

# Investigating the ecotoxicity of construction product eluates as multicomponent mixtures

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## Additional information

### SI 1: Basic analysis methods

TOC and TN were determined by a TOC-VCPH Analyzer (NDIR detector, Shimadzu) according to DIN EN 1484 [36]. The pH was determined according to DIN EN ISO 10523:2012 [37] using a SenTix41 or Sentix81 pH electrode (WTW), conductivity was determined according to DIN EN 27888 [38] using a TetraCON<sup>®</sup> 96 or TetraCon<sup>®</sup> 325 electrode (WTW), and turbidity was determined by a 2100AN IS turbidimeter (Hach) according to DIN EN ISO 7027 [39].

### SI 2: Inorganic anions and cations methods

The concentrations of anions in the eluates were determined by ion chromatography according to DIN EN ISO 10304-1 [40] by an 883 Basic C plus ion chromatograph (Metrohm) using a Metrosep A Supp 5 (250 mm · 4 mm) column. An eluent of carbonate and bicarbonate in water (8 mmol L<sup>-1</sup> and 1 mmol L<sup>-1</sup>) was applied for isocratic separation of the anions.

### Limits of quantification (LOQs) for anions

Anion	LOQ for analysis of DF4 to DF7, F10 to F14, WPC1 to WPC3, MOE1, SG1 to SG3, KG1 to KG3 in mg L <sup>-1</sup>	LOQ for analysis of DM1 to DM10 and WEG in mg L <sup>-1</sup>
F <sup>-</sup>	0,014	0,267
Cl <sup>-</sup>	0,544	0,095
Br <sup>-</sup>	0,010	0,076
NO <sub>2</sub> <sup>-</sup>	0,015	0,105
NO <sub>3</sub> <sup>-</sup>	0,114	0,271
PO <sub>4</sub> <sup>3-</sup>	0,032	0,266
SO <sub>4</sub> <sup>2-</sup>	0,811	0,187

**Limits of quantification (LOQs) for cations**

Cation	LOQ ICP-OES for analysis of DF4 to DF7, F10 to F14, WPC1 to WPC3, MOE1, SG1 to SG3, KG1 to KG3 in $\mu\text{g L}^{-1}$	LOQ ICP-OES for analysis of DM1 to DM10 and WEG in $\mu\text{g L}^{-1}$	LOQ ICP-MS for analysis of DF4 to DF7, F10 to F14, WPC1 to WPC3, MOE1, SG1 to SG3, KG1 to KG3 in $\mu\text{g L}^{-1}$	LOQ ICP-MS for analysis of DM1 to DM10 and WEG in $\mu\text{g L}^{-1}$
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
Hg			0,05	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	474	34		
Ca	80	67		
Fe	62	86		
K	77	167		
Mg	95	51		
Na	171	4120		0,46
B	93	11		
P	19	13		
S	23	13		0,014
Se			0,18	1,50
Si	250	4930		0,05
Ti	8400	2458		
Tl			0,022	

**SI 3: Organic screening methods**

(The following methods are also described in the supplementary information in [35]).

**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  $\mu\text{l}$ ) 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  $\text{L}^{-1}$ ). 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  $\mu\text{L}^{-1}$

d5-Chlorbenzol 20 ng  $\mu\text{L}^{-1}$

d34-Hexadecan 10 ng  $\mu\text{L}^{-1}$

d8-Naphthalin 10 ng  $\mu\text{L}^{-1}$

d10-Phenanthren 20 ng  $\mu\text{L}^{-1}$

d5-Phenol 80 ng  $\mu\text{L}^{-1}$

d62-Squalan 80 ng  $\mu\text{L}^{-1}$

### GC-MS method

GC-MS-System:	Agilent GC/MS-system 6890N
Detector:	Agilent MSD 5973 Network Mass Selective Detector
Column:	Rtx-5MS, 60 m · 0.25 mm ID, 0.25 µm
Carrier gas:	Helium
Flow rate:	He, 1.5 ml 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 [44], 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 · 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  $[M+H]^+$  or  $[M-H]^-$  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 · 2 mm, 3 $\mu$ m, Macherey Nagel)
Injection volume	20 $\mu$ L (direct injection)
Flow	0.45 mL min <sup>-1</sup>
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: Quantitative analysis of selected organic substances

In eluates of the cork granules, selected phenols that were identified in screening tests and available as a reference substance were quantified by BAM. The eluates were diluted in a ratio of 1-to-2 with water, filtered with a 0.2  $\mu$ m regenerated cellulose filter and analyzed by LC-DAD (Agilent Infinity 1290). The separation was carried out on a Poroshell 120 EC-C18 column (100 mm · 4.6 mm, 2.7  $\mu$ m) with pre-column by a gradient of acetonitrile and water (Acetonitrile: 5% for 1 min, then increase to 10% within 4 min, increase to 30% within 4 min, increase to 50% within 2 min, hold for 1 min, lower again to 5% within 3 min) with a flow rate of 0.75 mL min<sup>-1</sup> at 40 °C. The quantification was carried out by means of external calibration on the diode array detector.

For the analysis of isothiazolinones in eluates of sealants and coatings, about 1.2 mL of eluate were filtered with a 0.2  $\mu$ m cellulose filter and quantified using LC-DAD (Agilent Infinity 1290). The separation was carried out as described above, except for a different gradient of acetonitrile and water (Acetonitrile: 10% for 1 min, then increase to 90 % within 4 min, hold for 1 min, lower again to 10% within 0.2 min and hold for 1.8 min).

## SI 5: Results of organic screenings

Figure SI 5a gives an overview of the proportion of H-phrases for the substances found by GC and LC screening.

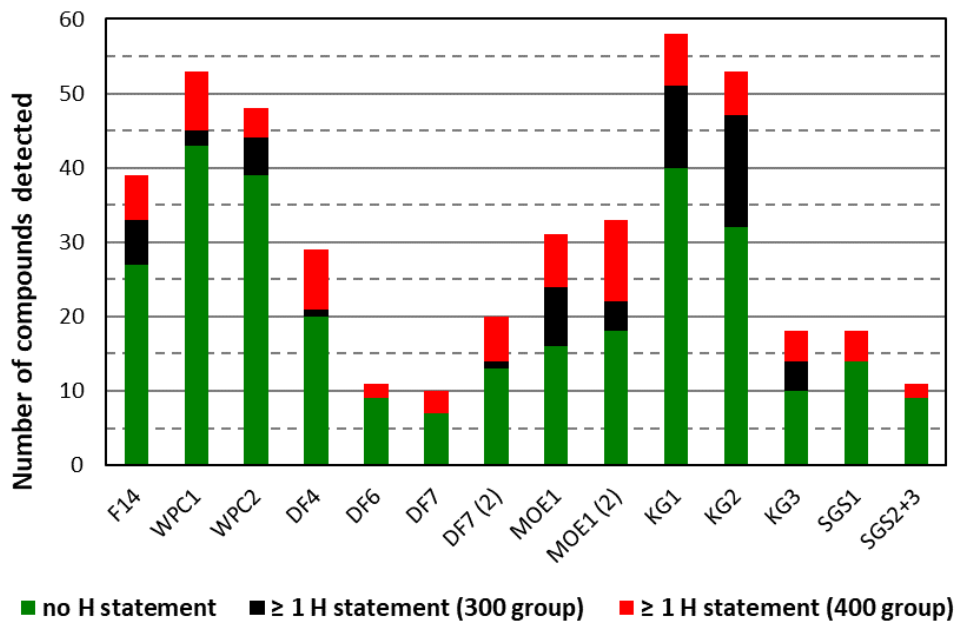


Figure SI 5a: Number of substances without and with H-statements from the 300 and 400 groups.

### Results LC-DAD measurements

Figures 5b, 5c and 5d show examples of the LC-DAD measurements.

The qualitative comparison shows that even with a high injection volume of 100  $\mu\text{L}$ , the signals are comparatively small for the foam glass SG 1 and SG 2/SG 3 with a height of approx. 10 mAU.

In contrast, the cork eluates KG 1, KG 2 and KG 3 showed very large signals. Despite the low injection volume of 5  $\mu\text{L}$ , the signals reach a level of approx. 100 mAU. The broad signal in the range of 4 min to 8 min is probably a combination of many individual compounds that cannot be resolved via the reversed phase separation column.

