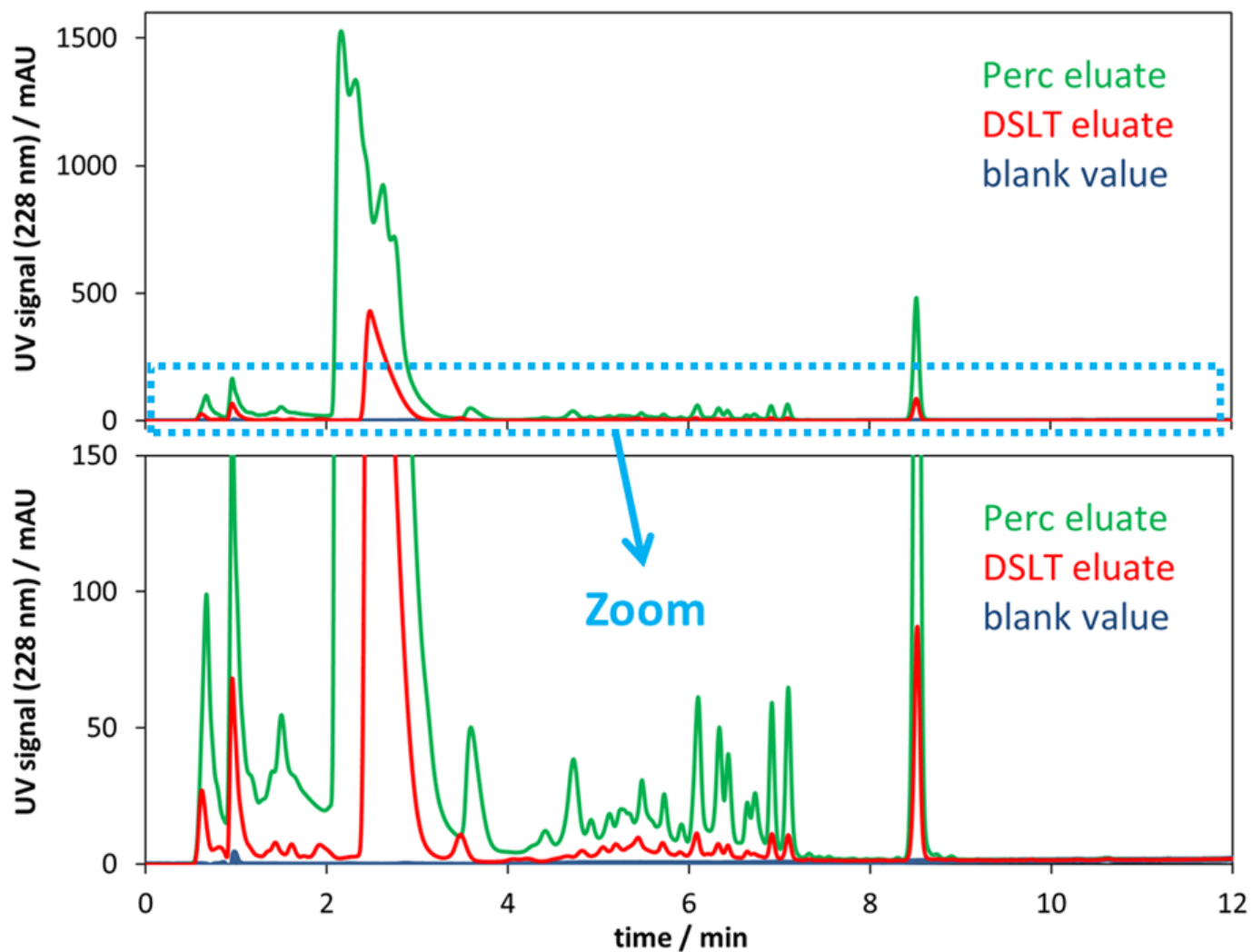


Figure SI 12-2: LC-DAD measurement of the two eluates of sample MOE1 and the laboratory blank sample (20  $\mu$ L injection volume). The perc eluate has significantly higher signals compared to the DSLT-eluate. The measurement serves only for the qualitative comparison of the samples. No standards were used for a possible elucidation of the signals.

