

GC/MS Screening of Substances Released from Post-Consumer Recycled HDPE Pellets into 95% Ethanol: Reproducibility and Variation between Production Batches

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Supplementary information. Example detailed results of the GC/MS analysis

Table S1: Results of the repeated measurement of reference sample REF-A1.

RT	RI	Compound	CAS	Group	Concentration / mg / kg of pellets														
					REF-A1- 2-1	REF-A1- 2-2	REF-A1- 3-3	REF-A1- 3-1	REF-A1- 3-2	REF-A1- 3-3	REF-A1- 4-1	REF-A1- 4-2	REF-A1- 4-3	REF-A1- 6-1	REF-A1- 6-2	REF-A1- 6-3	REF-A1- 8-1	REF-A1- 8-2	REF-A1- 8-3
6.687	783	unidentified															0.131	0.165	0.177
10.069	888	unidentified				0.134					0.130								
10.063	889	unidentified						0.145				0.134	0.148	0.149	0.139	0.134	0.151	0.155	0.172
10.681	908	unidentified															0.189	0.296	0.244
11.646	936	a-Pinene	80-56-8	IAS/NIAS	0.139	0.119	0.119	0.135	0.122	0.134	0.136	0.116	0.141	0.139	0.114	0.145	0.130	0.137	0.152
13.163	981	β-Pinene	127-91-3	IAS/NIAS		0.125	0.088												
13.134	981	unidentified										0.153							
14.640	1028	p-Cymene	99-87-6	IAS/NIAS	0.102	0.087	0.092	0.083	0.102	0.095					0.096				
14.804	1034	Limonene	5989-27-5	IAS/NIAS	0.308	0.306	0.301	0.308	0.304	0.320	0.280	0.297	0.305	0.303	0.328	0.325	0.333	0.338	0.337
14.928	1038	Eucalyptol	470-82-6	IAS/NIAS	0.175	0.139	0.145	0.175	0.135	0.188	0.156	0.155	0.153	0.149	0.163	0.177	0.215	0.185	0.204
18.134	1153	Benzoic acid	65-85-0	IAS/NIAS				0.175	0.141										
19.316	1200	Dodecane	112-40-3	ALK												0.139			
21.469	1294	Isobornyl Acetate	125-12-2	IAS/NIAS	0.881	0.698	0.865	0.836	0.675	0.879	0.906	0.652	0.836	0.909	0.774	0.948	1.015	0.845	0.991
21.527	1297	unidentified					0.079												
21.592	1300	Tridecane	629-50-5	ALK	0.088	0.063		0.058	0.071	0.071		0.066		0.094	0.107	0.144	0.151	0.080	0.097
		4-tert-Butylcyclohexyl acetate	1900-69-2	IAS/NIAS															
22.304	1339	trans						0.081											
22.563	1352	unidentified			0.206	0.145	0.130	0.173											
22.974	1374	4-tert-Butylcyclohexyl acetate cis	10411-92-4	IAS/NIAS	0.196	0.163	0.170	0.149	0.137	0.157	0.153		0.159	0.162	0.141	0.174	0.185	0.186	0.173
22.951	1374	unidentified										0.131							
23.286	1392	unidentified												0.112					
23.457	1400	Tetradecane	629-59-4	ALK	0.331	0.276	0.299	0.312	0.318	0.343	0.347	0.303	0.346	0.393	0.353	0.429	0.421	0.368	0.421
23.663	1413	Diphenyl Ether	101-84-8	IAS/NIAS	0.836	0.788	0.830	0.806	0.782	0.785	0.766	0.813	0.756	0.816	0.791	0.866	0.806	0.832	0.812
23.963	1432	Indan-1,3-diol monoacetate		IAS/NIAS	0.254	0.245	0.242	0.231	0.208	0.215	0.181	0.186	0.205	0.185		0.224			
23.927	1432	unidentified													0.209		0.205	0.209	0.227
24.339	1456	unidentified					0.137												
24.533	1468	2-Methoxy naphthalene	93-04-9	IAS/NIAS	0.337	0.354	0.360	0.343	0.331	0.324	0.305	0.323	0.309	0.312	0.322	0.359	0.314	0.388	0.344
25.027	1500	Pentadecane	629-62-9	ALK	0.180	0.169		0.168	0.171	0.159	0.199	0.167	0.182	0.206	0.183	0.209	0.216	0.192	0.214
25.157	1509	2,4-Di-tert-Butylphenol	96-76-4	IAS/NIAS	0.353	0.392		0.281	0.302	0.310	0.125	0.306		0.250			0.272	0.347	0.401
25.162	1509	BHT	128-37-0	IAS/NIAS			0.327				0.147		0.273						
25.127	1509	unidentified													0.300	0.266			
25.457	1531	Herbal propionate	17511-60-3	IAS/NIAS	0.375	0.320	0.360	0.317	0.299	0.308	0.293	0.271	0.265			0.334		0.298	
25.427	1531	unidentified												0.326	0.293		0.329		0.296
25.539	1536	Lilial	80-54-6	IAS/NIAS	0.129	0.129	0.149	0.115	0.111	0.108	0.125	0.086	0.117	0.090	0.112	0.137	0.152	0.112	0.091
25.563	1538	5-Phenyldecane	4537-11-5	IAS/NIAS	0.178	0.132	0.186	0.174	0.164	0.167	0.150	0.150	0.157	0.204	0.144	0.184	0.148	0.155	0.195
25.621	1542	Naphthalene, 2-ethoxy-	93-18-5	IAS/NIAS	1.148	1.177	1.203	1.114	1.059	1.118	1.048	1.042	1.082	1.062	1.082	1.213	1.173	1.118	1.148
25.704	1548	4-Phenyldecane	4537-12-6	IAS/NIAS	0.256	0.222	0.277	0.252		0.242	0.271	0.243	0.227	0.285	0.211	0.255	0.259	0.238	0.264

