

## Supplementary material

Table S1 Information on 173 kinds of volatiles of infant formula from NIST retrieval

No.	Compound	Formula	R.T. (s)	RI	RI*	Unique mass	Match
1	3-methyl-1-butanol	C5H12O	292 , 3.920	832.2	697	70	803
2	2-ethyl-1-decanol	C12H26O	1088 , 1.150	1422.8	1393	57	800
3	1-heptanol	C7H16O	464 , 1.310	972.59	960	70	889
4	1-hexadecanol	C16H34O	1128 , 1.150	1454.7	1854	68	874
5	1-octanol	C8H18O	608 , 1.340	1074.6	1059	56	913
6	1-octen-3-ol	C8H16O	480 , 1.290	984.56	969	57	941
7	1-pentanol	C5H12O	252 , 3.500	777.07	761	41	884
8	2,4-decadien-1-OL	C10H18O	920 , 1.720	1295	1274	83	796
9	Trans-2-Decen-1-OL	C10H20O	800 , 1.530	1208.5	1266	57	907
10	Furfuryl alcohol	C5H6O2	324 , 1.300	859.68	885	81	925
11	3-octanol	C8H18O	504 , 1.270	1002.3	979	83	769
12	4-ethylcyclohexanol	C8H16O	560 , 1.340	1041.2	1068	58	840
13	Cis-4-Heptenal	C7H12O	372 , 1.420	903.76	913	84	882
14	(R)-(+)-2-methyl-1-phenyl-1-propanol	C10H14O	964 , 1.490	1327.9	1351	107	811
15	2-methylcyclohexanol	C7H14O	980 , 1.480	1340.1	969	57	822
16	Phenethyl alcohol	C8H10O	672 , 1.470	1119.1	1136	91	939
17	Dimethylsilanediol	C2H8O2Si	240 , 1.050	743.38	409	77	921
18	N-formylpiperidine	C6H11NO	716 , 2.370	1150.3	1021	113	864
19	Gamma-nonanolactone	C9H16O2	1016 , 2.350	1368	1284	85	892
20	Trans, Trans -2,4-decadienal	C10H16O	1036 , 2.020	1382.9	1220	54	860
21	(2E,4E)-2,4-decanedienal	C10H16O	956 , 1.800	1298	1220	66	900
22	(E,E)-2,4-dodecadienal	C12H20O	1060 , 1.660	1400.8	1418	83	863
23	Trans,trans-2,4-heptadienal	C7H10O	416 , 1.530	1013.8	921	81	832
24	(E,E)-2,4-hexadienal	C6H8O	392 , 1.750	918.99	822	81	910
25	Trans,trans-2,4-nonadienal	C9H14O	812 , 1.790	1217.3	1120	81	943
26	(2E,4E)-2,4-octadienal	C8H12O	664 , 1.820	1113.8	1021	81	861
27	Crotonaldehyde	C4H6O	184 , 3.230	695.98	615	70	854
28	Trans-2-dodecenal	C12H22O	1148 , 1.620	1471	1410	70	893
29	5-methyl furfural	C6H6O2	456 , 1.870	967.02	920	109	883
30	2-propyl-2-heptenal	C10H18O	904 , 1.590	1283.4	1189	125	780
31	2-ethyl-2-hexenal	C8H14O	516 , 1.590	1010.9	990	111	817
32	(E)-2-Octenal	C8H14O	592 , 1.810	1063.8	1013	57	875
33	(E)-2-butyloct-2-enal	C12H22O	1028 , 1.550	1567.3	1023	111	755
34	Trans-2-Pentenal	C5H8O	232 , 3.790	763.99	715	83	898
35	2-Furanacrolein	C7H6O2	668 , 1.930	1116.6	1038	122	823
36	2-Pyridinecarboxaldehyde	C6H5NO	444 , 1.600	957.83	976	52	807
37	2-Undecenal	C11H20O	996 , 1.610	1367.5	1311	70	849
38	Trans-2-Undecenal	C11H20O	1020 , 1.890	1370.7	1311	36	845

No.	Compound	Formula	R.T. (s)	RI	RI*	Unique mass	Match
39	3-Cyclohexene-1-carboxaldehyde	C7H10O	536 , 1.670	1024.8	1008	110	829
40	3-Furaldehyde	C5H4O2	292 , 1.060	829.52	831	95	912
41	3-Hexen-2-One	C6H10O	308 , 1.580	844.98	762	83	820
42	Trans-4-Nonenal	C9H16O	644 , 1.510	1099.7	924	69	889
43	5-ethyl-2-furaldehyde	C7H8O2	584 , 1.850	1058.3	1020	109	962
44	5-Norbornene-2-carboxaldehyde	C8H10O	776 , 1.640	1191.5	973	66	821
45	Benzaldehyde	C7H6O	416 , 1.740	966.84	982	106	828
46	2-Ethylbenzaldehyde	C9H10O	720 , 1.600	1152.6	1195	133	836
47	Salicylaldehyde	C7H6O2	576 , 1.580	1052.5	1203	122	928
48	4-Ethylbenzaldehyde	C9H10O	744 , 1.670	1169.3	1195	105	862
49	Anisic aldehyde	C8H8O2	876 , 1.850	1263.4	1171	135	825
50	Phenylacetaldehyde	C8H8O	572 , 1.680	1049.8	1081	91	874
51	Trans-Cinnamaldehyde	C9H8O	900 , 1.860	1280.7	1189	131	798
52	Cis-4-Decenal	C10H18O	788 , 1.510	1199.8	1212	41	901
53	(Z)-4-Undecenal	C11H20O	928 , 1.490	1300.7	1123	84	864
54	Dodecyl aldehyde	C12H24O	1072 , 1.470	1410.3	1402	82	943
55	Furfural	C5H4O2	300 , 1.550	859.88	831	66	953
56	Heptaldehyde	C7H14O	376 , 1.480	906.8	905	70	933
57	Caproaldehyde	C6H12O	260 , 3.950	817.89	806	56	907
58	1-Nonanal	C9H18O	656 , 1.600	1108.1	1104	98	824
59	Octanal	C8H16O	512 , 1.560	1008.1	1005	57	865
60	Valeraldehyde	C5H10O	200 , 0.530	718.45	707	41	827
61	(E)-4-Undecenal	C11H20O	1120 , 2.290	1449.2	1158	84	773
62	Undecanal	C11H22O	940 , 1.490	1309.8	1303	56	954
63	Trans-2-Octenoic acid	C8H14O2	820 , 1.570	1222.9	1199	73	906
64	2-Hydroxycinnamic acid	C9H8O3	1120 , 2.170	1449.1	1577	118	903
65	Acetic acid glacial	C2H4O2	188 , 3.060	763.38	576	59	896
66	Benzoic acid	C7H6O2	904 , 1.260	1219.9	1150	105	767
67	(3R,4S)-1-Benzoyl-3-(1-methoxy-1-methylethoxy)-4-phenyl-2-azetidinone	C4H8O2	376 , 1.100	807.2	2640	60	788
68	Isovaleric acid	C5H10O2	344 , 1.230	878.33	811	74	812
69	Geranic acid	C10H16O2	1016 , 1.450	1367.3	1342	69	829
70	Heptanoic acid	C7H14O2	620 , 1.480	1083	1073	60	927
71	Hexanoic acid	C6H12O2	520 , 1.600	1013.7	974	60	906
72	Capric acid	C10H20O2	1020 , 1.550	1403.8	1372	129	824
73	Nonanoic acid	C9H18O2	892 , 1.430	1283.4	1272	60	883
74	Octanoic acid	C8H16O2	764 , 1.490	1183.1	1173	60	929
75	Valeric acid	C5H10O2	396 , 1.260	889.72	875	60	916
76	Propionic acid	C3H6O2	244 , 1.030	730.15	676	74	897
77	Trans-2-Decenoic acid	C10H18O2	1020 , 1.490	1370.4	1380	86	817
78	Delta-Nonalactone	C9H16O2	1052 , 2.380	1395.3	1304	99	836

