

Accession_Retired	data_file	BlobID	RT1	RT2	Description	Internal_N Name	UID
	20181204_	65	57.46	0.69	cis-Vaccenic Acid, TM	cis-Vaccenic Acid, TM	
	20181204_	663	29.32	0.53	citronellol	citronellol	
	20181204_	686	30.04	0.65	cycloisolongifolene	cycloisolongifolene	
	20181204_	674	78.9	0.97	deoxycholic Acid (ma	deoxycholic Acid (ma	
	20181204_	681	77.79	1.52	dibenz(ah)anthracene	dibenz(ah)anthracene	
	20181204_	648	34	0.9	dimethyl Glutaric Acid	dimethyl Glutaric Acid	
	20181204_	9	48.66	0.62	dodecyl benzene	dodecyl benzene	
	20181204_	40	60.54	0.55	eicosanol, TMS	eicosanol, TMS	
	20181204_	673	78.06	0.84	ergosterol	ergosterol	
	20181204_	66	46.15	0.55	farnesol	farnesol	
	20181204_	694	41.62	0.84	galactosan	galactosan	
	20181204_	79	42.42	1.9	gamma dodecalacton	gamma dodecalacton	
	20181204_	357	42.61	1.97	beta-caryophyllene al	beta-caryophyllene al	
	20181204_	704	36.82	0.54	SESQ7	SESQ7	
	20181204_	716	37.93	0.5	SESQ8	SESQ8	
	20181204_	109	52.47	0.93	beta-caryophyllinic ac	beta-caryophyllinic ac	
	20181204_	91	48.97	1.33	beta-caryophyllonic a	beta-caryophyllonic a	
	20181204_	23	54.18	1.25	beta-nocaryophyllinic	beta-nocaryophyllinic	
	20181204_	64	43.9	0.27	beta-nocaryophyllon	beta-nocaryophyllone	
	20181204_	45	50.49	1.73	beta-nocaryophylloni	beta-nocaryophylloni	
	20181204_	661	79.89	0.87	beta-sitosterol	beta-sitosterol	
	20181204_	654	44.32	0.56	bisabolol	bisabolol	
	20181204_	100	25.78	0.62	borneol	borneol	
	20181204_	78	76.61	0.84	cholesterol	cholesterol	
	20181204_	136	63.63	1.3	chrysene	chrysene	
	20181204_	695	27.34	0.72	C8 acid	C8 acid	
	20181204_	16	45.88	0.95	C9 Diacid (azelaic acid	C9 Diacid (azelaic acid	
	20181204_	711	31.22	0.69	C9 acid	C9 acid	
	20181204_	62	38.99	1.79	DEET	DEET	
	20181204_	14	49.69	0.73	FAME16 (Methyl Paln	FAME16 (Methyl Paln	
	20181204_	25	55.06	0.72	FAME18 (Methyl Stea	FAME18 (Methyl Stea	
	20181204_	4	44.51	0.98	MBTCA	MBTCA	
	20181204_	83	39.72	0.83	Me-OH-glutatric acid	Me-OH-glutatric acid	
	20181204_	74	81.14	1.06	a-Amyrin	a-Amyrin	
	20181204_	44	62.26	0.84	abietic acid	abietic acid	
	20181204_	119	51.37	1.45	anthraquinone	anthraquinone	
	20181204_	42	41.01	1.18	benzophenone	benzophenone	
	20181204_	12	48.7	0.94	C10 diacid (sebacic ac	C10 diacid (sebacic ac	
	20181204_	24	53.99	0.91	C12 diacid	C12 diacid	
	20181204_	21	44.51	0.69	C13 acid	C13 acid	
	20181204_	54	58.83	0.89	C14 Diacid	C14 Diacid	
	20181204_	2	52.93	0.69	C16 Acid	C16 Acid	
	20181204_	88	55.48	0.67	C17 acid	C17 acid	
	20181204_	1	57.95	0.7	C18 Acid	C18 Acid	
	20181204_	76	66.83	0.69	C22 acid	C22 acid	
	20181204_	87	70.79	0.7	C24 acid	C24 acid	