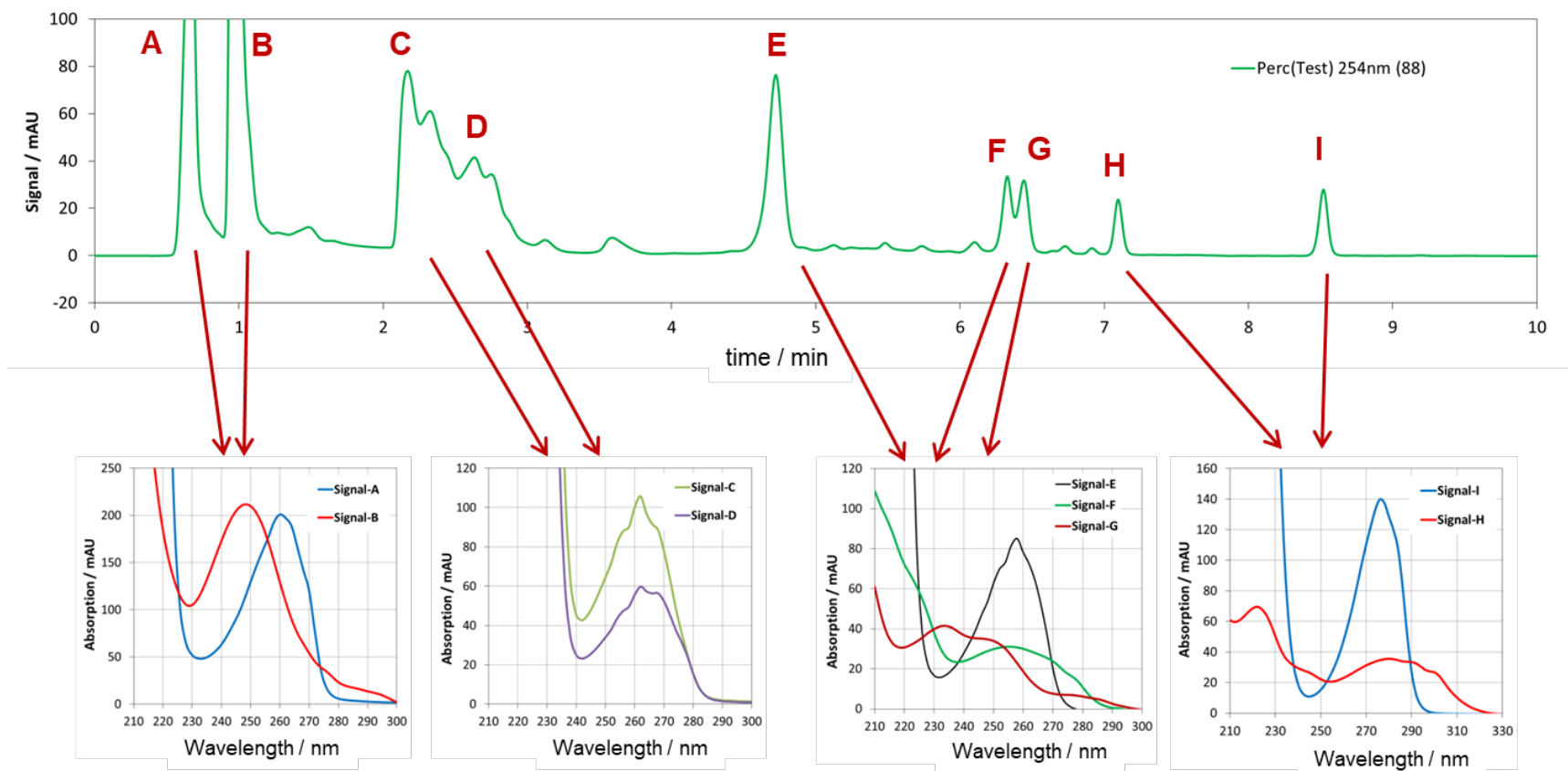


Figure SI 12-3: Top: LC-DAD-chromatogram of the perc eluate of MOE1 at a detection wavelength of 254 nm. Bottom: Extracted spectra from selected signals.

## References

Heisterkamp I, Ratte M, Schoknecht U, Gartiser S, Kalbe U, Ilvonen O (2021) Ecotoxicological evaluation of construction products: inter-laboratory test with DSLT and percolation test eluates in an aquatic biotest battery. *Environ Sci Eur* 33:75, 1-14. doi.org/10.1186/s12302-021-00514-x