No.	Compound	Formula	R.T. (s)	RI	RI*	Unique mass	Match
79	Gamma-Octanoic lactone	C8H14O2	872 , 2.460	1261	1184	85	882
80	4-Hexanolide	C6H10O2	584 , 2.660	1058.8	986	85	926
81	G-Decalactone	C10H18O 2	1148 , 2.220	1471.5	1383	85	817
82	4-hydroxyoxolan-2-one	C4H6O3	736 , 2.610	1164.4	879	44	834
83	4-Heptanolide	C7H12O2	724 , 2.580	1156	1085	85	871
84	Dihydroactinidiolide	C11H16O 2	1232 , 2.850	1541.4	1426	111	845
85	δ -Lauro lactone	C12H22O 2	1428 , 2.070	1712.7	1602	99	882
86	5-Hexanolide	C6H10O2	644 , 2.840	1100.6	1006	42	856
87	5-Decanolide	C10H18O 2	1180 , 2.270	1497	1404	99	846
88	5-Hydroxyoctanoic acid lactone	C8H14O2	912 , 2.500	1289.8	1205	99	867
89	(3Z)-3-Hexenyl benzoate	C13H16O 2	1276 , 1.430	1577.4	1565	67	840
90	Vinyl acetate	C4H6O2	344 , 1.940	878.99	576	43	881
91	Hexyl benzoate	C13H18O 2	1284 , 1.430	1584.2	1557	105	863
92	Butyl benzoate	C11H14O 2	1032 , 1.490	1379.5	1359	105	915
93	Dibutyl phthalate	C16H22O 4	1680 , 1.600	1958.5	2037	149	938
94	Diethyl phthalate	C12H14O 4	1292 , 1.760	1591.2	1639	149	907
95	Dimethyl phthalate	C10H10O 4	1124 , 1.880	1452.1	1440	163	896
96	Heptylformiat	C8H16O2	544 , 1.440	1030.2	1081	70	929
97	Methyl isoheptadecanoate	C18H36O 2	1444 , 1.310	1727	1914	74	784
98	Pentyl hexanoate	C11H22O 2	912 , 1.380	1289	1282	43	874
99	Methyl salicylate	C8H8O3	788 , 1.560	1199.8	1281	120	930
100	Hexanoic acid vinyl ester	C8H14O2	592 , 1.820	1063.8	974	99	864
101	Methyl 14-Methyl pentadecanoate	C17H34O 2	1648 , 1.290	1925.2	1814	74	885
102	Cis-4-Decene	C10H20	1044 , 1.140	1388.3	1023	70	797
103	Decane	C10H22	648 , 1.110	1536.5	1015	57	908
104	3-Methyldecane	C11H24	1060 , 1.140	1400.4	1051	57	887
105	Dodecane	C12H26	792 , 1.120	1502.7	1214	57	936
106	Heptane	C7H16	204 , 3.000	723.67	717	70	776
107	1-Chloroheptane	C7H15Cl	452 , 1.240	1066.2	942	91	851
108	N-Octane	C8H18	372 , 3.400	809.05	816	43	813
109	1,2-Epoxyheptane	C7H14O	380 , 1.350	909.7	807	58	853
110	1-Chloropentane	C5H11Cl	232 , 3.220	763.19	743	70	872
111	1-Nitropropane	C3H7NO2	204 , 2.420	722.86	701	43	840
112	n-Tridecane	C13H28	932 , 1.130	1303.4	1313	57	908
113	3-Methyltridecane	C14H30	1024 , 1.140	1373.1	1349	57	879

No.	Compound	Formula	R.T. (s)	RI	RI*	Unique mass	Match
114	1-Octen-3-one	C8H14O	476 , 1.530	981.75	943	70	819
115	2(5H)-Furanone	C4H4O2	400 , 2.640	925.65	807	55	948
116	Beta-Angelica Lactone	C5H6O2	432 , 2.700	949.66	868	55	845
117	2-Cyclohexen-1-one	C6H8O	420 , 1.840	940.03	873	68	945
118	2-Cyclopentenone	C5H6O	304 , 1.690	841.34	753	82	897
119	2-Decanone	C10H20O	780 , 1.590	1194.3	1151	58	872
120	2-Dodecanone	C12H24O	1180 , 1.490	1496.4	1350	58	872
121	2-Heptanone	C7H14O	364 , 1.520	897.31	853	58	937
122	3-Methyl-5-Hexanone	C7H14O	492 , 1.610	993.79	799	58	798
123	2-Hexanoylfuran	C10H14O 2	792 , 1.670	1202.8	1275	110	871
124	Alpha-Pyrone	C5H4O2	476 , 2.310	982.33	909	68	894
125	5-Hydroxy-2-Decenoic acid Lactone	C10H16O 2	1160 , 2.300	1481.1	1386	97	852
126	Delta-Heptalactone	C7H12O2	776 , 2.640	1192.2	1105	99	813
127	2-N-Hexylcyclopentanone	C11H20O	704 , 1.660	1141.5	1329	84	836
128	2-Nonanone	C9H18O	636 , 1.620	1094.2	1052	58	894
129	Hydroxyacetone	C3H6O2	212 , 3.500	735.57	698	43	904
130	3-Decanone	C10H20O	772 , 1.530	1188.7	1151	57	848
131	3-Nonen-2-one	C9H16O	704 , 1.760	1141.6	1060	55	860
132	3-Octen-2-One	C8H14O	560 , 1.790	1041.6	960	55	907
133	Trans-3-Penten-2-one	C5H8O	220 , 1.400	743.84	662	69	893
134	3-Tridecanone	C13H26O	1172 , 1.450	1490	1499	72	804
135	4-Cyclopentene-1,3-Dione	C5H4O2	356 , 2.010	890.28	958	96	883
136	2,3-Dihydro-3,5-dihydroxy-6-methyl-4(H)-pyran-4-one	C6H8O4	716 , 1.580	1149.8	1269	101	842
137	4-Octanone	C8H16O	468 , 1.520	975.75	952	58	795
138	6,10-Dimethyl-5,9-undecadien-2-one	C13H22O	1120 , 1.510	1448.6	1446	43	823
139	2-Methylacetophenone	C9H10O	776 , 1.750	1191.6	1142	119	839
140	Levogluosenone	C6H6O3	668 , 2.220	1116.8	993	98	816
141	3-Hydroxy-2-methyl-4H-pyran-4-one	C6H6O3	668 , 1.900	1116.6	1063	126	840
142	4'-Hydroxypropiophenone	C9H10O2	912 , 1.730	1289.3	1349	121	828
143	Ethyl-O-Tolyl ketone	C10H12O	876 , 1.640	1263.3	1257	119	813
144	4-(2,6,6-Trimethyl-1-cyclohexenyl)-3-buten-2-one	C13H20O	1168 , 1.680	1487	1556	177	834
145	Ocimene	C10H16	572 , 1.170	1049.5	976	93	864
146	1-Decene	C10H20	968 , 1.510	1331	1005	140	825
147	(+)- $\alpha$ -funebrene	C15H24	1096 , 1.240	1429.2	999	119	845
148	1-(2-methyl-1-cyclopentenyl)ethanone	C8H12O	656 , 1.890	1108.3	996	109	856
149	4-Chlorophenol	C6H5ClO	796 , 1.370	1205.5	1081	128	861
150	2-Ethyl-6-Methylphenol	C9H12O	580 , 1.250	1055.1	1227	121	798

No.	Compound	Formula	R.T. (s)	RI	RI*	Unique mass	Match
151	1-(2-Furyl)Butan-1-one	C8H10O2	648 , 1.680	1102.6	1077	110	865
152	2-Methyl-5-Propionyl-Furan	C8H10O2	600 , 1.520	1069.1	1067	109	823
153	5-Methyl-2-acetylfuran	C7H8O2	1000 , 1.460	1355.2	967	109	832
154	2-Butylfuran	C8H12O	360 , 3.670	895.58	941	81	903
155	2-N-Heptylfuran	C11H18O	780 , 1.220	1194	1239	81	918
156	3-Acetyl-2,5-Dimethylfuran	C8H10O2	680 , 1.840	1172.3	1057	123	796
157	Dibenzofuran	C12H8O	1220 , 1.460	1530	1483	168	864
158	2-Ethylbenzofuran	C10H10O	920 , 1.430	1294.8	1207	131	852
159	2-(2-Propenyl)furan	C7H8O	544 , 1.870	1030.5	1460	77	834
160	2-Ethylfuran	C6H8O	200 , 3.070	718.17	742	81	816
161	2-Ethyl-5-Methyl Furan	C7H10O	388 , 1.730	915.98	831	110	843
162	2-Hexylfuran	C10H16O	636 , 1.220	1093.9	1139	81	882
163	2-Pentylfuran	C9H14O	492 , 1.200	993.48	1040	53	776
164	2-Propylfuran	C7H10O	552 , 1.720	1008.2	841	110	861
165	2,3-Dimethylmaleic anhydride	C6H6O3	552 , 3.010	1036.9	1158	54	910
166	Butylbenzene	C10H14	592 , 1.230	1063.4	1092	134	895
167	Phenylpentane	C11H16	732 , 1.250	1160.7	1191	92	811
168	Butyric anhydride	C8H14O3	336 , 3.680	873.13	1120	71	879
169	1,7-Dimethylnaphthalene	C12H12	1096 , 1.430	1429.4	1458	141	897
170	1-Methylnaphthalene	C11H10	936 , 1.430	1306.7	1345	142	911
171	O-Cymene	C10H14	544 , 1.190	1030	1042	119	917
172	2-N-Hexylthiophene	C10H16S	884 , 1.250	1268.8	1292	97	855
173	2-N-Pentylthiophene	C9H14S	740 , 1.250	1166.2	1192	97	867

RI: retention time; RI\*:RI in NIST

Table S2 The relative content of volatiles in six infant formula(n=3).