20181204_	108	74.48	0.72 C26 acid	C26 acid
20181204_	110	77.98	0.74 C28 acid	C28 acid
20181204_	655	23.15	0.77 C7 acid	C7 acid
20181204_	1045	33.74	1.63 SESQ2	SESQ2
20181204_	22	61.72	0.55 C24	C24
20181204_	46	63.93	0.56 C25	C25
20181204_	32	66.1	0.57 C26	C26
20181204_	47	68.16	0.57 C27	C27
20181204_	48	70.14	0.58 C28	C28
20181204_	52	72.08	0.59 C29	C29
20181204_	67	73.95	0.6 C30	C30
20181204_	57	75.74	0.62 C31	C31
20181204_	77	77.45	0.63 C32	C32
20181204_	80	79.16	0.64 C33	C33
20181204_	102	82.63	0.72 C35	C35
20181204_	680	34.8	0.69 C10 carboxylic acid	C10 carboxylic acid
20181204_	58	44.28	1.57 4-nitrocatechol	4-nitrocatechol
20181204_	685	23.88	0.78 4-terpineol (?)	4-terpineol (?)
20181204_	107	44.55	1.39 9H-Florenone	9H-Florenone
20181204_	667	32.82	0.47 C14	C14
20181204_	71	39.83	0.49 C16	C16
20181204_	56	43.07	0.49 C17	C17
20181204_	20	46.11	0.5 C18	C18
20181204_	13	49.04	0.51 C19	C19
20181204_	10	51.79	0.52 C20	C20
20181204_	8	54.45	0.52 C21	C21
20181204_	11	56.96	0.54 C22	C22
20181204_	18	59.4	0.55 C23	C23
20181204_	41	62.29	0.7 12-OH C18 Acid, TMS	12-OH C18 Acid, TMS
20181204_	85	61.42	0.69 16-OH C16 Acid, TMS	16-OH C16 Acid, TMS
20181204_	692	39.91	0.8 2-Ketoglutaric acid, tr	2-Ketoglutaric acid, tr
20181204_	63	36.4	0.88 3-5-dimethoxyphenol	3-5-dimethoxyphenol
20181204_	183	58.26	1.45 4, 4 dimethoxy-benzc	4, 4 dimethoxy-benzo
20181204_	82	40.59	0.89 4-hydroxybenzoic aci	4-hydroxybenzoic aci
20181204_	781	29.93	0.69 glyceric acid (?)	glyceric acid (?)
20181204_	241	56.36	1.23 hexadecanamide	hexadecanamide
20181204_	7	50.61	0.53 hexadecanol, TMS	hexadecanol, TMS
20181204_	15	52.32	0.93 homosalate, TMS	homosalate, TMS
20181204_	650	32.75	0.73 hydroquinone	hydroquinone
20181204_	701	33.74	1.34 ionone	ionone
20181204_	1019	33.51	0.64 SESQ3	SESQ3
20181204_	856	33.81	0.66 SESQ4	SESQ4
20181204_	665	38.69	0.78 isoeugenol	isoeugenol
20181204_	26	60.43	0.87 isopimaric acid	isopimaric acid
20181204_	140	36.56	1.33 ketopinic acid	ketopinic acid
20181204_	97	42.95	0.85 levoglucosan	levoglucosan
20181204_	92	57.12	0.7 linoleic Acid, TMS	linoleic Acid, TMS