The comparison of the eluates of the grout MOE1 from two elution techniques shows clearly different signal intensities. Significantly smaller signals are found in the DSLT eluate (i.e. lower contents are contained). This result is consistent with the trends from the screening procedures and the results from the toxicological tests.

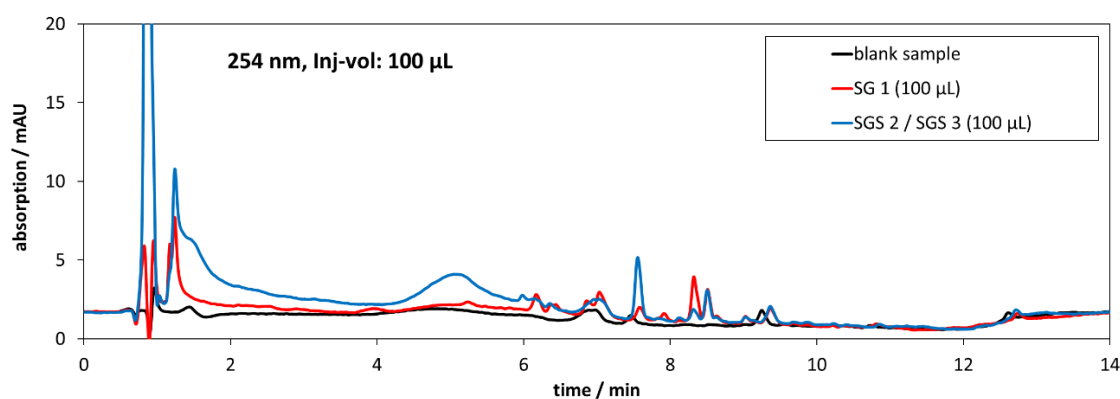
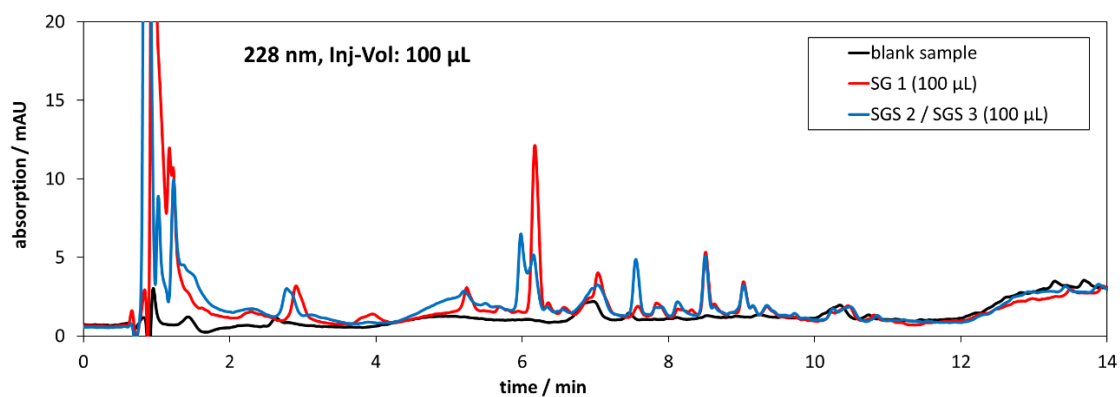


Figure SI 5b: Characterization of eluate samples from form glass aggregates by LC-DAD (sample volume = 100 µL, detection at 228 nm and 254 nm)

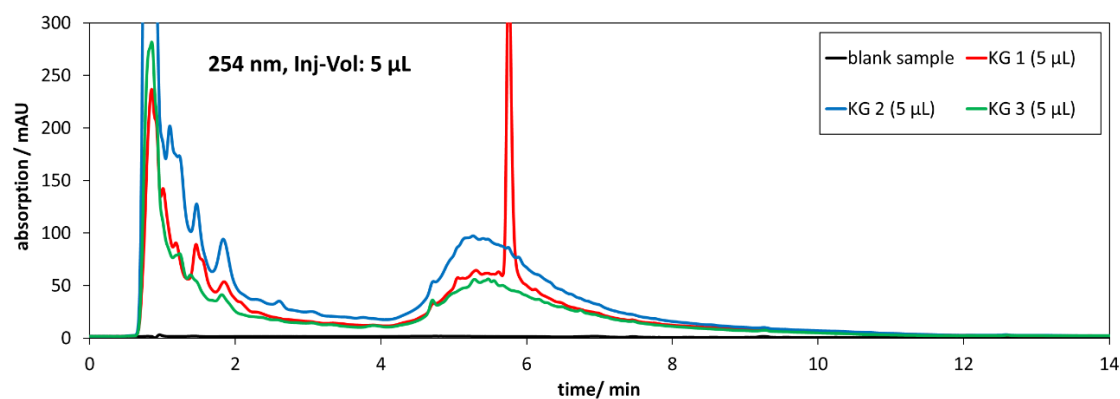
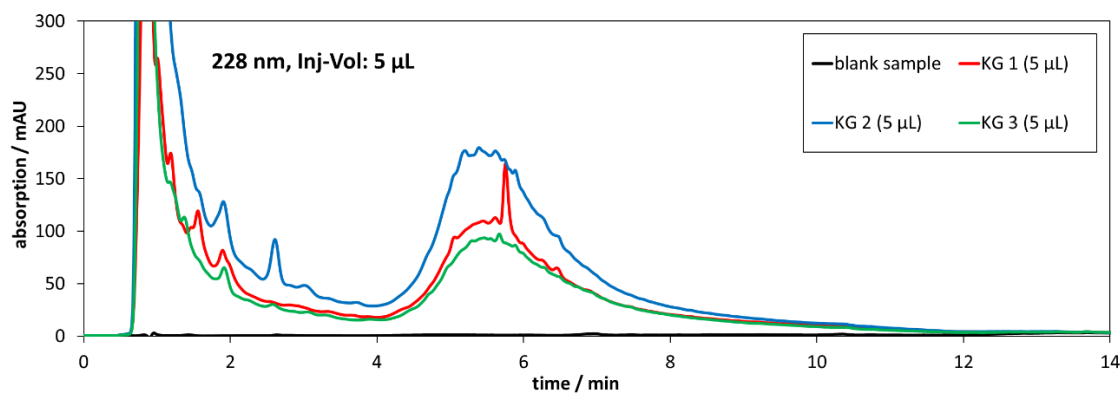
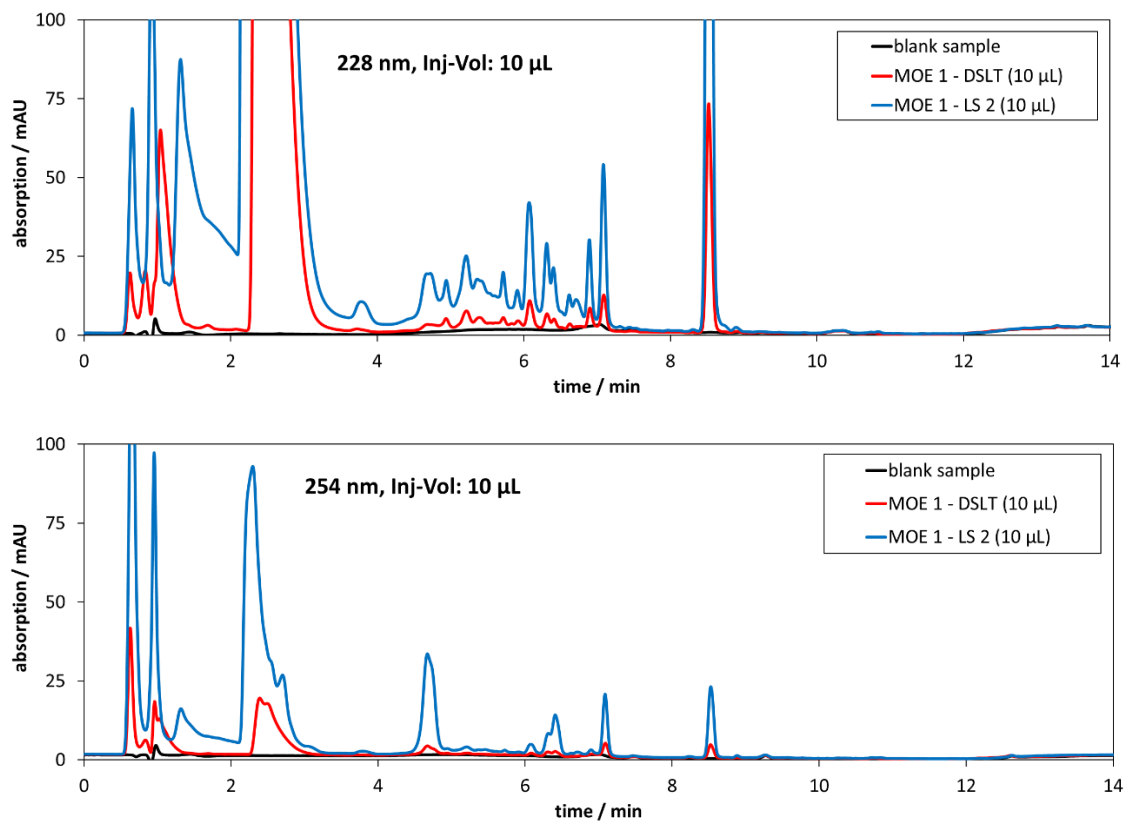