No.	Compound	Infant formula											
		1		2		3		4		5		6	
1	3-methyl-1-butanol	98.23	± 4.07	10.82	± 0.30	ND		76.29	± 1.27	20.75	± 0.20	94.21	± 4.43
2	2-ethyl-1-decanol	102.05	± 4.53	ND		369.87	± 10.38	ND		ND		ND	
3	1-heptanol	105.01	± 6.63	80.98	± 2.87	50.40	± 2.36	32.12	± 0.93	31.92	± 0.09	26.70	± 0.36
4	1-hexadecanol	101.67	± 2.57	151.3 <sub>8</sub>	± 1.41	123.40	± 4.07	125.64	± 1.78	57.92	± 1.40	89.80	± 1.67
5	1-octanol	101.04	± 3.16	94.66	± 3.22	70.19	± 0.72	3.75	± 0.01	2.57	± 0.04	21.78	± 0.08
6	1-octen-3-ol	101.67	± 2.49	96.84	± 0.87	64.91	± 1.16	46.28	± 1.59	45.53	± 0.41	47.90	± 1.50
7	1-pentanol	100.24	± 1.39	83.54	± 1.54	51.39	± 1.16	69.57	± 0.88	ND		70.66	± 1.32
8	2,4-decadien-1-OL	91.65	± 9.73	62.01	± 2.12	13.51	± 0.73	65.47	± 1.42	36.28	± 1.50	21.78	± 1.10
9	Trans-2-Decen-1-OL	104.39	± 4.79	77.26	± 2.89	40.67	± 0.35	56.68	± 1.78	57.68	± 1.98	55.81	± 1.11
10	Furfuryl alcohol	109.12	± 9.82	108.5 <sub>1</sub>	± 0.40	118.99	± 5.47	151.03	± 2.89	62.84	± 1.38	63.34	± 2.03
11	3-octanol	97.09	± 3.79	71.81	± 3.44	ND		99.92	± 3.92	127.67	± 5.69	126.60	± 0.95
12	4-ethylcyclohexanol	109.43	± 10.8 <sub>5</sub>	99.18	± 3.52	8.41	± 0.16	21.19	± 0.43	133.32	± 0.71	7.90	± 0.14
13	Cis-4-Heptenal	96.93	± 4.79	74.85	± 1.88	38.89	± 0.35	102.96	± 3.24	18.84	± 0.65	156.99	± 1.21
14	(R)-(+)-2-methyl-1-phenyl-1-propanol	107.23	± 7.43	ND		ND		44.45	± 1.60	ND		19.31	± 0.79

No.	Compound	Infant formula											
		1		2		3		4		5		6	
15	2-methylcyclohexanol	99.09	± 4.00	67.24	± 1.52	9.51	± 0.23	8.31	± 0.19	85.35	± 2.41	3.27	± 0.13
16	Phenethyl alcohol	98.27	± 3.71	44.66	± 0.70	28.44	± 0.16	21.67	± 0.02	17.37	± 0.15	13.19	± 0.26
17	Dimethylsilanediol	94.35	± 6.11	ND		ND		ND		57.56	± 1.59	19.62	± 0.68
18	N-formylpiperidine	92.51	± 8.58	281.9 <sub>1</sub>	± 7.78	310.52	± 3.25	132.22	± 2.88	94.98	± 1.44	88.87	± 1.25
19	Gamma-nonanolactone	96.18	± 4.96	98.64	± 4.19	28.46	± 0.59	38.43	± 0.56	40.97	± 0.28	39.88	± 1.00
20	Trans, Trans -2,4-decadienal	104.52	± 4.80	4068.08	± 154.6 <sub>8</sub>	373.78	± 10.86	742.96	± 7.42	706.51	± 7.37	494.01	± 21.1 <sub>2</sub>
21	(2E,4E)-2,4-decanedial	102.66	± 3.28	23.74	± 0.72	1.84	± 0.02	3.33	± 0.15	3.50	± 0.14	2.58	± 0.07
22	(E,E)-2,4-dodecadienal	103.88	± 4.18	48.28	± 0.88	10.14	± 0.15	18.09	± 0.38	13.32	± 0.05	10.58	± 0.16
23	Trans,trans-2,4-heptadienal	97.20	± 4.25	0.05	± 0.00	43.63	± 1.49	51.98	± 2.56	41.22	± 0.51	28.24	± 0.45
24	(E,E)-2,4-hexadienal	102.86	± 4.67	119.9 <sub>3</sub>	± 2.99	54.54	± 0.69	46.54	± 0.90	19.06	± 0.05	7.10	± 0.17
25	Trans,trans-2,4-nonadienal	103.45	± 3.39	860.2 <sub>2</sub>	± 13.91	363.94	± 14.02	493.60	± 17.9 <sub>4</sub>	384.99	± 7.80	192.71	± 4.31
26	(2E,4E)-2,4-octadienal	102.42	± 3.79	83.23	± 3.71	33.94	± 1.54	36.10	± 0.76	25.07	± 0.02	19.37	± 0.36
27	Crotonaldehyde	97.56	± 4.96	102.9 <sub>6</sub>	± 2.90	91.82	± 1.58	48.35	± 1.80	ND		ND	
28	Trans-2-dodecenal	104.09	± 5.28	57.36	± 1.72	4.70	± 0.14	18.08	± 0.37	10.81	± 0.06	7.52	± 0.18

No.	Compound	Infant formula											
		1		2		3		4		5		6	
29	5-methyl furfural	104.59	± 5.86	129.8 <sub>8</sub>	± 3.64	80.28	± 0.47	67.85	± 0.73	69.28	± 1.14	80.30	± 1.69
30	2-propyl-2-heptenal	97.49	± 3.53	443.9 <sub>0</sub>	± 4.88	142.23	± 6.44	3.54	± 0.14	122.23	± 3.03	151.97	± 1.02
31	2-ethyl-2-hexenal	96.38	± 5.16	335.4 <sub>3</sub>	± 5.30	167.10	± 7.23	77.52	± 3.90	54.85	± 0.28	0.72	± 0.00
32	(E)-2-Octenal	103.46	± 5.38	126.5 <sub>4</sub>	± 2.88	107.84	± 4.19	1101.98	± 16.9 <sub>1</sub>	ND		343.10	± 5.33
33	(E)-2-butyl-2-enal	99.55	± 0.63	301.4 <sub>1</sub>	± 3.49	ND		73.79	± 2.26	26.65	± 0.41	ND	
34	Trans-2-Pentenal	102.47	± 3.49	78.81	± 3.25	49.17	± 1.42	2.35	± 0.05	54.10	± 0.78	ND	
35	2-Furanacrolein	94.73	± 7.12	116.2 <sub>9</sub>	± 1.20	14.05	± 0.02	27.83	± 1.16	475.44	± 1.64	13.17	± 0.65
36	2-Pyridinecarboxaldehyde	97.54	± 3.47	1154.75	± 13.94	3121.38	± 71.04	47.01	± 1.89	37.96	± 0.62	23.91	± 1.23
37	2-Undecenal	106.59	± 8.59	123.7 <sub>3</sub>	± 0.99	29.28	± 0.42	45.41	± 0.36	17.55	± 0.04	24.36	± 0.59
38	Trans-2-Undecenal	105.34	± 7.75	95.24	± 1.03	30.87	± 0.24	23.49	± 1.07	216.41	± 5.52	ND	
39	3-Cyclohexene-1-carboxaldehyde	108.69	± 9.17	97.04	± 1.94	37.15	± 0.34	ND		1360.34	± 55.96	ND	
40	3-Furaldehyde	92.16	± 8.19	666.3 <sub>6</sub>	± 11.25	ND		ND		ND		17.21	± 0.69
41	3-Hexen-2-One	98.64	± 1.91	95.04	± 4.69	38.71	± 0.18	ND		126.83	± 0.55	ND	



No.	Compound	Infant formula											
		1		2		3		4		5		6	
42	Trans-4-Nonenal	99.80	± 3.98	91.44	± 0.85	29.87	± 0.66	ND		90.35	± 3.32	ND	
43	5-ethyl-2-furaldehyde	94.86	± 8.93	146.0 <sub>9</sub>	± 7.04	78.90	± 2.73	13.65	± 0.14	15.21	± 0.70	10.79	± 0.37
44	5-Norbornene-2-carboxaldehyde	107.92	± 7.45	55.76	± 2.53	14.19	± 0.49	9.18	± 0.17	ND		16.76	± 0.36
45	Benzaldehyde	98.98	± 2.23	75.88	± 1.81	98.90	± 3.05	106.49	± 3.68	82.58	± 0.50	77.84	± 0.92
46	2-Ethylbenzaldehyde	98.88	± 3.23	139.5 <sub>8</sub>	± 0.85	99.87	± 0.17	94.95	± 3.77	50.57	± 2.29	84.16	± 0.41
47	Salicylaldehyde	102.15	± 3.55	100.1 <sub>1</sub>	± 1.28	50.55	± 0.18	46.46	± 1.76	25.42	± 0.47	38.11	± 1.48
48	4-Ethylbenzaldehyde	102.45	± 3.77	110.1 <sub>1</sub>	± 2.13	31.83	± 0.50	84.49	± 1.42	121.25	± 1.75	41.19	± 0.38
49	Anisic aldehyde	96.24	± 4.38	154.1 <sub>6</sub>	± 4.76	118.52	± 2.93	411.74	± 10.8 <sub>3</sub>	10.76	± 0.42	202.67	± 1.53
50	Phenylacetaldehyde	97.58	± 3.40	40.76	± 0.57	22.77	± 0.76	ND		11.02	± 0.01	ND	
51	Trans-Cinnamaldehyde	98.78	± 3.28	152.1 <sub>8</sub>	± 4.74	65.71	± 1.45	10.62	± 0.06	144.68	± 0.33	113.36	± 4.76
52	Cis-4-Decenal	91.20	± 2.81	26.93	± 1.02	8.05	± 0.33	373.44	± 2.32	4.64	± 0.14	61.74	± 1.57
53	(Z)-4-Undecenal	100.20	± 1.59	21.60	± 0.24	2.28	± 0.09	6.46	± 0.24	5.29	± 0.16	9.02	± 0.30
54	Dodecyl aldehyde	102.13	± 2.49	126.6 <sub>4</sub>	± 0.69	52.41	± 2.59	166.85	± 4.28	106.33	± 2.96	97.64	± 0.78

