

Table S1. Identification of organic contaminants (unexpected substances) of rubber material by LLE-GC-MS from the analysis of water from the 1st migration (3rd day) and its quantification by a semi-quantitative method (S/V = 5).

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	C_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MTCTap
							(μg/l)				
1	8.607	2,2-dimethoxy-propane	77-76-9	739	761	68.4	0.891	0.0594	0.00119	0.000594	1.0
2	8.801	benzene	71-43-2	830	897	74.7	1.50	0.1003	0.00201	0.00100	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	---
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	---
5	17.436	cyclohexylamine	108-91-8	953	956	92.7	46.8	3.118	0.0624	0.0312	2.1
6	19.197	cyclohexanone	108-94-01	931	932	72.7	7.7	0.5155	0.0103	0.00515	1.0
7	22.540	benzaldehyde	100-52-7	970	970	82	62.8	4.1864	0.0837	0.0419	1.0
8	23.546	benzonitrile	100-47-0	879	903	50.4	2.4	0.1619	0.00324	0.00162	0.1
9	24.015	isocyanate-cyclohexane	3173-53-3	967	968	94.1	82.0	5.4640	0.1092	0.0546	1.0
10	24.550	benzylamine	100-46-09	911	931	59.8	6.1	0.4080	0.00816	0.00408	1.0
11	25.007	2-ethyl-1-hexanol	104-76-7	870	901	52.8	3.0	0.1978	0.00395	0.00198	1500
12	25.219	benzyl alcohol	100-51-6	913	829	46.6	1.5	0.1012	0.00202	0.00101	1.0
13	26.206	unknown	---	---	---	---	1.8	0.1218	0.00243	0.00121	1.0
14	27.017	methyl benzoate	95-58-3	874	924	69	2.3	0.1553	0.00310	0.00155	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	---
16	28.748	benzoic acid	65-85-0	931	945	52.8	10.0	0.6678	0.01336	0.00668	1.0
17	29.777	2-phenoxy-ethanol	122-99-6	837	868	85.1	1.0	0.06808	0.00136	0.000681	1.0
18	30.034	benzothiazole	95-16-9	933	933	75.5	110.2	7.3494	0.14698	0.073494	0.1
19	30.157	isothiocyanate-cyclohexane	1122-82-03	921	922	96.5	62.0	4.1365	0.08273	0.041366	1.0
20	30.236	benzylazetidine	7730-39-4	824	849	63.7	3.0	0.1995	0.00399	0.001996	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.492	N-cyclohexyl-formamide	766-93-8	935	938	97	22.7	1.5150	0.03030	0.015151	1.0
23	31.057	N-cyclohexyl-acetamide	1124-53-4	931	935	96.8	6.7	0.4476	0.00895	0.00448	1.0
24	31.711	benzamide	55-21-0	878	908	62.6	4.3	0.2881	0.00576	0.00288	1.0
25	31.910	t-butyl-p-cresol	2409-55-4	947	947	34.6	3.7	0.2456	0.00493	0.00246	1.0
26	32.016	unknown	---	---	---	---	0.4	0.02707	0.00054	0.000271	1.0
27	32.308	benzyl isothiocyanate	622-78-6	930	941	75.7	11.2	0.7451	0.01490	0.00745	1.0
28		6-tert-Butyl-2,4-xylenol	1879-09-0	---	---	---	---	---	---	---	---

29	32.716	N-benzylformamide	6343-54-0	945	962	93.6	10.9	0.7269	0.01454	0.00727	1.0
30	32.850	unknown	---	---	---	---	0.7	0.04969	0.00099	0.00049	1.0
31	32.939	unknown	---	---	---	---	0.8	0.05086	0.00101	0.00050	1.0
32	33.231	N-benzylacetamide	588-46-5	854	914	74.4	2.1	0.1387	0.002775	0.00139	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina	147-47-7	---	---	---	---	---	---	---	1.0
34	33.580	1-dodecanol	112-53-8	962	963	32.3	12.6	0.8396	0.01679	0.00839	1.0
35	33.668	unknown	---	---	---	---	1.7	0.11175	0.002235	0.001117	1.0
36	34.190	unknown	---	---	---	---	0.7	0.04979	0.000995	0.000497	1.0
37	34.653	dodecanoic acid	143-07-7	877	924	78	2.2	0.1466	0.00293	0.00147	1.0
38	35.040	N-phenylcyclohexylamine	1821-36-9	814	887	88.1	0.9	0.06330	0.00126	0.000633	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40	35.103	N-(phenylmethylene)-cyclohexamine	2211-66-7	922	923	97.4	8.0	0.5356	0.0107	0.0053	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.659	2-(methylthio)-benzothiazole	615-22-5	949	949	87.3	15.5	1.0352	0.0207	0.0103	1.0
43	35.762	tributylphosphate	126-73-8	737	883	66.8	0.4	0.02550	0.00051	0.000255	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45	36.082	unknown	---	---	---	---	1.7	0.11137	0.00222	0.001113	1.0
46	36.307	2-benzothiazolone	934-34-9	921	928	94.3	11.7	0.7807	0.0156	0.00780	0.1
47	36.432	Dibenzylmethylamine	102-05-6	884	917	91.6	0.3	0.02115	0.000423	0.000212	1.0
48	36.571	Lauryl ethoxylate	4536-30-5	909	918	58.5	2.6	0.1715	0.00343	0.00171	1.0
49	36.936	Dibenzylamine	103-49-1	920	923	91.3	70.7	4.7125	0.0942	0.0471	1.0
50	37.150	Dibenzylhydroxylamine	621-07-8	939	940	55.9	17.8	1.1894	0.0237	0.0118	1.0
51		N-Benzylidenebenzylamine	780-25-6	---	---	---	---	---	---	---	1.0
52		N-butylbenzenesulfonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53	37.845	Benthiazole	21564-17-0	723	809	45	7.8	0.5177	0.0103	0.00517	1.0
54	37.995	unknown	---	---	---	---	1.0	0.06628	0.00132	0.000662	1.0
55	38.573	N-cyclohexylbenzamide	1759-68-8	932	932	93	34.3	2.2852	0.0457	0.0228	1.0
56	38.904	N-methylbenzothiazoline-2-thione	2254-94-6	847	890	83.7	5.8	0.3869	0.00773	0.00386	1.0
57	39.181	Methyl-o-benzoylbenzoate	606-28-0	626	686	35.5	2.7	0.1805	0.00361	0.00180	1.0
58	39.722	2-mercaptobenzothiazole	149-30-4	932	936	96.5	184.5	12.3007	0.246	0.123	100
59	39.965	N-benzylformamide	6343-54-0	765	808	55	90.2	6.0159	0.120	0.0601	1.0
60	40.125	N-benzylbenzamide	1485-70-7	933	935	76.6	33.6	2.2415	0.0448	0.0224	1.0
61	40.428	Benzenesulfanilide	1678-25-7	819	875	94.6	1.7	0.1115	0.00223	0.00111	1.0

62	40.396	1,3-dicyclohexylurea	2387-23-7	905	922	97.3	32.6	2.174	0.0434	0.0217	1.0
63	40.666	unknown	---	---	---	---	22.6	1.507	0.03014	0.0150	1.0
64	40.851	2,3-diphenylmaleic anhydride	4808-48-4	809	893	85.3	1.8	0.1200	0.002402	0.00120	1.0
65	41.039	unknown	---	---	---	---	29.6	1.972	0.039457	0.019728	1.0
66	41.247	unknown	---	---	---	---	80.3	5.350	0.107019	0.053509	1.0
67	41.362	N,N'-dicyclohexyloxamide	3299-64-7	871	920	96.7	7.8	0.5223	0.010447	0.00522	1.0
68	41.642	2-cyclohexylamino-benzothiazole	28291-75-0	832	928	90.9	5.4	0.3577	0.007155	0.00357	1.0
69	41.750	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	893	928	95.1	16.2	1.0807	0.021615	0.0108	1.0
70	42.109	N-benzyl-benzenecarbothiamide	14309-89-8	909	956	95.6	208.6	13.904	0.2780	0.139	1.0
71	42.218	unknown	---	---	---	---	1.9	0.12371	0.00247	0.00123	1.0
72	42.262	Ethyl 9-fluorenyldeneacetate	27973-36-0	688	768	69	2.4	0.1624	0.00328	0.00162	1.0
73	42.557	unknown	---	---	---	---	2.8	0.18806	0.00376	0.00188	1.0
74	42.625	unknown	---	---	---	---	1.3	0.08617	0.00172	0.000861	1.0
75		unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77	43.055	N,N'-dibenzilureia	1466-67-7	737	848	61.8	3.1	0.2036	0.00407	0.00203	1.0
78	43.395	Antioxidant BKF	119-47-1	804	814	92.9	1.9	0.12504	0.00250	0.00125	75
79	43.565	unknown	---	---	---	---	65.6	4.3720	0.08744	0.04372	1.0
80	44.987	unknown	---	---	---	---	7.1	0.47006	0.009401	0.00470	1.0
81	45.433	unknown	---	---	---	---	2.5	0.16644	0.003328	0.00166	1.0
82	46.155	unknown	---	---	---	---	6.0	0.39718	0.007943	0.00397	1.0
83	46.419	unknown	---	---	---	---	15.8	1.05391	0.021078	0.0105	1.0
84	46.927	unknown	---	---	---	---	1.1	0.07645	0.001529	0.000764	1.0
85	47.974	unknown	---	---	---	---	5.3	0.3550	0.007101	0.00355	1.0
86	48.542	2,2'-tiobis-benzotiazol	402147	836	892	97.4	3.4	0.2270	0.00454	0.00227	1.0
87	56.149	Cl-5808	332370	883	888	91.2	3.6	0.2413	0.00483	0.00241	1.0

Table S2. Identification of organic contaminants (unexpected substances) of rubber material by LLE-GC-MS from the analysis of water from the 1st migration (3rd day) and its quantification by a semi-quantitative method (S/V = 5). Analysis of duplicate.

	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	$MTCTap$
							(μg/l)				
1	8.802	2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2	8.801	benzene	71-43-2	836	913	71	1.2	0.0797	0.001593	0.000797	1.0
3	11.062	1,1-diethoxy-ethane	105-57-7	884	893	93.5	4.0	0.2670	0.00534	0.00267	2.1
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.426	cyclohexylamine	108-91-8	952	953	94.1	34.6	2.3041	0.046082	0.023041	1.0
6	19.186	cyclohexanone	108-94-01	933	935	72.6	7.1	0.4718	0.009437	0.004718	1.0
7	22.542	benzaldehyde	100-52-7	965	965	81.8	57.9	3.8599	0.077197	0.038599	1.0
8	23.538	benzonitrile	100-47-0	893	936	63.8	2.1	0.1384	0.002768	0.001384	0.1
9	24.015	isocyanate-cyclohexane	3173-53-3	971	971	94	64.5	4.2978	0.085957	0.042978	1.0
10	24.555	benzylamine	100-46-09	917	939	64.6	4.4	0.2954	0.005908	0.002954	1.0
11	25.003	2-ethyl-1-hexanol	104-76-7	876	915	53.3	3.2	0.2109	0.0042181	0.002109	1500
12	25.215	benzyl alcohol	100-51-6	879	907	45	1.8	0.1172	0.0023442	0.001172	1.0
13	26.204	unknown	---	---	---	---	2.3	0.1503	0.0030059	0.001502	1.0
14	27.013	methyl benzoate	95-58-3	891	943	70.9	2.3	0.1516	0.003033	0.001516	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16	28.817	benzoic acid	65-85-0	969	970	60.6	10.6	0.7075	0.0141492	0.007074	1.0
17	29.783	2-phenoxy-ethanol	122-99-6	804	858	78	1.0	0.0697	0.001393	0.000697	1.0
18	30.043	benzothiazole	95-16-9	926	926	75	89.4	5.9610	0.1192192	0.059609	0.1
19	30.161	isothiocyanate-cyclohexane	1122-82-03	920	921	97.7	44.9	2.9943	0.059885	0.029943	1.0
20	30.236	benzylazetidine	7730-39-4	809	832	56.9	3.2	0.2109	0.004218	0.002109	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.501	N-cyclohexyl-formamide	766-93-8	942	944	97.3	18.2	1.2154	0.024307	0.012154	1.0
23	31.062	N-cyclohexyl-acetamide	1124-53-4	938	942	97	5.2	0.3491	0.006982	0.003491	1.0
24	31.717	benzamide	55-21-0	880	912	58.6	3.5	0.2337	0.004674	0.002337	1.0

25	31.911	t-butyl-p-cresol	2409-55-4	947	947	27.2	3.3	0.2225	0.004451	0.002225	1.0
26	32.015	unknown	---	---	---	---	0.4	0.0259	0.0005187	0.000259	1.0
27	32.308	benzyl isothiocyanate	622-78-6	932	943	78	8.1	0.5401	0.010802	0.005401	1.0
28	32,527	6-tert-Butyl-2,4-xyleneol	1879-09-0	878	879	77.3	1.0	0.0650	0.0013002	0.000650	1.0
29	32.721	N-benzylformamide	6343-54-0	945	965	94.2	9.3	0.6208	0.012416	0.006208	1.0
30	32.850	unknown	---	---	---	---	1.1	0.0703	0.0014068	0.000703	1.0
31	32.939	unknown	---								1.0
32	33.233	N-benzylacetamide	588-46-5	859	921	77.6	1.9	0.1274	0.002548	0.001274	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina	147-47-7	---	---	---	---	---	---	---	1.0
34	33.580	1-dodecanol	112-53-8	936	949	26.1	10.2	0.6816	0.013631	0.006816	1.0
35	33.668	unknown	---	---	---	---	1.4	0.0912	0.0018241	0.000912	1.0
36	34.190	unknown	---	---	---	---	0.7	0.0480	0.0009605	0.000480	1.0
37	34.661	dodecanoic acid	143-07-7	902	943	85.4	4.7	0.3138	0.006276	0.003138	1.0
38	35.040	N-phenylcyclohexylamine	1821-36-9	781	877	81.1	1.0	0.0665	0.00133	0.000665	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40	35.103	N-(phenylmethylene)-cyclohexamine	2211-66-7	915	917	96.4	6.1	0.4061	0.008123	0.004061	1.0
41	35.385	N-methyl-2-benzothiazolinone	2786-62-1	916	922	86.1	0.5	0.0323	0.000646	0.000323	1.0
42	35.661	2-(methylthio)-benzothiazole	615-22-5	956	958	88.5	13.5	0.9017	0.018035	0.009017	1.0
43	35.76	tributylphosphate	126-73-8	734	889	64.6	0.4	0.0245	0.00049	0.000245	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45	36.081	unknown	---	---	---	---	1.7	0.1103	0.002205	0.001103	1.0
46	36.323	2-benzothiazolone	934-34-9	923	931	94.2	9.7	0.6464	0.012928	0.006464	0.1
47	36.43	Dibenzylmethylamine	102-05-6	841	912	92.5	0.2	0.0155	0.00031	0.000155	1.0
48	36.571	Lauryl ethoxylate	4536-30-5	907	908	54.3	2.4	0.1628	0.003257	0.001628	1.0
49	36.939	Dibenzylamine	103-49-1	912	916	90.1	51.5	3.4352	0.068703	0.034352	1.0
50	37.151	Dibenzylhydroxylamine	621-07-8	938	939	78.9	16.5	1.0993	0.021986	0.010993	1.0
51		N-Benzylidenebenzylamine	780-25-6	---	---	---	---	---	---	---	1.0
52		N-butylbenzenesulfonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53	37.844	Benthiazole	21564-17-0	709	803	68.3	16.5	1.0993	0.021986	0.010993	1.0

54	37.995	unknown	---	---	---	---	0.9	0.0578	0.0011556	0.000577	1.0
55	38.577	N-cyclohexylbenzamide	1759-68-8	929	929	92.3	27.1	1.8083	0.036167	0.018083	1.0
56	38.904	N-methylbenzothiazoline-2-thione	2254-94-6	837	886	81.7	5.1	0.3395	0.00679	0.003395	1.0
57	39.180	Methyl-o-benzoylbenzoate	606-28-0	604	664	62	2.1	0.1433	0.002866	0.001433	1.0
58	39.756	2-mercaptobenzothiazole	149-30-4	930	943	96.4	147.7	9.8482	0.196963	0.098482	100
59	39.978	N-benzylformamide	6343-54-0	761	808	46.8	70.5	4.7004	0.094008	0.047004	1.0
60	40.141	N-benzylbenzamide	1485-70-7	936	947	77.7	26.8	1.7834	0.035668	0.017834	1.0
61	40.261	Benzenesulfanilide	1678-25-7	788	807	95.8	1.3	0.0841	0.001681	0.000841	1.0
62	40.407	1,3-dicyclohexylurea	2387-23-7	895	927	97.7	24.1	1.6064	0.032127	0.016064	1.0
63	40.671	unknown	---				17.8	1.1889	0.023778	0.011889	1.0
64	40.854	2,3-diphenylmaleic anhydride	4808-48-4	869	914	83.9	0.9	0.0611	0.001222	0.000611	1.0
65	41.043	unknown	---	---	---	---	24.9	1.6598	0.0331962	0.016598	1.0
66	41.253	unknown	---	---	---	---	62.6	4.1710	0.0834198	0.041709	1.0
67	41.367	N,N'-dicyclohexyloxamide	3299-64-7	872	923	96.4	6.1	0.4069	0.0081382	0.004069	1.0
68	41.650	2-cyclohexylamino-benzothiazole	28291-75-0	843	906	95.9	4.4	0.2915	0.0058300	0.002915	1.0
69	41.758	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	862	912	93.2	12.4	0.8285	0.0165701	0.008285	1.0
70	42.115	N-benzyl-benzenecarbothiamide	14309-89-8	903	956	97	17.1	1.1427	0.0228546	0.011427	1.0
71	42.22	unknown	---				1.5	0.1004	0.0020086	0.001004	1.0
72	42.263	Ethyl 9-fluorenyldeneacetate	27973-36-0	720	781	87.5	2.0	0.1306	0.0026111	0.001305	1.0
73	42.391	unknown	---	---	---	---	0.7	0.0483	0.0009658	0.000482	1.0
74	42.56	unknown	---	---	---	---	2.4	0.1580	0.0031596	0.001579	1.0
75		unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77	43.06	N,N'-dibenzilureia	1466-67-7	747	924	72.2	26.1	1.7421	0.0348412	0.017420	1.0
78	43.393	Antioxidant BKF	119-47-1	816	824	89.8	1.1	0.0724	0.0014478	0.000723	75
79	43.567	unknown	---				45.2	3.0128	0.0602566	0.030128	1.0
80	44.99	unknown	---	---	---	---	5.9	0.3910	0.0078208	0.003910	1.0
81	45.434	unknown	---	---	---	---	1.8	0.1224	0.0024476	0.001223	1.0

82	46.161	unknown	---	---	---	---	5.0	0.3313	0.0066260	0.003313	1.0
83	46.422	unknown	---	---	---	---	13.5	0.8993	0.0179853	0.008992	1.0
84	46.926	unknown	---	---	---	---	1.0	0.0693	0.0013861	0.000693	1.0
85	47.978	unknown	---	---	---	---	4.2	0.2822	0.0056433	0.002821	1.0
86	48.544	2,2'-tiobis-benzotiazol	402147	768	859	90.9	3.6	0.2378	0.004755	0.002378	1.0
87	56.147	Cl-5808	332370	826	860	84.4	3.7	0.2465	0.004931	0.002465	1.0

Table S3. Identification of organic contaminants (unexpected substances) of rubber material by LLE-GC-MS from the analysis of water from the 1st migration (3rd day) and its quantification by a semi-quantitative method (S/V = 10).