Figure SI 5c: Characterization of eluate samples from form cork granules by LC-DAD (sample volume = 5 µL, detection at 228 nm and 254 nm)



**Figure SI 5d: Characterization of eluate samples from form grouts by LC-DAD (sample volume = 10 µL, detection at 228 nm and 254 nm)**



## GC- and LC-screening results

**Table SI 5-1: GC- and LC-screening results for sample DF4**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Octanoic acid	124-07-2	H314, H412	yes	10000 - 100000
2	2,3-dihydro- <i>N</i> -methyl-1 <i>H</i> -Inden-2-amine	24445-44-1		no	
3	2-(Benzyloxy)propanal	53346-05-7		no	
4	p-Toluenesulfonic acid	104-15-4	H314	yes	10000 - 100000
5	2,4-Bis(1,1-dimethylethyl)-phenol	96-76-4	H315, H318, H410, H411	yes	100 - 1000
6	4-(1,1,3,3-Tertamethylbutyl)phenol	140-66-9	H315, H318, H410	yes	10000 - 100000
7	2,6-Di-tert-butyl-4-hydroxymethylphenol	88-26-6	H315, H319, H335, H412	yes	0 – 10
8	3,5-Di-tert-butyl-2-hydroxybenzaldehyde	1620-98-0		no	
9	3,5-Di-tert-butylbenzoic acid	16225-26-6		no	
10	Butyl isobutyl glutarate	-			
11	Diisobutyl glutarate	71195-64-7		no	
12	3,5-Di-tert-butyl-4-hydroxyacetophenone	14035-33-7	H412	no	
13	Tetrapropylene glycol (PPG-4)	-			
14	p-Anisil	1226-42-2		no	
15	7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione	82304-66-3		no	
16	Dibutyl phthalate	84-74-2	H360, H400, H410	yes	1000 - 10000
17	Diisobutylphthalat	84-69-5	H360, H410	yes	0 – 10
18	Bis(phenoxyethoxy)methane	13879-32-8		no	
19	Metilox	6386-38-5	H411	yes	10 – 100
20	13-Hydroxyoctadecadienoic acid	10219-69-9		no	
21	Coronaric acid	16833-56-0		no	
22	Decylbenzenesulfonic acid	140-60-3		no	
23	Ricinoleic acid	141-22-0		no	
24	2,4-Ditert-butylphenyl 5-hydroxypentanoate	166273-38-7		no	
25	Octaethylene glycol (PEG-8)	488-69-7		no	
26	Nonaethylene glycol (PEG-9)	5117-19-1		no	

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
27	Decaethylene glycol (PEG-10)	5579-66-8		no	
28	Undecaethylene glycol (PEG-11)	6809-70-7		no	
29	Dodecaethylene glycol (PEG-12)	6790-09-6		no	

**Table SI 5-2: GC- and LC-screening results for sample DF6**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Acetophenon	98-86-2		yes	10000 - 100000
2	Ethyl-1-hexanol	104-76-7		yes	100000 - 1000 000
3	Benzothiazol	95-16-9		yes	10 - 100
4	Terpineol	98-55-5		yes	100 - 1000
5	Oxononanal	-			
6	Propylheptanol	10042-59-8	H412	yes	10000+
7	2,6-Di-tert-butyl-4-methylphenol	128-37-0	H410	yes	10000 - 100000
8	2-Hydroxychalcone	42224-53-3		no	
9	Decylbenzenesulfonic acid	140-60-3		no	
10	Ricinoleic acid	141-22-0		no	
11	2,4-Ditert-butylphenyl 5-hydroxypentanoate	166273-38-7		no	

**Table SI 5-3: GC- and LC-screening results for sample DF7**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Ethyl-1-hexanol	104-76-7		yes	100000 - 1000 000
2	Tert-butylphenol (isomer)	-			
3	Cyclododecanon	830-13-7	H411	yes	10 – 100
4	Di-tert-Butylphenol (isomer)	-			
5	D_6-tert-Butyl-4-methylcoumarin	17874-32-7		no	
6	4-tert-Octyl-o-cresol	2219-84-3	H413	no	
7	Butylated hydroxytoluene	128-37-0	H410	yes	10000 - 100000
8	Farnesal	19317-11-4		no	
9	Hexapropylene glycol (PPG-6)	74388-92-4		no	
10	Heptapropylene glycol (PPG-7)	14362-16-4		no	

**Table SI 5-4: GC- and LC-screening results for sample DF7 – sample after 30 days elution**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	2-tert-Butylphenol	88-18-6	H411	yes	100 - 1 000
2	4-Tert-Butylphenol	98-54-4	H410	yes	10000 - 100000
3	Phenylglyoxylic acid	611-73-4		no	
4	4-tert-Butyl-2-Methylphenol	98-27-1		no	
5	Cyclododecanone	830-13-7	H411	yes	10 – 100
6	Di-tert-Butylphenol	-			
7	6-tert-Butyl-4-methylcoumarin	17874-32-7		no	
8	2,3-Cyclododecenopyridin	6571-43-3		no	
9	Butylated hydroxytoluene	128-37-0	H410	yes	10000 - 100000
10	2-Methyl-4-tert-octylphenol	2219-84-3	H413	no	
11	Farnesal	19317-11-4		no	
12	4-tert-Octyl-o-cresol	2219-84-3		no	
13	2,6-Di-tert-butyl-4-hydroxymethylphenol	88-26-6	H315, H319, H335, H412	yes	0 – 10
14	7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-dien-2,8-dion	82304-66-3		no	
15	3,5-Di-tert-Butyl-4-hydroxyphenylpropanoic acid	20170-32-5		no	
16	Lauric acid diethanolamide	120-40-1	H411	yes	> 100
17	Pentapropylene glycol (PPG-5)	21482-12-2		no	
18	Hexapropylene glycol (PPG-6)	74388-92-4		no	
19	Heptapropylene glycol (PPG-7)	14362-16-4		no	
20	Octapropylene glycol (PPG-8)	25322-69-4			
21	Nonapropylene glycol (PPG-9)	25322-69-4		yes	10000 - 100000

**Table SI 5-5: GC- and LC-screening results for sample F14**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Benzoic acid	65-85-0	H315, H318, H372	yes	100000 - 1000000
2	2,2-Dimethyl-4-pentenoic acid	16386-93-9		no	
3	2-Phenoxyethanol	122-99-6	H302, H319	yes	10000 - 100000
4	Octanoic acid	124-07-2	H314, H412	yes	10000 - 100000