No.	Compound	Infant formula														
		1		2		3		4		5		6				
55	Furfural	102.58	± 4.80	ND		ND		ND		ND		209.17	± 10.5	6		
56	Heptaldehyde	92.03	± 8.70	80.46	± 1.39	61.82	± 1.02	19.88	± 0.54	31.98	± 1.12	36.75	± 1.03			
57	Caproaldehyde	97.82	± 4.93	ND		ND		75.68	± 0.53	110.21	± 4.09	ND				
58	1-Nonanal	91.09	± 9.12	68.43	± 1.91	71.46	± 2.25	52.48	± 0.14	60.65	± 0.90	53.67	± 0.09			
59	Octanal	100.03	± 3.76	71.88	± 0.31	31.55	± 1.32	53.62	± 2.27	61.95	± 2.16	52.93	± 2.24			
60	Valeraldehyde	98.63	± 3.28	52.82	± 0.70	30.97	± 0.69	49.12	± 1.29	41.05	± 1.11	34.33	± 1.31			
61	(E)-4-Undecenal	102.95	± 2.53	96.20	± 3.50	24.28	± 0.12	31.10	± 1.35	24.38	± 0.45	18.63	± 0.10			
62	Undecanal	102.23	± 5.50	121.5	± 0.17	2	± 0.72	53.13	± 0.72	100.04	± 3.29	70.40	± 0.23	72.21	± 1.85	
63	Ttrans-2-Octenoic acid	99.71	± 4.45	93.35	± 4.35	1.67	± 0.01	40.63	± 1.23	8.56	± 0.32	17.65	± 0.26			
64	2-Hydroxycinnamic acid	107.89	± 7.90	67.31	± 2.28	27.51	± 0.40	570.04	± 23.4	6	± 0.68	40.74	± 0.68	494.75	± 14.3	7
65	Acetic acid glacial	94.75	± 6.74	26.16	± 0.69	3.69	± 0.08	ND		103.90	± 3.20	ND				
66	Benzoic acid	97.80	± 4.69	13.15	± 0.39	13.61	± 0.39	28.75	± 1.54	70.81	± 2.44	ND				
67	(3R,4S)-1-Benzoyl-3-(1-methoxy-1-methylethoxy)-4-phenyl-2-azetidinone	102.55	± 4.75	219.7	± 2.40	5	± 3.62	158.01	± 3.62	78.73	± 0.00	39.83	± 0.21	104.69	± 1.00	
68	Isovaleric acid	102.35	± 3.29	113.6	± 2.41	ND		21.96	± 1.00	64.27	± 0.44	ND				

No.	Compound	Infant formula									
		1	2	3	4	5	6				
69	Geranic acid	104.27 ± 5.20	142.0 <sub>9</sub> ± 6.56	ND	50.07 ± 1.53	52.09 ± 1.39	ND				
70	Heptanoic acid	102.37 ± 3.27	246.3 <sub>8</sub> ± 6.58	133.64 ± 5.97	241.42 ± 10.9 <sub>2</sub>	67.04 ± 1.59	105.13 ± 4.76				
71	Hexanoic acid	96.87 ± 4.07	194.4 <sub>3</sub> ± 5.23	25.12 ± 0.88	ND	ND	112.08 ± 3.46				
72	Capric acid	102.72 ± 4.22	80.37 ± 0.86	34.33 ± 1.68	129.12 ± 3.22	ND	110.78 ± 5.61				
73	Nonanoic acid	92.50 ± 8.65	ND	ND	ND	7.83 ± 0.26	ND				
74	Octanoic acid	102.61 ± 4.75	92.52 ± 2.76	68.87 ± 2.47	ND	ND	ND				
75	Valeric acid	102.93 ± 4.98	114.7 <sub>8</sub> ± 3.79	43.37 ± 0.70	60.18 ± 1.38	42.80 ± 0.17	ND				
76	Propionic acid	102.66 ± 3.26	ND	ND	ND	ND	ND				
77	Trans-2-Decenoic acid	97.97 ± 3.08	ND	230.69 ± 8.64	ND	ND	ND				
78	Delta-Nonalactone	102.00 ± 4.37	94.05 ± 4.42	16.40 ± 0.06	32.41 ± 1.49	29.73 ± 1.37	26.06 ± 0.32				
79	Gamma-Octanoic lactone	106.70 ± 5.76	88.62 ± 0.16	25.77 ± 0.35	54.98 ± 1.90	51.10 ± 1.89	50.94 ± 1.83				
80	4-Hexanolide	96.45 ± 4.15	125.4 <sub>0</sub> ± 5.75	61.44 ± 0.74	65.93 ± 1.90	60.54 ± 0.41	64.56 ± 0.70				
81	G-Decalactone	101.05 ± 2.93	179.7 <sub>6</sub> ± 8.12	44.00 ± 1.44	204.78 ± 2.32	128.99 ± 4.33	114.41 ± 0.38				
82	4-hydroxyoxolan-2-	102.58 ± 2.75	ND	ND	ND	ND	ND				

No.	Compound	Infant formula											
		1		2		3		4		5		6	
	one												
83	4-Heptanolide	100.99	± 4.59	155.7 9	± 0.76	74.33	± 1.18	63.78	± 0.26	54.67	± 0.33	56.34	± 1.73
84	Dihydroactinidiolide	96.61	± 4.43	124.1 9	± 1.68	87.35	± 3.61	154.85	± 5.06	186.91	± 6.36	196.38	± 6.92
85	δ-Laurolactone	102.39	± 3.79	193.8 5	± 3.17	7.02	± 0.24	138.40	± 4.29	22.09	± 0.37	107.37	± 3.22
86	5-Hexanolide	97.21	± 3.77	118.7 7	± 4.15	83.90	± 0.03	104.97	± 4.08	97.22	± 2.91	23.73	± 0.52
87	5-Decanolide	101.13	± 1.90	154.8 6	± 1.01	93.71	± 2.81	142.52	± 6.42	ND		90.67	± 1.73
88	5-Hydroxyoctanoic acid lactone	98.28	± 4.84	ND		ND		ND		50.46	± 1.48	48.26	± 1.94
89	(3Z)-3-Hexenyl benzoate	99.85	± 1.38	41.12	± 0.22	ND		45.74	± 1.65	ND		58.26	± 0.85
90	Vinyl acetate	102.89	± 4.27	ND		ND		91.88	± 2.58	109.42	± 1.41	79.61	± 3.54
91	Hexyl benzoate	102.45	± 4.65	52.92	± 1.19	ND		84.99	± 4.19	121.25	± 4.29	69.49	± 2.74
92	Butyl benzoate	96.56	± 4.90	176.5 9	± 7.12	80.66	± 1.89	154.44	± 4.65	13.51	± 0.60	140.55	± 5.96
93	Dibutyl phthalate	103.76	± 4.67	49.92	± 1.67	20.37	± 0.43	578.36	± 0.53	70.15	± 3.18	288.02	± 7.93
94	Diethyl phthalate	102.78	± 3.65	147.5 0	± 6.36	66.50	± 2.60	179.76	± 1.05	55.66	± 0.26	102.05	± 3.00
95	Dimethyl phthalate	101.08	± 2.84	151.4 6	± 6.19	58.48	± 0.86	85.21	± 3.62	79.71	± 1.41	57.28	± 2.53