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MTCTap
							(μg/l)				
1	8.602	2,2-dimethoxy-propane	77-76-9	805	818	81.6	1.4	0.0463	0.000926	0.000463	1.0
2	8.801	benzene	71-43-2	---	---	---	---	---	---	---	1.0
3	11.610	1,1-diethoxy-ethane	105-57-7	899	904	94.2	3.8	0.1274	0.00254	0.00127	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.428	cyclohexylamine	108-91-8	953	954	94.2	57.8	1.9266	0.03853	0.01926	2.1
6	19.192	cyclohexanone	108-94-01	935	936	68.5	14.8	0.4934	0.00986	0.00493	1.0
7	22.566	benzaldehyde	100-52-7	965	965	80.3	102.5	3.4151	0.06830	0.03415	1.0
8	23.542	benzonitrile	100-47-0	913	923	68.7	3.4	0.1135	0.00227	0.00113	0.1
9	24.031	isocyanate-cyclohexane	3173-53-3	971	971	94	100.4	3.3476	0.066952	0.033476	1.0
10	24.597	benzylamine	100-46-09	859	896	48.2	2.5	0.0818	0.00163	0.00081	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12	25.223	benzyl alcohol	100-51-6	913	928	47.8	4.3	0.1449	0.00289	0.00144	1.0
13	26.192	unknown	---	---	---	---	6.1	0.2041	0.00408	0.00204	1.0
14	27.018	methyl benzoate	95-58-3	816	923	62.6	1.3	0.0431	0.00086	0.00043	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16	28.846	benzoic acid	65-85-0	958	961	53.7	11.5	0.3833	0.00766	0.00383	1.0
17	29.795	2-phenoxy-ethanol	122-99-6	848	871	86.1	0.9	0.0299	0.00059	0.00029	1.0
18	30.036	benzothiazole	95-16-9	925	928	78.2	115.1	3.8377	0.07675	0.03837	0.1
19	30.168	isothiocyanate-cyclohexane	1122-82-03	929	930	98.4	50.9	1.6964	0.03392	0.01696	1.0
20	30.236	benzylazetidine	7730-39-4	828	852	56.6	2.9	0.0968	0.00193	0.00096	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.525	N-cyclohexyl-formamide	766-93-8	938	940	97.2	29.0	0.9663	0.01932	0.00966	1.0
23	31.075	N-cyclohexyl-acetamide	1124-53-4	941	944	97.4	8.2	0.2723	0.00544	0.00272	1.0
24	31.738	benzamide	55-21-0	904	925	72.1	6.2	0.2066	0.00413	0.00206	1.0
25	31.919	t-butyl-p-cresol	2409-55-4	941	941	28.1	4.0	0.1323	0.00264	0.00132	1.0
26	32.019	unknown	---	---	---	---	1.2	0.0414	0.00082	0.00041	1.0
27	32.310	benzyl isothiocyanate	622-78-6	935	946	81.7	11.0	0.3654	0.00730	0.00365	1.0
28	32.531	6-tert-Butyl-2,4-xyleneol	1879-09-0	874	886	59.9	1.2	0.0394	0.00078	0.00039	1.0

29	32.739	N-benzylformamide	6343-54-0	950	966	94.3	16.4	0.5457	0.01091	0.00545	1.0
30	32.852	unknown	---	---	---	---	0.8	0.0257	0.00051	0.00025	1.0
31	32.942	unknown	---	---	---	---	0.6	0.0186	0.00037	0.00018	1.0
32	33.246	N-benzylacetamide	588-46-5	879	931	80	2.9	0.0973	0.00194	0.00097	1.0
33	33.470	2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	814	881	61.5	1.0	0.0349	0.00069	0.00034	1.0
34	33.584	1-dodecanol	112-53-8	954	955	32.4	12.2	0.4062	0.00812	0.00406	1.0
35	33.674	unknown	---	---	---	---	2.2	0.0750	0.0015	0.00075	1.0
36	34.192	unknown	---	---	---	---	1.1	0.0381	0.00076	0.00038	1.0
37	34.678	dodecanoic acid	143-07-7	922	951	88.2	11.0	0.3651	0.00730	0.00365	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39	35.045	unknown	---	---	---	---	1.3	0.0423	0.00084	0.00042	1.0
40	35.103	N-(phenylmethylene)-cyclohexamine	2211-66-7	917	917	96.1	12.6	0.4194	0.00838	0.00419	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.659	2-(methylthio)-benzothiazole	615-22-5	955	955	88.9	11.1	0.3690	0.00738	0.00369	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45	36.083	unknown	---	---	---	---	1.9	0.0640	0.00128	0.00064	1.0
46	36.361	2-benzothiazolone	934-34-9	876	910	92.5	13.9	0.4633	0.00926	0.00463	0.1
47	36.431	Dibenzylmethylamine	102-05-6	674	844	84.1	0.3	0.0097	0.00019	9.67E-05	1.0
48	36.574	Lauryl ethoxylate	4536-30-5	898	909	57.5	2.5	0.0818	0.00163	0.00081	1.0
49	36.938	Dibenzylamine	103-49-1	918	925	91.6	41.8	1.3945	0.02788	0.01394	1.0
50		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51	37.160	N-Benzylidenebenzylamine	780-25-6	944	946	82	21.2	0.7070	0.01414	0.00707	1.0
52		N-butylbenzenesulfonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53	37.847	Benthiazole	21564-17-0	696	790	64.2	6.1	0.2022	0.00404	0.00202	1.0
54	37.997	unknown	---	---	---	---	0.8	0.0278	0.00055	0.00027	1.0
55	38.593	N-cyclohexylbenzamide	1759-68-8	937	938	94.9	33.7	1.1237	0.02247	0.01123	1.0
56	38.908	N-methylbenzothiazoline-2-thione	2254-94-6	844	890	74.9	5.8	0.1941	0.00388	0.00194	1.0
57	39.182	Methyl-o-benzoylbenzoate	606-28-0	888	879	87.8	1.9	0.0618	0.00123	0.00061	1.0
58	39.857	2-mercaptobenzothiazole	149-30-4	927	933	96.3	183.5	6.1177	0.12235	0.06117	100
59	40.019	N-benzylformamide	6343-54-0	765	816	53	80.3	2.6766	0.05353	0.02676	1.0
60	40.223	N-benzylbenzamide	1485-70-7	943	944	76.5	34.7	1.1573	0.02314	0.01157	1.0
61	40.356	Benzenesulfanilide	1678-25-7	940	943	98.3	44.0	1.4667	0.02933	0.01466	1.0

62	40.449	1,3-dicyclohexylurea	2387-23-7	928	939	98	23.1	0.7685	0.01537	0.00768	1.0
63	40.692	unknown	---	---	---	---	16.7	0.5582	0.01116	0.00558	1.0
64	40.866	2,3-diphenylmaleic anhydride	4808-48-4	684	851	45.6	1.9	0.0628	0.00125	0.00062	1.0
65	41.051	unknown	---	---	---	---	20.8	0.6933	0.01386	0.00693	1.0
66	41.261	unknown	---	---	---	---	54.0	1.7992	0.03598	0.01799	1.0
67	41.382	N,N'-dicyclohexyloxamide	3299-64-7	839	909	95.2	7.1	0.2368	0.00473	0.00236	1.0
68	41.666	2-cyclohexylamino-benzothiazole	28291-75-0	832	927	91.5	3.8	0.1282	0.00256	0.00128	1.0
69	41.785	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	869	913	93	13.7	0.4552	0.00910	0.00455	1.0
70	42.131	N-benzyl-benzenecarbothiamide	14309-89-8	904	956	97.3	16.0	0.5343	0.01068	0.00534	1.0
71	42.231	unknown	---	---	---	---	1.7	0.0576	0.00115	0.00057	1.0
72	42.268	Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	1.1	0.0360	0.00072	0.00036	1.0
73	42.395	unknown	---	---	---	---	0.6	0.0202	0.00040	0.00020	1.0
74	42.572	unknown	---	---	---	---	3.0	0.0997	0.00199	0.00099	1.0
75	42.625	unknown	---	---	---	---	3.8	0.1283	0.00256	0.00128	1.0
76	42.706	unknown	---	---	---	---	1.6	0.0541	0.00108	0.00054	1.0
77	43.077	N,N'-dibenzilureia	1466-67-7	816	944	89.5	3.3	0.1087	0.00217	0.00108	1.0
78	43.391	Antioxidant BKF	119-47-1	847	852	96.8	1.4	0.0472	0.00094	0.00047	75
79	43.577	unknown	---	---	---	---	39.5	1.3174	0.02634	0.01317	1.0
80	44.997	unknown	---	---	---	---	4.4	0.1477	0.002954	0.001477	1.0
81	45.439	unknown	---	---	---	---	1.0	0.0321	0.000641	0.000320	1.0
82	46.165	unknown	---	---	---	---	4.2	0.1391	0.002782	0.001391	1.0
83	46.426	unknown	---	---	---	---	10.8	0.3604	0.007208	0.003604	1.0
84	46.929	unknown	---	---	---	---	0.8	0.0267	0.000534	0.000267	1.0
85	47.991	unknown	---	---	---	---	5.1	0.1709	0.003417	0.001708	1.0
86	48.559	2,2'-tiobis-benzotiazol	402147	830	889	97.1	7.3	0.2443	0.004886	0.002443	1.0
87	56.149	Cl-5808	332370	864	887	89.7	6.0	0.2012	0.004024	0.002012	1.0

Table S4. Identification of organic contaminants (unexpected substances) of rubber material by LLE-GC-MS from the analysis of water from the 1st migration (3rd day) and its quantification by a semi-quantitative method (S/V = 10). Analysis of duplicate.

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MTCTap
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3	11.613	1,1-diethoxy-ethane	105-57-7	885	887	93.2	1.2	0.0411	0.000821	0.000410	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.431	cyclohexylamine	108-91-8	951	952	95.7	54.6	1.8189	0.036378	0.018189	2.1
6	19.194	cyclohexanone	108-94-01	946	948	73.7	14.2	0.4739	0.009477	0.004738	1.0
7	22.576	benzaldehyde	100-52-7	969	969	81.5	104.0	3.4672	0.069343	0.034671	1.0
8	23.543	benzonitrile	100-47-0	953	955	76.3	3.1	0.1020	0.002039	0.001019	0.1
9	24.032	isocyanate-cyclohexane	3173-53-3	970	970	92.8	91.8	3.0591	0.061181	0.030590	1.0
10	24.602	benzylamine	100-46-09	914	919	72	2.4	0.0784	0.001568	0.000784	1.0
11	25.007	2-ethyl-1-hexanol	104-76-7	875	903	130	5.3	0.1779	0.003557	0.001778	1500
12	25.224	benzyl alcohol	100-51-6	905	921	49	43.1	1.4377	0.028753	0.014376	1.0
13	26.199	unknown	---	---	---	---	5.3	0.1779	0.003557	0.001778	1.0
14	27.017	methyl benzoate	95-58-3	843	933	67.9	1.3	0.0423	0.000845	0.000422	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16	28.865	benzoic acid	65-85-0	971	974	58.4	12.2	0.4066	0.008132	0.004066	1.0
17	29.799	2-phenoxy-ethanol	122-99-6	848	871	84.1	1.0	0.0323	0.000646	0.000323	1.0
18	30.060	benzothiazole	95-16-9	923	926	77.4	119.7	3.9904	0.079807	0.039903	0.1
19	30.171	isothiocyanate-cyclohexane	1122-82-03	923	928	97.8	52.3	1.7435	0.034870	0.017435	1.0
20	30.238	benzylazetidine	7730-39-4	795	845	59.1	3.2	0.1082	0.002163	0.001081	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	
22	30.529	N-cyclohexyl-formamide	766-93-8	939	941	97.3	29.0	0.9659	0.019317	0.009658	1.0
23	31.079	N-cyclohexyl-acetamide	1124-53-4	934	937	97.2	8.1	0.2700	0.005399	0.002699	1.0

24	31.745	benzamide	55-21-0	897	918	66.2	6.3	0.2094	0.004187	0.002093	1.0
25	31.919	t-butyl-p-cresol	2409-55-4	929	938	35.3	4.1	0.1363	0.002725	0.001362	1.0
26	32.019	unknown	---	---	---	---	1.7	0.0551	0.001101	0.000550	1.0
27	32.311	benzyl isothiocyanate	622-78-6	941	952	84.7	10.7	0.3578	0.007156	0.003578	1.0
28	32.531	6-tert-Butyl-2,4-xlenol	1879-09-0	859	864	61.3	1.6	0.0520	0.001040	0.000520	1.0
29	32.742	N-benzylformamide	6343-54-0	952	968	95.5	17.9	0.5956	0.011911	0.005955	1.0
30	32.852	unknown	---	---	---	---	1.5	0.0511	0.001022	0.000511	1.0
31	32.943	unknown	---	---	---	---	1.4	0.0459	0.000918	0.000459	1.0
32	33.250	N-benzylacetamide	588-46-5	880	933	81.5	3.6	0.1192	0.002383	0.001191	1.0
33	33.470	2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	745	827	46.1	1.4	0.0466	0.000931	0.000465	1.0
34	33.584	1-dodecanol	112-53-8	931	931	25.9	12.5	0.4157	0.008313	0.004156	1.0
35	33.674	unknown	---	---	---	---	2.3	0.0766	0.001531	0.000765	1.0
36	34.191	unknown	---	---	---	---	1.2	0.0415	0.000830	0.000415	1.0
37	34.683	dodecanoic acid	143-07-7	924	952	89	12.5	0.4177	0.008354	0.004177	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39	35.043	unknown	---	---	---	---	1.6	0.0542	0.001083	0.000541	1.0
40	35.108	N-(phenylmethylene)-cyclohexamine	2211-66-7	915	916	95.7	11.3	0.3776	0.007551	0.003775	1.0
41	35.389	N-methyl-2-benzothiazolinone	2786-62-1	840	873	62.6	0.9	0.0286	0.000571	0.000285	1.0
42	35.663	2-(methylthio)-benzothiazole	615-22-5	950	950	87.7	12.6	0.4197	0.008393	0.004196	1.0
43	35.762	tributylphosphate	126-73-8	714	894	55.4	0.3	0.0102	0.000203	0.000101	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45	36.083	unknown	---	---	---	---	2.3	0.0750	0.001500	0.000750	1.0
46	36.37	2-benzothiazolone	934-34-9	875	916	90.1	15.8	0.5267	0.010534	0.005267	0.1
47	36.432	Dibenzylmethylamine	102-05-6	607	734	87.5	0.4	0.0123	0.000246	0.000123	1.0
48	36.574	Lauryl ethoxylate	4536-30-5	867	893	53.6	2.9	0.0953	0.001906	0.000953	1.0
49	36.939	Dibenzylamine	103-49-1	918	925	92.3	35.7	1.1909	0.023817	0.011908	1.0
50		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0

51	37.160	N-Benzylidenebenzylamine	780-25-6	935	937	81.6	27.9	0.9303	0.018606	0.009303	1.0
52	37.577	N-butylbenzenesulfonamide	3622-84-2	730	786	71.1	4.0	0.1338	0.002676	0.001338	1.0
53	37.847	Benthiazole	21564-17-0	694	791	65.4	6.7	0.2242	0.004484	0.002242	1.0
54	37.997	unknown	---	---	---	---	1.0	0.0322	0.000643	0.000321	1.0
55	38.596	N-cyclohexylbenzamide	1759-68-8	933	933	93.9	38.0	1.2663	0.025325	0.012662	1.0
56	38.909	N-methylbenzothiazoline-2-thione	2254-94-6	804	878	83.5	6.2	0.2059	0.004118	0.002059	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.871	2-mercaptobenzothiazole	149-30-4	933	936	96.4	206.1	6.8713	0.137425	0.068712	100
59	40.026	N-benzylformamide	6343-54-0	763	815	49.7	90.8	3.0253	0.060505	0.030252	1.0
60	40.231	N-benzylbenzamide	1485-70-7	943	944	76.6	39.1	1.3029	0.026058	0.013029	1.0
61	40.366	Benzenesulfanilide	1678-25-7	935	941	98.2	49.8	1.6585	0.033170	0.016585	1.0
62	40.454	1,3-dicyclohexylurea	2387-23-7	943	954	97.9	24.2	0.8054	0.016107	0.008053	1.0
63	40.696	unknown	---	---	---	---	18.4	0.6141	0.012282	0.006141	1.0
64	40.869	2,3-diphenylmaleic anhydride	4808-48-4	688	862	45.2	2.0	0.0668	0.001335	0.000667	1.0
65	41.053	unknown	---	---	---	---	23.5	0.7831	0.015661	0.007830	1.0
66	41.263	unknown	---	---	---	---	60.0	2.0014	0.040028	0.020014	1.0
67	41.382	N,N'-dicyclohexyloxamide	3299-64-7	860	910	95.8	7.6	0.2520	0.005039	0.002519	1.0
68	41.67	2-cyclohexylamino-benzothiazole	28291-75-0	790	919	77.2	4.2	0.1406	0.002811	0.001405	1.0
69	41.789	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	869	914	93.5	14.9	0.4952	0.009904	0.004952	1.0
70	42.133	N-benzyl-benzenecarbothiamide	14309-89-8	902	954	97.6	18.1	0.6041	0.012082	0.006041	1.0
71	42.232	unknown	---	---	---	---	1.9	0.0620	0.001239	0.000619	1.0
72	42.269	Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	1.1	0.0362	0.000723	0.000361	1.0
73	42.395	unknown	---	---	---	---	0.6	0.0207	0.000414	0.000207	1.0
74	42.574	unknown	---	---	---	---	3.3	0.1112	0.002224	0.001112	1.0
75	42.627	unknown	---	---	---	---	0.4	0.0139	0.000278	0.000139	1.0

76	42.708	unknown	---	---	---	---	1.9	0.0647	0.001294	0.000647	1.0
77	43.078	N,N'-dibenzilureia	1466-67-7	769	931	80.8	3.7	0.1247	0.002493	0.001246	1.0
78	43.39	Antioxidant BKF	119-47-1	857	862	97	1.8	0.0595	0.001190	0.000595	75
79	43.577	unknown	---	---	---	---	41.1	1.3712	0.027423	0.013711	1.0
80	44.998	unknown	---	---	---	---	4.9	0.1646	0.003291	0.001645	1.0
81	45.439	unknown	---	---	---	---	1.0	0.0339	0.000677	0.000338	1.0
82	46.166	unknown	---	---	---	---	4.5	0.1508	0.003016	0.001508	1.0
83	46.426	unknown	---	---	---	---	12.2	0.4079	0.008157	0.004078	1.0
84	46.93	unknown	---	---	---	---	0.9	0.0291	0.000581	0.000290	1.0
85	47.99	unknown	---	---	---	---	5.5	0.1841	0.003682	0.001841	1.0
86	48.56	2,2'-tiobis-benzotiazol	402147	836	894	97.2	8.7	0.2891	0.005782	0.002891	1.0
87	56.165	Cl-5808	332370	862	883	90.5	7.0	0.2329	0.004658	0.002329	1.0

Table S5. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 2nd, 6-day migration, and their quantification by semi-quantitative method (S/V = 5).