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
5	2,2,4-Trimethyl-1,3-pentandiol	144-19-4	H319	yes	100 - 1 000
6	Benzylisothiazolinon/ Benzisothiazolinon	2634-33-5	H302, H315, H318, H317, H400, H411	yes	100 - 1000
7	Tetraethylenglycol (PEG-4)	112-60-7		yes	100 - 1000
8	Dodeca-2(E),4(E)-dienoic acid	24738-48-5		no	
9	Octylmethacrylat	2157-01-9	H314, H319, H335	yes	10 - 100
10	2-Ethylhexylmethacrylat	688-84-6	H315, H319, H335, H412	yes	1000 - 10000
11	N-Butyl-4-chlorbenzamid	1455-99-8		no	
12	3-Hydroxy-2,2,4-trimethylpentylisobutyrat	77-68-9		no	
13	2,2,4-Trimethyl-1,3-pentanediol 1-isobutyrate	25265-77-4		yes	10000 - 100000
14	3-Ethyl-5-methylphenyl trifluoracetate	-			
15	3,5-Di-tert-butyl-2-hydroxybenzaldehyd	37942-07-7	H315, H319, H335	yes	Intermediate Use Only
16	Tri(propylene glycol) butyl ether (PPG-3 butyl ether)	55934-93-5		yes	1000+
17	p-Anisil	1226-42-2		no	
18	Dibutylphthalat	84-74-2	H360, H400, H410	yes	1000 - 10000
19	Diisobutylphthalat	84-69-5	H360, H410	yes	0 – 10
20	2,2,4-Trimethyl-1,3-pentadienol diisobutyrate	6846-50-0	H361, H412	yes	1000 - 10000
21	4,8,12,16-Tetraoxaeicosan-1-ol	-			
22	Heptaethylglycol	5617-32-3		no	
23	Tri(3-chloropropyl) phosphate	1067-98-7		no	
24	Octaethylglycol	5117-19-1		no	
25	D-Fructose 1,6-bisphosphate	488-69-7		no	
26	Hexapropylene glycol (PPG-6)	25322-69-4		yes	1000 - 100000
27	Octaethylene glycol (PEG-8)	25322-68-3		yes	100 - 1000
28	Nonaethylene glycol (PEG-9)	3386-18-3		no	
29	Diocetyl sulfosuccinate	577-11-7	H315, H318	yes	10000+
30	Hexapropylene glycol monobutyl ether (PPG-6 butyl ether)	-			

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
31	Heptapropylene glycol (PPG-7)	25322-69-4		yes	10000 - 100000
32	Decaethylene glycol (PEG-10)	5579-66-8		no	
33	Heptapropylene glycol monobutyl ether (PPG-7 butyl ether)	-			
34	Octapropylene glycol (PPG-8)	25322-69-4		yes	10000 - 100000
35	Octapropylene glycol monobutyl ether (PPG-8 butyl ether)	-			
36	Nonapropylene glycol (PPG-9)	25322-69-4		yes	10000 - 100000
37	Decapropylene glycol (PPG-10)	25322-69-4		yes	10000 - 100000
38	Undecapropylene glycol (PPG-11)	25322-69-4		yes	10000 - 100000
39	Dodecapropylene glycol (PPG-12)	25322-69-4		yes	10000 - 100000

**Table SI 5-6: GC- and LC-screening results for sample WPC1**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Pyrrolaldehyd	1003-29-8		no	
2	Acetylpyrrol	1072-83-9		no	
3	Caprolactam	105-60-2		yes	1000000 - 10000000
4	Hexanoic acid	142-62-1			
5	Hydroxybenzaldehyd	90-02-8	H411	yes	10 - 100 t
6	Benzoic acid	65-85-0	H315, H318, H372	yes	100000 - 1000000
7	Hydroxybenzaldehyd	123-08-0		yes	10 – 100
8	4-Methoxyphenol	150-76-5		yes	100 - 10000
9	Ethylhexanoic acid	149-57-5		yes	10000 - 100000
10	Phenyl-2-propenoic acid	621-82-9		no	
11	2-(4-Methylphenyl)-2-propanol	1197-01-9		no	
12	2-Methoxy-4-vinylphenol	7786-61-0		no	
13	4-Hydroxy-3-methoxybenzaldehyd	121-33-5		yes	1000 - 10000
14	Dimethoxyphenol	91-10-1		yes	Intermediate Use Only
15	<i>N,N</i> -Dibutylformamid	761-65-9	H412	yes	10 - 100
16	Pentanedioic acid dimethyl ester	1119-40-0		yes	1 000+

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
17	Acetylacetophenon	1009-61-6		no	
18	2-Methoxy-4-allylphenol	97-53-0		yes	1000 - 1000
19	2-Methoxy-4-propylphenol	2785-87-7		yes	10 – 100
20	3-Methoxy-4-hydroxyacetophenon	498-02-2		no	
21	2,6-Dimethoxy-p-benzochinon	530-55-2		no	
22	Dimethoxyhydrochinon	15233-65-5		no	
23	Dekanoic acid	334-48-5	H412	yes	10000 - 100000
24	Hexanedioic acid dimethyl ester	627-93-0		yes	1000 - 10000
25	1-[4-(1-hydroxy-1-methylethyl)phenyl]-ethanon	54549-72-3		no	
26	(4-Hydroxy-3-methoxyphenyl)-2-propen-1-on	2983-65-5		no	
27	3-Methoxy-4-hydroxycinnamaldehyd	458-36-6		no	
28	4-Hydroxy-3-methoxyphenylpropan-2-on	2503-46-0		no	
29	3,5-Dimethoxy-4-hydroxybenzaldehyd	134-96-3		yes	Intermediate Use Only
30	Trimethoxyphenol	642-71-7		no	
31	Dodeca-2(E),4(E)-dienoic acid	24738-48-5		no	
32	3,5-Dimethoxy-4-hydroxyacetophenon	2478-38-8		no	
33	Dodekanedioic acid	143-07-7		yes	10000 - 100000
34	Isophorone diisocyanate	4098-71-9	H411	yes	10000 - 100000
35	Diethyl phthalate	84-66-2		yes	1000 - 10000
36	Bisphenol A	80-05-7	H411	yes	100000 - 1000 000
37	3,5-Di-tert-butyl-2-hydroxybenzaldehyd	37942-07-7	H315, H319, H335	yes	Intermediate Use Only
38	2,6-Di-tert-butyl-4-hydroxymethylphenol	88-26-6	H315, H319, H335, H412	yes	0 – 10
39	Methyl 2-cyano-3-(2,3-dihydro-2-methyl-1H-indol-1-yl)acrylat	22560-84-5		no	
40	Pentandioic acid butyl isobutyl ester /Butyl isobutyl glutarate	-			
41	Hexadekanedioic acid	57-10-3		yes	10000 - 100000
42	Dibutyl phthalate	84-74-2	H360, H400, H410	yes	1000 - 10000
43	Diisobutylphthalat	84-69-5	H360, H410	yes	0 – 10

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
44	Oktadekaneic acid	57-11-4		yes	10000 - 100000
45	Terephthalic acid di(2-chloroethyl) ester	1026-93-3		no	
46	Pentapropylene glycol (PPG-5)	21482-12-2		no	
47	Hexapropylene glycol (PPG-6)	74388-92-4		no	
48	Heptapropylene glycol (PPG-7)	14362-16-4		no	
49	Octapropylene glycol (PPG-8)	25322-69-4		yes	10000 - 100000
50	Nonapropylene glycol (PPG-9)	25322-69-4		yes	10000 - 100000
51	Decapropylene glycol (PPG-10)	25322-69-4		yes	1000 - 100000
52	Undecapropylene glycol (PPG-11)	25322-69-4		yes	10000 - 100000
53	Dodecapropylene glycol (PPG-12)	25322-69-4		yes	10000 - 100000

**Table SI 5-7: GC- and LC-screening results for sample WPC2**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Hexanal	66-25-1		yes	100 - 1 000
2	Caprolactam	105-60-2		yes	1000000 - 10000000
3	Dihydrobenzofuran	496-16-2		yes	Intermediate Use Only
4	Benzoic acid	65-85-0	H315, H318, H372	yes	100000 - 100000
5	Hydroxybenzaldehyd	123-08-0		yes	10 - 100
6	4-Methoxyphenol	150-76-5		yes	100 - 10000
7	2-Octenal	2548-87-0		no	
8	1-Methoxy-2-propyl acetat	108-65-6		yes	10000 - 100000
9	Phenoxyethanol	122-99-6	H302, H319	yes	10000 - 100000
10	Ethylhexanoic acid	149-57-5		yes	10000 - 100000
11	2-Methyl-5-hydroxybenzofuran	6769-56-8		no	
12	2-Methoxy-4-vinylphenol	7786-61-0		no	
13	4-Hydroxy-2-methylacetophenone	875-59-2		no	
14	2-(4-Methylphenyl)-2-propanol	1197-01-9		no	
15	2-Pinen-4-on	80-57-9		no	
16	3-Phenoxy-1-Propanol	6180-61-6		no	
17	4-Hydroxy-3-methoxybenzaldehyd	121-33-5		yes	1000 - 10000

