

Supporting Information

For

# **Contribution of Professional Cleaning to Indoor Air and Sewage Pollution**

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Table S 1: ITEX program for adsorbtion and desorbtion of volatile compounds from water and product samples.

Syringe temperature	60 °C
Adsorbtion start temperature	35 °C
Extraction volume	1000 µl
Extraktion strokes	20
Extraktion velocity	100 µl/s
Pull up retarding	5000 ms
Desorption	500 µl/s at 250 °C
Adsorber cleaning	120 s at 320 °C

Table S 2: Selected fragment ions for GC/MS sim mode

M/Z: 29, 31, 32, 34, 39, 41, 42, 43, 44, 45, 46, 52, 55, 56, 57, 59, 65, 69, 73, 76, 77, 78, 87

Table S 3: Potentially harmful substances in the different cleaning products

*Table S3 a: Product 1 (diluted, 1 %)*

<b>Ret. time [min]</b>	<b>CAS No.</b>	<b>Identified compound</b>	<b>concentration [µg/l]</b>
<b>1.808</b>	64-17-5	Ethanol	796
<b>2.058</b>	67-63-0	Isopropanol	409
<b>3.242</b>	78-93-3	2-Butanone	114
<b>3.800</b>	141-78-6	Ethyl acetate	6
<b>6.050</b>	107-87-9	2-Pentanone	6
<b>20.733</b>	50871-05-1	3-Methyl-1,6-heptadien	11
<b>21.450</b>	10281-55-7	Citronellen	111
<b>22.142</b>	2807-34-3	5-Methyl-4-nonen	8
<b>22.633</b>	4057-42-5	2,6-Dimethyl-2-octen	17
<b>23.233</b>	500-00-5	3-Menthene	10
<b>24.325</b>	96100-29-7	1-Methyl-4-propyl-7-oxabicyclo[2,2,1]heptane	46
<b>24.650</b>	535-77-3	m-Cymene	464
<b>24.883</b>	500-00-5	p-Menthene	10
<b>25.000</b>	470-82-6	Eucalyptol, (1,8-Cineol)	965
<b>25.633</b>	3452-97-9	3,5,5-Trimethyl-1-Hexanol	70
<b>26.617</b>	18479-58-8	2,6-Dimethyl-7-octen-2-ol	1537
<b>27.458</b>	18479-57-7	2,6-Dimethyl-2-octanol	545
<b>27.683</b>	2983-37-1	ethyl-2-ethylhexanoate	43
<b>27.767</b>	137255-07-3	2-Ethyl-1,3,3-trimethylbicyclo[2,2,1]hept-5-en-2-ol	100
<b>28.208</b>	3613-33-0	Ethoxycitronellal	11
<b>28.650</b>	112-54-9	Dodecanal	24
<b>29.875</b>	66998-67-2	[[[(2-Chlorethyl)sulfonyl]methyl]benzol	9
<b>30.367</b>	19780-33-7	2-Ethyl-1-dodecanol	84
<b>30.492</b>	21078-65-9	2-Ethyl-1-decanol	92
<b>Total number:</b>		24	5488

Table S 3 b: Product 2 (diluted, 1 %)

Ret. time [min]	CAS No.	Identified compound	concentration [µg/l]
1.808	64-17-5	Ethanol	10749
2.067	67-63-0	Isopropanol	720
2.328	75-65-0	tert,-Butanol	59
3.250	78-93-3	2-Butanone	373
5.425	71-36-3	1-Butanol	176
9.333	105-57-7	1,1-Diethoxyethane	13
16.092	7452-79-1	Ethyl-2-methylbutanoate	138
17.120	111-27-3	1-Hexanol	20
20.650	54004-42-1	Ethyl-2,3Dimethylbutanoate	59
20.858	7785-70-8	alpha-Pinen	66
21.150	123-05-7	2-Ethylhexanal	11
22.492	110-93-0	6-Methyl-5-hepten-2-on	16
22.567	3387-41-5	4-Methylen-1-(1-methylethyl)-bicyclo[3,1,0]hexane	32
22.742	18172-67-3	β-Pinen	88
24.142	124-18-5	n-Decane	26
24.825	104-76-7	2-Ethyl-1-hexanol	22244
25.015	470-82-6	Eucalyptol, (1,8-Cineol)	2893
25.092	5989-27-5	D-Limonen	653
27.383	106-30-9	Ethyl-heptanoate	10
28.008	1423-46-7	2,4,6-Trimethyl-3-cyclohexen-1-carboxaldehyde	23
28.267	97-62-1	Ethylisobutanoate	99
28.300	89-80-5	trans-Menthone	91
28.425	491-07-6	Isomenthone	30
28.525	89-78-1	Menthol	17
28.592	142-19-8	Allylheptanoate	512
28.983	629-50-5	n-Tridecan	22
29.650	98-54-4	4-tert-Butylcyclohexylacetat	847
30.150	20279-29-2	Phenylisobutanoate	9
30.367	127-41-3	alpha-Ionon	8
<b>Total number:</b>		29	40004