N	t _R (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} 2	MTC _{tap} *
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4	16.72	4-hydroxy-4-methyl-2-pentanone	123-42-2	907	908	94.5	0.4	0.0271	0.000542	0.000271	
5	17.440	cyclohexylamine	108-91-8	954	955	95.2	3.9	0.2600	0.0052	0.0026	2.1
6	19.209	cyclohexanone	108-94-01	840	855	64.6	0.1	0.0070	0.000140	7.03E-05	1.0
7	22.533	benzaldehyde	100-52-7	963	963	81.5	3.8	0.2528	0.005055	0.002527	1.0
8	23.542	benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.020	isocyanate-cyclohexane	3173-53-3	969	970	92.4	6.4	0.4257	0.008513	0.004256	1.0
10	24.597	benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		1-hexanol-2-ethyl	104-76-7	---	---	---	---	---	---	---	1500
12	25.223	benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13	26.192	unknown	---	---	---	---	---	---	---	---	1.0
14	27.018	methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	
16	28.923	benzoic acid	65-85-0	935	947	56.9	2.6	0.1716	0.003432	0.001716	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.034	benzothiazole	95-16-9	925	925	78.2	94.7	6.3123	0.126246	0.063123	0.1
19	30.161	isothiocyanate-cyclohexane	1122-82-03	920	921	97.7	45.5	3.0327	0.060653	0.030326	1.0
20		benzylazetidine	7730-39-4	---	---	---	---	---	---	---	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	
22	30.515	N-cyclohexyl-formamide	766-93-8	932	937	97.3	21.1	1.4042	0.028084	0.014042	1.0
23	31.069	N-cyclohexyl-acetamide	1124-53-4	937	941	97.4	6.3	0.4198	0.008396	0.004198	1.0
24	31.727	benzamide	55-21-0	906	913	67.3	5.0	0.3351	0.006701	0.003350	1.0
25	31.913	t-butyl-p-cresol	2409-55-4	936	936	33.6	4.7	0.3149	0.006297	0.003148	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0

27	32.308	benzyl isothiocyanate	622-78-6	926	926	77.9	9.0	0.6015	0.012030	0.006015	1.0
28	32.531	tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.724	N-benzylformamide	6343-54-0	955	960	94.8	11.8	0.7891	0.015781	0.007890	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32	33.237	N-benzylacetamide	588-46-5	856	903	73.3	4.3	0.2855	0.005709	0.002854	1.0
33	33.470	2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37	34.678	dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38	35.040	N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39	35.045	unknown	---	---	---	---	---	---	---	---	1.0
40	35.100	N-(phenylmethylene)-cyclohexamine	2211-66-7	875	875	93.1	4.2	0.2830	0.005659	0.002829	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	
42	35.660	2-(methylthio)-benzothiazole	615-22-5	952	952	88.7	12.5	0.8341	0.016682	0.008341	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	
45	36.083	unknown	---	---	---	---					1.0
46	36.340	2-benzothiazolone	934-34-9	910	923	94.6	13.7	0.9113	0.018226	0.009113	0.1
47		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.944	Dibenzylamine	103-49-1	907	929	92.9	51.5	3.4306	0.068612	0.034306	1.0
50		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51	37.151	Benzaldehyde N-benzylimine	780-25-6	931	932	80.2	14.9	0.9911	0.019822	0.009911	1.0
52		N-butylbenzenesulfonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53	37.843	Benthiazole	21564-17-0	688	784	57.8	4.3	0.2872	0.005744	0.002872	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.584	N-cyclohexylbenzamide	1759-68-8	927	927	94	32.2	2.1436	0.042872	0.021436	1.0
56	38.908	N-methylbenzothiazoline-2-thione	2254-94-6	835	898	76	5.8	0.3889	0.007777	0.003888	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0

58	39.744	2-mercaptobenzothiazole	149-30-4	927	928	96.8	119.7	7.9801	0.159601	0.079800	100
59	39.977	N-benzylformamide	6343-54-0	751	797	53.9	74.9	4.9940	0.099880	0.049940	1.0
60	40.141	N-benzylbenzamide	1485-70-7	925	925	54.9	31.7	2.1130	0.042260	0.021130	1.0
61		Benzenesulfanilide	1678-25-7	---	---	---	---	---	---	---	1.0
62	40.403	1,3-dicyclohexylurea	2387-23-7	912	940	94.9	25.5	1.7008	0.034016	0.017008	1.0
63		unknown	---	---	---	---	18.8	1.2526	0.025052	0.012526	1.0
64	40.866	2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.044	unknown	---	---	---	---	26.5	1.7644	0.035288	0.017644	1.0
66	41.254	unknown	---	---	---	---	64.6	4.3083	0.086166	0.043083	1.0
67	41.365	N,N'-dicyclohexyloxamide	3299-64-7	847	854	97	7.3	0.4869	0.009738	0.004869	1.0
68	41.651	2-cyclohexylamino-benzothiazole	28291-75-0	764	824	77.7	4.9	0.3256	0.006512	0.003256	1.0
69	41.759	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	880	903	95.3	13.9	0.9300	0.018599	0.009299	1.0
70	42.117	N-benzyl-benzenecarbothiamide	14309-89-8	903	956	97	18.6	1.2420	0.024840	0.012420	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	
74		unknown	---	---	---	---	---	---	---	---	1.0
75		unknown	---	---	---	---	---	---	---	---	
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.560	unknown	---	---	---	---	37.3	2.4846	0.049692	0.024846	1.0
80	44.990	unknown	---	---	---	---	10.1	0.6726	0.013451	0.006725	1.0
81		unknown	---	---	---	---	---	---	---	---	1.0
82		unknown	---	---	---	---	---	---	---	---	1.0
83		unknown	---	---	---	---	---	---	---	---	1.0
84		unknown	---	---	---	---	---	---	---	---	1.0
85		unknown	---	---	---	---	---	---	---	---	1.0
86	48.559	2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	---
87	56.149	Cl-5808	332370	---	---	---	---	---	---	---	---

Table S6. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 2nd, 6-day migration, and their quantification by semi-quantitative method (S/V = 5). Analysis of duplicate.

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MTC_{tap}^*
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4	16.737	4-hydroxy-4-methyl-2-pentanone	123-42-2	931	931	96.5	0.18	0.0121	0.000242	0.000121	1.0
5	17.425	cyclohexylamine	108-91-8	954	955	95.2	3.90	0.2600	0.0052	0.0026	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7	22.528	benzaldehyde	100-52-7	963	963	81.5	0.89	0.0593	0.001186	0.000593	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.006	isocyanate-cyclohexane	3173-53-3	964	964	91.4	1.36	0.0908	0.001816	0.000908	1.0
10	24.524	benzylamine	100-46-09	944	946	69.9	0.41	0.0271	0.000542	0.000271	1.0
11		1-hexanol-2-ethyl	104-76-7	---	---	---	---	---	---	---	1500
12	25.223	benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14	27.016	methyl benzoate	95-58-3	820	930	63.1	0.06	0.0039	7.78E-05	3.89E-05	1.0
15	27.543	2,2,6,6-tetramethyl-4-piperidone	826-36-8	891	891	93.8	0.07	0.0046	9.17E-05	4.58E-05	1.0
16		benzoic acid	65-85-0	---	---	---	---	---	---	---	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.034	benzothiazole	95-16-9	920	923	71.6	123.1	8.2119	0.164238	0.082119	0.1
19	30.156	isothiocyanate-cyclohexane	1122-82-03	915	920	97.9	57.58	3.8389	0.076777	0.038388	1.0
20	30.236	benzylazetidine	7730-39-4	823	846	55.6	28.58	1.9052	0.038103	0.019051	1.0
21	30.494	N-benzyl-3-pyrrolidinone	775-16-6	822	842	68.7	23.14	1.5426	0.030852	0.015426	1.0
22		N-cyclohexyl-formamide	766-93-8	---	---	---	---	---	---	---	1.0
23	31.060	N-cyclohexyl-acetamide	1124-53-4	937	941	97.4	6.54	0.4363	0.008725	0.004362	1.0
24	31.711	benzamide	55-21-0	906	913	67.3	4.63	0.3086	0.006171	0.003085	1.0
25	31.913	t-butyl-p-cresol	2409-55-4	936	938	38.2	4.68	0.3119	0.006238	0.003119	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0

27	32.306	benzyl isothiocyanate	622-78-6	920	920	77.7	4.69	0.3126	0.006251	0.003125	1.0
28		6-tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.121	N-benzylformamide	6343-54-0	956	961	96.2	12.20	0.8131	0.016261	0.008130	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40	35.106	N-(phenylmethylene)-cyclohexamine	2211-66-7	911	913	96.3	10.19	0.6796	0.013592	0.006796	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.659	2-(methylthio)-benzothiazole	615-22-5	953	953	88.8	13.86	0.9238	0.018476	0.009238	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45	36.083	unknown	---	---	---	---	---	---	---	---	1.0
46	36.344	2-benzothiazolone	934-34-9	903	923	95.7	10.17	0.6780	0.013559	0.006779	0.1
47		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.971	Dibenzylamine	103-49-1	901	906	88.9	121.8	8.1242	0.162483	0.081241	1.0
50		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51	37.161	Benzaldehyde N-benzylimine	780-25-6	939	941	80.2	26.83	1.7889	0.035778	0.017889	1.0
52		N-butylbenzenesulfonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53	37.855	Benthiazole	21564-17-0	702	794	50.3	15.51	1.0342	0.020683	0.010341	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.578	N-cyclohexylbenzamide	1759-68-8	929	930	93.2	37.62	2.5077	0.050154	0.025077	1.0
56	38.908	N-methylbenzothiazoline-2-thione	2254-94-6	874	885	75.4	4.88	0.3254	0.006508	0.003254	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0

58	39.681	2-mercaptobenzothiazole	149-30-4	936	939	96.9	78.04	5.2024	0.104047	0.052023	100
59	39.959	N-benzylformamide	6343-54-0	764	817	62.8	93.00	6.1999	0.123998	0.061999	1.0
60	40.114	N-benzylbenzamide	1485-70-7	918	922	55.3	36.80	2.4534	0.049068	0.024534	1.0
61		Benzenesulfanilide	1678-25-7	---	---	---	---	---	---	---	1.0
62	40.395	1,3-dicyclohexylurea	2387-23-7	906	920	96.3	30.72	2.0482	0.040964	0.020482	1.0
63	40.666	unknown	---	---	---	---	21.25	1.4169	0.028337	0.014168	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.039	unknown	---	---	---	---	28.05	1.8699	0.037398	0.018699	1.0
66	41.246	unknown	---	---	---	---	76.30	5.0867	0.101734	0.050867	1.0
67	41.36	N,N'-dicyclohexyloxamide	3299-64-7	843	906	95.2	6.17	0.4115	0.008230	0.004115	1.0
68	41.637	2-cyclohexylamino-benzothiazole	28291-75-0	788	920	79.2	44.00	2.9333	0.058666	0.029333	1.0
69	41.759	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	880	903	95.3	15.81	1.0538	0.021075	0.010537	1.0
70	42.109	N-benzyl-benzenecarbothiamide	14309-89-8	908	949	95.6	19.71	1.3138	0.026275	0.013137	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	1.0
74		unknown	---	---	---	---	---	---	---	---	1.0
75		unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.578	unknown	---	---	---	---	95.05	6.3370	0.126739	0.063369	1.0
80	44.992	unknown	---	---	---	---	5.86	0.3909	0.007818	0.003909	1.0
81	45.444	7-benzyloxyindole	20289-27-4	651	807	46.7	8.10	0.5400	0.010799	0.005399	1.0
82		unknown	---	---	---	---	---	---	---	---	1.0
83		unknown	---	---	---	---	---	---	---	---	1.0
84		unknown	---	---	---	---	---	---	---	---	1.0
85		unknown	---	---	---	---	---	---	---	---	1.0
86		2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87	56.258	Cl-5808	332370	919	922	92.8	37.55	2.5033	0.050065	0.025032	1.0

Table S7. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 2nd, 6-day migration, and their quantification by semi-quantitative method (S/V = 10).

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MT_{Ctap}^*
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4	16.737	4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.443	cyclohexylamine	108-91-8	938	938	95.4	67.6	2.2518	0.045035	0.022517	2.1
6	19.203	cyclohexanone	108-94-01	916	922	76	5.5	0.1819	0.003637	0.001818	1.0
7	22.528	benzaldehyde	100-52-7	964	964	81.7	9.6	0.3190	0.006380	0.003190	1.0
8	23.542	benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.024	isocyanate-cyclohexane	3173-53-3	972	972	92.9	107.7	3.5889	0.071777	0.035888	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		1-hexanol-2-ethyl	104-76-7	---	---	---	---	---	---	---	1500
12	25.223	benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13	26.189	unknown	---	---	---	---	21.2	0.7054	0.014107	0.007053	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16	29.040	benzoic acid	65-85-0	922	925	78.2	77.4	2.5795	0.051589	0.025794	1.0
17	29.795	2-phenoxy-ethanol	122-99-6	922	931	97.9	33.8	1.1263	0.022526	0.011263	1.0
18	30.062	benzothiazole	95-16-9	823	848	58	9.6	0.3202	0.006404	0.003202	0.1
19		isothiocyanate-cyclohexane	1122-82-03	---	---	---	---	---	---	---	1.0
20		benzylazetidine	7730-39-4	---	---	---	---	---	---	---	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.569	N-cyclohexyl-formamide	766-93-8	930	931	96.6	24.7	0.8236	0.016471	0.008235	1.0
23	31.103	N-cyclohexyl-acetamide	1124-53-4	922	932	96.9	7.2	0.2390	0.004780	0.002390	1.0
24	31.775	benzamide	55-21-0	914	915	65	5.6	0.1858	0.003716	0.001858	1.0
25	31.925	t-butyl-p-cresol	2409-55-4	937	945	34.7	2.7	0.0891	0.001782	0.000891	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0

27	32.306	benzyl isothiocyanate	622-78-6	932	947	86.7	6.3	0.2090	0.004180	0.002090	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.754	N-benzylformamide	6343-54-0	956	958	95.3	13.0	0.4329	0.008657	0.004328	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32	33.256	N-benzylacetamide	588-46-5	891	936	81.3	2.9	0.0974	0.001947	0.000973	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40	35.105	N-(phenylmethylene)-cyclohexamine	2211-66-7	902	909	94.3	2.6	0.0866	0.001731	0.000865	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.663	2-(methylthio)-benzothiazole	615-22-5	948	949	87.8	9.8	0.3281	0.006561	0.003280	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45		unknown	---	---	---	---	---	---	---	---	1.0
46	36.403	2-benzothiazolone	934-34-9	903	918	93.5	16.2	0.5412	0.010824	0.005412	0.1
47		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.941	Dibenzylamine	103-49-1	924	928	92.5	25.9	0.8626	0.017251	0.008625	1.0
50	37.153	Dibenzylhydroxylamine	621-07-8	924	931	56.7	8.7	0.2907	0.005813	0.002906	1.0
51		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0
52		N-butylbenzenesulfonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53	37.848	Benthiazole	21564-17-0	692	782	35	4.9	0.1620	0.003240	0.001620	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.607	N-cyclohexylbenzamide	1759-68-8	925	925	93.7	33.0	1.1010	0.022019	0.011009	1.0
56	38.915	N-methylbenzothiazoline-2-thione	2254-94-6	881	902	73.9	4.6	0.1520	0.003040	0.001520	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0

58	39.896	2-mercaptobenzothiazole	149-30-4	923	933	96.4	124.4	4.1475	0.082949	0.041474	100
59	40.032	N-benzylformamide	6343-54-0	761	817	58	76.5	2.5513	0.051026	0.025513	1.0
60	40.229	N-benzylbenzamide	1485-70-7	928	930	70.7	36.2	1.2051	0.024101	0.012050	1.0
61	40.357	Benzenesulfanilide	1678-25-7	907	920	97.1	26.6	0.8874	0.017748	0.008874	1.0
62	40.481	1,3-dicyclohexylurea	2387-23-7	919	937	97.9	28.2	0.9402	0.018803	0.009401	1.0
63	40.700	unknown	---	---	---	---	15.0	0.4999	0.009998	0.004999	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.055	unknown	---	---	---	---	18.3	0.6114	0.012227	0.006113	1.0
66	41.261	unknown	---	---	---	---	45.9	1.5288	0.030575	0.015287	1.0
67	41.38	N,N'-dicyclohexyloxamide	3299-64-7	853	908	94.6	6.1	0.2030	0.004059	0.002029	1.0
68	41.671	2-cyclohexylamino-benzothiazole	28291-75-0	781	919	76.7	3.0	0.1011	0.002022	0.001011	1.0
69	41.799	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	864	914	97.9	12.4	0.4141	0.008281	0.004140	1.0
70	42.14	N-benzyl-benzenecarbothiamide	14309-89-8	899	956	97.5	14.6	0.4877	0.009753	0.004876	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73	42.395	unknown	---	---	---	---	---	---	---	---	1.0
74	42.576	unknown	---	---	---	---	2.7	0.0905	0.001809	0.000904	1.0
75		unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77	43.09	N,N'-dibenzilureia	1466-67-7	812	949	89	3.1	0.1039	0.002077	0.001038	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.58	unknown	---	---	---	---	32.0	1.0675	0.021350	0.010675	1.0
80	45.004	unknown	---	---	---	---	4.8	0.1603	0.003206	0.001603	1.0
81		7-benzylxyindole	---	---	---	---	---	---	---	---	1.0
82	46.165	unknown	---	---	---	---	2.8	0.0918	0.001835	0.000917	1.0
83		unknown	---	---	---	---	---	---	---	---	1.0
84		unknown	---	---	---	---	---	---	---	---	1.0
85	48.002	unknown	---	---	---	---	4.9	0.1620	0.003239	0.001619	1.0
86	48.56	2,2'-tiobis-benzotiazol	402147	859	914	97	4.8	0.1587	0.003173	0.001586	1.0
87	56.182	Cl-5808	332370	864	887	89.7	5.0	0.1678	0.003356	0.001678	1.0

Table S8 . Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 2nd, 6-day migration, and their quantification by semi-quantitative method (S/V = 10). Analysis of duplicate.

