

Supplementary materials

Development of a Method for the Measurement of Human Scent Samples Using Comprehensive Two-dimensional Gas Chromatography with Mass Detection

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Table S1. The list of the standards in a model mixture of human skin scent and measured retention indices on systems with a 2 m pre-column, a 30 m primary column and a 1 m secondary column.

Compounds	Molecular weight	Chemical family	Retention indices			
			Rxi-5ms /Rxi-17Sil MS	Rxi-5ms /Rtx-200 MS	Rxi-17Sil MS /TG-5HT	Rtx-200 MS /TG-5HT
Hexanoic acid	116.16	Acids	1011.3	1015.1	1112.9	1130.8
2-Octanone	128.21	Ketones	991.33	994.00	1108.3	1190.3
Octanal	128.21	Aldehydes	1002.5	1004.6	1119.7	1178.4
Heptanoic acid	130.18	Acids	1098.0	1107.2	1206.3	1233.3
2-Nonanone	142.24	Ketones	1093.5	1091.8	1210.9	1290.7
Decane	142.29	Alkanes	1000.0	1000.0	1000.0	1000.0
Octanoic acid	144.21	Acids	1192.2	1197.9	1300.5	1326.0
Nonanal	145.24	Aldehydes	1104.8	1102.6	1220.2	1283.0
2-Decanone	156.27	Ketones	1193.4	1193.4	1309.3	1398.2
Decanal	156.27	Aldehydes	1205.0	1207.3	1321.8	1385.8
Undecane	156.31	Alkanes	1100.0	1100.0	1100.0	1100.0
Nonanoic acid	158.24	Acids	1290.7	1288.6	1401.9	1424.6
2-Undecanone	170.29	Ketones	1293.0	1293.3	1412.1	1502.6
Undecanal	170.29	Aldehydes	1307.7	1305.4	1424.9	1493.9
Dodecanal	170.29	Aldehydes	1408.3	1408.4	1524.3	1598.1
Dodecane	170.33	Alkanes	1200.0	1200.0	1200.0	1200.0
Decanoic acid	172.26	Acids	1385.2	1387.4	1499.3	1530.2
1-Chlorodecane	176.73	Chlorinated hydrocarbons	1264.4	1265.2	1344.5	1349.0
2-Dodecanone	184.32	Ketones	1392.7	1395.2	1513.2	1607.8
Tridecane	184.37	Alkanes	1300.0	1300.0	1300.0	1300.0
Undecanoic acid	186.29	Acids	1478.6	1484.0	1596.5	1628.3
1-Dodecanol	186.34	Alcohols	1475.9	1475.8	1582.7	1585.1
Caffeine	194.19	Others	1855.2	1857.4	2342.4	2250.8
6,10-Dimethyl-5,9-undecadien-2-one (isomer 1)	194.32	Ketones	1435.5	1435.4	1588.1	1637.9
6,10-Dimethyl-5,9-undecadien-2-one (isomer 2)	194.32	Ketones	1454.4	1451.7	1613.4	1662.8
2-Tridecanone	198.34	Ketones	1494.8	1497.6	1616.5	1717.8
Tridecanal	198.35	Aldehydes	1512.0	1511.7	1627.9	1707.9
Tetradecane	198.39	Alkanes	1400.0	1400.0	1400.0	1400.0
Dodecanoic acid	200.32	Acids	1579.7	1577.4	1696.5	1733.3
1-Chlorododecane	204.78	Chlorinated hydrocarbons	1470.4	1470.4	1549.5	1558.0

hydrocarbons						
Pentadecane	212.42	Alkanes	1500.0	1500.0	1500.0	1500.0
N,N-Dimethyldodecylamine	213.40	Amines	1508.9	1511.5	1549.7	1544.9
Tridecanoic acid	214.34	Acids	1674.5	1673.7	1796.3	1835.0
1-Tetradecanol	214.39	Alcohols	1680.2	1679.5	1787.3	1793.6
2-Pentadecanone	226.4	Ketones	1700.2	1700.3	1818.7	1925.4
Hexadecane	226.41	Alkanes	1600.0	1600.0	1600.0	1600.0
Benzyl salicylate	228.24	Others	1877.7	1880.4	2221.8	2120.6
Oxybenzone	228.25	Others	2037.1	2037.6	2465.2	2355.4
Tetradecanoic acid	228.37	Acids	1771.2	1774.4	1902.6	1936.9
Chlorinated hydrocarbons						
1-Chlorotetradecane	232.83		1677.3	1676.6	1757.1	1768.8
ns						
Heptadecane	240.47	Alkanes	1700.0	1700.0	1700.0	1700.0
N,N-Dimethyltetradecylamine	241.46	Amines	1706.5	1706.5	1748.2	1744.4
Pentadecanoic acid	242.40	Acids	1873.6	1873.5	1999.3	2035.2
1-Hexadecanol	242.44	Alcohols	1883.5	1883.5	1992.7	1998.5
2-Ethylhexyl salicylate	250.33	Others	1810.4	1813.7	1992.5	2027.0
Pentacosane	252.69	Alkanes	2500.0	2500.0	2500.0	2500.0
Octadecane	254.49	Alkanes	1800.0	1800.0	1800.0	1800.0
Hexadecanoic acid	256.42	Acids	1972.7	1970.2	2110.0	2144.1
Chlorinated hydrocarbons						
1-Chlorohexadecane	260.90		1883.6	1883.4	1966.2	1976.5
ns						
Homosalate	262.36	Others	1893.8	1897.1	2099.1	2128.4
2-Octadecanone	268.48	Ketones	2007.4	2004.0	2127.9	2242.6
Nonadecane	268.52	Alkanes	1900.0	1900.0	1900.0	1900.0
N,N-Dimethylhexadecylamine	269.51	Amines	1906.9	1910.0	1946.4	1943.9
Heptadecanoic acid	270.45	Acids	2071.7	2070.5	2203.1	2243.1
Isopropyl myristate	270.46	Esters	1826.8	1830.2	1909.4	1981.4
1-Octadecanol	270.49	Alcohols	2085.9	2089.0	2199.4	2207.3
Oleic Acid	282.47	Acids	2169.5	2146.3	2311.2	2331.1
Eicosane	282.55	Alkanes	2000.0	2000.0	2000.0	2000.0
Octadecanoic acid	284.48	Acids	2169.5	2169.4	2311.2	2347.9
2-Ethylhexyl 4-methoxycinnamate (isomer 1)	290.40	Others	2170.1	2169.6	2482.1	2424.4
2-Ethylhexyl 4-methoxycinnamate (isomer 2)	290.40	Others	2322.7	2325.5	2652.0	2646.4
Heneicosane	296.57	Alkanes	2100.0	2100.0	2100.0	2100.0
N,N-Dimethyloctadecanamine	297.56	Amines	2107.8	2111.6	2149.7	2138.0