No.	Compound	Infant formula											
		1		2		3		4		5		6	
96	Heptylformiat	92.64	± 8.35	36.17	± 0.67	19.06	± 0.71	37.08	± 0.96	29.34	± 0.50	22.74	± 0.51
97	Methyl isoheptadecanoate	97.14	± 4.06	815.6 <sub>1</sub>	± 29.34	107.65	± 2.81	125.41	± 5.70	ND		48.13	± 0.14
98	Pentyl hexanoate	103.25	± 5.69	71.06	± 0.68	ND		ND		ND		ND	
99	Methyl salicylate	95.63	± 5.81	38.57	± 0.06	19.85	± 0.17	291.43	± 7.44	113.98	± 4.79	8.87	± 0.27
100	Hexanoic acid vinyl ester	94.61	± 8.97	111.6 <sub>7</sub>	± 4.39	26.31	± 0.92	42.41	± 1.32	36.72	± 0.64	32.06	± 0.60
101	Methyl 14-Methyl pentadecanoate	104.22	± 5.56	67.87	± 1.63	22.80	± 0.53	40.23	± 0.07	20.25	± 0.22	17.38	± 0.88
102	Cis-4-Decene	102.49	± 2.64	306.4 <sub>9</sub>	± 7.18	230.05	± 1.86	4.63	± 0.16	6.97	± 0.03	2.50	± 0.03
103	Decane	101.81	± 3.83	239.1 <sub>8</sub>	± 10.63	309.59	± 5.01	252.31	± 4.31	45.95	± 1.90	137.54	± 4.78
104	3-Methyldecane	103.21	± 4.01	354.6 <sub>1</sub>	± 10.48	256.41	± 8.23	85.00	± 0.21	16.82	± 0.16	42.70	± 1.34
105	Dodecane	99.95	± 1.31	244.1 <sub>6</sub>	± 8.29	156.18	± 1.54	87.80	± 2.20	143.98	± 2.73	92.18	± 1.79
106	Heptane	96.98	± 4.27	42.72	± 1.89	34.92	± 1.20	ND		ND		23.06	± 0.17
107	1-Chloroheptane	99.03	± 3.45	ND		ND		92.69	± 0.59	105.95	± 1.14	ND	
108	N-Octane	98.82	± 3.74	22.53	± 0.69	1.24	± 0.06	1.38	± 0.01	ND		3.47	± 0.07
109	1,2-Epoxyheptane	104.30	± 4.25	25.60	± 0.22	11.08	± 0.15	22.57	± 0.16	ND		ND	

No.	Compound	Infant formula											
		1		2		3		4		5		6	
110	1-Chloropentane	102.12	± 4.42	45.11	± 0.51	20.68	± 0.77	35.99	± 0.32	41.62	± 0.32	39.81	± 1.52
111	1-Nitropropane	99.63	± 1.14	ND		ND		ND		ND		ND	
112	n-Tridecane	104.12	± 4.57	195.7 <sub>8</sub>	± 0.27	289.42	± 3.85	270.57	± 8.34	134.81	± 0.65	198.79	± 8.58
113	3-Methyltridecane	97.76	± 2.76	360.6 <sub>5</sub>	± 9.52	567.85	± 2.54	459.50	± 5.91	176.04	± 2.43	308.06	± 10.3 <sub>3</sub>
114	1-Octen-3-one	102.73	± 4.13	102.2 <sub>1</sub>	± 0.80	127.28	± 3.79	148.68	± 4.38	138.64	± 1.77	163.55	± 4.27
115	2(5H)-Furanone	98.77	± 2.69	ND		ND		ND		ND		ND	
116	Beta-Angelica Lactone	101.76	± 4.98	ND		ND		ND		ND		ND	
117	2-Cyclohexen-1-one	97.32	± 3.39	60.02	± 1.54	38.66	± 0.76	25.65	± 0.71	26.48	± 0.49	17.87	± 0.24
118	2-Cyclopentenone	101.14	± 2.21	60.07	± 1.33	20.49	± 0.73	63.19	± 1.48	87.69	± 0.43	115.67	± 5.21
119	2-Decanone	100.08	± 0.53	87.31	± 0.26	45.22	± 1.45	70.89	± 0.42	63.56	± 0.33	92.91	± 0.95
120	2-Dodecanone	99.79	± 4.81	144.6 <sub>3</sub>	± 4.94	83.14	± 2.71	97.67	± 2.18	26.44	± 1.02	29.42	± 0.54
121	2-Heptanone	107.54	± 8.02	85.17	± 0.17	45.33	± 1.54	52.41	± 2.38	149.30	± 2.14	156.50	± 0.63
122	3-Methyl-5-Hexanone	97.06	± 3.87	109.4 <sub>9</sub>	± 0.40	81.77	± 3.99	96.21	± 3.98	31.17	± 0.88	27.82	± 0.85
123	2-Hexanoylfuran	98.99	± 4.09	122.8 <sub>9</sub>	± 3.24	16.99	± 0.19	36.52	± 0.53	94.17	± 5.01	99.57	± 0.90
124	Alpha-Pyrone	102.27	± 4.34	227.3	± 1.01	24.13	± 0.89	65.03	± 0.62	93.65	± 1.88	53.84	± 0.12

No.	Compound	Infant formula											
		1		2		3		4		5		6	
				4									
125	5-Hydroxy-2-Decenoic acid Lactone	92.85	± 9.42	303.6 6	± 13.67	154.20	± 1.86	114.66	± 3.05	29.27	± 1.04	95.29	± 3.20
126	Delta-Heptalactone	101.46	± 2.00	122.1 9	± 4.56	69.85	± 0.41	106.34	± 3.46	83.48	± 3.49	26.05	± 0.48
127	2-N-Hexylcyclopentanone	93.78	± 8.30	59.27	± 2.28	15.86	± 0.53	14.97	± 0.30	58.36	± 1.20	59.43	± 2.00
128	2-Nonanone	103.34	± 4.00	118.2 0	± 0.86	108.18	± 2.41	69.99	± 0.72	604.32	± 21.28	82.84	± 1.45
129	Hydroxyacetone	101.73	± 2.16	ND		ND		113.93	± 5.09	16.42	± 0.10	41.28	± 1.32
130	3-Decanone	97.22	± 3.91	145.3 2	± 7.27	36.86	± 1.50	272.94	± 1.58	15.76	± 0.16	ND	
131	3-Nonen-2-one	102.41	± 3.32	160.0 3	± 5.07	72.33	± 1.36	ND		120.38	± 1.66	ND	
132	3-Octen-2-One	106.22	± 8.73	153.1 9	± 5.77	177.06	± 5.37	69.92	± 0.54	16.19	± 0.66	108.29	± 3.92
133	trans-3-Penten-2-one	96.39	± 5.68	223.0 2	± 5.60	81.11	± 1.55	51.21	± 1.69	807.65	± 20.07	21.38	± 0.94
134	3-Tridecanone	97.68	± 4.35	33.69	± 0.79	27.69	± 1.10	745.47	± 21.6 8	22.13	± 0.87	728.02	± 15.3 8
135	4-Cyclopentene-1,3-Dione	102.50	± 2.90	191.0 7	± 7.20	223.76	± 8.91	21.26	± 0.05	10.29	± 0.20	42.00	± 1.27
136	2,3-Dihydro-3,5-dihydroxy-6-	103.03	± 3.75	155.3	± 0.63	123.30	± 1.69	16.73	± 0.86	ND		13.16	± 0.37

No.	Compound	Infant formula									
		1	2	3	4	5	6				
			8								
137	methyl-4(H)-pyran-4-one 4-Octanone	94.62 ± 6.72	57.25 ± 0.40	ND	140.25 ± 4.69	62.54 ± 0.12	103.34 ± 2.51				
138	6,10-Dimethyl-5,9-undecadien-2-one	98.07 ± 4.27	91.74 ± 0.81	66.37 ± 2.06	77.70 ± 2.72	12.06 ± 0.44	51.92 ± 0.68				
139	2-Methylacetophenone	92.44 ± 8.11	134.2 <sub>3</sub> ± 2.84	52.31 ± 1.57	25.98 ± 0.08	ND	ND				
140	Levogluconone	95.37 ± 6.75	ND	26.63 ± 1.20	316.13 ± 14.5 <sub>2</sub>	585.66 ± 12.55	ND				
141	3-Hydroxy-2-methyl-4H-pyran-4-one	95.16 ± 5.57	206.8 <sub>2</sub> ± 8.73	400.85 ± 5.10	16.98 ± 0.79	9.34 ± 0.30	643.36 ± 7.69				
142	4'-Hydroxypropiophenone	96.63 ± 4.01	159.9 <sub>9</sub> ± 0.50	45.02 ± 0.70	75.71 ± 3.71	58.91 ± 0.17	47.19 ± 1.74				
143	Ethyl-O-Tolyl ketone	96.04 ± 6.38	88.79 ± 1.91	14.54 ± 0.09	25.39 ± 0.99	18.08 ± 0.27	ND				
144	4-(2,6,6-Trimethyl-1-cyclohexenyl)-3-buten-2-one	96.96 ± 7.20	102.7 <sub>1</sub> ± 2.79	92.24 ± 4.39	162.82 ± 5.97	193.34 ± 7.02	144.08 ± 0.24				
145	Ocimene	92.43 ± 10.6 <sub>2</sub>	38.65 ± 0.87	26.50 ± 0.89	ND	ND	ND				
146	1-Decene	103.68 ± 5.92	ND	ND	ND	ND	ND				
147	(+)-Alpha-Funebrene	101.60 ± 2.09	331.8 <sub>2</sub> ± 4.46	501.33 ± 12.97	170.38 ± 1.05	80.18 ± 0.37	103.17 ± 4.73				
148	1-(2-methyl-1-cyclopentenyl)eth	99.98 ± 0.25	137.0 <sub>9</sub> ± 3.02	100.87 ± 3.22	155.84 ± 0.24	16.90 ± 0.01	115.09 ± 0.40				