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	C_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	$MTCap^*$
							(µg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	19.21	cyclohexylamine	108-91-8	953	954	95.3	47.9	1.5981	0.031962	0.015981	2.1
6	22.576	cyclohexanone	108-94-01	910	918	70.8	2.3	0.0757	0.001514	0.000757	1.0
7	22.528	benzaldehyde	100-52-7	934	939	80.8	3.8	0.1257	0.002514	0.001257	1.0
8	23.543	benzonitrile	100-47-0	953	955	76.3	0.0	---	---	---	0.1
9	24.015	isocyanate-cyclohexane	3173-53-3	964	965	93.9	61.4	2.0453	0.040906	0.020453	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13	26.189	unknown	---	---	---	---	12.9	0.4313	0.008626	0.004313	1.0
14		methyl benzoate	95-58-3	---	---	---	---				1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16	29.029	benzoic acid	65-85-0	914	942	51.9	23.9	0.7951	0.015902	0.007951	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.046	benzothiazole	95-16-9	933	935	73	58.1	1.9360	0.038719	0.019359	0.1
19	30.167	isothiocyanate-cyclohexane	1122-82-03	917	922	98	29.9	0.9964	0.019928	0.009964	1.0
20	30.247	benzylazetidine	7730-39-4	828	853	62.8	11.0	0.3672	0.007343	0.003671	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.553	N-cyclohexyl-formamide	766-93-8	925	937	97.5	21.3	0.7096	0.014191	0.007095	1.0
23	31.094	N-cyclohexyl-acetamide	1124-53-4	942	945	97.6	6.2	0.2074	0.004147	0.002073	1.0
24	31.754	benzamide	55-21-0	898	920	64.2	5.0	0.1672	0.003344	0.001672	1.0

25	31.924	t-butyl-p-cresol	2409-55-4	879	895	28.4	2.4	0.0791	0.001581	0.000790	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.309	benzyl isothiocyanate	622-78-6	912	940	83.8	4.1	0.1353	0.002705	0.001352	1.0
28	32.531	tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.749	N-benzylformamide	6343-54-0	933	962	94.5	11.8	0.3950	0.007899	0.003949	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32	33.257	N-benzylacetamide	588-46-5	888	932	81.1	3.6	0.1209	0.002418	0.001209	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40	35.106	N-(phenylmethylene)-cyclohexamine	2211-66-7	900	908	95.6	1.9	0.0633	0.001265	0.000632	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.662	2-(methylthio)-benzothiazole	615-22-5	947	947	86.3	7.3	0.2446	0.004891	0.002445	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45		unknown	---	---	---	---	---	---	---	---	1.0
46	36.390	2-benzothiazolone	934-34-9	865	915	91	12.7	0.4234	0.008468	0.004234	0.1
47		Dibenzylmethylaniline	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.952	Dibenzylamine	103-49-1	951	956	95.3	37.6	1.2520	0.025040	0.012520	1.0
50		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51		N-Benzylidenebenzylamine	780-25-6	---	---	---	---	---	---	---	1.0
52	37.587	N-butylbenzenesulphonamide	3622-84-2	750	803	60.9	2.7	0.0889	0.001778	0.000889	1.0

53	37.852	Benthiazole	21564-17-0	699	786	54.8	5.9	0.1971	0.003941	0.001970	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.601	N-cyclohexylbenzamide	1759-68-8	926	927	94.9	26.9	0.8958	0.017916	0.008958	1.0
56	38.913	N-methylbenzothiazoline-2-thione	2254-94-6	867	886	74.4	3.7	0.1241	0.002481	0.001240	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.841	2-mercaptobenzothiazole	149-30-4	927	932	96.2	103.1	3.4352	0.068704	0.034352	100
59	40.019	N-benzylformamide	6343-54-0	675	725	33.5	62.5	2.0842	0.041683	0.020841	1.0
60	40.211	N-benzylbenzamide	1485-70-7	935	938	75	29.0	0.9678	0.019356	0.009678	1.0
61	40.340	Benzenesulfanilide	1678-25-7	917	927	97	21.5	0.7163	0.014326	0.007163	1.0
62	40.476	1,3-dicyclohexylurea	2387-23-7	917	937	97.8	25.2	0.8386	0.016771	0.008385	1.0
63	40.694	unknown	---	---	---	---	12.1	0.4042	0.008084	0.004042	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.051	unknown	---	---	---	---	14.7	0.4900	0.009800	0.004900	1.0
66	41.261	unknown	---	---	---	---	37.9	1.2648	0.025295	0.012647	1.0
67	41.377	N,N'-dicyclohexyloxamide	3299-64-7	833	902	92.5	4.6	0.1540	0.003080	0.001540	1.0
68	41.666	2-cyclohexylamino-benzothiazole	28291-75-0	783	920	77.4	2.4	0.0787	0.001574	0.000787	1.0
69	41.793	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	867	915	95.5	10.3	0.3432	0.006863	0.003431	1.0
70	42.135	N-benzyl-benzenecarbothiamide	14309-89-8	901	955	97.4	11.8	0.3950	0.007899	0.003949	1.0
71	42.231	unknown	---	---	---	---	1.3	0.0417	0.000834	0.000417	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73	42.398	unknown	---	---	---	---	0.4	0.0137	0.000274	0.000137	1.0
74	42.573	unknown	---	---	---	---	2.2	0.0733	0.001465	0.000732	1.0
75	42.706	unknown	---	---	---	---	1.1	0.0361	0.000721	0.000360	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77	43.094	N,N'-dibenzilureia	1466-67-7	839	956	92.5	2.4	0.0811	0.001622	0.000811	1.0
78	43.394	Antioxidant BKF	119-47-1	764	775	87.6	0.6	0.0188	0.000375	0.000187	75
79	43.589	unknown	---	---	---	---	36.0	1.2017	0.024033	0.012016	1.0
80	45.003	unknown	---	---	---	---	4.1	0.1381	0.002762	0.001381	1.0

81	45.447	unknown	---	---	---	---	1.6	0.0545	0.001089	0.000544	1.0
82	46.169	unknown	---	---	---	---	3.3	0.1100	0.002199	0.001099	1.0
83	46.422	unknown	---	---	---	---	1.0	0.0344	0.000688	0.000344	1.0
84	46.932	unknown	---	---	---	---	0.5	0.0156	0.000311	0.000155	1.0
85	47.997	unknown	---	---	---	---	4.0	0.1344	0.002688	0.001344	1.0
86	48.554	2,2'-tiobis-benzotiazol	402147*	831	900	97.1	2.8	0.0920	0.001839	0.000919	1.0
87	56.214	Cl-5808	332370*	910	915	93.3	9.3	0.3088	0.006175	0.003087	1.0

Table S9. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 3rd, 9-day migration, and their quantification by semi-quantitative method (S/V = 5).

N	tR (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	C_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MT_{Ctap}
							(µg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4	16.737	4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	
5	17.456	cyclohexylamine	108-91-8	954	955	95.2	3.9	0.2600	0.0052	0.0026	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7	22.521	benzaldehyde	100-52-7	946	947	76.7	2.6	0.1751	0.003501	0.001750	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.006	isocyanate-cyclohexane	3173-53-3	969	970	94.2	11.2	0.7494	0.014988	0.00749	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	
16	28.921	benzoic acid	65-85-0	916	933	41.4	7.5	0.4982	0.009964	0.004982	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.038	benzothiazole	95-16-9	935	937	7305	80.0	5.3365	0.106729	0.053364	0.1
19	30.157	isothiocyanate-cyclohexane	1122-82-03	918	922	98.3	35.9	2.3945	0.047890	0.023945	1.0
20	30.250	benzylazetidine	7730-39-4	817	852	56.4	2.7	0.1785	0.003569	0.001784	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	
22	30.497	N-cyclohexyl-formamide	766-93-8	935	940	97.5	9.0	0.6024	0.012047	0.006023	1.0
23	31.060	N-cyclohexyl-acetamide	1124-53-4	930	939	97	2.7	0.1813	0.003626	0.001813	1.0
24	31.716	benzamide	55-21-0	868	902	55.4	2.2	0.1460	0.002920	0.001460	1.0
25	31.908	t-butyl-p-cresol	2409-55-4	943	948	34.5	3.5	0.2361	0.004722	0.002361	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.307	benzyl isothiocyanate	622-78-6	939	940	84.8	6.0	0.3999	0.007997	0.003998	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0

29	32.710	N-benzylformamide	6343-54-0	948	965	94.1	4.8	0.3219	0.006437	0.003218	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41	35.659	2-(methylthio)-benzothiazole	615-22-5	946	946	88.8	15.3	1.0221	0.020442	0.010221	1.0
42		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
43		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	
44		unknown	---	---	---	---	---	---	---	---	1.0
45	36.297	2-benzothiazolone	934-34-9	922	933	95.2	8.0	0.5357	0.010713	0.005356	0.1
46		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
47		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
48	36.941	Dibenzylamine	103-49-1	913	943	90.9	62.1	4.1379	0.082758	0.041379	1.0
49		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51	37.160	N-Benzylidenebenzylamine	780-25-6	931	932	80.2	10.0	0.6664	0.013327	0.00663	1.0
52		N-butylbenzenesulphonamide	3622-84-2	---	---	---	---	---	---	---	
53		Benthiazole	21564-17-0	---	---	---	---	---	---	---	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.566	N-cyclohexylbenzamide	1759-68-8	936	936	92.4	221.2	14.7435	0.294869	0.147434	1.0
56	38.903	N-methylbenzothiazoline-2-thione	2254-94-6	848	883	73.4	5.2	0.3451	0.006902	0.003451	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.667	2-mercaptobenzothiazole	149-30-4	931	932	96.7	99.5	6.6314	0.132627	0.066313	100
59	39.947	N-benzylformamide	6343-54-0	753	798	45.5	70.9	4.7285	0.094570	0.047285	1.0
60	40.103	N-benzylbenzamide	1485-70-7	925	928	63.5	23.0	1.5329	0.030657	0.015328	1.0
61		Benzenesulfanilide	1678-25-7	---	---	---	---	---	---	---	1.0
62	40.403	1,3-dicyclohexylurea	2387-23-7	923	924	93.5	16.6	1.1047	0.022093	0.011046	1.0

63	40.659	unknown	---	---	---	---	19.8	1.3198	0.026395	0.013197	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.036	unknown	---	---	---	---	30.9	2.0607	0.041213	0.020606	1.0
66	41.246	unknown	---	---	---	---	79.2	5.2783	0.105565	0.052782	1.0
67	41.353	N,N'-dicyclohexyloxamide	3299-64-7	847	854	97	6.0	0.4020	0.008039	0.004019	1.0
68	41.637	2-cyclohexylamino-benzothiazole	28291-75-0	781	920	77	5.0	0.3316	0.006631	0.00331	1.0
69	41.731	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	854	907	93.9	9.0	0.6004	0.012008	0.006004	1.0
70	42.103	N-benzyl-benzenecarbothiamide	14309-89-8	898	936	94.8	19.0	1.2683	0.025366	0.012683	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	
74		unknown	---	---	---	---	---	---	---	---	1.0
75		unknown	---	---	---	---	---	---	---	---	
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.553	unknown	---	---	---	---	45.9	3.0613	0.061225	0.030612	1.0
80		unknown	---	---	---	---	---	---	---	---	1.0
81		unknown		---	---	---	---	---	---	---	1.0
82	44.98	unknown	---	---	---	---	10.1	0.6721	0.013441	0.006720	1.0
83	45.426	unknown	---	---	---	---	4.9	0.3236	0.006471	0.003235	1.0
84	46.149	unknown	---	---	---	---	5.1	0.3414	0.006827	0.003413	1.0
85	47.964	unknown	---	---	---	---	3.5	0.2343	0.004686	0.002343	1.0
86		2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87		Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S10. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 3rd, 9-day migration, and their quantification by semi-quantitative method (S/V = 5). Analysis of duplicate.

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MT_{Ctap}
							(µg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4	16.737	4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.454	cyclohexylamine	108-91-8	898	898	91.1	3.9	0.2600	0.0052	0.0026	2.1
6	19.204	cyclohexanone	108-94-01	873	881	56.4	0.3	0.0206	0.000411	0.000205	1.0
7	22.522	benzaldehyde	100-52-7	964	964	77.8	1.8	0.1218	0.002435	0.001217	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.010	isocyanate-cyclohexane	3173-53-3	962	962	93.1	10.2	0.6830	0.013659	0.006829	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	
16	28.964	benzoic acid	65-85-0	926	934	48.8	6.7	0.4499	0.008998	0.004499	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.034	benzothiazole	95-16-9	933	936	66.2	80.8	5.3834	0.107667	0.053833	0.1
19	30.161	isothiocyanate-cyclohexane	1122-82-03	915	919	97.6	42.0	2.8022	0.056043	0.028021	1.0
20	30.252	benzylazetidine	7730-39-4	829	863	61.7	3.6	0.2424	0.004848	0.002424	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22		N-cyclohexyl-formamide	766-93-8	---	---	---	---	---	---	---	1.0
23		N-cyclohexyl-acetamide	1124-53-4	---	---	---	---	---	---	---	1.0
24		benzamide	55-21-0	---	---	---	---	---	---	---	1.0

25		t-butyl-p-cresol	2409-55-4	---	---	---	---	---	---	---	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27		benzyl isothiocyanate	622-78-6	---	---	---	---	---	---	---	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29		N-benzylformamide	6343-54-0	---	---	---	---	---	---	---	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		2-(methylthio)-benzothiazole	615-22-5	---	---	---	---	---	---	---	1.0
42		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
43		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
44		unknown	---	---	---	---	---	---	---	---	1.0
45		2-benzothiazolone	934-34-9	---	---	---	---	---	---	---	0.1
46		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
47		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
48		Dibenzylamine	103-49-1	---	---	---	---	---	---	---	1.0
49		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51		N-Benzylidenebenzylamine	780-25-6	---	---	---	---	---	---	---	1.0
52		N-butylbenzenesulphonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53		Benthiazole	21564-17-0	---	---	---	---	---	---	---	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0

55		N-cyclohexylbenzamide	1759-68-8	---	---	---	---	---	---	---	1.0
56		N-methylbenzothiazoline-2-thione	2254-94-6	---	---	---	---	---	---	---	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58		2-mercaptobenzothiazole	149-30-4	---	---	---	---	---	---	---	100
59		N-benzylformamide	6343-54-0	---	---	---	---	---	---	---	1.0
60		N-benzylbenzamide	1485-70-7	---	---	---	---	---	---	---	1.0
61		Benzenesulfanilide	1678-25-7	---	---	---	---	---	---	---	1.0
62		1,3-dicyclohexylurea	2387-23-7	---	---	---	---	---	---	---	1.0
63		unknown	---	---	---	---	---	---	---	---	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65		unknown	---	---	---	---	---	---	---	---	1.0
66		unknown	---	---	---	---	---	---	---	---	1.0
67		N,N'-dicyclohexyloxamide	3299-64-7	---	---	---	---	---	---	---	1.0
68		2-cyclohexylamino-benzothiazole	28291-75-0	---	---	---	---	---	---	---	1.0
69		N-benzyl-N'-cyclohexyl-isourea	25855-24-7	---	---	---	---	---	---	---	1.0
70		N-benzyl-benzenecarbothiamide	14309-89-8	---	---	---	---	---	---	---	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	1.0
74		unknown	---	---	---	---	---	---	---	---	1.0
75		unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79		unknown	---	---	---	---	---	---	---	---	1.0
80		unknown	---	---	---	---	---	---	---	---	1.0
81		7-benzyloxyindole		---	---	---	---	---	---	---	1.0
82		unknown	---	---	---	---	---	---	---	---	1.0

83	46.422	unknown	---	---	---	---	---	---	---	---	1.0
84	46.932	unknown	---	---	---	---	---	---	---	---	1.0
85	47.997	unknown	---	---	---	---	---	---	---	---	1.0
86	48.554	2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87	56.214	Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S11. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 3rd, 9-day migration, and their quantification by semi-quantitative method (S/V = 10).