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
18	Terpinol	98-55-5		yes	100 - 1000
19	Butoxyethoxyethanol	112-34-5		yes	1000 - 100000
20	Acetylacetophenon	1009-61-6		no	
21	2-(Benzyloxy)propanal	53346-05-7		no	
22	2-Methoxy-4-propylphenol	2785-87-7		yes	10 – 100
23	3-Methoxy-4-hydroxyacetophenon	498-02-2		no	
24	Hydroxycarvotanaceton	7712-46-1		no	
25	Decalacton	706-14-9		yes	100 - 1000
26	4-(1-Hydroxy-1-methylethyl)-1-methylcyclohexanol	80-53-5		yes	Intermediate Use Only
27	Dekanoic acid	334-48-5	H412	yes	10000 - 100000
28	Oxononanoic acid	2553-17-5		no	
29	1-[4-(1-hydroxy-1-methylethyl)phenyl]-ethanon	54549-72-3		no	
30	(4-Hydroxy-3-methoxyphenyl)-2-propen-1-on	2983-65-5		no	
31	3-Methoxy-4-hydroxycinnamaldehyd	458-36-6		no	
32	4-Hydroxy-3-methoxy-benzenpropanol	2305-13-7		no	
33	3,5-Dimethoxy-4-hydroxybenzaldehyd	134-96-3		yes	Intermediate Use Only
34	2,4'-Dihydroxy-3'-methoxyacetophenon	18256-48-9		no	
35	3-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-1-propanon	2196-18-1		no	
36	Butoxyethoxyethylacetat	124-17-4		yes	10000 - 100000
37	Hexanoic acid anhydride	2051-49-2		yes	Intermediate Use Only
38	Glycerintriacetat	102-76-1		yes	10000 - 100000
39	Diethyl phthalate	84-66-2		yes	1000 - 10000
40	Diisopropyl adipat	6938-94-9		yes	100 - 1000
41	2,6-Di-tert-butyl-4-hydroxymethylphenol	88-26-6	H315, H319, H335, H412	yes	0 - 10
42	7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione	82304-66-3		no	
43	Dibutyl phthalate	84-74-2	H360, H400, H410	yes	1000 - 10000



#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
44	Diisobutyl phthalate	84-69-5	H360, H410	yes	0 - 10
45	Bis(phenoxyethoxy)methane	13879-32-8		no	

**Table SI 5-8: GC- and LC-screening results for sample MOE1 – DSLT**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Benzaldehyd	100-52-7	H302	yes	10000 - 100000
2	Benzylalkohol	100-51-6	H302, H332	yes	10000 - 100000
3	Methylphenol	95-48-7	H412, H301, H311, H314	yes	10000 - 100000
4	2-Phenylacetamide	103-81-1	H302, H319	no	
5	3-Propionylperazine	1570-48-5	H302, H312, H332, H315, H319, H335	no	
6	Propylphenol	644-35-9	H302, H312, H315, H319, H332, H335	no	
7	Octanoic acid	124-07-2	H412, H314	yes	10000 - 100000
8	o-Propylanisol	13629-73-7		no	
9	4-tert-Butylphenol	98-54-4	H410, H315, H318, H361f	yes	10000 - 100000
10	<i>N,N</i> -Dibutylformamid	761-65-9	H412	yes	10 – 100
11	2-Phenylbutyric acid	90-27-7	H302	yes	
12	3-Phenylbutyric acid	4593-90-2		no	
13	2-(Benzyloxy)propanal	53346-05-7		no	
14	2-Mercaptobenzothiazole	149-30-4	H410, H317	yes	1000 - 10000
15	Benzylphosphonic acid	6881-57-8		no	
16	p-Toluenesulfonic acid	104-15-4		yes	100 - 1000
17	2-(Benzylmethylamino)ethanol N-oxide	15831-63-7	H302	no	
18	Tripropylene glycol (PPG-3)	-			
19	Tetraethylene glycol (PEG-4)	112-60-7		yes	100 - 1000
20	3,4-Dihydroxymandelic acid	775-01-9		no	
21	Sebacic acid	111-20-6		yes	10000 - 100000
22	Laurylguanidine	112-65-2		no	
23	7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione	82304-66-3		no	

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
24	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	H412, H361	yes	1000 - 10000
25	Benzylododecyldimethylammonium cation	7281-04-1	Biozidbestandteil	No	
26	Pentapropylene glycol (PPG-5)	21482-12-2		no	
27	Prostaglandin A1 methyl ester	26771-94-8		no	
28	2-Ethylhexyl maleate	142-16-5	H410, H373	yes	1000 - 10000
29	Bis(2-ethylhexyl)-(2E)-2-butendioat	141-02-6	H411	yes	1000 - 1000
30	Decamethylcyclopentasiloxane	541-02-6		yes	10000 - 100000
31	Decapropylene glycol (PPG-10)	25322-69-4		yes	10000 - 100000

**Table SI 5-9: GC- and LC-screening results for sample MOE1 – Perc.**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Benzaldehyd	100-52-7	H302	yes	10000 - 100000
2	Benzylalkohol	100-51-6	H302, H332	yes	10000 - 100000
3	Methylphenol	95-48-7	H412, H301, H311, H314	yes	10000 - 100000
4	2-Butoxyethanol	111-76-2	H302, H312, H332, H315, H319	yes	100000 - 1000 000
5	4-tert-Butylphenol	98-54-4	H410, H315, H318, H361f	yes	10000 - 100000
6	<i>N,N</i> -Dibutylformamid	761-65-9	H412	yes	10 – 100
7	2-(Benzyloxy)propanal	53346-05-7	H410, H411, H315, H318	no	
8	2-Phenylbutyric acid	90-27-7	H302	yes	Intermediate Use Only
9	3-Phenylbutyric acid	4593-90-2		no	
10	Glycidyl-2-methylphenylether	2210-79-9	H411, H341, H315, H317	yes	1000+
11	2-Mercaptobenzothiazole	149-30-4	H410, H317	yes	1000 - 10000
12	Benzylphosphonic acid	6881-57-8		no	
13	p-Toluenesulfonic acid	104-15-4		yes	100 - 1000
14	2-(Benzylmethylamino)ethanol N-oxide	15831-63-7		no	
15	3-(Octylamino)propionitril	29504-89-0		no	
16	Tripropylene glycol (PPG-3)	-			

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
17	Tetraethylene glycol (PEG-4)	112-60-7		yes	100 - 1000
18	Sebacic acid	111-20-6		yes	10000 - 100000
19	<i>N,N</i> -Dimethyl-n-dodecylamin	112-18-5	H410, H302, H314	yes	100 - 1000
20	Laurylguanidine	112-65-2		no	
21	3-Ethyl-5-methylphenyl trifluoroacetate	-			
22	4-Amino-7-diethylamino-chromen-2-one	107995-76-6		no	
23	Tetrapropylene glycol (PPG-4)	-			
24	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	H412, H361	yes	1000 - 10000
25	Benzyl-dodecyl-dimethylammonium cation	7281-04-1	Biozidbestandteil	no	
26	Clomipramine	303-49-1	H410, H302, H336, H370	yes	Intermediate Use Only
27	2-Ethylhexyl maleate	142-16-5	H410, H373	yes	1000 - 10000
28	Bis(2-ethylhexyl)-(2E)-2-butendioat	141-02-6	H411	yes	1000 - 10000
29	Hexapropylene glycol (PPG-6)	74388-92-4		no	
30	Heptapropylene glycol (PPG-7)	14362-16-4		no	
31	Octapropylene glycol (PPG-8)	25322-69-4		yes	10000 - 100000
32	Nonapropylene glycol (PPG-9)	2172326-56-4		no	
33	Decapropylene glycol (PPG-10)	25322-69-4		yes	10000 - 100000