25.727	1552	unidentified											0.142	0.136	0.158	0.144	0.160	0.216
25.774	1553	Dodecanoic acid	143-07-7	FAE		0.186					0.257	0.248	0.225					
25.774	1553	unidentified			0.148		0.178											
25.763	1554	unidentified						0.171		0.170								
25.992	1569	3-Phenyldecane	4621-36-7	IAS/NIAS	0.315	0.423	0.392	0.295	0.326	0.341	0.473	0.321	0.345	0.524	0.462	0.357	0.375	0.365
26.027	1572	unidentified			0.137										0.136			0.523
26.210	1585	Amyl salicylate	2050-08-0	IAS/NIAS	0.787	0.583	0.773	0.790	0.584	0.593	0.505	0.561	0.568	0.601	0.582	0.605	0.669	0.704
26.315	1592	Hexadecene	629-73-2	ALK	3.319	2.894	3.106	2.793	2.651	2.813	2.819	2.637	2.798	2.869	2.933	3.301	3.136	3.046
26.415	1600	Hexadecane	544-76-3	ALK	7.214	6.752	7.148	7.434	6.924	7.450	7.961	7.370	7.706	8.519	7.979	8.875	9.059	8.748
26.504	1607	2-Phenyldecane	4537-13-7	IAS/NIAS	1.238	1.220	1.282	1.287	1.264	1.285	1.360	1.313	1.344	1.325	1.302	1.337	1.425	1.487
26.592	1616	unidentified															0.331	0.358
26.633	1617	unidentified			0.252	0.253	0.272	0.266	0.251	0.257	0.273	0.267	0.291	0.300	0.301	0.339	0.326	
26.751	1626	unidentified			0.222		0.214											
26.780	1629	p-Octylacetophenone	10541-56-7	IAS/NIAS	0.194	0.227	0.263	0.532	0.530	0.619	0.727	0.795	0.846	0.593	0.764	1.179	0.641	0.756
26.839	1633	6-Phenylundecane	4537-14-8	IAS/NIAS	0.446	0.410	0.448	0.426	0.396	0.480	0.569	0.444	0.444	0.504	0.444	0.640	0.469	0.463
26.886	1637	5-Phenylundecane	4537-15-9	IAS/NIAS	1.513	1.447	1.552	1.550	1.507	1.575	1.491	1.528	1.525	1.541	1.527	1.634	1.594	1.585
27.027	1648	4-Phenylundecane	4536-86-1	IAS/NIAS	1.927	1.783	1.892	1.798	1.813	1.953	1.825	1.824	1.809	1.840	1.842	1.897	1.922	1.879
		Methyl (3-oxo-2-pentylcyclopentyl)acetate isomer 2	24851-98-7	IAS/NIAS														
27.098	1654				0.529	0.371	0.510	0.480	0.419	0.627	0.489	0.484	0.632	0.557	0.511	0.677	0.487	0.501
27.139	1657	a-Pentylcinnamaldehyde isomer	122-40-7	IAS/NIAS	1.273	1.290	1.352	1.041	1.022	1.050	0.947	1.007	1.022	0.932	0.976	1.049	0.998	1.042
27.209	1663	Di-n-Octylether	629-82-3	IAS/NIAS	0.793	0.669	0.655	0.657	0.788	0.819	0.833	0.826	0.873	0.876	0.900	0.805	0.963	1.152
27.321	1672	Benzene, (1-ethynonyl)-	4536-87-2	IAS/NIAS	2.213	2.162	2.279	2.314	2.261	2.396	2.260	2.392	2.339	2.507	2.403	2.409	2.612	2.559
27.392	1677	1-Tetradecanol	112-72-1	IAS/NIAS	0.783		0.722	0.551		0.572								2.512
27.398	1678	unidentified			0.650				0.501		0.478	0.560	0.562	0.498	0.571	0.256	0.308	0.294
27.457	1683	Amberonne	68155-66-8	IAS/NIAS	2.951	2.766	3.010	2.686	2.611	2.802	2.507	2.525	2.657	2.599	2.680	2.929	2.857	2.967
27.545	1690	n-Hexyl salicylate	6259-76-3	IAS/NIAS	8.006	8.002	8.352	8.260	8.236	8.615	7.464	8.698	8.595	7.901	8.599	8.669	9.618	9.615
27.668	1700	Heptadecane	629-78-7	ALK	1.102	1.055	1.239	1.089	1.074	0.913	1.138	1.127	1.194	1.391	1.402	1.333	1.705	1.374
27.692	1703	unidentified									0.431	0.344						1.133
27.698	1704	unidentified						0.149					0.443	0.374	0.403	0.169	0.169	0.186
27.792	1710	2-Phenylundecane	4536-88-3	IAS/NIAS	3.335	3.354	3.564	3.532	3.463	3.477	3.710	3.733	3.806	3.851	3.769	3.688	3.690	3.665
27.874	1717	Amberonne Isomer	68155-66-8	IAS/NIAS	1.680	1.684												3.762
27.874	1717	unidentified					1.706	1.619										
		Ethylene glycol monododecyl ether	4536-30-5	IAS/NIAS					1.601	1.707	1.487	1.781	1.873	1.800	2.162	1.962	1.957	1.843
27.862	1718								0.609	0.667	0.554	0.585	0.610	0.603	0.634	0.647	0.676	0.697
27.927	1722	Methyl myristate	124-10-7	FAE	0.644	0.688	0.670	0.648	0.609	0.667	0.554	0.585	0.610	0.603	0.634	0.647	0.676	0.697
28.039	1732	6-Phenylundecane	2719-62-2	IAS/NIAS	1.817	1.789	1.873	1.879	1.853	1.895	1.806	1.858	1.891	2.024	1.958	2.015	2.017	1.968
28.092	1736	5-Phenylundecane	2719-63-3	IAS/NIAS	2.096	1.917	2.099	2.078	2.202	2.072	2.089	2.197	2.109	2.153	2.211	2.335	2.253	2.229
28.180	1744	unidentified			0.243	0.294	0.283	0.281	0.269	0.289	0.269	0.301	0.288	0.291	0.287	0.296	0.315	0.350
28.256	1751	4-Phenylundecane	2719-64-4	IAS/NIAS	2.105	2.097	2.161	2.184	2.148	2.220	2.160	2.262	2.280	2.441	2.329	2.414	2.393	2.370
28.351	1759	a-Hexylcinnamaldehyde trans	101-86-0	IAS/NIAS	11.922	12.019	12.200	11.001	11.179	11.254	9.882	10.979	10.746	10.555	10.976	11.368	11.068	11.409
28.427	1765	unidentified			0.502	0.555	0.571	0.487	0.502	0.540	0.452	0.477	0.542	0.487	0.519	0.550	0.568	0.575
28.533	1775	3-Phenylundecane	2400-00-2	IAS/NIAS	3.206	3.121	2.910	3.195	3.427	3.149	3.241	3.458	3.466	3.329	3.626	3.219	3.269	3.320
28.651	1785	a-Hexylcinnamaldehyde cis	101-86-0	IAS/NIAS	1.188	1.110	1.238	1.375	1.271	1.328	1.116	1.529	1.345	1.365	1.557	1.076	1.294	1.390
28.668	1786	Benzyl benzoate	120-51-4	IAS/NIAS	1.389	1.441	1.791	1.169	0.990	1.344	1.178	1.211	1.863	1.256	1.240	1.237	1.150	1.250
28.745	1793	1-Octadecene	112-88-9	ALK	6.385	6.351	6.490	6.140	6.055	6.322	6.027	6.448	6.605	6.691	6.865	7.143	6.987	7.126
28.821	1800	Octadecane	593-45-3	ALK	9.488	9.225	9.603	9.941	9.793	10.221	10.001	10.606	10.776	11.311	10.972	11.255	11.919	11.797
28.986	1815	2-Phenylundecane	2719-61-1	IAS/NIAS	4.289	4.515	4.552	4.723	4.650	4.853	4.582	4.787	4.974	4.964	4.982	5.087	5.112	5.210
29.051	1821	Isopropyl myristate	110-27-0	FAE	13.033	12.839	13.464	13.114	13.204	13.533	12.965	14.227	13.764	13.860	13.955	14.480	14.397	15.109
29.098	1827	unidentified								0.495		0.350	0.513	0.444	0.453		0.690	0.180
29.157	1830	6-Phenyltridecane	4534-49-0	IAS/NIAS	1.985	2.056	2.633	2.150	2.134	2.165	2.002	2.289	2.171	2.220	2.200	2.231	2.343	2.229
29.233	1838	5-Phenyltridecane	4534-50-3	IAS/NIAS	1.216	1.291	1.277	1.320	1.299	1.339	1.325	1.391	1.390	1.389	1.291	1.380	1.453	1.395
29.386	1852	4-Phenyltridecane	4534-51-4	IAS/NIAS	1.799	1.820	1.829	1.881	1.866	1.856	1.821	1.938	2.005	1.968	1.965	2.073	2.055	2.023
29.492	1861	unidentified			0.737	0.692	0.697	0.735	0.718	0.734	0.718	0.797	0.762			0.790	0.802	0.847
29.462	1862	unidentified												0.755	0.752	0.854		
29.539	1866	Galaxolide	1222-05-5	IAS/NIAS	6.948	7.382	7.374	7.371	7.160	7.346	6.544	7.215	7.294	7.104	7.241	7.601	7.601	6.854
29.598	1871	Tonalid	21145-77-7	IAS/NIAS	0.621	0.666	0.691	0.586	0.606	0.610	0.503	0.588	0.578	0.586	0.609	0.640	0.630	0.638
29.668	1878	3-Phenyltridecane	4534-52-5	IAS/NIAS	1.456	1.445	1.448	1.525	1.494	1.543	1.507	1.656	1.622	1.625	1.576	1.783	1.677	1.648
29.709	1882	1-Hexadecanol	36653-82-4	IAS/NIAS	1.307	1.397	1.443	1.314	0.952	1.310	1.113	1.256	1.343	1.224	1.325	1.417	1.500	1.495
29.851	1895	Benzyl salicylate	118-58-1	IAS/NIAS	2.051	2.235	2.240	2.605	2.455	2.733	2.219	2.717	2.733	2.088	2.265	2.453	2.598	2.847
29.904	1899	Nonadecane	629-92-5	ALK	1.023	1.048	1.083	0.783	0.837	0.888	0.852	0.976	0.664	1.119	1.008	1.068	1.317	1.321