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MTCtap
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4	16.737	4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.428	cyclohexylamine	108-91-8	941	941	95	39.3	2.6179	0.052358	0.026179	2.1
6	19.187	cyclohexanone	108-94-01	940	941	75.6	8.8	0.5891	0.011782	0.005891	1.0
7	22.523	benzaldehyde	100-52-7	959	959	78.3	16.1	1.0729	0.021458	0.010720	1.0
8	23.534	benzonitrile	100-47-0	923	925	66.6	3.6	0.2384	0.004767	0.002383	0.1
9	24.013	isocyanate-cyclohexane	3173-53-3	954	954	92.7	59.7	3.9806	0.079612	0.039806	1.0
10	24.549	benzylamine	100-46-09	938	939	68.9	6.9	0.4630	0.009259	0.004629	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone		---	---	---	---	---	---	---	1.0
16		benzoic acid	65-85-0	---	---	---	---	---	---	---	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.056	benzothiazole	95-16-9	923	926	70.5	111.6	7.4383	0.148766	0.074383	0.1
19	30.166	isothiocyanate-cyclohexane	1122-82-03	914	919	97.7	40.4	2.6939	0.053878	0.026939	1.0
20	30.238	benzylazetidine	7730-39-4	822	847	49.5	2.6	0.1716	0.003432	0.001716	1.0
21		N-benzyl-3-pyrrolidinone		---	---	---	---	---	---	---	1.0
22	30.504	N-cyclohexyl-formamide	766-93-8	924	924	96.4	17.4	1.1611	0.023222	0.011611	1.0
23	31.061	N-cyclohexyl-acetamide	1124-53-4	907	907	96.4	4.9	0.3235	0.006470	0.003235	1.0

24	31.717	benzamide	55-21-0	910	919	70.2	3.9	0.2601	0.005201	0.002600	1.0
25	31.913	t-butyl-p-cresol	2409-55-4	927	927	32.3	3.9	0.2632	0.005263	0.002631	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.307	benzyl isothiocyanate	622-78-6	937	937	84.8	5.3	0.3532	0.007063	0.003531	1.0
28	32.531	tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.722	N-benzylformamide	6343-54-0	957	962	95.3	10.1	0.6736	0.013471	0.006735	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32	33.257	N-benzylacetamide		---	---	---	---	---	---	---	1.0
33	33.470	2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40	35.101	N-(phenylmethylene)-cyclohexamine	2211-66-7	907	913	95.2	3.4	0.2272	0.004543	0.002271	1.0
41	35.66	2-(methylthio)-benzothiazole	615-22-5	955	955	89.7	14.6	0.9741	0.019481	0.009740	1.0
42		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
43		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	
44	36.083	unknown	---	---	---	---	---	---	---	---	1.0
45	36.35	2-benzothiazolone	934-34-9	898	923	93.4	14.7	0.9793	0.019585	0.009792	0.1
46		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
47		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
48	36.946	Dibenzylamine	103-49-1	895	917	92.5	64.8	4.3169	0.086337	0.043168	1.0
49		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51	37.150	N-Benzylidenebenzylamine	780-25-6	890	891	84.6	13.3	0.8859	0.017717	0.008858	1.0
52	37.575	N-butylbenzenesulphonamide	3622-84-2	875	893	90.2	6.7	0.4458	0.008915	0.004457	
53	37.845	Benthiazole	21564-17-0	692	782	35	4.0	0.2667	0.005333	0.002666	1.0

54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.581	N-cyclohexylbenzamide	1759-68-8	936	937	92.9	34.1	2.2719	0.045438	0.022719	1.0
56		N-methylbenzothiazoline-2-thione	2254-94-6	---	---	---	---	---	---	---	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.794	2-mercaptobenzothiazole	149-30-4	938	939	96.3	170.4	11.3594	0.227188	0.113594	100
59	39.999	N-benzylformamide	6343-54-0	762	813	52.6	100.9	6.7252	0.134504	0.067252	1.0
60	40.175	N-benzylbenzamide	1485-70-7	935	946	77.1	35.3	2.3562	0.047123	0.023561	1.0
61	40.307	Benzenesulfanilide	1678-25-7	927	934	98.2	30.0	1.9983	0.039966	0.019983	1.0
62	40.408	1,3-dicyclohexylurea	2387-23-7	930	944	98	22.4	1.4952	0.029904	0.014952	1.0
63	40.679	unknown	---				21.5	1.4305	0.028610	0.014305	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.044	unknown	---	---	---	---	28.9	1.9277	0.038554	0.019277	1.0
66	41.253	unknown	---	---	---	---	73.3	4.8858	0.097715	0.048857	1.0
67	41.37	N,N'-dicyclohexyloxamide	3299-64-7	883	924	97.6	8.7	0.5776	0.011552	0.005776	1.0
68	41.656	2-cyclohexylamino-benzothiazole	28291-75-0	795	922	78.4	5.6	0.3762	0.007523	0.003761	1.0
69	41.758	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	867	909	97.7	13.7	0.9160	0.018320	0.009160	1.0
70		N-benzyl-benzenecarbothiamide	14309-89-8	---	---	---	---	---	---	---	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	1.0
74	42.565	unknown	---	---	---	---	50.4	3.3617	0.067233	0.033616	1.0
75		unknown	---	---	---	---	---	---	---	---	
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79		unknown	---	---	---	---	---	---	---	---	1.0
80		unknown	---	---	---	---	---	---	---	---	1.0
81		unknown	---	---	---	---	---	---	---	---	1.0

82	44.98	unknown	---	---	---	---	7.4	0.4948	0.009895	0.004947	1.0
83		unknown	---	---	---	---	---	---	---	---	1.0
84	46.155	unknown	---	642	886	38.1	5.5	0.3681	0.007362	0.003681	1.0
85	47.975	unknown	---	677	873	39.7	5.0	0.3304	0.006607	0.003303	1.0
86	48.54	2,2'-tiobis-benzotiazol	402147	847	913	96.6	4.5	0.2998	0.005996	0.002998	1.0
87		Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S12. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 3rd, 9-day migration, and their quantification by semi-quantitative method (S/V = 10). Analysis of duplicate.

N	t _R (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} 2	MT _{Ctap}
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4	16.737	4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	
5	17.432	cyclohexylamine	108-91-8	917	917	91.9	38.0	2.5331	0.050662	0.025331	2.1
6	19.188	cyclohexanone	108-94-01	936	938	72.4	8.7	0.5787	0.011573	0.005786	1.0
7	22.521	benzaldehyde	100-52-7	948	949	80.7	17.9	1.1945	0.023890	0.011945	1.0
8	23.532	benzonitrile	100-47-0	918	924	66.7	3.3	0.2199	0.004397	0.002198	0.1
9		isocyanate-cyclohexane	3173-53-3	961	962	93.2	68.1	4.5386	0.090771	0.045385	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	
16		benzoic acid	65-85-0	---	---	---	---	---	---	---	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.041	benzothiazole	95-16-9	932	934	71.9	117.6	7.8380	0.156760	0.078380	0.1
19	30.156	isothiocyanate-cyclohexane	1122-82-03	922	926	97.7	42.3	2.8228	0.056456	0.028228	1.0
20		benzylazetidine	7730-39-4	---	---	---	---	---	---	---	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	
22	30.489	N-cyclohexyl-formamide	766-93-8	926	926	96.5	16.3	1.0841	0.021681	0.010840	1.0
23	31.054	N-cyclohexyl-acetamide	1124-53-4	934	934	97.3	4.4	0.2962	0.005924	0.002962	1.0
24	31.706	benzamide	55-21-0	859	896	54.4	3.3	0.2227	0.004454	0.002227	1.0
25	31.909	t-butyl-p-cresol	2409-55-4	936	939	28.5	3.7	0.2448	0.004896	0.002448	1.0

26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.306	benzyl isothiocyanate	622-78-6	952	954	89.3	8.6	0.5745	0.011489	0.005744	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.713	N-benzylformamide	6343-54-0	954	958	96.5	9.2	0.6156	0.012312	0.006156	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	---	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.657	2-(methylthio)-benzothiazole	615-22-5	963	963	90.6	13.8	0.9214	0.018427	0.009213	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45		unknown	---	---	---	---	---	---	---	---	1.0
46	36.320	2-benzothiazolone	934-34-9	938	938	97.4	13.6	0.9092	0.018184	0.009092	0.1
47	36.431	Dibenzylmethylamine	102-05-6	918	936	92.5	59.0	3.9351	0.078702	0.039351	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49		Dibenzylamine	103-49-1	---	---	---	---	---	---	---	1.0
50		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51		N-Benzylidenebenzylamine	780-25-6	---	---	---	---	---	---	---	1.0
52	37.563	N-butylbenzenesulphonamide	3622-84-2	883	899	90.6	5.4	0.3589	0.007178	0.003589	1.0
53	37.842	Bentthiazole	21564-17-0	687	777	28.3	5.9	0.3903	0.007806	0.003903	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.573	N-cyclohexylbenzamide	1759-68-8	936	936	92.5	34.6	2.3065	0.046130	0.023065	1.0
56	38.903	N-methylbenzothiazoline-2-thione	2254-94-6	862	889	73.5	6.3	0.4213	0.008429	0.004213	1.0

57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.733	2-mercaptobenzothiazole	149-30-4	939	946	97.2	175.1	11.6762	0.233523	0.116761	10
59	39.971	N-benzylformamide	6343-54-0	748	793	44	103.7	6.9162	0.138323	0.069161	1.0
60	40.143	N-benzylbenzamide	1485-70-7	900	900	51.7	35.2	2.3454	0.046908	0.023454	1.0
61	40.276	Benzenesulfanilide	1678-25-7	935	939	98	29.3	1.9524	0.039047	0.019523	1.0
62	40.381	1,3-dicyclohexylurea	2387-23-7	916	936	97.8	22.6	1.5069	0.0301	0.015068	1.0
63	40.666	unknown	---	---	---	---	21.6	1.4423	0.028846	0.014423	1.0
64	40.869	2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.037	unknown	---	---	---	---	28.6	1.9072	0.038144	0.019072	1.0
66	41.243	unknown	---	---	---	---	78.3	5.2217	0.104434	0.052217	1.0
67	41.356	N,N'-dicyclohexyloxamide	3299-64-7	874	926	95.7	7.8	0.5226	0.010451	0.005225	1.0
68	41.641	2-cyclohexylamino-benzothiazole	28291-75-0	798	920	81	5.3	0.3559	0.007118	0.003559	1.0
69	41.741	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	867	907	97.7	14.1	0.9432	0.018863	0.009431	1.0
70	42.106	N-benzyl-benzenecarbothiamide	14309-89-8	907	945	95.6	20.6	1.3756	0.027511	0.013755	1.0
71	42.231	unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73	42.398	unknown	---	---	---	---	---	---	---	---	
74	42.573	unknown	---	---	---	---	---	---	---	---	1.0
75	42.706	unknown	---	---	---	---	---	---	---	---	
76		unknown	---	---	---	---	---	---	---	---	1.0
77	43.094	N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78	43.394	Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.554	unknown	---	---	---	---	56.3	3.7514	0.07502	0.03751	1.0
80		unknown	---	---	---	---	---	---	---	---	1.0
81		unknown	---	---	---	---	---	---	---	---	1.0
82		unknown	---	---	---	---	---	---	---	---	1.0
83	46.402	unknown	---	---	---	---	4.4	0.2923	0.005845	0.002922	1.0
84	46.900	unknown	---	---	---	---	5.3	0.3523	0.007046	0.003523	1.0
85	47.964	unknown		694	868	57.1	4.3	0.2876	0.005751	0.002875	1.0

86		2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87		Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S13. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 4th, 15-day migration, and their quantification by semi-quantitative method (S/V = 5).

N	t _R (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} ²	MTC _{tap}
							(µg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4	16.737	4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	
5	17.053	cyclohexylamine	108-91-8	857	894	82.4	3.9	0.2600	0.0052	0.0026	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7		benzaldehyde	100-52-7	---	---	---	---	---	---	---	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.002	isocyanate-cyclohexane	3173-53-3	964	964	93.2	21.2	1.4120	0.028239	0.014119	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	
16	28.801	benzoic acid	65-85-0	946	947	49.6	8.4	0.5617	0.011234	0.005617	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.026	benzothiazole	95-16-9	933	957	62.7	62.2	4.1455	0.082909	0.041454	0.1
19	30.150	isothiocyanate-cyclohexane	1122-82-03	915	915	97.7	27.6	1.8425	0.036849	0.018424	1.0
20		benzylazetidine	7730-39-4	---	---	---	---	---	---	---	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.476	N-cyclohexyl-formamide	766-93-8	924	931	96.4	6.2	0.4105	0.008209	0.004104	1.0
23		N-cyclohexyl-acetamide	1124-53-4	---	---	---	---	---	---	---	1.0
24		benzamide	55-21-0	---	---	---	---	---	---	---	1.0
25	31.906	t-butyl-p-cresol	2409-55-4	944	948	34.3	2.6	0.1763	0.003525	0.001762	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.306	benzyl isothiocyanate	622-78-6	930	931	83.7	4.3	0.2863	0.005725	0.002862	1.0

28	32.305	tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.703	N-benzylformamide	6343-54-0	945	963	93.6	2.6	0.1762	0.003523	0.001761	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.656	2-(methylthio)-benzothiazole	615-22-5	955	955	89	15.9	1.0601	0.021202	0.010601	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45	36.083	unknown	---	---	---	---	---	---	---	---	1.0
46	36.28	2-benzothiazolone	934-34-9	895	916	92	6.0	0.4028	0.008056	0.004028	0.1
47		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.934	Dibenzylamine	103-49-1	921	923	91.5	59.1	3.9403	0.078805	0.039402	1.0
50		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0
52		N-butylbenzenesulfonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53		Benthiazole	21564-17-0	---	---	---	---	---	---	---	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.556	N-cyclohexylbenzamide	1759-68-8	928	928	93.3	17.2	1.1460	0.022919	0.011459	1.0
56	38.900	N-methylbenzothiazoline-2-thione	2254-94-6	847	887	77.9	4.6	0.3097	0.006194	0.003097	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.617	2-mercaptobenzothiazole	149-30-4	947	950	97.4	85.7	5.7139	0.114277	0.057138	10
59	39.928	N-benzylformamide	6343-54-0	758	803	44.8	60.4	4.0280	0.080560	0.040280	1.0

60	40.085	N-benzylbenzamide	1485-70-7	922	938	76.8	17.9	1.1929	0.023857	0.011928	1.0
61		Benzenesulfanilide	1678-25-7	---	---	---	---	---	---	---	1.0
62	40.381	1,3-dicyclohexylurea	2387-23-7	---	---	---	---	---	---	---	1.0
63	40.649	unknown	---	---	---	---	17.5	1.1638	0.023275	0.011637	1.0
64	40.869	2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.032	unknown	---	---	---	---	30.9	2.0576	0.041151	0.020575	1.0
66	41.246	unknown	---	---	---	---	82.3	5.4879		0.054878	1.0
67	41.347	N,N'-dicyclohexyloxamide	3299-64-7	863	919	96	4.4	0.2925	0.005849	0.002924	1.0
68	41.627	2-cyclohexylamino-benzothiazole	28291-75-0	765	919	73.7	4.3	0.2847	0.005693	0.002846	1.0
69	41.716	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	820	888	92.5	6.2	0.4140	0.008279	0.004139	1.0
70	42.094	N-benzyl-benzenecarbothiamide	14309-89-8	906	955	97.4	16.3	1.0860	0.021720	0.010860	1.0
71	42.231	unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73	42.398	unknown	---	---	---	---	---	---	---	---	1.0
74	42.573	unknown	---	---	---	---	---	---	---	---	1.0
75	42.706	unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77	43.094	N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78	43.394	Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.537	unknown	---	---	---	---	19.0	1.2663	0.025326	0.012663	1.0
80	44.974	unknown	---	---	---	---	4.4	0.2953	0.005906	0.002953	1.0
81		unknown		---	---	---	---	---	---	---	1.0
82		unknown	---	---	---	---	---	---	---	---	1.0
83	46.146	unknown	---	---	---	---	3.2	0.2142	0.004283	0.002141	1.0
84		unknown	---	---	---	---	---	---	---	---	1.0
85	47.955	unknown		---	---	---	2.7	0.1824	0.003648	0.001824	1.0
86	48.554	2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87	56.214	Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S14. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 4th, 15-day migration, and their quantification by semi-quantitative method (S/V = 5). Analysis of duplicate.

N	t _R (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} 2	MTCTap
							(µg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.417	cyclohexylamine	108-91-8	926	929	90.5	3.9	0.2600	0.0052	0.0026	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7		benzaldehyde	100-52-7	---	---	---	---	---	---	---	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.001	isocyanate-cyclohexane	3173-53-3	966	966	93.1	3.8	0.2556	0.005112	0.002556	1.0
10	24.542	benzylamine	100-46-09	927	935	61	0.6	0.0416	0.000832	0.000416	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16		benzoic acid	65-85-0	---	---	---	---	---	---	---	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.029	benzothiazole	95-16-9	931	934	71.7	66.3	4.4203	0.088405	0.044202	0.1
19	30.153	isothiocyanate-cyclohexane	1122-82-03	920	921	98.3	30.5	2.0319	0.040638	0.020319	1.0
20	30.237	benzylazetidine	7730-39-4	829	851	64.5	9.6	0.6415	0.012829	0.006414	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.479	N-cyclohexyl-formamide	766-93-8	914	928	96.1	7.6	0.5094	0.010187	0.005093	1.0
23	31.050	N-cyclohexyl-acetamide	1124-53-4	907	931	95.4	2.5	0.1670	0.003339	0.001669	1.0
24	31.703	benzamide	55-21-0	842	881	43.5	1.5	0.1031	0.002061	0.001030	1.0
25	31.908	t-butyl-p-cresol	2409-55-4	936	948	31.7	3.1	0.2092	0.004184	0.002092	1.0

26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.304	benzyl isothiocyanate	622-78-6	901	923	86	1.4	0.0930	0.001860	0.000930	1.0
28	32.531	tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.706	N-benzylformamide	6343-54-0	918	957	92	3.4	0.2285	0.004569	0.002284	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.658	2-(methylthio)-benzothiazole	615-22-5	954	954	88	14.3	0.9563	0.019125	0.009562	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45		unknown	---	---	---	---	---	---	---	---	1.0
46	36.311	2-benzothiazolone	934-34-9	915	925	95	5.1	0.3405	0.006809	0.003404	0.1
47		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.977	Dibenzylamine	103-49-1	906	910	89.2	104.4	6.9574	0.139149	0.069574	1.0
50		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0
52		N-butylbenzenesulphonamide	3622-84-2	---	---	---	---	---	---	---	
53		Benthiazole	21564-17-0	---	---	---	---	---	---	---	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.561	N-cyclohexylbenzamide	1759-68-8	919	920	91.7	16.2	1.0772	0.021543	0.010771	1.0
56	38.903	N-methylbenzothiazoline-2-thione	2254-94-6	859	882	76	4.5	0.2976	0.005951	0.002975	1.0

57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.640	2-mercaptobenzothiazole	149-30-4	944	952	97.2	75.8	5.0517	0.101034	0.050517	10
59	39.938	N-benzylformamide	6343-54-0	757	806	49.4	56.1	3.7368	0.074735	0.037367	1.0
60	40.093	N-benzylbenzamide	1485-70-7	921	937	75.5	16.5	1.1027	0.022053	0.011026	1.0
61		Benzenesulfanilide	1678-25-7	---	---	---	---	---	---	---	1.0
62	40.355	1,3-dicyclohexylurea	2387-23-7	903	935	97.7	10.8	0.7208	0.014416	0.007208	1.0
63	40.654	unknown	---	---	---	---	16.6	1.1081	0.022162	0.011081	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.035	unknown	---	---	---	---	28.7	1.9144	0.038287	0.019143	1.0
66	41.245	unknown	---	---	---	---	72.5	4.8364	0.096727	0.048363	1.0
67	41.351	N,N'-dicyclohexyloxamide	3299-64-7	845	907	95.4	3.7	0.2496	0.004992	0.002496	1.0
68	41.63	2-cyclohexylamino-benzothiazole	28291-75-0	804	919	84.1	4.1	0.2760	0.005519	0.002759	1.0
69	41.724	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	807	889	91.8	5.7	0.3830	0.007660	0.003830	1.0
70	42.099	N-benzyl-benzenecarbothiamide	14309-89-8	904	954	97.3	15.6	1.0393	0.020786	0.010393	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	1.0
74		unknown	---	---	---	---	---	---	---	---	1.0
75		unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.554	unknown	---	---	---	---	42.9	2.8607	0.057213	0.028606	1.0
80	45.003	unknown	---	---	---	---	5.4	0.3628	0.007256	0.003628	1.0
81		unknown	---	---	---	---	---	---	---	---	1.0
82	45.428	unknown	---	---	---	---	2.6	0.1721	0.003441	0.001720	1.0
83	46.153	unknown	---	---	---	---	5.3	0.3544	0.007088	0.003544	1.0
84	46.402	unknown	---	---	---	---	5.4	0.3628	0.007256	0.003628	1.0
85	47.961	unknown	---	---	---	---	3.0	0.1996	0.003991	0.001995	1.0

86		2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87		Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S15. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 4th, 9-day migration, and their quantification by semi-quantitative method (S/V = 10).