**Table SI 5-10: GC- and LC-screening results for sample KG1**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Methylphenol	95-48-7	H412, H301, H311, H314	yes	10000 - 100000
2	5-Methyl-3-methylenedihydro-2(3H)-furanon	62873-16-9		no	
3	4-Methyl-2,3-dihydropyran-6-on	2381-87-5		no	
4	Methylisothiazolinon	2682-20-4	H410, H301, H311, H314, H317, H330	Biozid	
5	1,2,3-Benzenetriol	87-66-1	H412, H302, H312, H332, H341	yes	10 - 100
6	Anisaldehyde	123-11-5	H412	yes	1000 - 10000

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
7	Protocatechuic aldehyde	139-85-5		no	
8	2-Methoxy-4-vinylphenol	7786-61-0		no	
9	4-Hydroxy-2-methylacetophenone	875-59-2		no	
10	Bornanon	464-49-3	H315, H319, H335	yes	100 - 1000
11	4-Hydroxy-3-methoxybenzaldehyd	121-33-5		yes	1000 - 10000
12	Protocatechuic acid	99-50-3		no	
13	2-(Benzyloxy)propanal	53346-05-7		no	
14	Bornanedion	4230-32-4		no	
15	Hydroxy-3-methoxyacetophenon	498-02-2		no	
16	6-Pentyl-5,6-dihydro-2H-pyran-2-on	54814-64-1	H315, H317, H319	no	
17	Gallic acid	149-91-7	H315, H319, H335	yes	10 - 100
18	7-Methoxycoumarin	531-59-9	H315, H319, H335	no	
19	Esculetin	305-01-1		no	
20	3,4-Dihydro-8-hydroxy-3-methyl-(1H)-2-benzopyran-1-on	1200-93-7	H315, H319, H335	no	
21	4-Hydroxy-2-methoxycinnamaldehyd	127321-19-1		no	
22	Caffeic acid	331-39-5	H315, H319, H335, H351	no	
23	4-Hydroxy-3-methoxybenzenoic acid	306-08-1		no	
24	3,5-Dimethoxy-4-hydroxybenzaldehyd	134-96-3		yes	Intermediate Use Only
25	Azelaic acid	123-99-9	H315, H319	yes	1000 - 10000
26	Ethyl ferulate	4046-02-0		no	
27	Isoscopoletin	776-86-3		no	
28	Scopoletin	92-61-5		no	
29	Isofraxidin	486-21-5		no	
30	Fraxinol	486-28-2	H302	no	
31	6,7-Dihydroxycoumarin-4-acetic acid	88404-14-2		no	
32	3,5-Di-tert-butyl-4-hydroxyacetophenone	14035-33-7	H315, H319, H335	no	
33	p-Anisil	1226-42-2		no	

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
34	Nandrolone	434-22-0	H351	yes	Intermediate Use Only
35	Pinolenic acid	16833-54-8		no	
36	Catechin	18829-70-4		no	
37	Epicatechin	490-46-0		no	
38	9-Oxo-10E,12Z,15Z-octadecatrienoic acid	125559-74-2		no	
39	Metilox	6386-38-5	H411	yes	10 - 100
40	9-Oxo-10E,12Z-octadecadienoic acid	54232-59-6		no	
41	12(13)-Epoxy-9Z-octadecenoic acid	6799-85-5		no	
42	Oleic acid methyl ester	112-62-9	H410, H304, H315, H336	no	
43	Ellagic acid	476-66-4	H302	no	
44	9-Oxo-11-(3-pentyl-2-oxiranyl)-10E-undecenoic acid	478931-82-7		no	
45	Desogestrel	54024-22-5	H410	no	
46	9,10-Dihydroxy-12Z-octadecenoic acid	263399-34-4		no	
47	12,13-Dihydroxy-9Z-octadecenoic acid	263399-35-5		no	
48	Hydroxyprostanazol	-			
49	Arachidonic acid ethyl ester	1808-26-0		no	
50	2-Ethylhexyl undecyl sulfite	-			
51	Propofol Glucuronide	114991-26-3		no	
52	Hexapropylene glycol (PPG-6)	74388-92-4		no	
53	Diisooctyl phthalate	27554-26-3		no	
54	Heptapropylene glycol (PPG-7)	14362-16-4		no	
55	Quercetin 7-rhamnoside	22007-72-3		no	
56	Octapropylene glycol (PPG-8)	25322-69-4		yes	10000 - 10000
57	Nonapropylene glycol (PPG-9)	25322-69-4		no	
58	Procyanidin B2	29106-49-8		no	

**Table SI 5-11: GC- and LC-screening results for sample KG2**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Benzylalkohol	100-51-6	H302, H332	yes	10000 - 100000
2	Methylphenol	95-48-7	H412, H301, H311, H314	yes	10000 - 100000

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
3	5-Methyl-3-methylenedihydro-2(3H)-furanon	62873-16-9		no	
4	4-Methyl-2,3-dihydropyran-6-on	2381-87-5		no	
5	Methoxyphenol	90-05-1	H315, H319, H302	yes	1000 - 10000
6	1,2,3-Benzenetriol	87-66-1	H412, H302, H332, H341	yes	10 – 100
7	Anisaldehyde	123-11-5	H412	yes	1000 - 10000
8	2-Phenoxyethanol	122-99-6	H302, H319	yes	10000 - 100000
9	Bornanon	464-49-3	H315, H319, H335	yes	100 - 1000
10	4-Hydroxy-3-methoxybenzaldehyd	121-33-5		yes	100 - 10000
11	Protocatechuic acid	99-50-3		no	
12	2-(Benzyloxy)propanal	53346-05-7		no	
13	Bornanedion	4230-32-4		no	
14	Hydroxy-3-methoxyacetophenon	498-02-2		no	
15	6-Pentyl-5,6-dihydro-2H-pyran-2-on	54814-64-1	H315, H317, H319	no	
16	Gallic acid	149-91-7	H315, H319, H335	yes	10 - 100
17	7-Methoxycoumarin	531-59-9	H315, H319, H335	no	
18	3,4-Dihydro-8-hydroxy-3-methyl-(1H)-2-benzopyran-1-on	1200-93-7	H315, H319, H335	no	
19	4-Hydroxy-2-methoxycinnamaldehyd	127321-19-1		no	
20	Caffeic acid	331-39-5	H315, H319, H335, H351	no	
21	4-Hydroxy-3-methoxybenzenoic acid	306-08-1		no	
22	3,5-Dimethoxy-4-hydroxybenzaldehyd	134-96-3		yes	Intermediate Use Only
23	Azelaic acid	123-99-9	H315, H319	yes	1000 - 10000
24	6,7-Dihydroxycoumarin-4-acetic acid	88404-14-2		no	
25	Isoscapoletin	776-86-3		no	
26	Ethyl ferulate	4046-02-0		no	
27	Fraxidin	525-21-3		no	
28	Isofraxidin	486-21-5		no	

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
29	Fraxinol	486-28-2	H302	no	
30	3,5-Di-tert-butyl-4-hydroxyacetophenone	14035-33-7	H315, H319, H335	no	
31	p-Anisil	1226-42-2		no	
32	Nandrolone	434-22-0	H351	yes	Intermediate Use Only
33	Catechin	154-23-4	H315, H319, H335	no	
34	9-Oxo-10E,12Z,15Z-octadecatrienoic acid	125559-74-2		no	
35	Metilox	6386-38-5	H411	yes	10 - 100
36	9-Oxo-10E,12Z-octadecadienoic acid	54232-59-6		no	
37	9(10)-Epoxy-12Z-octadecenoic acid	16833-56-0		no	
38	Ellagic acid	476-66-4	H302	no	
39	9-Oxo-11-(3-pentyl-2-oxiranyl)-10E-undecenoic acid	478931-82-7		no	
40	Desogestrel	54024-22-5	H410	no	
41	9,10-Dihydroxy-12Z-octadecenoic acid	263399-34-4		no	
42	12,13-Dihydroxy-9Z-octadecenoic acid	263399-35-5		no	
43	Hydroxyprostanazol	-			
44	Arachidonic acid ethyl ester	1808-26-0		no	
45	2-Ethylhexyl undecyl sulfite	-			
46	Hexapropylene glycol (PPG-6)	74388-92-4		no	
47	Diisooctyl phthalate	27554-26-3		no	
48	Diocetyl phthalate	117-84-0	H413	no	
49	Heptapropylene glycol (PPG-7)	14362-16-4		no	
50	Quercetin 7-rhamnoside	22007-72-3		no	
51	Octapropylene glycol (PPG-8)	25322-69-4		yes	10000 - 100000
52	Nonapropylene glycol (PPG-9)	2172326-56-4		no	
53	Procyanidin B2	29106-49-8		no	