29.992	1908	Homosalate	118-56-9	IAS/NIAS	0.603	0.644	0.635	0.562	0.659	0.617	0.596	0.704	0.719	0.617		0.634	0.689	0.739	0.843
29.956	1908	unidentified													0.684				
30.098	1919	2-Phenyltridecane	4534-53-6	IAS/NIAS	3.099	3.557	3.314	3.430	3.535	3.570	3.223	3.700	3.601	3.328	3.500	3.517	3.512	3.830	3.760
30.145	1923	Methyl Palmitate	112-39-0	FAE	6.891	6.864	7.006	6.968	6.705	7.335	6.400	7.185	7.325	7.267	7.220	7.464	8.082	7.789	8.349
30.239	1932	unidentified			0.342														
30.245	1933	unidentified				0.320	0.332	0.344	0.350	0.376	0.337	0.375	0.331			0.321	0.354	0.340	0.345
30.215	1934	unidentified												0.324	0.341				
30.280	1940	unidentified												0.346		0.345			
30.339	1942	unidentified				0.133													
30.345	1943	unidentified			0.137			0.130									0.137	0.151	
30.415	1950	unidentified			0.290	0.290	0.317	0.316	0.324	0.346		0.354					0.370	0.350	0.467
30.403	1951	unidentified									0.314		0.349	0.485	0.416	0.410			
30.474	1956	n-Hexadecanoic acid	57-10-3	IAS/NIAS	1.374	1.614	1.773	1.480	1.393	1.772	1.159	1.428	1.705	0.502	0.780	1.136	0.345	0.817	1.357
30.539	1962	Dibutyl phthalate	84-74-2	IAS/NIAS	1.257	1.358	1.397	1.318	1.540	1.594	1.282	1.349	1.675	1.185	1.502	1.243	1.306	1.635	1.884
30.556	1967	unidentified														0.192			
30.639	1972	unidentified			0.409	0.291	0.422	0.230	0.517	0.483	0.356	0.186	0.251	0.232	0.253	0.337	0.241	0.242	0.275
30.698	1977	unidentified			1.061	0.942		0.444	0.618	0.982								0.256	0.269
30.703	1978	unidentified					1.101				0.227	0.325	0.364	0.182	0.193	0.443	0.178		
30.856	1993	1-Eicosene	3452-07-1	ALK	7.850	8.048	8.585	8.508	7.489	8.488	7.315	7.851	8.698	9.008	8.379	9.202	9.116	8.682	10.156
30.915	1999	Eicosane	112-95-8	ALK	7.907	7.861	8.405	8.481	7.501	8.740	8.109	8.285	9.181	9.613	8.754	9.393	10.283	9.848	10.472
31.109	2019	Isopropyl palmitate	142-91-6	FAE	10.748	9.343	8.759	9.013	8.790	9.718	8.630	9.129	9.753	9.493	9.291	9.657	9.632	9.661	10.854
31.186	2027	unidentified					0.260	0.299		0.280			0.279	0.366			0.356	0.263	
31.339	2043	Ethylene brassylate	105-95-3	FAE	0.617	0.700	0.656	0.633	0.670	0.545	0.618	0.661	0.591	0.651	0.574	0.709	0.702	0.616	0.769
31.474	2057	unidentified			0.249	0.788	0.283	0.358	0.308							0.299			
31.451	2058	Eicosane, 2-methyl-	1560-84-5	ALK										0.603					
31.462	2058	unidentified									0.280	0.337	0.302		0.556		0.696	0.698	0.833
31.497	2059	unidentified			0.252				0.440										
31.503	2060	unidentified					0.273									0.258			
31.668	2077	unidentified			0.142	0.154	0.193	0.172			0.130	0.165	0.198	0.138			0.183	0.151	0.188
31.645	2078	unidentified													0.148				
31.756	2086	1-Octadecanol	112-92-5	FAE	1.888	2.053	1.943	1.937	1.691	1.951	1.487	1.912	1.891	1.667	1.953	2.010	2.175	2.260	2.634
31.845	2095	Methyl linoleate	112-63-0	FAE	0.759	0.817	0.778	0.814	0.660	0.759	0.725	0.826	0.809	0.825	0.825	0.959	0.963	0.952	1.080
31.898	2101	Methyl Oleate	112-62-9	FAE	5.650	5.854	5.814	5.689	5.292	6.057	5.198	5.924	6.318	6.064	6.097	6.275	6.709	6.706	7.365
31.945	2106	unidentified			1.132	0.907	0.930	0.860	0.816	0.906	0.942	0.956	1.177	1.164	1.189	1.251	1.397	1.417	1.224
32.115	2124	Methyl stearate	112-61-8	FAE	2.459	2.450	2.522	2.956	2.491	2.761	2.249	2.586	2.784	2.929	2.650	3.112	3.025	2.933	3.348
32.227	2137	Oleic Acid	112-80-1	FAE	1.914	1.436	1.181	0.748	0.798	1.099									
32.209	2137	unidentified									0.267	0.375	0.390	0.156	0.171	0.243	0.324	0.428	0.440
32.251	2141	unidentified						0.311				0.231	0.276				0.350		
32.256	2142	unidentified							0.226		0.175			0.239	0.271	0.288		0.597	0.485
32.344	2149	unidentified			0.481	0.241		0.287	0.259	0.299	0.242	0.253		0.320	0.316	0.348			
32.350	2150	unidentified					0.283						0.301				0.314	0.317	0.377
32.421	2158	Stearic acid	57-11-4	FAE	0.605	0.776	0.837	0.634	0.647	0.767	0.650	0.804	0.853		0.319	0.488		0.357	0.423
32.392	2158	unidentified												0.189			0.239		
32.462	2162	Ethyl Linoleate	544-35-4	FAE	0.766	0.794	0.819	0.794	0.742	0.828						0.878	0.674		
32.444	2162	unidentified											0.797	0.712	0.664				
32.433	2163	unidentified																0.905	0.944
32.474	2167	Ethyl Oleate	111-62-6	FAE														3.065	3.654
32.503	2167	Ethyl elaidate	6114-18-7	FAE	2.651	2.819	3.021	2.839	2.659	2.873	2.247	2.535	2.915	2.707	2.798	2.917	2.855		
32.556	2172	unidentified			1.199	1.225	1.302	1.217	1.261	1.267	1.132	1.316	1.327	1.252	1.249	1.298		1.477	1.530
32.527	2173	unidentified						0.241		0.243		0.436					1.379		
32.639	2183	unidentified																	
32.662	2184	unidentified			0.182	0.180	0.251		0.274		0.167		0.255	0.325	0.291	0.345	0.253	0.267	
32.633	2185	unidentified																	0.413
32.750	2194	1-Docosene	1599-67-3	ALK	5.246	5.131	5.963	5.993	4.768	5.715	4.725	5.114	6.200	6.408	5.359	6.267	6.040	5.641	7.584
32.797	2199	Docosane	629-97-0	ALK	4.132	3.498	4.504	4.752	3.780	4.744	3.844	3.758	4.848	5.128	4.176	4.814	5.330	4.714	5.927
32.862	2206	unidentified				0.159		0.146	0.155						0.150				
32.933	2214	Benzoic acid, dodecyl ester	2915-72-2	IAS/NIAS	0.529	0.589	0.528	0.561	0.535	0.562	0.464	0.555	0.608	0.669	0.564	0.582	0.573	0.593	0.629
32.980	2219	unidentified			0.235		0.264		0.192	0.313		0.219	0.220	0.199		0.263	0.255	0.258	0.291
32.986	2220	unidentified				0.216		0.167											
33.015	2227	unidentified																0.335	
33.050	2228	unidentified			0.303	0.287	0.308	0.329	0.252	0.339	0.265	0.311	0.338	0.380	0.314	0.361	0.339		0.398

33.168	2241	unidentified			0.212	0.213													
33.168	2245	unidentified																	0.171
33.291	2257	unidentified									0.220								
33.315	2258	unidentified			0.247	0.243	0.240	0.242	0.215	0.276	0.156	0.264		0.263	0.284	0.252	0.237	0.200	0.353
33.421	2270	unidentified			0.366	0.319		0.393	0.359	0.460	0.345	0.412	0.413	0.399	0.445		0.365		
33.397	2271	unidentified																0.424	
33.444	2272	unidentified					0.166									0.411			0.537
33.668	2298	unidentified			0.338			0.594	0.418		0.422	0.566	0.646		0.703	0.675	0.802		0.998
33.674	2299	unidentified				0.476	0.367			0.520				0.654				0.640	
33.762	2311	unidentified							0.366						0.487				
33.786	2312	unidentified			0.323	0.426	0.399	0.400		0.444	0.370	0.446	0.471	0.421		0.437	0.438	0.343	0.584
33.850	2319	Benzoic acid, tridecyl ester	29376-83-8	IAS/NIAS	0.727	0.888	0.781	0.792	0.799	0.902	0.688	0.881	0.854	0.851	0.939	0.909	0.937	0.979	1.093
33.974	2334	unidentified			1.186	1.310	1.282	1.418	1.187	1.470	1.086	1.257	1.354	1.423	1.391	1.335	1.397	1.365	1.671
34.097	2348	unidentified			0.315			0.461	0.321	0.461									
34.103	2349	unidentified				0.311	0.311				0.205	0.252	0.354	0.331	0.440	0.440	0.252	0.378	0.316
34.174	2359	unidentified									0.218								
34.197	2360	unidentified			0.303			0.389						0.216					
34.203	2361	unidentified				0.264	0.306		0.326	0.395	0.227		0.297		0.248	0.279	0.322	0.366	0.392
34.297	2372	unidentified			1.017	0.833	1.081	1.286	1.076	1.115	0.758	0.952	1.199	1.054	1.067	1.135	1.259	1.407	1.628
34.380	2383	unidentified								0.335	0.144	0.181	0.157			0.294			
34.403	2384	unidentified				0.181			0.351						0.327		0.190		
34.409	2385	unidentified					0.276											0.429	0.436
34.492	2395	1-Tetracosene	10192-32-2	ALK	2.171	2.267	2.890	2.392	1.900	2.270	1.546	1.825	2.300	2.687	2.331	2.466	2.461	2.218	3.196
34.527	2399	Tetracosane	646-31-1	ALK	1.804	1.447	1.924	2.143	1.564	1.920	1.353	1.597	1.915	2.419	1.805	1.843	2.228	1.958	2.317
34.568	2405	unidentified							0.194										
34.562	2406	unidentified															0.291		
34.709	2418	unidentified			0.169			0.213	0.214	0.233	0.148	0.184	0.169	0.188	0.247	0.196	0.232	0.257	
34.715	2419	unidentified				0.178	0.207												0.267
34.756	2423	Benzoic acid, tetradecyl ester	70682-72-3	IAS/NIAS	0.587	0.586	0.654												0.687
34.739	2423	unidentified						0.633	0.557	0.558									
34.744	2424	unidentified									0.458	0.509	0.608	0.579	0.581	0.633	0.714	0.640	
34.833	2431	unidentified			0.380			0.345	0.274	0.324	0.233	0.271	0.343	0.428	0.304	0.311	0.289		
34.838	2432	unidentified				0.307	0.307											0.170	0.351
35.015	2450	unidentified			0.769								0.931						
34.997	2451	unidentified						0.810	0.707	0.793	0.644	0.706		0.969	0.775	0.860	0.941	0.939	1.078
35.027	2452	unidentified				0.743	0.825												
35.191	2469	unidentified			0.751			0.833	0.852	0.898	0.553	0.707	0.762	0.704	0.720	0.787	0.764	0.898	0.989
35.197	2470	unidentified				0.835	0.923												
35.274	2478	unidentified			0.427			0.576	0.623	0.418	0.606	0.709	0.661	0.765	0.858	0.850		0.966	
35.285	2479	unidentified				0.409	0.438										1.256		1.224
35.468	2498	unidentified			1.229														
35.480	2499	unidentified				1.309	1.597	1.599	1.337	1.338	1.272	1.283	1.370	1.273	1.503	1.499	1.505	1.510	1.744
35.785	2527	unidentified			0.264														
35.768	2528	unidentified						0.259			0.217			0.334					0.650
35.780	2529	unidentified								0.640		0.526	0.590		0.640			0.698	
35.815	2530	unidentified				0.613	0.554		0.526							0.650	0.645		
35.886	2536	Dicyclohexyl phthalate	84-61-7	IAS/NIAS	0.364		0.774	0.550				0.456	0.513			0.611			0.561
35.897	2537	Diheptyl phthalate	117-81-7	IAS/NIAS		0.735				0.514									
35.868	2537	unidentified							0.403		0.340			0.246	0.438		0.263	0.587	
36.033	2553	unidentified													0.148	0.136			0.138
36.215	2566	Dodecyl Laurate	13945-76-1	FAE	5.416	5.675	6.146	5.839	4.910	5.648	4.411	5.165	5.940	5.986	5.615	6.022	6.419	6.327	7.626
36.397	2583	Bumetizole	3896-11-5	IAS/NIAS	14.873	15.408	16.473	17.211	14.995	17.180	13.642	15.484	17.121	17.134	16.033	16.852	17.467	16.842	19.398
36.521	2594	unidentified			0.450														
36.532	2595	unidentified				0.414	0.556	0.518	0.268	0.420	0.288	0.297	0.482	0.562	0.390	0.482	0.536	0.440	0.767
36.568	2598	unidentified			0.465														
36.526	2599	Hexacosane	630-01-3	ALK															0.805
36.580	2599	unidentified				0.481	0.657	0.596	0.470	0.541	0.565	0.481	0.643	0.749	0.512	0.580	0.631	0.609	
36.662	2608	unidentified						0.179											0.199
36.668	2609	unidentified												0.168		0.128	0.218		
37.021	2633	unidentified			0.130				0.137										
36.991	2634	unidentified												0.203					