N	t _R (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} ²	MTCTap
							(µg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.438	cyclohexylamine	108-91-8	936	938	91.1	47.8	1.5924	0.031848	0.015924	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7	22.522	benzaldehyde	100-52-7	895	933	76.2	16.4	0.5472	0.010944	0.005472	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.005	isocyanate-cyclohexane	3173-53-3	965	966	93.3	82.8	2.7616	0.055232	0.027616	1.0
10	24.543	benzylamine	100-46-09	929	937	59.9	11.4	0.3793	0.007586	0.003793	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	
16	28.904	benzoic acid	65-85-0	823	924	32.4	26.6	0.8864	0.017728	0.008864	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.040	benzothiazole	95-16-9	928	931	74.2	105.2	3.5070	0.070140	0.035070	0.1
19	30.156	isothiocyanate-cyclohexane	1122-82-03	911	915	97.6	40.7	1.3552	0.027103	0.013551	1.0
20	30.246	benzylazetidine	7730-39-4	782	862	41.3	1.3	0.0447	0.000893	0.000446	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	
22	30.492	N-cyclohexyl-formamide	766-93-8	927	932	96.5	14.4	0.4799	0.009597	0.004798	1.0
23	31.056	N-cyclohexyl-acetamide	1124-53-4	921	935	96	4.3	0.1428	0.002856	0.001428	1.0
24	31.711	benzamide	55-21-0	851	890	46.4	3.2	0.1057	0.002113	0.001056	1.0
25	31.909	t-butyl-p-cresol	2409-55-4	930	938	31.4	4.0	0.1333	0.002665	0.001332	1.0

26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.304	benzyl isothiocyanate	622-78-6	927	942	88.6	3.2	0.1081	0.002162	0.001081	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.714	N-benzylformamide	6343-54-0	936	961	92.6	7.3	0.2449	0.004898	0.002449	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40	35.102	N-(phenylmethylene)-cyclohexamine	2211-66-7	898	908	93.9	2.9	0.0982	0.001963	0.000981	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.657	2-(methylthio)-benzothiazole	615-22-5	954	954	88.8	15.5	0.5156	0.010311	0.005155	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45	36.083	unknown	---	---	---	---	---	---	---	---	1.0
46	36.336	2-benzothiazolone	934-34-9	929	936	95.2	12.2	0.4080	0.008160	0.004080	0.1
47		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.963	Dibenzylamine	103-49-1	912	915	90.5	104.4	3.4789	0.069578	0.034789	1.0
50	37.151	Dibenzylhydroxylamine	621-07-8	894	902	46.6	10.6	0.3542	0.007084	0.003542	1.0
51		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0
52	37.562	N-butylbenzenesulphonamide	3622-84-2	749	813	76.2	3.2	0.1059	0.002117	0.001058	1.0
53	37.848	Benthiazole	21564-17-0	692	782	35	10.0	0.3323	0.006646	0.003323	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.571	N-cyclohexylbenzamide	1759-68-8	919	920	92.5	29.8	0.9945	0.019889	0.009944	1.0

56	38.906	N-methylbenzothiazoline-2-thione	2254-94-6	877	906	73.3	6.1	0.2018	0.004036	0.002018	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.738	2-mercaptobenzothiazole	149-30-4	936	939	96.5	159.7	5.3234	0.106467	0.053233	10
59	39.976	N-benzylformamide	6343-54-0	758	808	46.5	104.4	3.4792	0.069584	0.034792	1.0
60	40.145	N-benzylbenzamide	1485-70-7	929	942	76	31.0	1.0325	0.020650	0.010325	1.0
61	40.281	Benzenesulfanilide	1678-25-7	931	937	98.2	28.5	0.9489	0.018978	0.009489	1.0
62	40.385	1,3-dicyclohexylurea	2387-23-7	910	937	97.8	19.2	0.6398	0.012796	0.006398	1.0
63	40.668	unknown	---	---	---	---	22.6	0.7548	0.015095	0.007547	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.039	unknown	---	---	---	---	31.7	1.0568	0.021136	0.010568	1.0
66	41.247	unknown	---	---	---	---	83.9	2.7979	0.055957	0.027978	1.0
67	41.359	N,N'-dicyclohexyloxamide	3299-64-7	875	924	96	7.1	0.2358	0.004716	0.002358	1.0
68	41.642	2-cyclohexylamino-benzothiazole	28291-75-0	787	921	80.6	4.7	0.1573	0.003146	0.001573	1.0
69	41.741	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	851	903	98	10.4	0.3473	0.006945	0.003472	1.0
70	42.11	N-benzyl-benzenecarbothiamide	14309-89-8	904	955	97.5	22.0	0.7318	0.014636	0.007318	1.0
71	42.216	unknown	---	---	---	---	2.2	0.0729	0.001457	0.000728	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	1.0
74	42.555	unknown	---				2.8	0.0918	0.001835	0.000917	1.0
75	42.706	unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77	43.094	N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78	43.394	Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.569	unknown	---	---	---	---	71.9	2.3982	0.047963	0.023981	1.0
80	45.003	unknown	---	---	---	---	7.4	0.2458	0.004915	0.002457	1.0
81		unknown		---	---	---	---	---	---	---	1.0
82	45.434	unknown	---	---	---	---	2.2	0.0720	0.001439	0.000719	1.0
83	46.154	unknown	---	---	---	---	6.2	0.2056	0.004112	0.002056	1.0

84	46.406	unknown	---	---	---	---	2.9	0.0978	0.001955	0.000977	1.0
85	47.968	unknown		---	---	---	4.7	0.1564	0.003127	0.001563	1.0
86	48.536	2,2'-tiobis-benzotiazol	402147	747	857	85.9	3.0	0.1014	0.002027	0.001013	1.0
87	56.162	Cl-5808	332370	838	857	88.7	10.3	0.3435	0.006869	0.003434	1.0

Table S16. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 4th, 15-day migration, and their quantification by semi-quantitative method (S/V = 10). Analysis of duplicate.

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MTCtap
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.445	cyclohexylamine	108-91-8	899	900	90.6	43.9	1.4637	0.029273	0.014636	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7		benzaldehyde	100-52-7	---	---	---	---	---	---	---	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.007	isocyanate-cyclohexane	3173-53-3	968	968	92.8	108.0	3.6000	0.072000	0.036000	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16		benzoic acid	65-85-0	---	---	---	---	---	---	---	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.030	benzothiazole	95-16-9	930	932	73.1	120.6	4.0191	0.080381	0.040190	0.1
19	30.154	isothiocyanate-cyclohexane	1122-82-03	921	921	98.2	57.8	1.9255	0.038510	0.019255	1.0
20		benzylazetidine	7730-39-4	---	---	---	---	---	---	---	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.491	N-cyclohexyl-formamide	766-93-8	934	937	96.5	17.4	0.5812	0.011624	0.005812	1.0
23	31.055	N-cyclohexyl-acetamide	1124-53-4	910	930	95.7	5.2	0.1722	0.003444	0.001722	1.0
24		benzamide	55-21-0	---	---	---	---	---	---	---	1.0

25		t-butyl-p-cresol	2409-55-4	---	---	---	---	---	---	---	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.305	benzyl isothiocyanate	622-78-6	947	958	87.9	8.3	0.2754	0.005507	0.002753	1.0
28	32.531	tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.712	N-benzylformamide	6343-54-0	936	961	92.9	9.7	0.3236	0.006471	0.003235	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.656	2-(methylthio)-benzothiazole	615-22-5	955	955	89	15.3	0.5088	0.010175	0.005087	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45		unknown	---	---	---	---	---	---	---	---	1.0
46	36.322	2-benzothiazolone	934-34-9	931	934	96.2	13.6	0.4548	0.009096	0.004548	0.1
47		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.937	Dibenzylamine	103-49-1	926	928	92.3	67.3	2.2432	0.044863	0.022431	1.0
50	37.145	Dibenzylhydroxylamine	621-07-8	911	920	51.8	8.7	0.2914	0.005828	0.002914	1.0
51		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0
52	37.559	N-butylbenzenesulphonamide	3622-84-2	819	861	83.5	2.3	0.0779	0.001557	0.000778	1.0
53	37.839	Benthiazole	21564-17-0	687	777	28.3	3.7	0.1230	0.002460	0.001230	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.569	N-cyclohexylbenzamide	1759-68-8	924	925	92.8	31.8	1.0594	0.021187	0.010593	1.0

56	38.904	N-methylbenzothiazoline-2-thione	2254-94-6	887	903	73.5	7.0	0.2325	0.004650	0.002325	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.739	2-mercaptobenzothiazole	149-30-4	934	942	96.5	184.2	6.1402	0.122803	0.061401	10
59	39.975	N-benzylformamide	6343-54-0	761	812	53.9	110.2	3.6748	0.073495	0.036747	1.0
60	40.144	N-benzylbenzamide	1485-70-7	938	947	76.6	32.9	1.0973	0.021946	0.010973	1.0
61	40.278	Benzenesulfanilide	1678-25-7	912	932	97.1	30.3	1.0094	0.020188	0.010094	1.0
62	40.380	1,3-dicyclohexylurea	2387-23-7	906	938	97.8	20.6	0.6875	0.013749	0.006874	1.0
63	40.666	unknown	---	---	---	---	23.9	0.7959	0.015918	0.007959	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.038	unknown	---	---	---	---	33.8	1.1280	0.022559	0.011279	1.0
66	41.247	unknown	---	---	---	---	91.6	3.0523	0.061046	0.030523	1.0
67	41.357	N,N'-dicyclohexyloxamide	3299-64-7	885	903	97.8	7.5	0.2490	0.004980	0.002490	1.0
68	41.64	2-cyclohexylamino-benzothiazole	28291-75-0	802	921	79.7	5.0	0.1661	0.003322	0.001661	1.0
69	41.739	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	815	900	95	11.1	0.3697	0.007394	0.003697	1.0
70	42.109	N-benzyl-benzenecarbothiamide	14309-89-8	906	955	97.3	23.1	0.7697	0.015394	0.007697	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	1.0
74	42.554	unknown	---	---	---	---	2.9	0.0973	0.001945	0.000972	1.0
75		unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.546	unknown	---	---	---	---	34.0	1.1328	0.022655	0.011327	1.0
80		unknown	---	---	---	---	---	---	---	---	1.0
81		unknown	---	---	---	---	---	---	---	---	1.0
82		unknown	---	---	---	---	---	---	---	---	1.0
83	46.145	unknown	---	611	849	53.2	40.9	1.3648	0.027296	0.013648	1.0
84	46.399	unknown	---				4.0	0.1334	0.002668	0.001334	1.0

85	47.963	unknown		694	868	57.1	4.4	0.1452	0.002904	0.001452	1.0
86	48.534	2,2'-tiobis-benzotiazol	402147	797	886	94.5	4.1	0.1351	0.002701	0.001350	1.0
87		Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S17. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 5th, 22-day migration, and their quantification by semi-quantitative method (S/V = 5).

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	C _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} 2	MTC _{tap}
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.479	cyclohexylamine	108-91-8	934	939	92.3	9.8	0.6563	0.013125	0.006562	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7		benzaldehyde	100-52-7	---	---	---	---	---	---	---	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.001	isocyanate-cyclohexane	3173-53-3	966	966	93.3	40.4	2.6963	0.053926	0.026963	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16	28.835	benzoic acid	65-85-0	943	950	51	10.4	0.6940	0.013879	0.006939	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.028	benzothiazole	95-16-9	932	935	73.1	64.8	4.3226	0.086452	0.043226	0.1
19	30.151	isothiocyanate-cyclohexane	1122-82-03	919	923	97.1	32.4	2.1578	0.043154	0.021576	1.0
20		benzylazetidine	7730-39-4	---	---	---	---	---	---	---	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.478	N-cyclohexyl-formamide	766-93-8	931	936	97.5	6.5	0.4336	0.008672	0.004336	1.0
23	31.052	N-cyclohexyl-acetamide	1124-53-4	909	931	96.5	18.7	1.2448	0.024896	0.012448	1.0

24		benzamide	55-21-0	---	---	---	---	---	---	---	1.0
25	31.905	t-butyl-p-cresol	2409-55-4	945	949	32.1	3.1	0.2094	0.004186	0.002092	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.303	benzyl isothiocyanate	622-78-6	946	947	87.9	3.7	0.247	0.00494	0.00247	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.705	N-benzylformamide	6343-54-0	939	963	93	3.0	0.1974	0.003948	0.001974	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.657	2-(methylthio)-benzothiazole	615-22-5	954	955	86.6	17.1	1.1414	0.022828	0.011414	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45		unknown	---	---	---	---	---	---	---	---	1.0
46	36.292	2-benzothiazolone	934-34-9	892	911	92.5	5.7	0.3826	0.00765	0.003824	0.1
47	36.428	Dibenzylmethylanine	102-05-6	924	941	93.9	2.8	0.1878	0.003756	0.001878	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.946	Dibenzylamine	103-49-1	913	916	90.8	71.5	4.768	0.09536	0.04768	1.0
50	37.145	Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0
51	37.148	Benzaldehyde N-benzylimine	780-25-6	902	902	82.3	6.1	0.4044	0.008086	0.004042	1.0

52	37.547	N-butylbenzenesulphonamide	3622-84-2	799	839	80.8	1.0	0.0666	0.00133	0.000664	1.0
53	37.837	Benthiazole	21564-17-0	671	757	22.5	3.3	0.2218	0.004434	0.002216	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.556	N-cyclohexylbenzamide	1759-68-8	926	928	92	15.5	1.034	0.020678	0.010338	1.0
56	38.900	N-methylbenzothiazoline-2-thione	2254-94-6	852	881	74.6	4.1	0.2736	0.005472	0.002736	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.632	2-mercaptobenzothiazole	149-30-4	943	945	97.6	81.0	5.401	0.108018	0.054008	10
59	39.931	N-benzylformamide	6343-54-0	762	810	51.9	56.4	3.7568	0.075136	0.037568	1.0
60	40.090	N-benzylbenzamide	1485-70-7	917	934	75	16.1	1.0758	0.021514	0.010756	1.0
61		Benzenesulfanilide	1678-25-7	---	---	---	---	---	---	---	1.0
62	40.345	1,3-dicyclohexylurea	2387-23-7	878	934	97.6	9.3	0.6206	0.01241	0.006204	1.0
63	40.651	unknown	---	---	---	---	17.7	1.1824	0.023648	0.011824	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.033	unknown	---	---	---	---	32.3	2.1504	0.043006	0.021502	1.0
66	41.242	unknown	---	---	---	---	79.9	5.3276	0.10655	0.053274	1.0
67	41.348	N,N'-dicyclohexyloxamide	3299-64-7	807	923	85.3	4.1	0.2704	0.005406	0.002702	1.0
68	41.628	2-cyclohexylamino-benzothiazole	28291-75-0	762	877	84.2	4.6	0.306	0.006118	0.003058	1.0
69	41.718	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	854	907	93.9	4.8	0.3198	0.006394	0.003196	1.0
70	42.095	N-benzyl-benzenecarbothiamide	14309-89-8	903	956	97.4	16.6	1.1036	0.02207	0.011034	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72	42.255	Ethyl 9-fluorenyldeneacetate	27973-36-0	744	781	83	1.9	0.1254	0.002508	0.001254	1.0
73		unknown	---	---	---	---	---	---	---	---	
74		unknown	---	---	---	---	---	---	---	---	1.0
75		unknown	---	---	---	---	---	---	---	---	
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.536	unknown	---	---	---	---	20.6	1.37	0.0274	0.0137	1.0
80	45.003	unknown	---	---	---	---	5.9	0.3962	0.007922	0.00396	1.0

81		7-benzyloxyindole		---	---	---	---	---	---	---	1.0
82	45.419	unknown	---	---	---	---	1.0	0.064	0.001278	0.000638	1.0
83	46.142	unknown	---	---	---	---	2.4	0.159	0.003178	0.001588	1.0
84		unknown	---	---	---	---	---	---	---	---	1.0
85	47.964	unknown	---	---	---	---	1.6	0.1056	0.002112	0.001056	1.0
86		2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87		Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S18. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 5th, 22-day migration, and their quantification by semi-quantitative method (S/V = 5). Analysis of duplicate.