Nonadecanoic acid	298.50	Acids	2269.5	2269.3	2411.7	2443.2
Docosane	310.60	Alkanes	2200.0	2200.0	2200.0	2200.0
Eicosanoic acid	312.53	Acids	2395.9	2370.9	2516.2	2557.4
Hexadecanoic acid, butyl ester	312.54	Esters	2188.7	2188.6	2287.9	2348.0
Tricosane	324.63	Alkanes	2300.0	2300.0	2300.0	2300.0
Tetracosane	338.65	Alkanes	2400.0	2400.0	2400.0	2400.0
Docosanamide	339.60	Amides	2810.8	2810.6	2777.3	2884.3
Octadecanoic acid, butyl ester	340.59	Esters	2391.5	2391.8	2491.1	2557.6
Octocrylene	361.48	Others	2678.7	2691.3	3123.2	3166.3
Tetraethylene glycol monododecyl ether	362.54	Ethers	2548.6	2550.3	2848.6	2786.9
Hexacosane	366.71	Alkanes	2600.0	2600.0	2600.0	2600.0
Heptacosane	380.73	Alkanes	2700.0	2700.0	2700.0	2700.0
Cholesterol	386.65	Others	3134.8	3133.8	3509.4	3379.7
Octacosane	394.77	Alkanes	2800.0	2800.0	2800.0	2800.0
Tetradecanoic acid, dodecyl ester	396.69	Esters	2770.3	2776.4	2870.9	2952.8
Pentaethylene glycol monododecyl ether	406.60	Ethers	2831.0	2830.3	3173.2	3096.3
Nonacosane	408.80	Alkanes	2900.0	2900.0	2900.0	2900.0
Squalene	410.73	Others	2835.4	2840.0	2977.8	2822.3
9-Hexadecenoic acid, dodecyl ester	422.73	Esters	2955.3	2960.2	3083.9	3140.0
Triacontane	422.82	Alkanes	3000.0	3000.0	3000.0	3000.0
Tetradecanoic acid, tetradecyl ester	424.74	Esters	2970.2	2975.2	3076.3	3154.4
Hentriacontane	436.85	Alkanes	3100.0	3100.0	3100.0	3100.0
Hexaethylene glycol monododecyl ether	450.65	Ethers	3101.4	3100.4	3508.9	3428.1
Dotriacontane	450.87	Alkanes	3200.0	3200.0	3200.0	3200.0
Tetradecanoic acid, hexadecyl ester	452.80	Esters	3166.9	3166.9	3266.9	3347.0
Octadecanoic acid, dodecyl ester	452.80	Esters	3166.9	3166.9	3266.9	3347.0
Trtriacontane	464.89	Alkanes	3300.0	3300.0	3300.0	3300.0
Tetratriacontane	478.93	Alkanes	3400.0	3400.0	3400.0	3400.0
Hexadecanoic acid, hexadecyl ester	480.85	Esters	3370.9	3366.9	3474.2	3563.2
Pentatriacontane	492.96	Alkanes	3500.0	3500.0	3500.0	3500.0
Hexatriacontane	506.97	Alkanes	3600.0	3600.0	3600.0	3600.0
Hexadecanoic acid, octadecyl ester	508.90	Esters	3569.2	3570.8	3674.0	3763.0
Heptatriacontane	520.99	Alkanes	3700.0	3700.0	3700.0	3700.0
Octatriacontane	535.03	Alkanes	3800.0	3800.0	3800.0	3800.0
Octadecanoic acid, octadecyl ester	536.96	Esters	3763.6	3772.6	3869.0	3962.8
Nonatriacontane	549.05	Alkanes	3900.0	3900.0	3900.0	3900.0
Tetracontane	563.08	Alkanes	4000.0	4000.0	4000.0	4000.0