37.009	2635	unidentified				0.132									0.168		
37.215	2648	unidentified	0.334				0.238	0.347	0.248	0.266	0.339			0.306	0.406	0.426	0.419
37.227	2649	unidentified		0.307	0.454	0.403						0.387	0.297				
37.444	2665	unidentified	0.852														
37.421	2666	unidentified				0.832	0.761	0.813	0.633	0.690	0.896	0.736	0.926	0.718	0.826	0.963	1.012
37.462	2667	unidentified		1.001	0.988												
37.579	2675	unidentified			0.205												
37.827	2699	unidentified													0.276		
37.903	2700	unidentified		0.157	0.202	0.276		0.238	0.160			0.212	0.143	0.236		0.260	0.283
38.362	2731	unidentified						0.154									
38.621	2745	unidentified	0.289				0.364	0.439			0.341						
38.644	2746	unidentified		0.323	0.421	0.353			0.297	0.314		0.413	0.313	0.321	0.341	0.547	0.670
38.932	2764	unidentified	1.977														
38.950	2765	unidentified		1.942	2.406	2.243	1.849	2.220	1.617	1.742	2.166	2.108	2.038	2.193	2.286	2.226	2.765
39.238	2783	unidentified		0.156				0.195					0.171	0.242	0.152	0.196	0.247
39.285	2789	unidentified				0.185	0.158										
39.315	2790	unidentified							0.135				0.157		0.154		
39.368	2794	unidentified				0.145		0.152									
39.344	2795	unidentified															0.134
39.827	2816	unidentified	0.431														
39.791	2817	unidentified				0.498	0.421	0.503	0.288	0.274	0.448		0.577	0.489		0.543	0.619
39.850	2818	unidentified		0.440	0.542							0.497			0.432		
42.991	2962	unidentified	0.667														
42.938	2963	unidentified						0.486	0.440	0.505	0.587		0.357	0.602		0.605	
43.032	2964	unidentified		0.653	0.642	0.718	0.460					0.633	0.285		0.689		0.819

Table S2: Results of the repeated measurement of reference sample REF-A2.

RT	RI	Compound	CAS	Group	Concentration / mg / kg of pellets																
					REF-A2-1-1	REF-A2-1-2	REF-A2-1-3	REF-A2-2-1	REF-A2-2-2	REF-A2-2-2	REF-A2-4-1	REF-A2-4-2	REF-A2-4-3	REF-A2-6-1	REF-A2-6-2	REF-A2-8-1	REF-A2-8-2	REF-A2-8-3	REF-A2-9-1	REF-A2-9-2	REF-A2-9-3
6.087	760	unidentified									0.187		0.193								
6.093	759	unidentified			0.325	0.401	0.208	0.192	0.238	0.134				0.160							0.147
6.675	782	unidentified															0.211	0.442			
6.681	783	unidentified																	0.251		
10.052	889	unidentified										0.144	0.138		0.151		0.163	0.165	0.137		0.159
10.305	896	Cyclohexanone	108-94-1	ALK	0.203															0.171	
10.681	908	unidentified													0.158	0.235	0.248	0.170			
10.698	909	unidentified													0.152						
10.957	917	unidentified				0.141															
14.663	1029	2-Ethylhexanol	104-76-7	IAS/NIAS	0.075		0.072	0.077	0.088	0.100	0.053	0.073	0.080	0.091	0.099	0.099	0.088	0.097	0.087	0.080	0.099
	5989-27-5			IAS/NIAS																	
14.804	1034	Limonene			0.041			0.038	0.054	0.056	0.027	0.049	0.044	0.050	0.058	0.063		0.061	0.058	0.046	0.039
14.857	1035	Benzyl alcohol	100-51-6	IAS/NIAS	0.162		0.161	0.140	0.133	0.157	0.120	0.130	0.154	0.176	0.178	0.187	0.198	0.205	0.187	0.308	0.258
14.893	1037	unidentified									0.065										
14.928	1038	Eucalyptol	470-82-6	IAS/NIAS			0.060	0.069						0.063		0.088	0.060	0.066	0.062	0.041	
14.928	1038	unidentified							0.084	0.084		0.069									0.049
15.875	1069	Acetophenone	98-86-2	IAS/NIAS	0.135																
16.869	1104	unidentified																			
19.351	1200	Dodecane	112-40-3	ALK	0.209	0.211	0.211	0.177	0.191	0.182	0.199	0.214	0.187	0.215	0.232	0.232	0.258	0.254	0.254	0.219	0.228
19.480	1205	unidentified				0.171	0.164	0.158	0.161	0.181						0.204	0.188		0.198	0.166	
19.457	1206	Decanal	112-31-2	IAS/NIAS							0.143				0.226			0.211			0.181
19.457	1206	unidentified										0.159	0.164	0.205							0.182
19.769	1218	unidentified			0.305	0.175															
20.780	1265	unidentified																	0.142		
21.033	1275	Ethyl Salicylate	118-61-6	IAS/NIAS	0.203	0.249	0.306	0.300	0.342	0.346	0.258	0.333	0.324	0.348	0.389	0.397	0.394	0.410	0.412	0.228	0.276
21.410	1292	2-Undecanone	112-12-9	ALK	0.064	0.064	0.085	0.089	0.105	0.091	0.075	0.092	0.088	0.098	0.104	0.103	0.102	0.130	0.098		0.319
21.369	1292	unidentified																		0.098	0.090
21.463	1294	Isobornyl Acetate	125-12-2	IAS/NIAS	0.265	0.320	0.272	0.261	0.269	0.281	0.239	0.311	0.324	0.255	0.270	0.262	0.285	0.372	0.243	0.319	0.359
		ortho tert-Butyl cyclohexyl acetate	88-41-5	IAS/NIAS																	0.340
21.480	1295	unidentified			0.822	1.035	0.414	0.361	0.343	0.349	0.359	0.304	0.330	0.455	0.440	0.452	0.460	0.360	0.468	0.446	0.406
21.527	1297	unidentified							0.096							0.029					0.396
21.586	1299	Tridecane	629-50-5	ALK	0.092		0.084	0.077	0.080	0.058	0.113	0.092	0.129	0.150	0.113	0.122	0.101	0.146	0.114	0.175	0.150
22.221	1333	Triacetin	102-76-1	IAS/NIAS	0.173	0.210	0.213	0.212	0.252	0.268	0.198	0.211	0.240	0.232	0.261	0.260	0.275	0.297	0.280	0.173	0.236
22.569	1352	unidentified						0.180	0.171	0.193			0.145	0.159	0.175	0.170	0.157	0.196	0.184		0.232
22.874	1368	unidentified			0.134	0.185	0.194	0.195	0.214	0.223	0.165	0.177	0.202	0.231	0.287	0.230	0.278	0.296	0.307		0.141
22.827	1369	unidentified																		0.173	0.231
		4-tert-Butylcyclohexyl acetate	10411-92-4	IAS/NIAS																	
22.974	1374	acetate cis			0.137	0.160	0.147	0.130	0.149	0.149	0.130	0.135	0.129	0.143	0.164	0.175	0.171	0.179	0.181	0.125	0.158
23.074	1379	unidentified			0.192	0.146														0.125	0.175
			1120-36-1	ALK																	
23.316	1392	1-Tetradecene			0.008		0.105	0.021	0.097		0.111				0.141	0.146	0.147	0.123	0.183	0.197	0.168
23.298	1392	unidentified										0.141	0.135								0.175
23.316	1392	unidentified				0.129				0.096				0.147							
23.457	1400	Tetradecane	629-59-4	ALK	0.638	0.646	0.646	0.516	0.535	0.546	0.566	0.615	0.605	0.650	0.689	0.681	0.659	0.738	0.708	0.664	0.690
23.616	1410	Dodecanal	112-54-9	IAS/NIAS	0.511	0.602	0.635	0.560	0.530	0.631	0.432	0.480	0.571	0.687	0.718	0.820	0.660	0.729	0.727	0.648	0.675
23.663	1413	Diphenyl Ether	101-84-8	IAS/NIAS	0.214	0.288	0.229	0.216	0.218	0.207	0.214	0.241	0.238	0.231	0.297	0.206	0.231	0.221	0.234	0.210	0.273
		Indan-1,3-diol		IAS/NIAS																	0.279
23.963	1432	monoacetate			0.173	0.221	0.221	0.242	0.254	0.263	0.187	0.236	0.238	0.268	0.276	0.272	0.271	0.269	0.304	0.183	0.218
24.333	1455	unidentified				0.141	0.141	0.201	0.209	0.217			0.185	0.180	0.192	0.224	0.196	0.223	0.211	0.182	0.235
24.315	1456	unidentified											0.160								0.183
24.539	1468	2-Methoxy naphthalene	93-04-9	IAS/NIAS	0.208	0.212	0.266	0.316	0.328	0.353	0.252	0.245	0.277	0.289	0.321	0.320	0.308	0.336	0.331	0.205	0.251
24.633	1474	unidentified						0.176	0.194	0.189											0.284
24.616	1475	unidentified			0.141	0.188	0.182				0.154	0.159	0.206	0.228	0.232	0.263	0.275	0.293	0.288	0.208	0.209
24.874	1493	unidentified																			0.129