No.	Compound	Infant formula									
		1	2	3	4	5	6				
	anone										
149	4-Chlorophenol	97.95 ± 4.51	202.3 <sub>7</sub> ± 0.17	ND	14.41 ± 0.72	110.49 ± 2.19	17.76 ± 0.88				
150	2-Ethyl-6-Methylphenol	96.85 ± 4.72	69.43 ± 3.53	14.43 ± 0.51	12.90 ± 0.20	20.63 ± 0.64	13.74 ± 0.01				
151	1-(2-Furyl)Butan-1-one	104.72 ± 5.45	53.69 ± 0.43	62.17 ± 1.76	62.76 ± 0.89	22.54 ± 0.81	ND				
152	2-Methyl-5-Propionyl-Furan	105.89 ± 7.45	104.2 <sub>0</sub> ± 0.52	36.80 ± 1.83	31.17 ± 0.51	22.00 ± 0.61	21.62 ± 0.90				
153	5-Methyl-2-acetylfuran	100.90 ± 1.69	116.3 <sub>7</sub> ± 2.15	12.87 ± 0.15	20.02 ± 0.44	11.08 ± 0.06	10.05 ± 0.26				
154	2-Butylfuran	103.72 ± 4.50	123.2 <sub>7</sub> ± 1.18	74.76 ± 0.43	60.69 ± 1.79	37.19 ± 1.24	28.44 ± 1.38				
155	2-N-Heptylfuran	107.87 ± 8.85	66.86 ± 1.52	25.95 ± 0.15	42.38 ± 0.05	14.72 ± 0.09	10.36 ± 0.49				
156	3-Acetyl-2,5-Dimethylfuran	91.10 ± 9.56	121.0 <sub>5</sub> ± 2.26	30.02 ± 0.10	158.42 ± 6.62	ND	182.76 ± 5.98				
157	Dibenzofuran	96.07 ± 7.90	105.7 <sub>2</sub> ± 5.24	73.03 ± 1.43	28.66 ± 0.73	265.14 ± 1.30	14.12 ± 0.09				
158	2-Ethylbenzofuran	90.92 ± 10.9 <sub>5</sub>	70.66 ± 3.58	11.50 ± 0.26	ND	ND	ND				
159	2-(2-Propenyl)furan	93.91 ± 9.21	70.91 ± 0.20	37.56 ± 0.66	31.39 ± 0.60	212.56 ± 1.70	11.84 ± 0.10				
160	2-Ethylfuran	104.40 ± 4.02	88.09 ± 3.11	31.74 ± 1.27	152.54 ± 3.54	67.90 ± 0.61	250.19 ± 0.51				
161	2-Ethyl-5-Methyl Furan	104.44 ± 5.48	127.0 <sub>7</sub> ± 1.64	118.73 ± 4.13	68.47 ± 0.18	57.76 ± 0.97	54.72 ± 0.28				

No.	Compound	Infant formula											
		1		2		3		4		5		6	
162	2-Hexylfuran	107.56	± 8.66	158.3 <sub>4</sub>	± 3.11	75.24	± 2.89	51.46	± 0.45	16.54	± 0.26	51.63	± 1.72
163	2-Pentylfuran	101.65	± 4.71	89.63	± 2.42	68.47	± 3.34	ND		491.71	± 5.88	ND	
164	2-Propylfuran	91.41	± 9.78	34.16	± 1.76	ND		39.31	± 0.64	143.71	± 1.72	929.86	± 15.4 <sub>1</sub>
165	2,3-Dimethylmaleic anhydride	108.45	± 8.88	121.3 <sub>5</sub>	± 2.34	83.33	± 0.74	115.43	± 5.26	56.25	± 2.46	46.97	± 1.06
166	Butylbenzene	95.72	± 5.17	58.19	± 0.92	25.90	± 1.00	65.30	± 3.10	29.08	± 0.74	56.83	± 2.78
167	Phenylpentane	100.87	± 1.77	105.8 <sub>9</sub>	± 3.68	50.17	± 0.23	36.56	± 1.09	ND		29.44	± 0.97
168	Butyric anhydride	109.70	± 10.1 <sub>1</sub>	ND		ND		210.00	± 7.00	168.68	± 1.82	78.06	± 4.08
169	1,7-Dimethylnaphthalene	98.67	± 4.84	342.4 <sub>6</sub>	± 11.57	202.82	± 4.97	181.37	± 3.95	80.34	± 3.02	127.35	± 4.14
170	1-Methylnaphthalene	99.41	± 3.25	262.5 <sub>6</sub>	± 2.35	206.90	± 4.00	88.67	± 2.12	85.25	± 2.52	89.90	± 1.11
171	O-Cymene	101.21	± 3.66	56.79	± 0.36	24.02	± 0.78	28.42	± 1.05	13.10	± 0.21	14.55	± 0.24
172	2-N-Hexylthiophene	95.38	± 6.24	58.32	± 3.05	651.64	± 23.14	1219.95	± 53.4 <sub>4</sub>	38.60	± 0.35	11.83	± 0.40
173	2-N-Pentylthiophene	104.98	± 5.25	58.60	± 0.48	81.95	± 2.07	55.44	± 0.29	112.71	± 3.34	97.27	± 2.62

ND: Non- detected

Table S3 Component matrix of six infant formula

No.	Compound	Principal components				
		1	2	3	4	5
1	3-methyl-1-butanol	-0.6565	-0.0343	-0.0845	0.1626	-0.1466
2	2-ethyl-1-decanol	-0.9836	-0.1337	-0.2480	0.1576	-0.1308
3	1-heptanol	-0.4502	0.4820	-0.0944	0.0865	0.1366
4	1-hexadecanol	-0.6875	-0.1223	-0.2350	-0.1145	-0.2358
5	1-octanol	-0.6013	-0.7757	-0.9892	-0.3941	0.4032
6	1-octen-3-ol	-1.0911	-0.0296	-0.1882	0.1132	-0.1136
7	1-pentanol	-0.6244	-0.0999	-0.1416	0.1000	-0.0497
8	2,4-decadien-1-OL	0.1755	0.1416	-0.2106	-0.0856	-0.0477
9	Trans-2-Decen-1-OL	-0.7293	-0.1928	-0.3401	0.2305	-0.0329
10	Furfuryl alcohol	-0.4605	-0.0716	-0.0957	0.1058	0.0086
11	3-octanol	0.6032	0.3239	0.2510	-0.2938	0.4242
12	4-ethylcyclohexanol	-0.3957	0.2391	-0.3171	0.1384	-0.0426
13	Cis-4-Heptenal	0.7332	-0.4633	-0.3485	-0.0785	0.0423
14	(R)-(+)-2-methyl-1-phenyl-1-propanol	-0.6488	-0.0916	-0.1567	0.1731	-0.1373
15	2-methylcyclohexanol	-0.4646	0.0375	0.0244	0.0958	-0.0153
16	Phenethyl alcohol	-0.2305	-0.0195	-0.0305	0.1132	0.0097
17	Dimethylsilanediol	0.5268	0.3943	0.2860	-0.1243	-0.0904
18	N-formylpiperidine	-1.0911	-0.0296	-0.1882	0.1132	-0.1136
19	Gamma-nonanolactone	-0.5239	-0.0353	-0.0473	0.1580	-0.0801
20	Trans, Trans -2,4-decadienal	-0.2414	-0.0873	-0.0629	0.1500	-0.0705
21	(2E,4E)-2,4-decanediinal	0.8647	0.4464	0.5924	-0.1497	0.6214
22	(E,E)-2,4-dodecadienal	-1.0911	-0.0296	-0.1882	0.1132	-0.1136
23	Trans,trans-2,4-heptadienal	-1.0911	-0.0296	-0.1882	0.1132	-0.1136
24	(E,E)-2,4-hexadienal	-0.6092	0.0479	-0.0664	0.0145	-0.2143
25	Trans,trans-2,4-nonadienal	11.5610	-2.7071	2.3932	4.8645	-3.4813
26	(2E,4E)-2,4-octadienal	-1.0237	-0.0469	-0.1767	0.1434	-0.1346
27	Crotonaldehyde	-0.6554	0.0537	-0.0907	-0.1406	-0.0072
28	Trans-2-dodecenal	-0.6267	-0.1554	-0.2185	0.1006	-0.2631
29	5-methyl furfural	3.5831	-0.3515	0.7728	-0.4243	-0.5535
30	2-propyl-2-heptenal	-0.6744	-0.0563	-0.1379	0.1079	-0.1527
31	2-ethyl-2-hexenal	-0.1328	0.0821	-0.1021	-0.1206	-0.1654
32	(E)-2-Octenal	-0.6718	-0.1681	-0.2204	0.1126	-0.1216
33	(E)-2-butyl-2-enal	-0.7614	-0.1230	-0.1665	0.2657	-0.2414
34	Trans-2-Pentenal	-0.6410	-0.2171	-0.3995	0.0398	-0.2687
35	2-Furanacrolein	-0.7415	-0.0804	-0.1469	0.1015	-0.0987
36	2-Pyridinecarboxaldehyde	-0.1697	0.3350	0.1691	0.1178	0.3298
37	2-Undecenal	-0.2357	0.1866	0.0004	0.1142	0.1423
38	Trans-2-Undecenal	-0.4238	0.0362	0.0046	0.0644	0.0581
39	3-Cyclohexene-1-carboxaldehyde	-0.3011	-0.0659	-0.2503	0.0272	-0.2773
40	3-Furaldehyde	-0.8760	-0.0436	-0.1431	0.1503	-0.1808
41	3-Hexen-2-One	-0.1127	0.0013	-0.0133	0.0853	0.1432
42	Trans-4-Nonenal	0.1052	0.2250	0.4502	0.1247	0.6180
43	5-ethyl-2-furaldehyde	0.7772	-0.4340	0.1921	1.0094	0.4590
44	5-Norbornene-2-	-0.3464	-0.0503	-0.2456	-0.0616	-0.2420