N	t _R (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} ²	MTC _{tap}
							(µg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.485	cyclohexylamine	108-91-8	908	908	92.7	10.3	0.6893	0.013786	0.006893	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7		benzaldehyde	100-52-7	---	---	---	---	---	---	---	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.007	isocyanate-cyclohexane	3173-53-3	961	961	92.5	47.2	3.1475	0.062950	0.031475	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16	28.812	benzoic acid	65-85-0	907	940	46.6	16.0	1.0685	0.021369	0.010684	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.026	benzothiazole	95-16-9	933	936	72	63.4	4.227	0.08454	0.04227	0.1
19	30.151	isothiocyanate-cyclohexane	1122-82-03	924	928	98.3	32.8	2.1882	0.043764	0.021882	1.0
20	30.247	benzylazetidine	7730-39-4	796	870	45.9	0.9	0.0602	0.001202	0.0006	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.479	N-cyclohexyl-formamide	766-93-8	921	927	96.5	6.2	0.411	0.00822	0.00411	1.0

23	31.052	N-cyclohexyl-acetamide	1124-53-4	914	929	96.4	1.7	0.1144	0.002286	0.001142	1.0
24		benzamide	55-21-0	---	---	---	---	---	---	---	1.0
25	31.904	t-butyl-p-cresol	2409-55-4	948	953	35.3	29.0	1.9306	0.03861	0.019304	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.303	benzyl isothiocyanate	622-78-6	942	942	86.5	4.8	0.323	0.006458	0.003228	1.0
28	32.531	tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.704	N-benzylformamide	6343-54-0	942	967	94	2.9	0.1946	0.003892	0.001946	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	---	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38	35.037	N-phenylcyclohexylamine	1821-36-9	808	898	72.3	0.9	0.0576	0.001152	0.000576	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.659	2-(methylthio)-benzothiazole	615-22-5	953	953	88.6	16.8	1.1232	0.022462	0.01123	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44	35.857	dipropylbenzamide	10546-70-0	870	944	86.8	1.1	0.076	0.00152	0.00076	1.0
45		unknown	---	---	---	---	---	---	---	---	1.0
46	36.285	2-benzothiazolone	934-34-9	891	910	92.7	5.8	0.389	0.00778	0.00389	0.1
47	36.429	Dibenzylmethylaniline	102-05-6	895	936	91.9	1.3	0.084	0.00168	0.00084	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.936	Dibenzylamine	103-49-1	927	929	93.1	59.4	3.9588	0.079176	0.039588	1.0
50		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0

51	37.148	Benzaldehyde N-benzylimine	780-25-6	914	914	78.2	2.9	0.1908	0.003814	0.001906	1.0
52		N-butylbenzenesulfonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53	37.839	Benthiazole	21564-17-0	640	727	52.1	1.7	0.1114	0.002228	0.001114	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.569	N-cyclohexylbenzamide	1759-68-8	927	928	92	15.6	1.04	0.0208	0.0104	1.0
56	38.904	N-methylbenzothiazoline-2-thione	2254-94-6	846	878	73.4	4.8	0.32	0.006398	0.003198	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.626	2-mercaptobenzothiazole	149-30-4	944	945	97	85.4	5.6918	0.113834	0.056916	10
59	39.929	N-benzylformamide	6343-54-0	759	805	45.6	56.5	3.7676	0.075352	0.037676	1.0
60	40.087	N-benzylbenzamide	1485-70-7	914	934	76.9	16.2	1.078	0.02156	0.01078	1.0
61		Benzenesulfanilide	1678-25-7	---	---	---	---	---	---	---	1.0
62	40.343	1,3-dicyclohexylurea	2387-23-7	878	920	97.6	9.4	0.6254	0.012508	0.006254	1.0
63	40.649	unknown	---	---	---	---	18.0	1.1976	0.023952	0.011976	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.032	unknown	---	---	---	---	33.2	2.2158	0.044314	0.022156	1.0
66	41.241	unknown	---	---	---	---	84.6	5.6406	0.11281	0.056404	1.0
67	41.347	N,N'-dicyclohexyloxamide	3299-64-7	833	909	95.9	3.9	0.2612	0.005224	0.002612	1.0
68	41.625	2-cyclohexylamino-benzothiazole	28291-75-0	794	922	79.8	4.7	0.314	0.00628	0.00314	1.0
69	41.716	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	799	889	91.3	5.0	0.3324	0.006646	0.003322	1.0
70	42.094	N-benzyl-benzenecarbothiamide	14309-89-8	905	956	96.8	16.8	1.1228	0.022456	0.011228	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73	42.398	unknown	---	---	---	---	---	---	---	---	
74	42.53	unknown	---	---	---	---	8.4	0.5574	0.01114747	0.00557373	1.0
75		unknown	---	---	---	---	---	---	---	---	
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79		unknown	---	---	---	---	---	---	---	---	1.0

80		unknown	---	---	---	---	---	---	---	---	1.0
81		unknown	---	---	---	---	---	---	---	---	1.0
82		unknown	---	---	---	---	---	---	---	---	1.0
83	46.145	unknown	---	---	---	---	2.0	0.1314	0.002628	0.001314	1.0
84		unknown	---	---	---	---	---	---	---	---	1.0
85	47.948	unknown	---	---	---	---	1.4	0.096	0.00192	0.00096	1.0
86		2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87		Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S19. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 5th, 22-day migration, and their quantification by semi-quantitative method (S/V = 10).

N	t _R (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} 2	MTC _{tap}
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4	16.737	4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.426	cyclohexylamine	108-91-8	917	917	91.9	43.4	1.4461	0.028921	0.014460	2.1
6	19.188	cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7	22.521	benzaldehyde	100-52-7	---	---	---	---	---	---	---	1.0
8	23.532	benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	23.999	isocyanate-cyclohexane	3173-53-3	966	966	94	54.9	1.8315	0.036629	0.018314	1.0
10	24.527	benzylamine	100-46-09	934	937	69.3	20.9	0.6953	0.013905	0.006952	1.0
11	25.007	2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12	25.224	benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13	26.189	unknown	---	---	---	---	---	---	---	---	1.0
14	27.017	methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15	27.543	2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16	28.921	benzoic acid	65-85-0	---	---	---	---	---	---	---	1.0
17	29.795	2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.034	benzothiazole	95-16-9	932	934	71.8	95.1	3.1713	0.063426	0.031713	0.1
19	30.155	isothiocyanate-cyclohexane	1122-82-03	918	922	98.3	43.3	1.4429	0.028858	0.014429	1.0
20	30.235	benzylazetidine	7730-39-4	829	853	62.6	9.8	0.3282	0.006563	0.003281	1.0
21	30.494	N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.488	N-cyclohexyl-formamide	766-93-8	922	928	96.4	13.3	0.4421	0.008841	0.004420	1.0

23	31.055	N-cyclohexyl-acetamide	1124-53-4	930	938	97.4	3.7	0.1223	0.002445	0.001222	1.0
24		benzamide	55-21-0	---	---	---	---	---	---	---	1.0
25	31.907	t-butyl-p-cresol	2409-55-4	946	951	38.4	4.2	0.1386	0.002772	0.001386	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27		benzyl isothiocyanate	622-78-6	---	---	---	---	---	---	---	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.852	N-benzylformamide	6343-54-0	951	967	94.4	6.6	0.2206	0.004411	0.002205	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide		---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40	35.098	N-(phenylmethylene)-cyclohexamine	2211-66-7	897	910	95.4	1.9	0.0620	0.001239	0.000619	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.655	2-(methylthio)-benzothiazole	615-22-5	951	951	87.7	11.0	0.3668	0.007336	0.003668	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45		unknown	---	---	---	---	---	---	---	---	1.0
46	36.331	2-benzothiazolone	934-34-9	904	919	92.9	7.4	0.2452	0.004904	0.002452	0.1
47		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.973	Dibenzylamine	103-49-1	905	912	89.2	83.6	2.7852	0.055704	0.027852	1.0
50	37.152	Dibenzylhydroxylamine	621-07-8	897	907	47.9	6.7	0.2229	0.004457	0.002228	1.0

51		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0
52		N-butylbenzenesulphonamide	3622-84-2	---	---	---	---	---	---	---	
53	37.847	Benthiazole	21564-17-0	688	780	29.2	8.9	0.2966	0.005931	0.002965	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.567	N-cyclohexylbenzamide	1759-68-8	922	924	93.5	18.9	0.6299	0.012597	0.006298	1.0
56		N-methylbenzothiazoline-2-thione	2254-94-6	---	---	---	---	---	---	---	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.716	2-mercaptobenzothiazole	149-30-4	911	914	89.6	95.8	3.1939	0.063877	0.031938	10
59	39.966	N-benzylformamide	6343-54-0	759	809	51.3	66.1	2.2035	0.044070	0.022035	1.0
60	40.133	N-benzylbenzamide	1485-70-7	939	948	77.3	19.0	0.6327	0.012653	0.006326	1.0
61	40.270	Benzenesulfanilide	1678-25-7	895	924	96.5	16.8	0.5609	0.011218	0.005609	1.0
62	40.370	1,3-dicyclohexylurea	2387-23-7	885	937	97.4	9.6	0.3190	0.006380	0.003190	1.0
63	40.663	unknown	---	---	---	---	15.9	0.5288	0.010576	0.005288	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.036	unknown	---	---	---	---	22.7	0.7574	0.015147	0.007573	1.0
66	41.245	unknown	---	---	---	---	58.6	1.9534	0.039068	0.019534	1.0
67	41.355	N,N'-dicyclohexyloxamide	3299-64-7	857	916	96	4.6	0.1546	0.003092	0.001546	1.0
68	41.635	2-cyclohexylamino-benzothiazole	28291-75-0	792	920	80.9	3.8	0.1279	0.002558	0.001279	1.0
69	41.733	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	833	900	92.7	6.3	0.2100	0.004199	0.002099	1.0
70	42.105	N-benzyl-benzenecarbothiamide	14309-89-8	903	953	97.4	15.1	0.5049	0.010097	0.005048	1.0
71	42.231	unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73	42.398	unknown	---	---	---	---	---	---	---	---	
74	42.562	unknown	---	---	---	---	45.7	1.5230	0.030459	0.015229	1.0
75		unknown	---	---	---	---	---	---	---	---	
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75

79		unknown	---	---	---	---	---	---	---	---	1.0
80	45.003	unknown	---	---	---	---	4.7	0.1553	0.003105	0.001552	1.0
81		unknown		---	---	---	---	---	---	---	1.0
82		unknown	---	---	---	---	---	---	---	---	1.0
83	46.145	unknown	---	---	---	---	2.3	0.0775	0.001549	0.000774	1.0
84	46.399	unknown	---	---	---	---	1.3	0.0446	0.000892	0.000446	1.0
85		unknown		---	---	---	---	---	---	---	1.0
86	48.527	2,2'-tiobis-benzotiazol	402147	643	864	42.2	1.4	0.0450	0.000900	0.000450	1.0
87	56.167	Cl-5808	332370	910	915	93.3	10.5	0.3504	0.007008	0.003504	1.0

Table S20. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 5th, 22-day migration, and their quantification by semi-quantitative method (S/V = 10). Analysis of duplicate

N	t _R (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} 2	MTC _{tap}
							(µg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5	17.438	cyclohexylamine	108-91-8	937	937	94.4	24.2	0.8076	0.016152	0.008076	2.1
6	19.187	cyclohexanone	108-94-01	938	941	74	6.0	0.2000	0.003999	0.001999	1.0
7	22.521	benzaldehyde	100-52-7	939	942	77.7	6.9	0.2299	0.004598	0.002299	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	24.008	isocyanate-cyclohexane	3173-53-3	966	967	92.4	56.6	1.8881	0.037762	0.018881	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16	28.881	benzoic acid	65-85-0	925	945	48.3	16.5	0.5484	0.010967	0.005483	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.051	benzothiazole	95-16-9	921	924	77.5	95.2	3.1724	0.063447	0.031723	0.1
19	30.165	isothiocyanate-cyclohexane	1122-82-03	916	920	97.7	41.1	1.3689	0.027378	0.013689	1.0
20	30.246	benzylazetidine	7730-39-4	812	872	62.9	1.8	0.0587	0.001174	0.000587	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.503	N-cyclohexyl-formamide	766-93-8	932	937	97.5	11.6	0.3850	0.007700	0.003850	1.0
23	31.064	N-cyclohexyl-acetamide	1124-53-4	929	937	96.9	3.2	0.1060	0.002119	0.001059	1.0

24		benzamide	55-21-0	---	---	---	---	---	---	---	1.0
25	31.909	t-butyl-p-cresol	2409-55-4	945	949	33.9	3.8	0.1277	0.002553	0.001276	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.305	benzyl isothiocyanate	622-78-6	945	948	87.7	5.7	0.1887	0.003773	0.001886	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.717	N-benzylformamide	6343-54-0	947	967	93.7	6.1	0.2028	0.004055	0.002027	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	
42	35.659	2-(methylthio)-benzothiazole	615-22-5	951	951	88	16.1	0.5365	0.010729	0.005364	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	
45	36.083	unknown	---	---	---	---	---	---	---	---	1.0
46	36.338	2-benzothiazolone	934-34-9	899	921	91.9	11.2	0.3723	0.007446	0.003723	0.1
47		Dibenzylmethylaniline	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.941	Dibenzylamine	103-49-1	916	944	91.5	604.4	20.1453	0.402905	0.201452	1.0
50	37.146	Dibenzylhydroxylamine	621-07-8	910	919	56.7	8.9	0.2960	0.005920	0.002960	1.0
51		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0

52	37.564	N-butylbenzenesulphonamide	3622-84-2	758	828	78.6	1.9	0.0631	0.001262	0.000631	1.0
53	37.839	Benthiazole	21564-17-0	677	766	25.4	4.1	0.1369	0.002738	0.001369	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.569	N-cyclohexylbenzamide	1759-68-8	925	926	93.8	25.1	0.8353	0.016705	0.008352	1.0
56	38.904	N-methylbenzothiazoline-2-thione	2254-94-6	884	905	73.7	5.9	0.1962	0.003923	0.001961	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.769	2-mercaptobenzothiazole	149-30-4	937	939	96.6	146.7	4.8907	0.097814	0.048907	10
59	39.987	N-benzylformamide	6343-54-0	758	809	50.7	89.7	2.9894	0.059787	0.029893	1.0
60	40.157	N-benzylbenzamide	1485-70-7	937	945	76.2	26.6	0.8868	0.017736	0.008868	1.0
61	40.291	Benzenesulfanilide	1678-25-7	930	936	98	23.9	0.7951	0.015902	0.007951	1.0
62	40.386	1,3-dicyclohexylurea	2387-23-7	904	933	98	13.8	0.4600	0.009200	0.004600	1.0
63	40.673	unknown	---	---	---	---	21.6	0.7209	0.014418	0.007209	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.042	unknown	---	---	---	---	31.3	1.0431	0.020861	0.010430	1.0
66	41.252	unknown	---	---	---	---	77.9	2.5973	0.051946	0.025973	1.0
67	41.362	N,N'-dicyclohexyloxamide	3299-64-7	860	918	96.4	6.5	0.2158	0.004315	0.002157	1.0
68	41.645	2-cyclohexylamino-benzothiazole	28291-75-0	781	921	79.2	4.8	0.1602	0.003203	0.001601	1.0
69	41.744	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	836	900	92	8.1	0.2702	0.005403	0.002701	1.0
70	42.114	N-benzyl-benzenecarbothiamide	14309-89-8	904	953	97.4	20.9	0.6974	0.013948	0.006974	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	1.0
74	42.555	unknown	---	---	---	---	2.3	0.0783	0.001565	0.000782	1.0
75		unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.544	unknown	---	---	---	---	20.5	0.6826	0.013652	0.006826	1.0

80	45.003	unknown	---	---	---	---	7.6	0.2536	0.005071	0.002535	1.0
81		unknown	---	---	---	---	---	---	---	---	1.0
82		unknown	---	---	---	---	---	---	---	---	1.0
83	46.145	unknown	---	---	---	---	2.4	0.0791	0.001582	0.000791	1.0
84	46.399	unknown	---	---	---	---	3.1	0.1034	0.002067	0.001033	1.0
85	47.963	unknown	---	---	---	---	19.6	0.6549	0.013097	0.006548	1.0
86	48.534	2,2'-tiobis-benzotiazol	402147	802	895	94.7	4.3	0.1424	0.002847	0.001423	1.0
87		Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S21. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 6^h, 29-day migration, and their quantification by semi-quantitative method (S/V = 5).

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	C_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MTCtap
							(μg/l)				
1			77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5		cyclohexylamine	108-91-8	---	---	---	---	---	---	---	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7		benzaldehyde	100-52-7	---	---	---	---	---	---	---	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	23.983	isocyanate-cyclohexane	3173-53-3	956	956	92.3	60.2	4.0118	0.080236	0.040118	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16		benzoic acid	65-85-0	---	---	---	---	---	---	---	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.012	benzothiazole	95-16-9	931	933	64.6	61.8	4.1229	0.082458	0.041229	0.1
19	30.141	isothiocyanate-cyclohexane	1122-82-03	915	918	97.1	61.8	4.1229	0.082458	0.041229	1.0
20		benzylazetidine	7730-39-4	---	---	---	---	---	---	---	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22		N-cyclohexyl-formamide	766-93-8	---	---	---	---	---	---	---	1.0
23		N-cyclohexyl-acetamide	1124-53-4	---	---	---	---	---	---	---	1.0

24		benzamide	55-21-0	---	---	---	---	---	---	---	1.0
25	31.896	t-butyl-p-cresol	2409-55-4	938	942	32.7	2.9	0.1958	0.003915	0.001957	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.296	benzyl isothiocyanate	622-78-6	935	936	82.4	4.7	0.3102	0.006203	0.003101	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29		N-benzylformamide	6343-54-0	---	---	---	---	---	---	---	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide		---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.648	2-(methylthio)-benzothiazole	615-22-5	957	957	88.9	14.7	0.9790	0.019579	0.009789	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45		unknown	---	---	---	---	---	---	---	---	1.0
46	36.421	2-benzothiazolone	934-34-9	897	918	95.5	4.5	0.2971	0.005941	0.002970	0.1
47	36.571	Dibenzylmethylaniline	102-05-6	932	934	94.1	2.7	0.1774	0.003548	0.001774	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.934	Dibenzylamine	103-49-1	918	920	91.8	62.9	4.1947	0.083894	0.041947	1.0
50	37.138	Dibenzylhydroxylamine	621-07-8	920	938	41.7	5.1	0.3417	0.006834	0.003417	1.0
51		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0

52		N-butylbenzenesulphonamide		---	---	---	---	---	---	---	1.0
53		Benthiazole	21564-17-0	---	---	---	---	---	---	---	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.546	N-cyclohexylbenzamide	1759-68-8	926	928	93.7	13.5	0.9004	0.018008	0.009004	1.0
56		N-methylbenzothiazoline-2-thione	2254-94-6	---	---	---	---	---	---	---	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.592	2-mercaptobenzothiazole	149-30-4	947	948	97.6	68.9	4.5911	0.091821	0.045910	10
59	39.912	N-benzylformamide	6343-54-0	763	808	50.1	47.6	3.1728	0.063455	0.031727	1.0
60	40.073	N-benzylbenzamide	1485-70-7	920	939	77.9	13.2	0.8802	0.017604	0.008802	1.0
61		Benzenesulfanilide	1678-25-7	---	---	---	---	---	---	---	1.0
62	40.403	1,3-dicyclohexylurea	2387-23-7	907	919	95.7	7.6	0.5052	0.010103	0.005051	1.0
63	40.638	unknown	---	---	---	---	15.3	1.0222	0.020444	0.010222	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.025	unknown	---	---	---	---	28.6	1.9080	0.038160	0.019080	1.0
66	41.246	unknown	---	---	---	---	72.2	4.8136	0.096271	0.048135	1.0
67	41.339	N,N'-dicyclohexyloxamide	3299-64-7	836	905	96	4.1	0.2711	0.005422	0.002711	1.0
68	41.618	2-cyclohexylamino-benzothiazole	28291-75-0	793	917	80.7	4.5	0.3027	0.006054	0.003027	1.0
69		N-benzyl-N'-cyclohexyl-isourea	25855-24-7	---	---	---	---	---	---	---	1.0
70	42.084	N-benzyl-benzenecarbothiamide	14309-89-8	903	957	96.1	13.9	0.9295	0.018590	0.009295	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	
74		unknown	---	---	---	---	---	---	---	---	1.0
75		unknown	---	---	---	---	---	---	---	---	
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79	43.524	unknown	---	---	---	---	12.2	0.8118	0.016236	0.008118	1.0

80		unknown	---	---	---	---	---	---	---	---	1.0
81		unknown	---	---	---	---	---	---	---	---	1.0
82	45.426	unknown	---	---	---	---	---	---	---	---	1.0
83	46.145	unknown	---	---	---	---	---	---	---	---	1.0
84	46.399	unknown	---	---	---	---	---	---	---	---	1.0
85	47.963	unknown		---	---	---	---	---	---	---	1.0
86	48.534	2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87	56.214	Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S22. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 6^h, 29-day migration, and their quantification by semi-quantitative method (S/V = 5). Analysis of duplicate