25.027	1499	Pentadecane	629-62-9	ALK	0.288	0.308	0.317	0.255	0.269	0.274	0.268	0.292	0.300	0.326	0.350	0.365	0.368	0.344	0.374	0.320	0.341	0.329
25.145	1508	2,4-Di-tert-Butylphenol	96-76-4	IAS/NIAS	0.101	0.156	0.183		0.175	0.217	0.149	0.159	0.176	0.215	0.191		0.203	0.203	0.210	0.121		0.218
25.163	1509	BHT	128-37-0	IAS/NIAS	0.127	0.156	0.175	0.410	0.258	0.184	0.119	0.161	0.146	0.172	0.228	0.482	0.218	0.241	0.224	0.155	0.351	0.205
25.204	1512	unidentified			0.062					0.072	0.068		0.065	0.093	0.072		0.085	0.069	0.099			0.123
25.457	1530	Herbal propionate	17511-60-3	IAS/NIAS	0.394	0.685	0.613	0.637	0.657	0.705	0.544	0.580	0.638	0.671	0.713	0.737	0.707	0.746	0.811	0.569	0.631	0.630
25.486	1532	unidentified			0.226																	
25.539	1536	Lilial	80-54-6	IAS/NIAS	0.465	0.551	0.486	0.505	0.530	0.565	0.402	0.437	0.591	0.642	0.574	0.591	0.578	0.728	0.604	0.543	0.557	0.564
25.557	1537	5-Phenyldecane	4537-11-5	IAS/NIAS	0.299	0.320	0.443	0.403	0.407	0.432	0.348	0.371	0.295	0.289	0.419	0.428	0.387	0.293	0.442	0.292	0.309	0.329
25.621	1542	Naphthalene, 2-ethoxy-	93-18-5	IAS/NIAS	0.450	0.525	0.528	0.456	0.518	0.587	0.414	0.453	0.485	0.508	0.533	0.531	0.538	0.593	0.561	0.627	0.691	0.671
25.645	1544	Isoamyl Salicylate	87-20-7	IAS/NIAS	0.145	0.177	0.179	0.260	0.200	0.192	0.239	0.208	0.215	0.231	0.275	0.270	0.226	0.219	0.286			
25.704	1548	4-Phenyldecane	4537-12-6	IAS/NIAS	0.244	0.303	0.235	0.290	0.264	0.283	0.274	0.262	0.277	0.305	0.302	0.325	0.322	0.286	0.332	0.274	0.311	0.324
25.786	1554	Dodecanoic acid	143-07-7	FAE	0.293	0.433	0.552	0.602	0.735	0.704	0.332	0.436	0.628	0.425	0.559	0.699	0.188	0.337	0.375		0.376	0.243
25.992	1569	3-Phenyldecane	4621-36-7	IAS/NIAS	0.389	0.473	0.369	0.378	0.367	0.549	0.356	0.333	0.379	0.388	0.461	0.417	0.413	0.404	0.384	0.480	0.354	0.365
26.027	1571	unidentified						0.173	0.148													
26.027	1571	unidentified												0.261				0.196	0.340			
25.986	1572	unidentified																			0.175	
26.010	1572	unidentified			0.185	0.192	0.207				0.155	0.246	0.182	0.187		0.176	0.162			0.155	0.166	
26.080	1578	Undecalactone	104-67-6	IAS/NIAS												0.176	0.162		0.133	0.163		
26.092	1578	unidentified					0.135						0.129		0.143	0.136	0.159				0.136	
26.209	1585	Amyl salicylate	2050-08-0	IAS/NIAS	0.741	1.089	1.271	1.073	1.243	1.183	0.842	1.017	1.358	1.101	1.740	1.568	1.511	1.353	1.502	0.754	0.948	1.026
26.298	1591	Ethyl Laurate	106-33-2	FAE	4.289	6.028	5.287	5.207	6.346	5.364	4.512	5.865	5.251	5.374	5.998	5.859	6	6.343	6.264	8.218	8.932	6.149
26.315	1592	Hexadecene	629-73-2	ALK	3.958	2.940	4.264	3.759	2.731	3.773	3.283	2.885	3.782	3.908	4.055	4.246	0.769	4.283	4.166			3.358
26.415	1600	Hexadecane	544-76-3	ALK	9.988	9.298	9.728	7.981	7.793	8.047	8.557	8.237	8.512	9.263	9.122	9.343	9.681	9.500	9.641	9.597	9.253	9.343
26.462	1603	unidentified							0.563	0.535								0.605	0.686			
26.433	1604	unidentified				0.500	0.711								0.597	0.599				0.522	0.510	
26.504	1607	2-Phenyldecane	4537-13-7	IAS/NIAS	1.388	1.315	1.366	1.181	1.205	1.156	1.217	1.241	1.258	1.272	1.280	1.279	1.299	1.326	1.320	1.306	1.296	1.312
26.586	1615	unidentified			0.230								0.218	0.329	0.354	0.353			0.619	0.635	0.705	
26.627	1616	unidentified				0.284	0.344	0.470	0.447	0.319							0.358	0.324	0.400			
26.610	1617	unidentified			0.264						0.269	0.305	0.267	0.323	0.330	0.341						
26.698	1622	unidentified					0.139										0.151					
26.668	1623	unidentified												0.159							0.173	
26.715	1626	unidentified				0.622											0.720	0.818	0.777		0.595	
26.751	1626	unidentified					0.966	0.704														
26.733	1627	unidentified											0.754		0.754	0.747				0.654		
26.756	1627	unidentified			0.501	0.603				0.707	0.970	0.684		0.723						0.690		
26.780	1629	p-Octylacetophenone	10541-56-7	IAS/NIAS	0.377	0.484	0.592		0.470	0.574		0.626	0.725	0.569	1.177	1.274	1.094	1.447	1.602	0.799	0.917	1.369
26.839	1633	6-Phenylundecane	4537-14-8	IAS/NIAS	0.532	0.506	0.664	0.826	0.824	0.774	0.720	0.612	0.699	0.527	0.896	0.858	0.754	0.956	0.809	0.765	0.738	0.785
26.880	1637	5-Phenylundecane	4537-15-9	IAS/NIAS	2.024	2.013	2.016	1.870	1.824	1.898	1.852	1.822	1.919	1.963	1.983	2.042	2.053	2.002	2.036	1.971	1.927	2.000
27.027	1648	4-Phenylundecane	4536-86-1	IAS/NIAS	2.058	2.437	2.086	2.241	2.179	2.004	2.149	2.199	2.125	2.027	2.431	2.552	2.114	2.480	2.178	2.240	1.996	2.430
27.098	1654	Methyl (3-oxo-2-pentylcyclopentyl)acetate isomer 2	24851-98-7	IAS/NIAS				1.195	1.147	1.068	0.881	1.096	0.953	0.966	1.312	1.111	1.092	1.422	1.177	0.955	0.888	1.273
27.104	1654	Methyl (3-oxo-2-pentylcyclopentyl)acetate isomer 1	24851-98-7	IAS/NIAS	0.823	1.085	0.994															
27.133	1657	a-Pentylcinnamaldehyde isomer	122-40-7	IAS/NIAS				0.649	0.675	0.690	0.490	0.548	0.608	0.606	0.666	0.701	0.656	0.697	0.739	0.583	0.640	0.699
27.145	1657	a-Pentylcinnamaldehyde	122-40-7	IAS/NIAS	0.541	0.588	0.663															
27.209	1663	Di-n-Octylether	629-82-3	IAS/NIAS	3.243	3.252	3.356	2.921	2.883	2.900	2.914	2.918	3.037	3.272	3.578	3.367	3.595	3.734	3.558	3.173	3.192	3.240