20181204_	68	81.22	1.04 lupeol	lupeol
20181204_	713	28.33	1.1 maltol	maltol
20181204_	687	42.3	0.86 mannosan	mannosan
20181204_	35	65.68	0.75 monopalmitin	monopalmitin
20181204_	188	68.92	0.71 monostearin TMS	monostearin TMS
20181204_	651	28.41	0.51 nonanol	nonanol
20181204_	59	52.36	0.87 octadecanal (?)	octadecanal (?)
20181204_	3	55.82	0.55 octadecanol	octadecanol
20181204_	19	51.71	0.85 octadecanone	octadecanone
20181204_	29	57.27	0.7 oleic Acid, TMS	oleic Acid, TMS
20181204_	86	37.05	0.97 p-anisic acid (4-methoxy)	p-anisic acid (4-methoxy)
20181204_	27	52.36	0.71 palmitoleic Acid	palmitoleic Acid
20181204_	50	42.95	0.95 pentadecanone	pentadecanone
20181204_	117	72.31	1.46 perylene	perylen
20181204_	55	42.57	1.11 phthalic acid	phthalic acid
20181204_	94	38.76	1.14 phthalimide	phthalimide
20181204_	33	41.89	0.97 pinic acid 1	pinic acid 1
20181204_	60	42.04	0.98 pinic acid 2	pinic acid 2
20181204_	103	37.28	1.47 pinonic acid	pinonic acid
20181204_	84	55.33	1.22 pyrene	pyrene
20181204_	659	29.36	0.68 pyrocatechol	pyrocatechol
20181204_	96	26.73	1.1 quinoline	quinoline
20181204_	132	31.99	0.73 resorcinol	resorcinol
20181204_	962	32.18	0.57 SESQ1	SESQ1
20181204_	49	57.65	1.05 retene	retene
20181204_	51	51.75	1.54 sinapinaldehyde	sinapinaldehyde
20181204_	70	70.44	0.6 squalene	squalene
20181204_	73	78.86	0.86 stigmasterol	stigmasterol
20181204_	17	42.95	1.33 syringaldehyde	syringaldehyde
20181204_	5	48.78	0.88 syringic acid	syringic acid
20181204_	154	32.67	0.82 syringol	syringol
20181204_	652	36.25	0.53 threitol	threitol
20181204_	93	36.52	0.54 erythreitol	erythreitol
20181204_	672	30.39	2.11 triacetin	triacetin
20181204_	529	36.82	0.93 tridecanal (?)	tridecanal (?)
20181204_	6	44.89	0.88 vanillic acid	vanillic acid
20181204_	69	37.55	1.34 vanillin	vanillin
20181204_	772	25.09	2.07 verbenone (-)	verbenone (-)
20181204_	125	48.24	1.38 xanthone	xanthone
20181204_	783	39.33	1.07 SESQ9	SESQ9
20181204_	818	35.3	0.62 SESQ6	SESQ6
20181204_	913	34.5	0.62 SESQ5	SESQ5

[illegible]

[illegible]

i-TMS
phenone
d

oxybenzoic acid)

[illegible]

Retention_d_alkane_n_alkane_RT2	VUV_Exact Instrumen Ionization Injection_1 Derivatizat GC_column
2259	2260
1338	1339
1355	1355
3347	3347
3280	3280
1456	1457
1920	1921
2390	2390
3296	3297
1832	1832
1684	1684
1709	1710
1715	1716
1537	1538
1569	1569
2060	2061
1931	1932
2127	2127
1757	1757
1985	1985
3406	3407
1770	1771
1254	1254
3209	3209
2531	2532
1293	1293
1822	1823
1381	1382
1600	1600
1957	1957
2161	2161
1776	1777
1623	1623
3479	3479
2468	2468
2017	2018
1664	1665
1922	1922
2120	2120
1776	1777
2317	2318
2078	2079
2177	2178
2280	2281
2684	2685
2886	2887

3088	3088
3291	3292
0	
1449	1449
2443	2444
2545	2546
2649	2649
2750	2751
2852	2853
2955	2956
3058	3058
3159	3159
3259	3260
3363	3363
3564	3565
1479	1480
1769	1770
1206	1207
1778	1778
1422	1423
1626	1627
1730	1730
1830	1831
1934	1934
2034	2034
2137	2138
2238	2239
2341	2342
2470	2470
2429	2430
1629	1629
1525	1526
2293	2294
1651	1651
1352	1353
2212	2213
1989	1989
2054	2055
1420	1421
1449	1449
1442	1443
1451	1451
1591	1591
2385	2385
1530	1530
1726	1727
2245	2245

3483	3484
1316	1316
1706	1706
2628	2628
2788	2789
1318	1318
2056	2056
2191	2191
2031	2031
2251	2252
1544	1544
2056	2056
1726	1727
2967	2968
1714	1715
1593	1593
1692	1693
1697	1698
1550	1551
2171	2172
1339	1340
1278	1278
1399	1399
1404	1404
2267	2268
2032	2033
2868	2869
3344	3345
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1418	1419
1521	1521
1528	1529
1362	1363
1537	1538
1789	1789
1558	1558
1237	1237
1906	1906
1610	1611
1493	1494
1471	1471

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Emily Barnes	148 41 4; 42
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