Table S 3 c: Product3 (diluted, 1 %)

Ret. time [min]	CAS No.	Identified compound	concentration [µg/l]
1.808	64-17-5	Ethanol	14080
2.067	67-63-0	Isopropanol	1061
3.242	78-93-3	2-Butanone	397
4.975	563-80-4	3-Methyl-2-butanone	19
7.773	142-82-5	n-Heptane	3
17.067	111-27-3	1-Hexanol	1017
20.550	106-68-3	3-Octanone	24
20.858	7785-70-8	alpha-Pinen	2
21.150	123-05-7	2-Ethylhexanal	23
22.925	106-67-2	2-Ethyl-4-methyl-1-pentanol	8
24.150	124-18-5	n-Decane	35
24.967	104-76-7	2-Ethyl-1-hexanol	122537
25.092	5989-27-5	D-Limonen	338
25.692	7146-60-3	2,3-Dimethyloctane	6
26.650	18479-58-8	2,6-Dimethyl-7-octen-2-ol	7522
28,983	629-50-5	n-Tridecane	23
29,650	32210-23-4	4-tert-Butylcyclohexylacetate	382
<b>Total number:</b>		17	147477

Table S 3 d: Product 4 (diluted, 1 %)

Ret. time [min]	CAS No.	Identified compound	concentration [µg/l]
1.817	64-17-5	Ethanol	28984
2.092	67-63-0	Isopropanol	4354
3.250	123-72-8	Butanal	1216
16.108	7452-79-1	Ethyl-2-methylbutanoate	20
20.733	59840-10-7	2,7-Dimethyl-1,7-octadien	19
21.450	10281-55-7	Citronellen	11
24.792	104-76-7	2-Ethyl-1-hexanol	10303
25.092	5989-27-5	D-Limonen	34
26.625	18479-58-8	2,6-Dimethyl-7-octen-2-ol	7064
28.292	101-41-7	Methyl-phenylacetate	11
28.583	19781-07-8	2,7-Dimethyl-2,7-octandiol	389
28.667	101-97-3	Ethyl-phenylacetate	9
29.092	7540-51-4	Citronellol	52
29.650	98-54-4	4-tert-Butylcyclohexylacetate	750
29.917	150-84-5	Citronellolacetate	80
31.333	6259-76-3	n-Hexylsalicylate	14

<b>Total number:</b>	16	53310
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*Table S 3 e: Experimental product 5 (diluted, 1 %)*

Ret. time [min]	CAS No.	Identified compound	concentration [µg/l]
1.924	67-63-0	Isopropanol	82
2.958	123-72-8	Butanal	10
5.068	71-36-3	1-Butanol	316
13.385	14850-23-8	4-Octen trans	7
13.769	13389-42-9	2-Octen trans	4
14.216	111-67-1	2-Octen cis	3
20.384	5131-66-8	1-Butoxy-2-propanol, (Propylenglycolmonobutylether)	3104
20.571	75-98-9	Pivalic acid	61
20.723	123-05-7	2-Ethylhexanal	13
20.926	6863-58-7	Di-sec-butylether	76
24.356	104-76-7	2-Ethyl-1-hexanol	7515
27.233	1569-01-3	2-(1-Methylethoxy)-1-propanol	41
27.942	818-81-5	2-Methyl-1-octanol	100
28.133	2370-14-1	2,2-Dimethyl-1-octanol	105
28.284	41884-28-0	Tetrahydrolavandulol	113
28.481	112-34-5	Butyldiglycol	98
28.614	10042-59-8	2-Propyl-1-heptanol	955
28.674	34019-17-5	2-Methyl-1-undecanol	818
28.741	106-21-8	3,7-Dimethyl-1-octanol (Dihydrocitronellol)	865
28.881	112-30-1	1-Decanol	470
29.522	32210-23-4	4-tert-Butylcyclohexylacetate	2
30.127	629-59-4	n-Tetradecane	16
30.400	112-53-8	1-Dodecanol	177
Total number:		23	14951

Table S 4: Release of potential harmful substances from different surface and floor materials  
Effect of artificial cleaning with different cleaning products

Table S 4 a: Laminate A

Ret. time [min]		Released Concentration [mg/kg]			
		before cleaning	Product 2	Product 3	Product 5
3.742	Acetic acid	20	25	33	31
12.633	Hexanal	10	1	1	1
13.992	Furfural	7	9	9	12