N	tr (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	C_n^T	M_n^T	C_{Tap}^1	C_{Tap2}	MTCtap
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5		cyclohexylamine	108-91-8	---	---	---	---	---	---	---	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7		benzaldehyde	100-52-7	---	---	---	---	---	---	---	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	23.986	isocyanate-cyclohexane	3173-53-3	958	960	92.9	37.2	2.4826	0.049651	0.024825	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16		benzoic acid	65-85-0	---	---	---	---	---	---	---	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.009	benzothiazole	95-16-9	936	938	74	64.0	4.2646	0.085291	0.042645	0.1
19	30.134	isothiocyanate-cyclohexane	1122-82-03	914	917	97	33.0	2.2027	0.044054	0.022027	1.0
20		benzylazetidine	7730-39-4	---	---	---	---	---	---	---	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.460	N-cyclohexyl-formamide	766-93-8	926	931	97.5	6.6	0.4367	0.008734	0.004367	1.0

23		N-cyclohexyl-acetamide	1124-53-4	---	---	---	---	---	---	---	1.0
24		benzamide	55-21-0	---	---	---	---	---	---	---	1.0
25	31.896	t-butyl-p-cresol	2409-55-4	933	940	27.6	3.0	0.2031	0.004061	0.002030	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.295	benzyl isothiocyanate	622-78-6	926	931	82.7	3.0	0.1970	0.003940	0.001970	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.694	N-benzylformamide	6343-54-0	918	957	92	2.7	0.1815	0.003630	0.001815	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41	35.647	2-(methylthio)-benzothiazole	615-22-5	953	953	88.2	15.2	1.0130	0.020259	0.010129	1.0
42		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
43		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
44		unknown	---	---	---	---	---	---	---	---	1.0
45	36.274	2-benzothiazolone	934-34-9	875	902	89.9	4.1	0.2750	0.005500	0.002750	0.1
46	36.421	Dibenzylmethylaniline	102-05-6	929	946	92.9	2.9	0.1900	0.003800	0.001900	1.0
47		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
48	36.953	Dibenzylamine	103-49-1	913	916	91.2	106.9	7.1286	0.142572	0.071286	1.0
49	37.142	Dibenzylhydroxylamine	621-07-8	938	945	71.2	6.8	0.4538	0.009076	0.004538	1.0
50		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0

51		N-Benzylidenebenzylamine	780-25-6	---	---	---	---	---	---	---	1.0
52		N-butylbenzenesulphonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53		Benthiazole	21564-17-0	---	---	---	---	---	---	---	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.544	N-cyclohexylbenzamide	1759-68-8	919	921	93.2	13.5	0.9001	0.018001	0.009000	1.0
56	38.891	N-methylbenzothiazoline-2-thione	2254-94-6	854	881	75.6	4.0	0.2672	0.005344	0.002672	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.570	2-mercaptobenzothiazole	149-30-4	948	949	97.6	67.9	4.5236	0.090472	0.045236	10
59	39.904	N-benzylformamide	6343-54-0	758	801	46.1	48.1	3.2091	0.064181	0.032090	1.0
60	40.067	N-benzylbenzamide	1485-70-7	920	939	77.9	12.7	0.8443	0.016886	0.008443	1.0
61		Benzenesulfanilide	1678-25-7	---	---	---	---	---	---	---	1.0
62	40.319	1,3-dicyclohexylurea	2387-23-7	835	912	97.3	6.3	0.4216	0.008431	0.004215	1.0
63	40.633	unknown	---	---	---	---	12.6	0.8371	0.016742	0.008371	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.021	unknown	---	---	---	---	26.8	1.7849	0.035697	0.017848	1.0
66	41.227	unknown	---	---	---	---	73.2	4.8767	0.097534	0.048767	1.0
67	41.337	N,N'-dicyclohexyloxamide	3299-64-7	842	910	96.3	3.1	0.2043	0.004086	0.002043	1.0
68	41.614	2-cyclohexylamino-benzothiazole	28291-75-0	779	921	81.4	3.7	0.2470	0.004939	0.002469	1.0
69	41.697	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	713	871	71	3.2	0.2123	0.004246	0.002123	1.0
70	42.079	N-benzyl-benzenecarbothiamide	14309-89-8	903	959	97.3	12.6	0.8387	0.016773	0.008386	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	1.0
74		unknown	---	---	---	---	---	---	---	---	1.0
75		unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75

79	43.521	unknown	---	---	---	---	5.0	0.3315	0.006629	0.003314	1.0
80	45.003	unknown	---	---	---	---	4.1	0.2705	0.005410	0.002705	1.0
81	45.447	unknown	---	---	---	---	---	---	---	---	1.0
82	45.426	unknown	---	---	---	---	---	---	---	---	1.0
83	46.145	unknown	---	---	---	---	---	---	---	---	1.0
84	46.399	unknown	---	---	---	---	---	---	---	---	1.0
85	47.963	unknown	---	---	---	---	---	---	---	---	1.0
86	48.534	2,2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87	56.214	Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S23. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 6^h, 29-day migration, and their quantification by semi-quantitative method (S/V = 10).

N	t _R (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} 2	MT _{Ctap}
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5		cyclohexylamine	108-91-8	---	---	---	---	---	---	---	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7		benzaldehyde	100-52-7	---	---	---	---	---	---	---	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	23.922	isocyanate-cyclohexane	3173-53-3	954	954	92.7	49.4	1.6460	0.032919	0.016459	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16		benzoic acid	65-85-0	---	---	---	---	---	---	---	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.027	benzothiazole	95-16-9	930	933	74	88.0	2.9347	0.058693	0.029346	0.1
19	30.145	isothiocyanate-cyclohexane	1122-82-03	918	921	98.3	38.8	1.2923	0.025846	0.012923	1.0
20		benzylazetidine	7730-39-4	---	---	---	---	---	---	---	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.479	N-cyclohexyl-formamide	766-93-8	935	938	97.4	11.0	0.3679	0.007357	0.003678	1.0

23	31.048	N-cyclohexyl-acetamide	1124-53-4	927	99	96.5	3.0	0.1001	0.002001	0.001000	1.0
24	31.701	benzamide	55-21-0	853	890	53.6	2.3	0.0759	0.001517	0.000758	1.0
25	31.898	t-butyl-p-cresol	2409-55-4	937	942	30.4	3.7	0.1217	0.002433	0.001216	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27	32.296	benzyl isothiocyanate	622-78-6	936	938	85.3	6.3	0.2115	0.004229	0.002114	1.0
28	32.531	tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29	32.701	N-benzylformamide	6343-54-0	950	968	94.5	5.3	0.1777	0.003554	0.001777	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1	---	---	---	---	---	---	---	1.0
42	35.648	2-(methylthio)-benzothiazole	615-22-5	949	951	87.6	15.4	0.5128	0.010256	0.005128	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	1.0
45		unknown	---	---	---	---	---	---	---	---	1.0
46	36.300	2-benzothiazolone	934-34-9	929	936	95.2	9.0	0.2995	0.005989	0.002994	0.1
47		Dibenzylmethylamine	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.929	Dibenzylamine	103-49-1	928	929	94.1	57.3	1.9090	0.038180	0.019090	1.0
50		Dibenzylhydroxylamine	621-07-8	---	---	---	---	---	---	---	1.0

51		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0
52		N-butylbenzenesulphonamide	3622-84-2	---	---	---	---	---	---	---	1.0
53		Benthiazole	21564-17-0	---	---	---	---	---	---	---	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.555	N-cyclohexylbenzamide	1759-68-8	927	929	93.5	22.8	0.7597	0.015194	0.007597	1.0
56	38.895	N-methylbenzothiazoline-2-thione	2254-94-6	876	908	74	5.7	0.1912	0.003823	0.001911	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.688	2-mercaptobenzothiazole	149-30-4	941	943	97.1	131.3	4.3760	0.087520	0.043760	10
59	39.948	N-benzylformamide	6343-54-0	758	803	47.4	80.0	2.6666	0.053332	0.026666	1.0
60	40.115	N-benzylbenzamide	1485-70-7	937	946	76.8	22.8	0.7614	0.015228	0.007614	1.0
61	40.251	Benzenesulfanilide	1678-25-7	918	937	97.8	19.8	0.6590	0.013180	0.006590	1.0
62	40.353	1,3-dicyclohexylurea	2387-23-7	884	927	97.6	11.4	0.3793	0.007585	0.003792	1.0
63	40.650	unknown	---	---	---	---	19.6	0.6524	0.013048	0.006524	1.0
64		2,3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.027	unknown	---	---	---	---	29.0	0.9661	0.019321	0.009660	1.0
66	41.236	unknown	---	---	---	---	77.0	2.5653	0.051306	0.025653	1.0
67	41.346	N,N'-dicyclohexyloxamide	3299-64-7	799	890	88.9	5.4	0.1813	0.003626	0.001813	1.0
68	41.626	2-cyclohexylamino-benzothiazole	28291-75-0	787	917	80.9	4.2	0.1392	0.002784	0.001392	1.0
69	41.720	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	813	900	89.3	6.0	0.2001	0.004002	0.002001	1.0
70	42.094	N-benzyl-benzenecarbothiamide	14309-89-8	901	955	97.5	18.8	0.6275	0.012549	0.006274	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	1.0
74		unknown	---	---	---	---	---	---	---	---	1.0
75		unknown	---	---	---	---	---	---	---	---	1.0
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N,N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75

79	43.529	unknown	---	---	---	---	17.6	0.5879	0.011758	0.005879	1.0
80	45.003	unknown	---	---	---	---	6.2	0.2060	0.004120	0.002060	1.0
81	45.447	unknown	---	---	---	---	---	---	---	---	1.0
82	45.426	unknown	---	---	---	---	---	---	---	---	1.0
83	46.145	unknown	---	---	---	---	---	---	---	---	1.0
84	46.399	unknown	---	---	---	---	---	---	---	---	1.0
85	47.963	unknown	---	---	---	---	---	---	---	---	1.0
86	48.509	2,2'-tiobis-benzotiazol	402147	707	888	72.6	2.0	0.0670	0.001339	0.000669	1.0
87	56.214	Cl-5808	332370	---	---	---	---	---	---	---	1.0

Table S24. Identification of organic contaminants (unexpected substances) from rubber material by LLE-GC-MS, from analysis of 6^h, 29-day migration, and their quantification by semi-quantitative method (S/V = 10). Analysis of duplicate

N	t _R (min)	Unexpected substances	CAS#	Match	Reverse match	Prob (%)	c _n ^T	M _n ^T	C _{Tap} ¹	C _{Tap} ²	MTC _{tap}
							(μg/l)				
1		2,2-dimethoxy-propane	77-76-9	---	---	---	---	---	---	---	1.0
2		benzene	71-43-2	---	---	---	---	---	---	---	1.0
3		1,1-diethoxy-ethane	105-57-7	---	---	---	---	---	---	---	1.0
4		4-hydroxy-4-methyl-2-pentanone	123-42-2	---	---	---	---	---	---	---	1.0
5		cyclohexylamine	108-91-8	---	---	---	---	---	---	---	2.1
6		cyclohexanone	108-94-01	---	---	---	---	---	---	---	1.0
7		benzaldehyde	100-52-7	---	---	---	---	---	---	---	1.0
8		benzonitrile	100-47-0	---	---	---	---	---	---	---	0.1
9	23.991	isocyanate-cyclohexane	3173-53-3	966	967	93.2	72.7	2.4223	0.048446	0.024223	1.0
10		benzylamine	100-46-09	---	---	---	---	---	---	---	1.0
11		2-ethyl-1-hexanol	104-76-7	---	---	---	---	---	---	---	1500
12		benzyl alcohol	100-51-6	---	---	---	---	---	---	---	1.0
13		unknown	---	---	---	---	---	---	---	---	1.0
14		methyl benzoate	95-58-3	---	---	---	---	---	---	---	1.0
15		2,2,6,6-tetramethyl-4-piperidone	826-36-8	---	---	---	---	---	---	---	1.0
16		benzoic acid	65-85-0	---	---	---	---	---	---	---	1.0
17		2-phenoxy-ethanol	122-99-6	---	---	---	---	---	---	---	1.0
18	30.028	benzothiazole	95-16-9	931	933	69	88.0	2.9323	0.058645	0.029322	0.1
19	30.146	isothiocyanate-cyclohexane	1122-82-03	924	928	98.4	37.6	1.2532	0.025064	0.012532	1.0
20		benzylazetidine	7730-39-4	---	---	---	---	---	---	---	1.0
21		N-benzyl-3-pyrrolidinone	775-16-6	---	---	---	---	---	---	---	1.0
22	30.482	N-cyclohexyl-formamide	766-93-8	924	932	96.4	10.6	0.3529	0.007057	0.003528	1.0

23		N-cyclohexyl-acetamide	1124-53-4	---	---	---	---	---	---	---	1.0
24		benzamide	55-21-0	---	---	---	---	---	---	---	1.0
25		t-butyl-p-cresol	2409-55-4	---	---	---	---	---	---	---	1.0
26		unknown	---	---	---	---	---	---	---	---	1.0
27		benzyl isothiocyanate	622-78-6	---	---	---	---	---	---	---	1.0
28		tert-butyl-2,4-xilenol	1879-09-0	---	---	---	---	---	---	---	1.0
29		N-benzylformamide	6343-54-0	---	---	---	---	---	---	---	1.0
30		unknown	---	---	---	---	---	---	---	---	1.0
31		unknown	---	---	---	---	---	---	---	---	1.0
32		N-benzylacetamide	588-46-5	---	---	---	---	---	---	---	1.0
33		2,2,4-trimetil-1,2-dihidroquinolina (Flectol A)	147-47-7	---	---	---	---	---	---	---	1.0
34		1-dodecanol	112-53-8	---	---	---	---	---	---	---	1.0
35		unknown	---	---	---	---	---	---	---	---	1.0
36		unknown	---	---	---	---	---	---	---	---	1.0
37		dodecanoic acid	143-07-7	---	---	---	---	---	---	---	1.0
38		N-phenylcyclohexylamine	1821-36-9	---	---	---	---	---	---	---	1.0
39		unknown	---	---	---	---	---	---	---	---	1.0
40		N-(phenylmethylene)-cyclohexamine	2211-66-7	---	---	---	---	---	---	---	1.0
41		N-methyl-2-benzothiazolinone	2786-62-1								
42	35.649	2-(methylthio)-benzothiazole	615-22-5	952	955	88.5	15.3	0.5106	0.010212	0.005106	1.0
43		tributylphosphate	126-73-8	---	---	---	---	---	---	---	1.0
44		dipropylbenzamide	10546-70-0	---	---	---	---	---	---	---	
45	36.083	unknown	---	---	---	---	---	---	---	---	1.0
46	36.338	2-benzothiazolone	934-34-9	918	925	96.2	9.7	0.3224	0.006448	0.003224	0.1
47		Dibenzylmethylaniline	102-05-6	---	---	---	---	---	---	---	1.0
48		Lauryl ethoxylate	4536-30-5	---	---	---	---	---	---	---	1.0
49	36.929	Dibenzylaniline	103-49-1	927	929	93	59.0	1.9653	0.039306	0.019653	1.0
50		Dibenzylhydroxylaniline	621-07-8	---	---	---	---	---	---	---	1.0

51		Benzaldehyde N-benzylimine	780-25-6	---	---	---	---	---	---	---	1.0
52		N-butylbenzenesulphonamide	3622-84-2	---	---	---	---	---	---	---	
53		Benthiazole	21564-17-0	---	---	---	---	---	---	---	1.0
54		unknown	---	---	---	---	---	---	---	---	1.0
55	38.556	N-cyclohexylbenzamide	1759-68-8	921	922	92.7	21.5	0.7152	0.014303	0.007151	1.0
56		N-methylbenzothiazoline-2-thione	2254-94-6	---	---	---	---	---	---	---	1.0
57		Methyl-o-benzoylbenzoate	606-28-0	---	---	---	---	---	---	---	1.0
58	39.692	2-mercaptobenzothiazole	149-30-4	932	939	96.9	129.3	4.3116	0.086231	0.043115	10
59	39.952	N-benzylformamide	6343-54-0	761	808	55.4	78.2	2.6058	0.052116	0.026058	1.0
60	40.117	N-benzylbenzamide	1485-70-7	927	938	74.9	22.2	0.7386	0.014772	0.007386	1.0
61	40.252	Benzenesulfanilide	1678-25-7	922	937	97.5	19.2	0.6402	0.012803	0.006401	1.0
62	40.354	1.3-dicyclohexylurea	2387-23-7	864	929	97.4	10.9	0.3621	0.007242	0.003621	1.0
63	40.652	unknown	---	---	---	---	19.6	0.6545	0.013089	0.006544	1.0
64		2.3-diphenylmaleic anhydride	4808-48-4	---	---	---	---	---	---	---	1.0
65	41.028	unknown	---	---	---	---	29.4	0.9811	0.019621	0.009810	1.0
66	41.237	unknown	---	---	---	---	76.3	2.5438	0.050876	0.025438	1.0
67	41.346	N.N'-dicyclohexyloxamide	3299-64-7	885	903	97.8	5.4	0.1814	0.003628	0.001814	1.0
68	41.627	2-cyclohexylamino-benzothiazole	28291-75-0	792	920	81	4.2	0.1413	0.002825	0.001412	1.0
69	41.721	N-benzyl-N'-cyclohexyl-isourea	25855-24-7	815	900	95	5.8	0.1932	0.003863	0.001931	1.0
70	42.095	N-benzyl-benzenecarbothiamide	14309-89-8	904	955	97.7	18.8	0.6272	0.012544	0.006272	1.0
71		unknown	---	---	---	---	---	---	---	---	1.0
72		Ethyl 9-fluorenyldeneacetate	27973-36-0	---	---	---	---	---	---	---	1.0
73		unknown	---	---	---	---	---	---	---	---	
74	42.529	unknown	---	---	---	---	17.2	0.5735	0.011469	0.005734	1.0
75		unknown	---	---	---	---	---	---	---	---	
76		unknown	---	---	---	---	---	---	---	---	1.0
77		N.N'-dibenzilureia	1466-67-7	---	---	---	---	---	---	---	1.0
78		Antioxidant BKF	119-47-1	---	---	---	---	---	---	---	75
79		unknown	---	---	---	---	---	---	---	---	1.0
80	45.003	unknown	---	---	---	---	6.3	0.2095	0.004190	0.002095	1.0

81		7-benzyloxyindole		---	---	---	---	---	---	---	1.0
82		unknown	---	---	---	---	---	---	---	---	1.0
83		unknown	---	---	---	---	---	---	---	---	1.0
84		unknown	---	---	---	---	---	---	---	---	1.0
85		unknown		---	---	---	---	---	---	---	1.0
86		2.2'-tiobis-benzotiazol	402147	---	---	---	---	---	---	---	1.0
87		Cl-5808	332370	---	---	---	---	---	---	---	1.0