27.321	1672	Benzene, (1-ethylnonyl)-	4536-87-2	IAS/NIAS	3.144	3.106	3.105	2.536	2.464	2.560	2.916	2.459	2.563	2.740	2.735	2.740	2.862	2.784	3.144	3.020	3.002	3.059
27.392	1677	1-Tetradecanol	112-72-1	IAS/NIAS	0.781	0.749	0.838	1.042	1.102	1.178	0.580	0.813	1.060	1.074	1.168	1.237	0.940		1.160	0.719		
27.362	1678	unidentified															0.969			1.006	0.909	
27.456	1683	Amberonne	68155-66-8	IAS/NIAS	6.056	6.135	6.436	6.733	6.119	6.500	5.465	5.885	6.249	6.639	6.810	7.157	6.897	6.851	7.521	6.063	6.514	6.622
27.545	1690	n-Hexyl salicylate	6259-76-3	IAS/NIAS	15.283	15.87	17.34	16.40	16.02	16.58	15.30	16.35	17.60	16.87	18.38	19.41	19.31	19.42	19.43	15.39	16.77	17.24
27.662	1699	Heptadecane	629-78-7	ALK		9	8	1	9	7	2	5	5	5	4	4	9	1	5	1	1	7
27.692	1703	unidentified			1.520	1.470	1.165	1.232	0.939	0.950	1.479	1.155	1.214	1.089	1.089	1.467	1.202	1.360	1.414	1.309	1.150	1.099
27.680	1704	unidentified					0.146					0.138	0.131				0.143	0.149	0.172		0.155	
														0.136	0.150	0.157					0.160	
27.792	1710	2-Phenylundecane	4536-88-3	IAS/NIAS	3.929	3.722	3.803	3.655	3.401	3.388	3.572	3.354	3.667	3.656	3.534	3.574	3.744	3.654	3.600	3.727	3.614	3.707
27.874	1717	Amberonne Isomer	68155-66-8	IAS/NIAS	3.700	3.767	4.177	4.087	3.962		3.250	3.817	3.263							4.424	4.440	4.282
27.874	1717	Ethylene glycol monododecyl ether	4536-30-5	IAS/NIAS						4.258				3.521	4.701	4.973	3.881	5.002	5.404			
27.927	1722	Methyl myristate	124-10-7	IAS/NIAS	0.526	0.544	0.616	0.557	0.560	0.621	0.509	0.524	0.566	0.592	0.570	0.666	0.623	0.678	0.659	0.539	0.595	0.586
			2719-62-2	IAS/NIAS																		
28.039	1732	6-Phenylldodecane	2719-63-3	IAS/NIAS	2.517	2.478	2.501	2.363	2.228	2.331	2.350	2.206	2.380	2.401	2.405	2.473	2.596	2.527	2.486	2.462	2.356	2.428
28.092	1736	5-Phenylldodecane	2719-63-3	IAS/NIAS	2.672	2.396	1.954	2.261	2.153	2.196	2.232	2.143	2.227	2.338	2.273	2.311	2.390	2.377	2.337	2.749	2.759	2.868
28.186	1742	unidentified			0.334	0.397	0.391															
28.180	1744	unidentified						0.384	0.333	0.353	0.297	0.378	0.355	0.432	0.351	0.427	0.369	0.419	0.404	0.383	0.385	0.325
28.256	1751	4-Phenylldodecane	2719-64-4	IAS/NIAS	2.608	2.477	2.540	2.325	2.205	2.230	2.365	2.232	2.317	2.425	2.430	2.435	2.612	2.526	2.483	2.523	2.427	2.455
		a-Hexylcinnamaldehyde																				
28.351	1759	trans	101-86-0	IAS/NIAS	33.610	1	35.25	34.30	33.81	34.52	30.57	30.25	32.82	33.46	35.06	35.67	36.29	35.53	35.61	34.36	34.67	35.01
28.433	1762	unidentified			0.652	0.641	0.714				5	5	4	1	7	8	0	9	2	5	9	6
28.427	1765	unidentified						0.648	0.639	0.660	0.604	0.587	0.638	0.659	0.689	0.702	0.684	0.700	0.691	0.676	0.684	0.688
28.533	1774	3-Phenylldodecane	2400-00-2	IAS/NIAS			4.187	3.882	3.710	3.674	3.857	3.598	3.740	4.028	3.988	4.017	4.289	4.137	4.032	4.170	3.973	4.103
		a-Hexylcinnamaldehyde																				
28.645	1784	cis	101-86-0	IAS/NIAS	4.126	4.202	4.354	3.838	3.930	3.945	3.479	3.396	4.015	3.713	3.947	3.930	4.114	4.623	3.682	4.110	3.905	4.091
28.674	1787	Benzyl benzoate	120-51-4	IAS/NIAS	1.986	1.722	2.063	2.303	2.178	2.158	2.266	1.911	1.622	1.867	2.073	2.013	2.009	1.694	3.001	2.462	2.325	2.749
28.750	1793	1-Octadecene	112-88-9	ALK	8.892	9.174	9.805	9.211	8.273	8.927	7.814	8.098	7.730	8.305	9.620	8.775	9.748	9.273	9.467	9.498	8.269	9.323
						13.14	14.56	11.75	10.42	10.94	11.36	10.69	11.28	11.97	13.22	12.28	13.07	12.59	12.50	14.60	12.66	12.63
28.821	1799	Octadecane	593-45-3	ALK	14.247	3	3	8	8	5	4	7		1	5	1	4	2	0	7	8	8
28.992	1815	2-Phenylldodecane	2719-61-1	IAS/NIAS	6.619	6.544	7.131	6.433	3.563	3.523	3.488	6.199	3.374	6.832	7.175	7.253	7.693	7.458	7.572	6.507	6.566	6.655
29.009	1817	Ethylhexyl Salicylate	118-60-5	IAS/NIAS					2.846	2.957	2.799		3.040									
						25.23	26.35	23.77	23.61	24.13	24.33	23.51	23.65	25.84	26.14	26.39	28.11	27.37	26.99	27.24	27.51	27.16
29.050	1821	Isopropyl myristate	110-27-0	FAE	26.613	4	2	9	6	2	3	5	5	9	4	2	1	1	9	1	6	3
29.121	1822	unidentified				0.722	0.589															
29.127	1823	unidentified			1.018																	
29.115	1827	unidentified						0.692	0.519	0.498	0.599	0.532	0.201	0.684	0.696	0.637	0.615	0.710	0.728	0.589	0.762	0.594
29.156	1830	6-Phenyltridecane	4534-49-0	IAS/NIAS	2.769	2.490	2.589	2.455	2.355	2.336	2.489	2.272	2.378	2.518	2.507	2.532	2.645	2.589	2.470	2.819	2.648	2.685
29.233	1837	5-Phenyltridecane	4534-50-3	IAS/NIAS	2.198	2.118	2.294	2.148	2.030	2.109	2.017	1.922	2.088	2.197	2.253	2.304	2.400	2.315	2.308	2.198	2.211	2.199
29.386	1852	4-Phenyltridecane	4534-51-4	IAS/NIAS	3.919	3.804	4.121	3.758	3.681	3.762	3.621	3.566	3.771	3.998	4.090	4.168	4.311	4.259	4.216	4.061	4.073	4.109
29.498	1859	unidentified				1.126	1.485															
29.503	1860	unidentified			1.301																	
29.492	1861	unidentified						1.205	1.228	1.186	1.137	1.111	1.208				1.510	1.702	1.391	1.209		
29.462	1862	unidentified																				
														1.288	1.405	1.372						
29.539	1866	Galaxolide	1222-05-5	IAS/NIAS	9.928	8.689	9.815	9.788	9.483	9.558	8.667	8.586	9.068	9.887	9.904	9.887	10.40	10.07	10.18	10.14	9.222	9.850
29.598	1871	Tonalid	21145-77-7	IAS/NIAS	1.277	1.346	1.484	1.379	1.406	1.450	1.158	1.177	1.300	1.404	1.399	1.479	1.550	1.713	1.439	1.385	1.446	1.511