**Table SI 5-12: GC- and LC-screening results for sample KG3**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	5-Methyl-3-methylenedihydro-2(3H)-furanon	62873-16-9		no	
2	Methoxyphenol	90-05-1	H315, H319, H302	yes	1000 - 10000
3	Anisaldehyde	123-11-5	H412	yes	1000 - 10000
4	2-Phenoxyethanol	122-99-6	H302, H3019	yes	10000 - 100000
5	Bornanediol	4230-32-4		no	
6	Esculetin	305-01-1		no	
7	Cyclododecanone	830-13-7	H411	yes	10 – 100
8	6,7-Dihydroxycoumarin-4-acetic acid	88404-14-2		no	
9	Isoscapoletin	776-86-3		no	
10	Scopoletin	92-61-5		no	
11	Ethyl ferulate	4046-02-0		no	
12	Isofraxidin	486-21-5		no	
13	Fraxinol	486-28-2	H302	no	
14	Dibutylphthalat	84-74-2	H400, H410, H360	yes	1000 - 10000
15	Diisobutylphthalat	84-69-5	H410, H360	yes	0 – 10
16	Ellagic acid	476-66-4	H302	no	
17	Hexapropylene glycol (PPG-6)	74388-92-4		no	
18	Diisooctyl phthalate	27554-26-3		no	
19	Heptapropylene glycol (PPG-7)	14362-16-4		no	
20	Octapropylene glycol (PPG-8)	25322-69-4		yes	10000 - 100000
21	Nonapropylene glycol (PPG-9)	25322-69-4		no	
22	Decapropylene glycol (PPG-10)	25322-69-4		no	

**Table SI 5-13: GC- and LC-screening results for sample SG1**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Nonanoic acid	112-05-0	H412, H315, H319	yes	1000 - 10000
2	1-(2-Butoxyethoxy)ethanol	54446-78-5		no	



#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
3	Butyldiglycol (PEG-2 Butyl Ether)	112-34-5		yes	10000 - 100000
4	2,2,4-Trimethyl-1,3-pentanediol 1-isobutyrate	25265-77-4		yes	10000 - 100000
5	Diethyl phthalate	84-66-2		yes	1000 - 10000
6	Butyl isobutyl glutarate	-			
7	Diisobutyl glutarat	71195-64-7		no	
8	Tridecanedioic acid	505-52-2	H412, H319	yes	1000 - 10000
9	Pentapropylene glycol (PPG-5)	21482-12-2		no	
10	2-Ethylhexyl maleate	142-16-5	H410, H373	yes	1000 - 10000
11	Bis(2-ethylhexyl)-(2E)-2-butendioat	141-02-6	H411	yes	1000 - 10000
12	Hexapropylene glycol (PPG-6)	74388-92-4		no	
13	Heptapropylene glycol (PPG-7)	14362-16-4		no	
14	Octapropylene glycol (PPG-8)	25322-69-4		yes	10000 - 100000
15	Nonapropylene glycol (PPG-9)	25322-69-4		no	
16	Decapropylene glycol (PPG-10)	25322-69-4		yes	10000 - 100000
17	Undecapropylene glycol (PPG-11)	25322-69-4		yes	10000 - 100000
18	Dodecapropylene glycol (PPG-12)	25322-69-4		yes	10000 - 100000

**Table SI 5-14: GC- and LC-screening results for sample SG2 + SG3**

#	compound	CAS	H- phrases	REACH	Total tonnage in t per year
1	Nonanoic acid	112-05-0	H412, H315, H319	yes	1000 - 10000
2	Diethyl phthalate	84-66-2		yes	1000 - 10000
3	Butyl isobutyl glutarate	-			
4	Diisobutyl glutarate	71195-64-7		no	
5	Tridecanedioic acid	505-52-2	H412, H319	yes	1000 - 10000
6	Hexapropylene glycol (PPG-6)	74388-92-4		no	
7	Heptapropylene glycol (PPG-7)	14362-16-4		no	
8	Octapropylene glycol (PPG-8)	25322-69-4		yes	10000 - 100000
9	Nonapropylene glycol (PPG-9)	25322-69-4		no	
10	Decapropylene glycol (PPG-10)	25322-69-4		yes	10000 - 100000
11	Undecapropylene glycol (PPG-11)	25322-69-4		yes	10000 - 100000
12	Dodecapropylene glycol (PPG-12)	25322-69-4		yes	10000 - 100000

**SI 6: Classification and ecotoxicity data of identified substances**

Substance	CAS	Hazard classification	Fish	Crustacea	Algae	Product group
Quinic acid = 1,3,4,5-tetrahydroxycyclohexanecarboxylic acid	77-95-2		LC50 >100 mg/L (read accross Shikimi acid)	LC50 = 116 mg/L (read accross Shikimi acid)	LC50 >100 mg/L (read accross Shikimi acid)	KG
Bisphenol A	80-05-7	H411	<i>Pimephales promelas</i> LC50 (96 h) = 4,6 mg/L	EC50 (48 h) = 10,2 mg/L	<i>Pseudokirchneriella subcapitata</i> EC50 (96 h) = 3,1 mg/L, EC10 (72 h) = 1,36 mg/L	WPC
Diisobutylphthalate	84-69-5	H410	Fathead minnows LC50 (96 h) = 0,90 mg/L	<i>Nitocra spinipes</i> LC50 (96 h) = 3,0 mg/L	<i>Desmodesmus subspicatus</i> EC50 (72 h) = 1,7 mg/L, NOEC (72 h) = 0,35 mg/L	DF + F+WPC
Dibutyl phthalate	84-74-2	H400, H410	bluegill sunfish LC50 (96 h) = 0,48mg/L	EC50 (48 h) = 3,4 mg/L	<i>Desmodesmus subspicatus</i> EC50 (72 h) = 1,2 mg/L	DF + F+WPC
2-tert-Butylphenol	88-18-6	H400, H411	<i>Oryzias latipes</i> LC50 (96 h) = 6 mg/L	LC50 (48 h) 3,2 mg/L	<i>Scendesmus subspicatus</i> EC50 (72 h) = 6,4 mg/L, EC10 (72 h) = 2,0 mg/L	DF
Hydroxybenzaldehyde = Salicylaldehyde	90-02-8	H411	No data	EC50 (48 h) = 2,6 mg/L	<i>Pseudokirchneriella subcapitata</i> EC50 (72 h) = 4,76 mg/L, NOEC (72 h) = 0.55 mg/L	WPC
1,3-Benzothiazol	95-16-9		<i>Oryzias latipes</i> LC50 (96 h) = 39 mg/L	EC50 (48 h) = 19 mg/L	<i>Desmodesmus subspicatus</i> EC50 (72 h) = 48,7 mg/l, NOEC (72 h) = 5,1 mg/L	DF