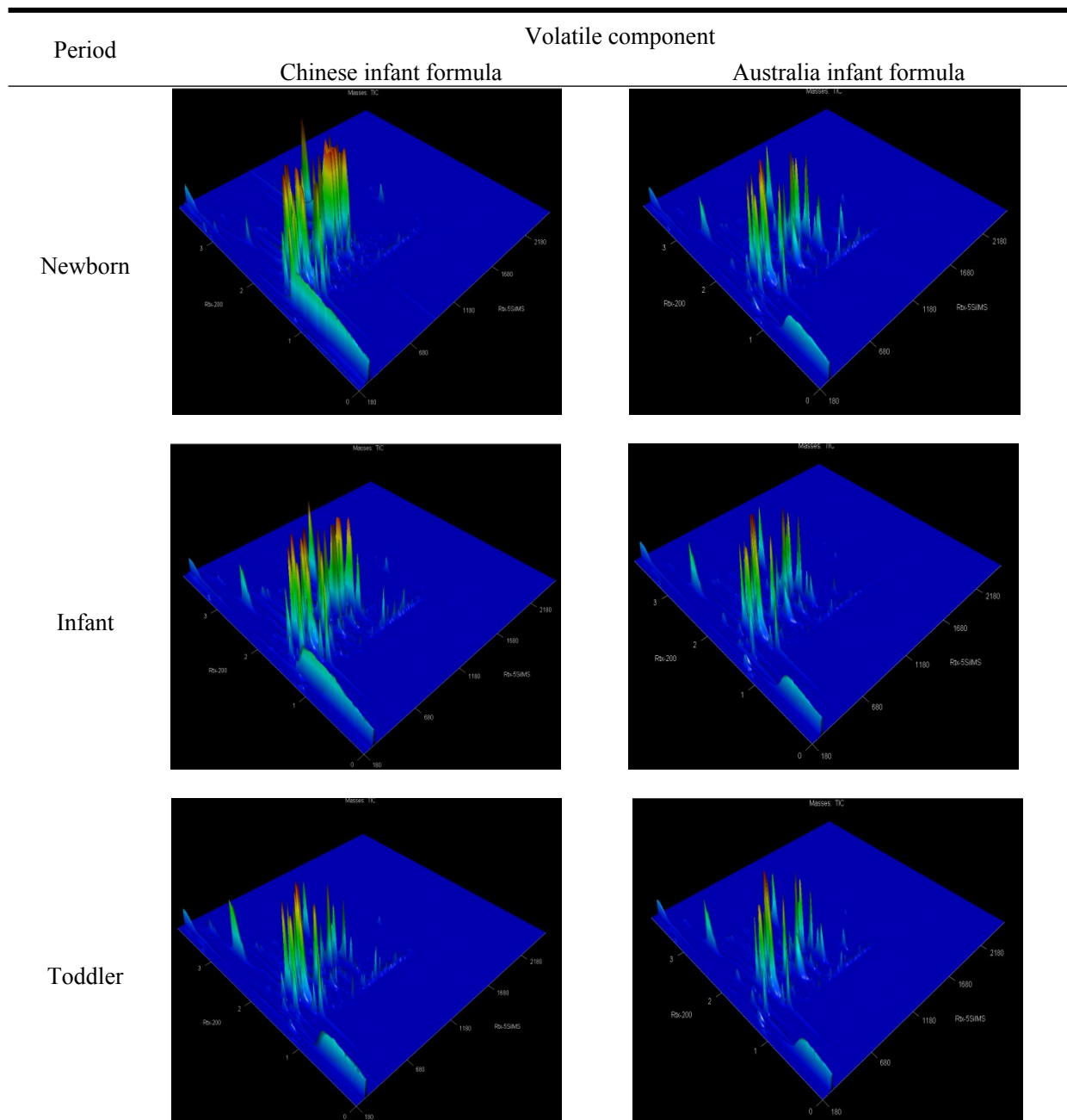
No.	Compound	Principal components				
		1	2	3	4	5
	carboxaldehyde					
45	Benzaldehyde	-0.1608	0.0942	0.2985	0.2749	0.2823
46	2-Ethylbenzaldehyde	0.0779	-0.6799	-0.2797	0.2154	-0.5151
47	Salicylaldehyde	-0.1627	-0.1352	0.1912	0.2734	-0.1438
48	4-Ethylbenzaldehyde	0.4242	-0.1434	-0.4032	0.3755	-0.1756
49	Anisic aldehyde	-0.2032	-0.1089	0.1080	-0.2079	-0.2155
50	Phenylacetaldehyde	0.0825	0.4497	-0.1231	0.2690	-0.2080
51	Trans-Cinnamaldehyde	-0.1671	-0.1514	0.0554	-0.2251	-0.2364
52	Cis-4-Decenal	0.0850	0.3576	-0.4294	0.0313	-0.1660
53	(Z)-4-Undecenal	-0.8162	0.0652	0.0739	0.1432	0.1983
54	Dodecyl aldehyde	-0.4177	-0.1436	-0.1764	0.0647	-0.1100
55	Furfural	-0.7588	-0.0458	-0.1824	0.0716	-0.1971
56	Heptaldehyde	-0.5802	0.0399	0.0575	0.2223	0.1693
57	Caproaldehyde	0.8795	-1.2972	2.9141	-1.0073	0.9962
58	1-Nonanal	3.9494	3.8046	-0.6938	-2.2128	-1.3707
59	Octanal	-0.3240	-0.2644	-0.0784	0.4454	-0.6835
60	Valeraldehyde	-0.7200	0.0161	-0.1609	0.1840	-0.2694
61	(E)-4-Undecenal	-0.8004	-0.3243	-0.0200	0.0979	-0.0799
62	Undecanal	-0.5571	0.3833	-0.1264	-0.1607	-0.1969
63	Trans-2-Octenoic acid	0.1849	-1.2284	2.5022	-0.6666	0.4945
64	2-Hydroxycinnamic acid	3.0103	3.4786	-0.2021	-0.4088	0.8241
65	Acetic acid glacial	5.7561	-8.0507	-7.2167	-2.2077	2.9532
66	Benzoic acid	-0.5886	-0.0382	-0.1617	0.1963	-0.2034
67	(3R,4S)-1-Benzoyl-3-(1-methoxy-1-methylethoxy)-4-phenyl-2-azetidinone	-0.4442	-0.6117	0.8677	-0.2224	0.0513
68	Isovaleric acid	0.4265	0.9766	-0.3005	0.3059	0.2436
69	Geranic acid	-0.6376	-0.3326	-0.3750	0.2481	-0.2774
70	Heptanoic acid	1.6389	-3.4296	7.3237	-2.3964	1.9555
71	Hexanoic acid	0.1796	0.4304	-0.2681	-0.6478	-1.1259
72	Capric acid	0.2058	-0.7860	-0.1853	1.5831	-0.9876
73	Nonanoic acid	-0.6755	0.2620	-0.2000	0.1904	-0.0290
74	Octanoic acid	-0.6608	-0.4884	0.3576	0.0442	-0.0204
75	Valeric acid	-0.3686	0.6865	-0.2110	0.1471	0.2333
76	Propionic acid	-0.5088	-0.6403	0.2886	0.0907	-0.0324
77	Trans-2-Decenoic acid	0.0722	0.4149	0.4272	0.0036	0.2716
78	Delta-Nonalactone	0.0152	0.0585	-0.4717	0.2025	0.2793
79	Gamma-Octanoic lactone	1.1049	-2.0313	3.8877	-1.0967	0.8107
80	4-Hexanolide	4.5933	5.2043	-0.3368	-0.3058	1.6802
81	G-Decalactone	-0.2688	-0.4560	-0.6046	0.1839	0.1126
82	4-hydroxyoxolan-2-one	-0.5929	-0.3638	0.4938	-0.0172	-0.0520
83	4-Heptanolide	0.0078	0.6565	-0.2028	0.2568	0.3282
84	Dihydroactinidiolide	-0.5517	-0.3672	-0.4783	0.2024	-0.1205
85	δ-Lauro lactone	-0.7517	-0.3793	0.1935	0.1020	-0.0726