29.668	1878	3-Phenyltridecane	4534-52-5	IAS/NIAS	1.613	1.593	1.729	1.381	1.311	1.628	1.611	1.511	1.584	1.688	1.468	1.766	1.889	1.819	1.786	1.722	1.595	1.640
29.709	1882	1-Hexadecanol	36653-82-4	IAS/NIAS	7.387	7.970	9.486	10.04	10.81	10.93				10.46	12.54	12.39	11.63	12.63	12.92			
29.851	1895	Benzyl salicylate	118-58-1	IAS/NIAS	6.433	6.263	7.251	6.812	7.006	7.269	7.140	6.877	7.760	7.269	8.058	8.406	8.588	8.561	8.404	5.817	6.874	6.860
29.903	1899	Nonadecane	629-92-5	ALK	1.168	1.039	1.002	0.760	0.768	0.773	1.235	1.098	1.053	0.835	0.969	0.905	1.044	0.843	0.869	1.296	1.097	1.105
29.992	1908	Homosalate	118-56-9	IAS/NIAS	1.811	1.848	2.052	1.875	1.909	1.967	1.847	1.845	2.011	2.012	2.167	2.243	2.404	2.330	2.352	1.881	2.009	2.062
30.092	1918	2-Phenyltridecane	4534-53-6	IAS/NIAS		3.290	4.296	4.786	4.690	4.461	4.475	4.257	4.380	4.705	4.850	4.849	5.326	5.192	5.012	4.107	4.133	4.372
30.145	1923	Methyl Palmitate	112-39-0	FAE	5.710	5.724	6.473	5.733	5.663	5.850	5.613	5.392	5.779	6.136	6.471	6.697	6.821	6.716	6.662	6.215	6.235	6.219
30.239	1932	unidentified						0.416	0.413								0.425	0.424	0.400			
30.244	1933	unidentified			0.439	0.422	0.440			0.367	0.428	0.368	0.370	0.443	0.398	0.396				0.473	0.424	0.446
30.339	1942	unidentified						0.409	0.397	0.427	0.420	0.380	0.381				0.468	0.746	0.452	0.595		
30.309	1943	unidentified			0.456	0.542	0.453							0.438	0.471	0.381					0.491	0.425
30.433	1951	unidentified			1.010	1.061	1.172	1.065	1.027	1.059							1.208	1.213	1.212	1.108		
30.415	1952	unidentified									0.963	0.860	0.932	1.118	1.106	1.132					1.103	1.154
30.474	1955	n-Hexadecanoic acid	57-10-3	FAE	0.662	1.087	1.510	1.759	1.921	1.875	0.726	1.076	1.483	1.305	1.894	1.707	1.551	1.727	1.677	0.632	0.826	
30.539	1962	unidentified			3.779	3.811	4.342	4.133	4.183	4.500	3.786	3.639	4.136	4.342	4.806	4.921	5.311	5.107	5.196	3.948	4.167	4.236
30.639	1972	unidentified			0.497	0.502	0.549	0.442	0.460	0.476	0.496			0.569	0.557	0.556	0.719	0.672	0.626	0.633	0.552	0.639
30.627	1973	unidentified										0.426	0.510									
30.698	1977	unidentified				0.868		2.025	1.848	1.737							0.931	1.137	1.117	0.399		
30.680	1978	unidentified			0.710		1.276				0.961	1.236	1.358	1.046	1.423						0.985	0.653
30.674	1979	unidentified														1.435						
30.827	1990	Ethyl Palmitate	628-97-7	FAE	2.831	3.012	3.492	2.967	2.762	2.892	3.161	3.071	3.360	3.015	3.279	3.741	3.548	4.165	3.498	3.226	3.414	3.479
30.856	1993	1-Eicosene	3452-07-1	ALK	7.161	6.207	8.051	6.742	6.416	6.826	5.422	5.405	6.113	7.163	7.379	6.951	8.077	7.268	8.252	7.061	7.123	7.236
30.921	1999	Eicosane	112-95-8	ALK			11.52								10.37	10.80	11.42	11.04		11.66	10.41	10.73
30.933	2005	unidentified			11.133	9.084	9	8.772	7.780	9.115	8.519	8.347	8.879	9.149	6	8	9	8	9.672	2	9	5
31.115	2020	Isopropyl palmitate	142-91-6	FAE	48.904	43.21	47.26	42.32	41.09	42.90	43.06	39.74	42.42	43.67	45.24	46.49	49.65	47.04	46.69	47.27	46.30	46.38
31.192	2027	unidentified			7	9		0	6	5	6	0	0	8	4	4	7	6	2	5	4	5
31.174	2028	unidentified			0.759	0.732	0.906	0.500	0.522	0.590												
31.339	2043	Ethylene brassylate	105-95-3	FAE	1.402	1.503	1.410	1.523	1.319	1.534	1.398	1.251	1.364	1.546	1.425	1.421	0.887	0.960	0.960	0.903	0.874	0.914
31.450	2054	unidentified					0.311	0.616	0.465	0.558				0.347		0.322	0.640	0.623	0.251	0.560		
31.433	2055	unidentified									0.261	0.436	0.441	0.272		0.583						0.614
31.439	2057	Eicosane, 2-methyl-	1560-84-5	ALK													0.281					
31.445	2057	unidentified					0.219							0.243								
31.668	2077	unidentified			0.319	0.323	0.392	0.414	0.471	0.410	0.325	0.380	0.392	0.435	0.441	0.379	0.412	0.477	0.433	0.299	0.371	0.384
31.756	2086	1-Octadecanol	112-92-5	IAS/NIAS	7.780	9.081	7	10.80	11.16	11.85	8.029	8.735	10.32	11.61	13.53	14.49	14.15	14.20	14.95	8.094	9.402	9.997
31.886	2099	1-Propylpentyl laurate	84713-06-4	FAE	7.565	7.419	8.065	7.325	6.936	6.594	3.655	6.524	6.917	8.540	7.628	8.213	9.189	8.141	8.996	8.279	8.595	7.924
31.880	2101	Methyl Oleate	112-62-9	FAE					0.644													
31.956	2107	unidentified																				
31.939	2108	unidentified													0.307	0.325						
31.974	2109	unidentified				0.275		0.307		0.282	0.227	0.218				0.314			0.311		0.177	0.183
31.939	2110	unidentified			0.400																	
32.109	2124	Didecyl methylamine	7396-58-9	IAS/NIAS	5.528	5.365	6.531	5.889	5.710	5.739	5.671	5.604	5.761	6.237	6.470	6.694	7.178	6.784	6.681	5.780	5.888	6.118
32.227	2137	Oleic Acid	112-80-1	FAE				0.841														
32.227	2137	unidentified				0.300	0.575		0.848	0.717	0.271	0.282	0.343	0.559	0.567	0.519	0.819	0.586	0.488	0.191	0.193	
32.197	2138	unidentified			0.199																	0.311
32.274	2142	unidentified			0.443	0.400	0.454	0.460	0.498	0.517	0.413	0.376	0.403	0.486	0.466	0.469	0.573	0.516	0.547	0.408	0.423	0.424
32.350	2150	Tributyl aconitate	7568-58-3	IAS/NIAS	0.549	0.535	0.644		0.556	0.582			0.548	0.645		0.689	0.765	0.752	0.761		0.583	
32.350	2150	unidentified						0.527			0.521	0.480			0.679					0.607		0.628
32.421	2158	Stearic acid	57-11-4	FAE	0.486	0.728	0.879	0.827	0.851	0.972			0.520	0.520	0.556	0.649	0.662	0.542	0.612	0.588		0.205
32.403	2158	unidentified									0.296											
32.427	2162	Ethyl Oleate	111-62-6	FAE														1.139			0.677	