Substance	CAS	Hazard classification	Fish	Crustacea	Algae	Product group
2,4-di-tert-butylphenol = 2,4-Bis(1,1-dimethylethyl)-phenol	96-76-4	H410	fathead minnow LC50 (96 h) = 1,4 mg/L	EC50 (48 h) = 0,5 mg/L, ECO (48 h) = 0,2 mg/L	<i>Desmodesmus subspicatus</i> EC50 (72 h) = 0,37 mg/L, NOEC (72 h) = 0,073 mg/L	DF
4-tert-butylphenol	98-54-4	H410	rainbow trout LD50 (96 h) = 5.1 mg/L	EC50 (48 h) = 3,9 mg/L	<i>Selenastrum capricornutum</i> EC50 (72 h) = 14 mg/L, EC10 or NOEC (72 h) = 0,32 mg/L	DF+MOE
Benzylalcohol	100-51-6		<i>Lepomis macrochirus</i> LC50 (96 h) = 10 mg/L	EC50 (48 h) = 360 mg/L	<i>Pseudokirchnerella subcapitata</i> EC50 (72 h) = 770 mg/L, NOEC (72 h) = 310 mg/L	MOE
N,N-Dimethyl-n-dodecylamine	112-18-5	H410	<i>Danio rerio</i> und <i>Oncorhynchus mykiss</i> LC50 (96 h) = 1,13 mg/L und 0,26 mg/L	EC50 (48 h) = 0,93 mg/L - 0,056 mg/L	different species EC50 (72 h) = 0,016 mg/L, EC10 or NOEC (72 h) = 0,0026 mg/L	MOE
2-(2-butoxyethoxy)ethanol = Butyldiglycol	112-34-5		<i>Leopomis macrochirus</i> LC50 (96 h) = 1300mg/L	EC50 (48 h) > 1000 mg/L	<i>Pseudokirchneriella subcapitata</i> EC50 (72 h) = 1101 mg/	DF
Oleic acid methyl ester = Methyloleat	112-62-9	H410	No data	No data	No data	KG
Lauric acid diethanolamide = N,N-bis(2-hydroxyethyl)dodecanamide	120-40-1	H411	<i>Oncorhynchus mykiss</i> LC50 (96 h) = 2,4 mg/L	EC50 (48 h) = 3,2 mg/L	<i>Selenastrum subspicatus</i> EC (72 h) = 3.9 mg/L, NOEC (72 h) = 0,3 mg/L	DF

Substance	CAS	Hazard classification	Fish	Crustacea	Algae	Product group
2,4,7,9-tetramethyldec-5-yne-4,7-diol = TMDD	126-86-3	H412	<i>Cyprinus carpio</i> LC50 (96 h) = 42 mg/L, LC0 (96 h) = 32 mg/L	EC50 (48 h) = 91 mg/L	<i>Pseudokirchneriella subcapitata</i> EC50 (72h) = 82 mg/L, EC10 (72 h) = 15 mg/L	
2,6-Di-tert-butyl-4-methylphenol = 2,6-di-tert-butyl-p-cresol	128-37-0	H410	<i>Oryzias latipes</i> LC50 (96 h) = 1,1 mg/L	EC50 (48 h) = 0,48 mg/L, NOEC (48 h) = 0,15 mg/L	<i>Pseudokirchneriella subcapitata</i> EC50 (72 h) > 0,24 mg/L, NOEC (72 h) = 0,24 mg/L	DF
4-(1,1,3,3-tetramethylbutyl)phenol	140-66-9	H410	<i>Leusiscus idus</i> LC50 (96 h) = 0,26 mg/L	<i>Gammarus pulex</i> LC50 (96 h) = 0,0133 mg/L	<i>Pseudokirchneriella subcapitata</i> EC50 (96 h) = 1,9 mg/L	DF
Bis(2-ethylhexyl)-(2E)-2-butendioat = Bis(2-ethylhexyl) fumarate	141-02-6	H411	No data	EC50 (48 h) > 100 mg/L	QSAR-Schätzung EC50 > 1,19 mg/L, NOEC ≥ 1,19 mg/L	MOE+SGS
2-Ethylhexylmaleat = Bis(2-ethylhexyl) maleate	142-16-5	H410	Zebra fish LC50 (96 h) >100 mg/L	EC50 (48 h) = 59,5 mg/L	verschiedene Spezies EC50 (72 h) >100 mg/L nominal bzw. 0,62 mg/L gemessen, NOEC (72 h) = 3,7 mg/L (nominal) bzw. 0,052 mg/L (gemessen)	MOE+SGS
Benzothiazole-2-thiol = 2-Mercaptobenzothiazol	149-30-4	H410	rainbow trout LC50 (96 h) = 0,73 mg/L.	EC50 (48 h) = 29,8 mg/L	<i>Selenastrum capricornutum</i> EC50 (72 h) = 0,5mg/L, NOEC (72 h) = 0,066 mg/L	MOE
2-Ethylhexan acid = 2-ethylhexanoic acid	149-57-5		<i>Oncorhynchus mykiss</i> EC50 (96 h) = 180 mg/L	EC50 (48 h) = 85,4 mg/L	<i>Desmodesmus subspicatus</i> EC50 (72 h) = 485,1 mg/L, EC10 or NOEC = 231,2 mg/L	MOE

Substance	CAS	Hazard classification	Fish	Crustacea	Algae	Product group
Gallic acid = 3,4,5-trihydroxybenzoic acid	149-91-7		<i>Danio rerio</i> LC50 96 h > 100 mg/L	EC50 (48h) = 19,1 mg/L	<i>Selenastrum capricornutum</i> EC50(72h) = 2,19 mg/L, NOEC (72 h) = >1-1,5 mg/L	KG
Esculetin = 6,7-dihydroxy-2-benzopyrone	305-01-1		No data	No data	No data	KG
Coniferylaldehyde = 4'-hydroxy-3'-methoxycinnamaldehyde	458-36-6		No data	No data	No data	KG
Ellagic acid	476-66-4		No data	No data	No data	KG
Cyclododecanon	830-13-7	H411	<i>Leuciscus idus</i> LC50 (48 h) = 10,8 mg/L	EC50 (48 h) = 2,5 mg/L	<i>Desmodesmus subspicatus</i> EC50 (72 h) 7,77 mg/L	DF
1,3-Benzoldimethanamin = m-phenylenebis(methylamine)	1477-55-0	H412	Rainbow trout LC50 (96 h) > 100 mg/L	EC50 (48 h) = 16 mg/L	<i>Desmodesmus subspicatus</i> EC50 (72h) = 12 mg/L, NOEC (72 h) = 6.25 mg/L	MOE
Glycidyl-2-methylphenylether	2210-79-9	H411	<i>Oncorhynchus mykiss</i> LC50 (96 h) = 2,8 - 5,1 mg/L	EC50 (48 h) = 3,3	No data	MOE
1,2-benzisothiazol-3(2H)-one	2634-33-5	H400, H411	<i>Oncorhynchus mykiss</i> LC50 (96 h) = 2,18 mg/L	EC50 (48 h) = 2,94 mg/L	<i>Selenastrum capricornutum</i> EC50 (72 h) = 0,15 mg/L, NOEC (72 h) = 0,055 mg/L	F
Methylisothiazolinon	2682-20-4	H400, H410	<i>Oncorhynchus mykiss</i> LC50 (96 h) = 4,77 mg/L	EC50 (48 h) = 0,934 mg/L	<i>Selenastrum capricornutum</i> EC50 (72 h) = 0,103 mg/L, NOEC (72 h) = 0,05 mg/L	KG

Substance	CAS	Hazard classification	Fish	Crustacea	Algae	Product group
Isophorone diisocyanate	4098-71-9	H411	<i>Danio rerio</i> LC50 (96 h) > 72 mg/L	EC50 (96 h) = 4,0 mg/L	<i>Desmodesmus subspicatus</i> EC50 (72 h) >70 mg/L, NOEC (72 h) = 4,4 mg/L	WPC
Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate = Metilox	6386-38-5	H411	Zebra-fish LC50 (96 h) = 5,6 mg/L	EC50 (24 h) = > 100 mg/L	<i>Scenedesmus subspicatus</i> EC50 (72 h) = 2,3 mg/L	KG + DF
Benzyl dodecyl dimethyl ammonium cation = Benzyl dodecyl dimethyl ammonium bromide	7281-04-1	H400	No data	No data	No data	MOE
2-Octyl-2H-isothiazol-3-on OIT	26530-20-1	H400, H410	EC50= 0,122 mg/L (QSAR)	EC50= 0,181 mg/L (QSAR)	EC50 = 0,15 mg/L, NOEC = 0,068 mg/L (QSAR)	DM
Desogestrel	54024-22-5	H410	<i>Lepomis macrochirus</i> LC50 (96 h) > 1,3 mg/L	EC50 (48 h) = 3,9 mg/L	<i>Selenastrum capricornutum</i> EC50 (8 d) > 4,5 mg/L, NOEC (8 d) = 4,5 mg/L	KG

DF= Roofing membranes, DM= Sealings & coatings, F= varnishes, KG= cork granules, MOE= grouts, SG= foam glass aggregates, WPC= Wood-plastic composites  
Data on crustacea refer to *Daphnia magna* if not stated otherwise