No.	Compound	Principal components				
		1	2	3	4	5
86	5-Hexanolide	-0.0951	0.4878	0.1210	-0.0654	-0.0069
87	5-Decanolide	-0.3887	0.0906	-0.2937	0.0625	-0.0925
88	5-Hydroxyoctanoic acid lactone	-0.6088	-0.3179	-0.2817	0.2656	-0.1774
89	(3Z)-3-Hexenyl benzoate	-0.8972	-0.0292	-0.2208	0.2071	-0.1112
90	Vinyl acetate	-0.8572	-0.3005	0.3477	-0.0251	0.0070
91	Hexyl benzoate	-0.2618	0.3058	0.4093	-0.1703	0.2323
92	Butyl benzoate	-0.0179	0.1053	0.0470	-0.1182	0.1815
93	Dibutyl phthalate	0.0131	0.0505	-0.1480	0.0878	0.0464
94	Diethyl phthalate	-0.5233	-0.0447	-0.1726	0.1322	-0.0832
95	Dimethyl phthalate	-0.2153	-0.0616	0.3345	-0.1174	-0.0845
96	Heptylformiat	1.3582	1.3638	-0.4798	-0.5888	-0.4309
97	Methyl isoheptadecanoate	0.1137	-1.1687	-0.6805	0.0392	0.1380
98	Pentyl hexanoate	-0.4749	0.1970	-0.1305	0.0923	-0.0076
99	Methyl salicylate	-0.6084	-0.0227	-0.3040	0.1947	-0.1627
100	Hexanoic acid vinyl ester	-0.9689	-0.1493	-0.1850	0.1487	-0.1244
101	Methyl 14-Methyl pentadecanoate	-0.8658	0.1749	-0.2007	0.0184	-0.1445
102	Cis-4-Decene	-0.8377	-0.1408	0.1111	-0.0999	-0.1086
103	Decane	-0.2499	0.1866	0.3902	-0.1177	0.0709
104	3-Methyldecane	0.2356	0.0209	-0.3434	0.2249	0.1948
105	Dodecane	-0.7230	-0.2436	0.1607	0.1216	-0.2226
106	Heptane	0.1532	0.4485	0.6446	-0.6295	-0.0411
107	1-Chloroheptane	0.4151	0.5617	-0.3611	0.1638	0.0089
108	N-Octane	-0.0431	-0.1615	0.3524	0.3193	0.4742
109	1,2-Epoxyheptane	0.2850	1.0280	-0.2773	-0.8026	-0.8445
110	1-Chloropentane	-0.2242	-0.8596	-0.6798	0.3443	-0.1653
111	1-Nitropropane	-0.9865	-0.0162	-0.1678	0.1417	-0.1096
112	n-Tridecane	-0.7763	-0.2803	0.2331	0.0593	-0.0767
113	3-Methyltridecane	0.4438	0.8869	0.2507	-0.3748	0.0395
114	1-Octen-3-one	1.1071	0.2302	-0.6338	-0.3167	0.0801
115	2(5H)-Furanone	0.3228	-0.6002	-0.7161	0.2231	-0.2036
116	Beta-Angelica Lactone	-0.2242	-0.7530	1.0112	-0.2904	0.2080
117	2-Cyclohexen-1-one	2.3408	2.6439	-0.0217	-1.1848	-0.3312
118	2-Cyclopentenone	1.0657	-0.7102	-0.8496	-0.3482	0.2726
119	2-Decanone	0.2595	0.3855	-0.0714	-0.1352	-0.1649
120	2-Dodecanone	-0.1784	-0.0250	0.0702	0.0373	-0.0963
121	2-Heptanone	0.3155	0.3530	0.2305	-0.2373	-0.0406
122	3-Methyl-5-Hexanone	0.4660	-0.3440	0.1664	0.1131	0.1521
123	2-Hexanoylfuran	0.2706	0.4794	-0.3556	0.0151	-0.0051
124	Alpha-Pyrone	-0.6875	-0.2503	-0.3205	0.2357	-0.3030
125	5-Hydroxy-2-Decenoic acid Lactone	-0.9440	-0.1429	-0.2132	0.2502	-0.2011
126	Delta-Heptalactone	-1.0214	-0.1184	0.0211	0.0406	-0.0548
127	2-N-Hexylcyclopentanone	0.0822	-0.4110	-0.0385	1.0391	-0.6355
128	2-Nonanone	-0.7371	0.0278	-0.0981	0.0477	-0.1051
129	Hydroxyacetone	-0.4145	-0.4977	0.7690	-0.2337	0.0835
130	3-Decanone	-0.1891	-0.1756	-0.1764	-0.0246	0.0554
131	3-Nonen-2-one	-0.3324	-0.0154	-0.2787	0.2471	-0.0535
132	3-Octen-2-One	0.0825	-1.4596	2.4473	-0.7793	0.6536
133	trans-3-Penten-2-one	2.7685	3.5014	0.5051	2.0324	4.2842

No.	Compound	Principal components				
		1	2	3	4	5
134	3-Tridecanone	-0.2153	0.9323	-0.1888	0.6781	0.9984
135	4-Cyclopentene-1,3-Dione	-0.6165	-0.1734	0.0608	0.1282	-0.3706
136	2,3-Dihydro-3,5-dihydroxy-6-methyl-4(H)-pyran-4-one	-0.5854	-0.1069	-0.1664	0.1684	0.0305
137	4-Octanone	-0.8793	-0.0423	-0.2583	0.2163	-0.0075
138	6,10-Dimethyl-5,9-undecadien-2-one	-0.6200	-0.0098	0.3015	-0.3762	-0.2530
139	2-Methylacetophenone	0.6974	0.2941	-0.1839	-0.1593	-0.3042
140	Levogluconone	1.0936	-0.7048	-0.4806	1.2790	-1.2418
141	3-Hydroxy-2-methyl-4H-pyran-4-one	-0.6835	-0.0777	0.3328	-0.3104	-0.1777
142	4'-Hydroxypropiophenone	-0.2965	0.1424	-0.2471	0.7404	0.1878
143	Ethyl-O-Tolyl ketone	-0.9746	-0.1091	-0.1879	0.2487	-0.2055
144	4-(2,6,6-Trimethyl-1-cyclohexenyl)-3-buten-2-one	0.9619	-0.4579	2.5298	-2.0200	-0.2752
145	Ocimene	2.5313	1.8983	-0.9776	1.6635	3.4924
146	1-Decene	0.0922	0.3317	0.3240	-0.9070	-0.7255
147	(+)-Alpha-Funebrene	0.4267	-0.3206	-0.1866	0.1272	0.1338
148	1-(2-methyl-1-cyclopentenyl)ethanone	-0.5321	-0.0427	-0.0742	0.1971	-0.1409
149	4-Chlorophenol	-0.0221	0.6728	-0.3010	0.0803	0.0401
150	2-Ethyl-6-Methylphenol	-0.3967	-0.0531	-0.0383	0.0076	0.0776
151	1-(2-Furyl)Butan-1-one	-1.0789	-0.0452	-0.1514	0.1005	-0.1033
152	2-Methyl-5-Propionyl-Furan	-0.4309	0.0555	0.0462	0.0634	0.0469
153	5-Methyl-2-acetylfuran	-1.0324	-0.0424	-0.1912	0.1619	-0.1318
154	2-Butylfuran	-0.8447	-0.2789	-0.3459	0.1873	-0.1298
155	2-N-Heptylfuran	-0.7921	-0.0322	-0.1757	0.1188	-0.1381
156	3-Acetyl-2,5-Dimethylfuran	-0.9663	-0.0269	-0.2190	0.0752	-0.1950
157	Dibenzofuran	-0.4138	-0.3940	0.3437	0.3639	-0.2113
158	2-Ethylbenzofuran	-0.2479	-0.0560	-0.0131	0.1426	-0.1999
159	2-(2-Propenyl)furan	-0.7061	-0.0087	-0.1411	0.0733	-0.1829
160	2-Ethylfuran	-0.6053	0.0229	-0.0649	0.0416	-0.0434
161	2-Ethyl-5-Methyl Furan	-0.6499	0.0561	-0.0261	0.0918	0.0299
162	2-Hexylfuran	-0.5842	-0.2177	-0.0684	0.0026	-0.2940
163	2-Pentylfuran	-0.8174	-0.0856	-0.1216	0.1954	-0.1261
164	2-Propylfuran	-0.8201	-0.0498	-0.1675	0.0983	-0.1099
165	2,3-Dimethylmaleic anhydride	-1.0911	-0.0296	-0.1882	0.1132	-0.1136
166	Butylbenzene	-0.8078	-0.1492	-0.1355	0.1748	-0.2646
167	Phenylpentane	-0.9205	-0.0597	0.0871	0.0686	0.0641
168	Butyric anhydride	4.0624	1.8712	-1.6815	-4.9241	-3.1032
169	1,7-Dimethylnaphthalene	-0.7621	-0.5308	-0.7263	-0.2276	0.2335
170	1-Methylnaphthalene	-0.7093	-0.0852	-0.1370	0.1586	-0.1602
171	O-Cymene	1.4332	0.4762	-0.1753	-0.4515	0.4367
172	2-N-Hexylthiophene	3.0219	0.3078	-0.6573	-0.8315	0.5465

No.	Compound	Principal components				
		1	2	3	4	5
173	2-N-Pentylthiophene	-0.1197	0.1076	0.0595	0.0011	-0.0092

Table S4 Volatile component stereograms of six infant formula



Note: The number and size of chromatography peak on behalf of the volatile component type and content