Table S 4 b: Laminate C

Ret. time [min]		Released Concentration [mg/kg]				
		before cleaning	Product 2	Product 3	Product 5	H <sub>2</sub> O only
3.250	2-Butanone	165	195	133	149	170
3.833	Ethyl acetate	1	2	1	2	2
5.457	1-Butanol	16	25	20	22	26
7.658	Methylmethacrylate	5	16	11	14	13
9.150	4-Methyl-2-pentanone	4	6	4	6	5
11.105	Toluene	1	4	4	3	2
13.211	3-Methylheptane	1	1	1	1	1
13.950	Butylacetate	3	7	5	6	6
17.210	Cyclohexanon	100	131	86	116	94
18.300	Butylacrylate	1	2	1	2	1
21.150	2-Ethylhexanal	1	1	1	1	1
23.883	Isododecane	35	64	38	78	47
24.142	n-Decane	1	1	1	1	1
24.758	Isooctanol, (2-Ethyl-1-Hexanol)	29	73	85	55	78
25.483	2,2,4,4-Tetramethyloctane	4	6	3	4	4
26.442	6-Methyldodecane	1	1	1	1	1
28.283	Octylacetate	1	2	1	1	1

Table S 4 c: Laminate D

Ret. time [min]		Released Concentration [mg/kg]				
		before cleaning	Product 2	Product 3	Product 5	H <sub>2</sub> O only
3.250	2-Butanon	141	247	151	221	194
3.548	2-Butanol	10	11	13	14	14
3.867	Ethyl acetate	29	91	37	57	73
5.474	1-Butanol	14	19	15	16	17
9.150	4-Methyl-2-pentanone	6	10	6	7	7
11.105	Toluene	18	83	86	124	52
12.650	Hexanal	4	1	1	1	1
13.950	Butylacetate	10	21	12	15	13
17.210	Cyclohexanone	3	4	2	3	2
23.883	Isododecane	1	1	1	1	1
24.758	Isooctanol. (2-Ethyl-1-Hexanol)	28	110	109	121	76
28.283	Octylacetate	4	6	4	5	2

Table S 4 d: Vinyl bue

Ret. time [min]		Released Concentration [mg/kg]			
		before cleaning	Product 2	Product 3	Product 5
4.186	Isobutanol	6	3	4	5
10.428	2,3,4-Trimethylpentane	1	1	1	1
10.659	2,3,3-Trimethylpentane	1	2	1	1
23.506	Isododecane	1	1	2	1
24.412	Isooctanol, (2-Ethyl-1-hexanol)	7	6	7	4

Table S 4 e: Vinyl grey

Ret. time [min]		Released Concentration [mg/kg]			
		before cleaning	Product 2	Product 3	Product 5
10.622	2,3,3-Trimethylpentane	1	2	2	1
12.597	2,2,5-Trimethylhexane	1	1	1	1
12.759	3-Methylenheptane	1	2	1	1
23.885	Isododecane	14	20	22	18
24.741	Isooctanol, (2-Ethyl-1-hexanol)	6	9	16	7
25.073	2,2,4,4-Tetramethyloctane	1	1	1	1



Table S 4 f: Vinyl mixed colored

Ret. time [min]		Released Concentration [mg/kg]			
		before cleaning	Product 2	Product 3	Product 5
<b>1.717</b>	Ethanol	123	125	105	86
<b>2.187</b>	n-Pentane	14	13	13	11
<b>2.492</b>	Formic acid	<1	10	<1	20
<b>2.683</b>	1-Propanol	<b>28</b>	22	19	18
<b>3.182</b>	Butanal	23	21	17	18
<b>3.484</b>	Acetic acid	1	9	3	3
<b>3.527</b>	n-Hexane	5	3	3	14
<b>5.442</b>	1-Butanol	43	32	26	28
<b>5.674</b>	2-Pentanone	2	3	2	2
<b>5.804</b>	1-Penten-3-ol	16	15	11	13
<b>6.412</b>	Pentanal	46	39	35	36
<b>6.824</b>	2-Ethylfuran	5	7	7	5
<b>7.794</b>	n-Heptane	12	10	11	10
<b>10.817</b>	1-Pentanol	16	24	12	19
<b>11.703</b>	2-Hexanone	1	2	1	1
<b>12.623</b>	Hexanal	74	82	62	63
<b>12.881</b>	1-Octene	1	1	1	1
<b>14.002</b>	n-Octane	12	11	11	10
<b>14.198</b>	Pentylformiate	2	3	1	2
<b>16.809</b>	Cyclohexanone	3	1	2	1
<b>17.394</b>	2-Heptanone	2	2	2	2
<b>18.350</b>	Heptanal	6	5	4	4
<b>18.413</b>	1-Nonene	1	1	1	1
<b>18.996</b>	n-Nonane	1	1	1	1
<b>20.420</b>	Benzaldehyde	2	2	1	2
<b>21.692</b>	1-Heptanol	2	3	1	3
<b>22.867</b>	Octanal	7	6	5	7
<b>27.182</b>	Nonanal	3	3	3	3
<b>27.809</b>	Decanol	1	2	1	1

Figure S 1 : Daily time course of the sewage concentration of different trace substances after cleaning with products 1 to 4 (summarized as reference) and the experimental product. The data show the mean from 10 individual measurements from Monday to Friday