32.462	2162	Ethyl Linoleate	544-35-4	FAE		0.589		0.667	0.724	0.829	0.497	0.580		0.811	1.040	0.947	0.964		1.239			
32.444	2162	unidentified			0.447								0.682									
32.427	2163	unidentified																	0.377		0.576	
			6114-18-7	FAE																		
32.509	2167	Ethyl elaidate			2.051	2.275	2.590	2.408	2.442	2.524	1.951	2.022	2.371	2.773	3.064	2.993	3.156	3.073	3.029	2.229	2.496	2.417
32.550	2172	unidentified			4.405	4.092	4.646	4.136	4.029	4.380	4.006	3.978	4.260	4.770	5.012	5.052	5.319	5.111	4.983	4.213	4.584	4.505
32.621	2183	unidentified				0.611	0.707												1.037			
32.662	2184	unidentified			0.404			0.591	0.617	0.653	0.405	0.656	0.819	0.928	1.131	0.925	0.746	1.090				
32.627	2185	unidentified																		0.601	0.914	0.995
			1599-67-3	ALK	4.288	3.588	4.969	4.713	4.480	4.288	3.733	3.600	4.019	4.544	4.569	4.887	5.764	4.693	5.496	4.473	4.537	4.812
32.756	2194	1-Docosene																				
32.803	2199	Docosane	629-97-0	ALK	6.254	5.614	6.559	4.557	4.418	4.640	5.033	4.421	4.947	5.107	5.580	5.993	6.122	5.719	5.856	5.650	5.490	5.738
32.856	2205	unidentified							0.306													
32.862	2206	unidentified						0.236		0.245										0.283	0.316	0.348
		Benzoic acid, dodecyl ester	2915-72-2	FAE																		
32.938	2215	unidentified			2.697	2.258	2.568	2.550	2.446	2.471	2.318	2.111	2.284	2.560	2.711	2.713	3.020	2.777	2.587	2.312	2.362	2.391
32.974	2219	unidentified			1.662	1.750	1.929	1.637	1.605	1.673	1.471	1.442	1.585	1.758	1.794	1.907	2.034	1.950	2.147	1.700	1.826	1.863
33.056	2227	unidentified				0.298																
33.050	2228	unidentified			0.360		0.386	0.311	0.330	0.315	0.360	0.298	0.358	0.362	0.344	0.413	0.464	0.358	0.369	0.411	0.387	0.366
33.097	2238	unidentified																		0.131		
33.168	2241	Tributyl acetyl	77-90-7	IAS/NIAS				0.460	0.522	0.493	0.338	0.243	0.220									
33.139	2241	unidentified																				
33.209	2246	unidentified			0.307	0.208	0.317	0.298	0.304	0.268	0.216	0.229	0.228	0.312	0.367	0.345	0.433	0.315	0.377	0.298	0.322	0.341
33.297	2254	unidentified				0.225																
33.303	2256	unidentified			0.221		0.173	0.143	0.179	0.165	0.160			0.165	0.159	0.175	0.216		0.169	0.151		
33.274	2257	unidentified																0.177			0.132	0.181
33.339	2264	unidentified																	0.140	0.145		
33.344	2265	unidentified																	0.157			
33.427	2270	unidentified			0.405	0.451			0.455		0.377									0.807	0.340	
33.403	2271	unidentified																				
33.444	2272	unidentified				0.365		0.382							0.913	0.428						
33.450	2273	unidentified			0.275			0.277	0.344		0.641	0.586		0.807			1.104	1.009	1.058			0.345
33.538	2282	unidentified				0.162																
33.568	2285	unidentified					0.214															
33.521	2286	unidentified																				0.210
33.556	2289	unidentified																				
33.638	2298	unidentified				1.574	1.845													2.482		
33.644	2299	Tricosane	638-67-5	ALK												2.164						
33.674	2299	unidentified			1.567			1.343	1.256	1.310	1.416	1.433	1.475	2.042			2.592	2.400		1.977	2.032	2.108
33.756	2310	unidentified				0.594					0.598			0.781	0.673		0.939		0.793			
33.780	2311	unidentified			0.548		0.654	0.659	0.669	0.569			0.598		0.754		0.813		0.759	0.722		
33.768	2312	unidentified										0.590										0.683
		Benzoic acid, tridecyl ester	29376-83-8	IAS/NIAS	2.967	2.971	3.427	3.275	3.187	3.162	2.981	2.898	3.043	3.568	3.609	3.663	4.109	3.802	3.783	3.246	3.334	3.475
33.856	2320		5466-77-3	IAS/NIAS																		
33.956	2332	Eusolex 2292			1.249	1.263	1.096	1.665	1.411	1.391	2.002	1.204	2.116	1.340	1.418	1.847	2.709	1.579	1.704	2.261	2.256	2.331
33.950	2334	unidentified			1.009	0.861	1.161							1.249	1.195							
33.985	2335	unidentified							0.797	0.754		0.849						0.930	0.920			
33.991	2336	unidentified						0.597									0.804					
34.050	2342	unidentified			0.156	0.243	0.141	0.354		0.165												
34.033	2343	unidentified									0.367		0.247	0.377	0.293	0.356	0.482	0.343	0.288		0.140	0.445
34.103	2349	unidentified			0.341	0.326	0.386	0.314	0.279	0.322	0.364	0.373	0.280	0.356	0.353	0.386	0.424	0.409	0.296			
34.068	2350	unidentified																		0.347	0.318	0.457
34.209	2360	unidentified				0.311																
34.209	2361	unidentified			0.337		0.422	0.453	0.379	0.425		0.348		0.460	0.476	0.484	0.481	0.503	0.488	0.367		
34.197	2362	unidentified									0.343		0.351								0.371	0.349
34.291	2371	unidentified			1.511	1.431	1.503	1.618	1.402	1.564			1.612		2.156	1.898			2.014			
34.280	2372	unidentified									1.264	1.295		1.854			2.253	2.117		1.816	1.506	1.646
34.409	2384	unidentified			0.420	0.394	0.298	0.560	0.580	0.620		0.455	0.459				0.706		0.692			
34.392	2385	unidentified									0.468			0.649	1.377	0.657		0.757		0.556	0.577	0.554

34.433	2390	Hexanedioic acid, bis(2-ethylhexyl) ester	103-23-1	FAE							0.513						0.717					
34.491	2394	1-Tetracosene	10192-32-2	ALK	2.005	2.232	2.440	2.125	1.911	2.151	1.594	1.444	1.713	2.117	2.130	2.482	2.549	2.401	2.369	1.751	1.774	1.914
34.533	2399	Tetracosane	646-31-1	ALK	2.585	2.597	2.433	1.886	2.031	1.905	1.818	1.573	2.069	1.989	2.020	2.097	1.988	2.054	2.290	2.239	2.416	2.067
34.591	2405	unidentified					0.188			0.206	0.283											
34.562	2406	unidentified															0.214	0.289	0.265			0.264
34.715	2417	unidentified				0.265																
34.715	2418	unidentified						0.220											0.250			
34.674	2419	unidentified																				0.206
34.762	2423	Benzoic acid, tetradecyl ester	70682-72-3	IAS/NIAS	2.117	2.168	2.522	2.473	2.318	2.347	2.250	1.948	2.098	2.752	2.941	2.728	3.224	3.170	2.907	2.116	2.569	2.409
34.838	2431	unidentified				0.311	0.312	0.388	0.435	0.336	0.411			0.451	0.417	0.460	0.343	0.431	0.446	0.297	0.386	
34.821	2432	unidentified									0.326	0.241	0.271									0.395
34.909	2439	unidentified						0.186		0.214												
35.021	2450	unidentified					1.936	1.806	1.605	1.764												
35.003	2451	unidentified									1.581	1.417	1.576	1.996	2.012	2.065	2.389	2.146	2.178	1.645	1.687	1.813
35.044	2452	unidentified			2.875																	
35.197	2469	unidentified			3.497	3.429	3.858	3.765	3.610	3.741	3.227	3.033	3.430	3.918	4.195	4.327	4.705	4.317	4.420	3.354	3.681	3.779
35.280	2478	unidentified			0.824	0.712	0.819	0.681	0.496	0.598	0.665	0.719	0.613	0.896	0.996	1.101	1.383	1.353	1.432			
35.238	2479	unidentified																		0.971	0.990	1.123
35.403	2489	unidentified				0.130																
35.480	2499	Octan-2-yl palmitate	55194-81-5	FAE	3.660	3.375	3.786	3.351	3.434	3.525	3.071	3.009	3.161	4.220	4.265	4.332	4.808	4.908	5.218	3.510	3.811	4.010
35.538	2509	unidentified																		0.136		
35.656	2515	unidentified					0.199	0.312	0.383	0.374	0.226	0.283					0.143	0.186				
35.639	2516	unidentified			0.176								0.265	0.130	0.229	0.200			0.161			
35.791	2527	Benzoic acid, pentadecyl ester	68411-27-8	IAS/NIAS	1.730	1.720	1.724	1.679	1.637	1.674	1.422	1.345	1.447	1.738	1.921	1.948	2.080	1.874	1.951	1.392	1.543	1.560
35.891	2536	Dicyclohexyl phthalate	84-61-7	IAS/NIAS	0.301		0.509			0.778						0.728	0.809		0.863			
35.891	2536	Diheptyl phthalate	117-81-7	IAS/NIAS				0.838	0.626				0.613	0.702	0.796			0.856				0.673
35.903	2536	Bis(2-ethylhexyl)phthalate	117-81-7	IAS/NIAS		0.880																
35.868	2537	unidentified									0.609	0.638								0.654	0.705	
35.938	2541	unidentified					0.290	0.378			0.290	0.272			0.329	0.345		0.368				
35.909	2542	unidentified												0.166						0.274		0.378
36.221	2566	Dodecyl Laurate	13945-76-1	FAE	10.120	9.576	11.148	11.091	10.444	10.826	9.161	8.340	9.551	11.003	11.640	12.392	13.371	12.182	12.479	10.565	10.886	
36.409	2583	Bumetrizole	3896-11-5	IAS/NIAS	1.715		1.072	0.970	0.954	0.926	0.931	0.766	0.830	1.071	1.073	1.155	1.160	1.150	1.131	0.750	0.872	0.982
36.538	2595	1-Hexacosene	18835-33-1	ALK		0.515	0.733	0.646	0.409	0.481	0.500	0.313	0.476	0.534	0.830	0.563			0.618		0.300	
36.574	2598	Hexacosane	630-01-3	ALK		1.211	1.438	0.770	0.909	0.678	0.735	0.446	0.688	0.846	1.030	0.901	1.103	1.239	1.385		0.684	
36.515	2599	unidentified			1.357														1.048		1.504	
36.691	2608	unidentified						0.183		0.131	0.161		0.191	0.225	0.148					0.196		
36.656	2609	unidentified			0.208											0.169	0.146	0.150	0.168			
36.986	2634	unidentified																0.140				
37.062	2640	unidentified												0.143			0.141					
37.144	2641	unidentified					0.132															
37.226	2648	unidentified			0.660	0.651			0.485	0.492	0.454	0.410	0.463		0.705	0.627	0.858	0.598	0.680			
37.232	2649	unidentified			0.612		0.680							0.486						0.447	0.435	0.529
37.462	2666	Octocrylene	6197-30-4	IAS/NIAS	2.516	2.556	3.008	3.184	3.297	3.111	2.147	2.330	2.400	2.759	3.571	3.289	3.712	3.436	3.642	2.615	2.881	2.744
37.491	2668	unidentified			2.320	1.938	2.110	2.479		2.378						2.953						
37.497	2669	unidentified							2.002		1.857	1.604	2.031		2.156		2.552	2.584	2.463			2.053
37.432	2670	unidentified																		1.415	1.785	
37.503	2674	unidentified				0.247											0.512					
37.573	2675	unidentified							0.338												0.396	
37.838	2699	unidentified				0.614																
37.903	2700	unidentified			0.788		1.026	0.908	0.904	0.863	0.600	0.659	0.775	0.930	1.104	0.991	1.040	1.070	0.963	0.667	0.853	0.740
38.244	2721	unidentified					0.222	0.292	0.211													

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