Creation of Libraries of Recurring Mass Spectra from Large Data Sets assisted by a Dual-Column Workflow

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Supporting Information

Detailed information on the filters used in AMDIS and in the post-processing of the results and details of the scoring procedure in AMDIS is included. Two figures showing, in figure S1 - the increase in number of instances of a molecule found by AMDIS vs what was found in when only high quality spectra were accepted, and in figure S2 – the distribution of identified vs recurrent unidentified compounds in the data.

Finally a table of the measured RI values and standard deviation for all identified compounds in both columns is given along with the number of times each compound is found in the two columns.

Introduction

As noted in the body of the paper, AMDIS was designed to ensure that even very small components of a target compound were detected. This means that the AMDIS algorithms look for ions that maximize within narrow windows of one another and then collects these ions into spectra to be compared against the target library. In order to be sure that no peak is missed, the criteria for what constitutes an extractable spectrum are deliberately liberal. The spectra that are extracted often have m/z values that arise from noise or m/z values that are poor matches to the time profile of other extracted m/z values. In the development of AMDIS and in extensive testing since then these techniques have not proven to produce false positive results, but they have yielded large number of components that have caused some confusion over the results.

The data from a large number of deconvolutions were examined and certain characteristics were noted in the "poor" deconvolutions. They typically had few model ions, low S/N ratios, few m/z values extracted in the spectrum, high levels of uncertain peaks, low minimum abundance – *i.e.* the smallest extracted m/z value was large compared to the base peak and in some cases very low purity.

What were judged to be the most useful of these parameters were then added to the AMDIS algorithm as filters to be used after the components failed to match the target library at the level specified by the user.

AMDIS Filters

The filters incorporated into AMDIS (Version 2.71) are noted below. Each non-identified spectrum is subject to four filters:

1. Numbers of model ions: AMDIS constructs a model peak, which represents the shape of the deconvoluted component in time. To do this the program finds the ion that rises and falls the fastest

and all other ions that rise and fall at 75% or more of the fastest. These ions are the model ions. The more such ions that rise and fall rapidly, the greater the confidence in having found a single component. The weighted sum of the model ions is used to create the model peak (or model total ion chromatogram) of the component.

2. Signal-to-Noise: The total area under the deconvoluted TIC (total ion chromatogram) relative to the noise level detected by AMDIS is the signal to noise (S/N). As the S/N increases, so does the confidence in having a reliable deconvolution.
3. Minimum Abundance: This parameter is a measure of the lowest peak relative to the base peak (=100) that can be extracted and is dependent on the noise and the relative strength of the base peak. It measures the dynamic range of the spectrum. For most purposes a value of 0.1% of the base peak is desirable - this is equivalent to the lowest level (1 part in 1000) at which both AMDIS and the NIST library retain mass spectral information.
4. Fraction of Spectrum Confidently Deconvoluted: AMDIS constructs a model peak shape as noted above. The shape of every ion is then compared to this shape. Ions with shapes poorly overlapping the model peak are rejected, and those with a strong similarity to the model peak are accepted. There is an intermediate range where a peak is flagged as uncertain. The fraction of spectral intensity from these uncertain peaks in a given spectrum is subtracted from 1 to give the fraction of peaks that are good – "Fraction Good"– as the fraction of peaks that are "good" increases in a given spectrum, the confidence in the deconvolution increase. The uncertain peaks arise from a number of sources, but one of the most common is the near overlap of components with common ions. These common ions can sometimes not be assigned to one or the component, and in some cases it is not clear if the ions belong to either component. When the ion is assigned as uncertain it is used in target searching to aid in identification, but when it there is no matching target it is not clear if the ion is part of the spectrum.

Table S1 shows the values of the threshold and weights for the AMDIS filters. For each filter F_i, the value is calculated as:

$$F_i = W_i * (\text{ExpValue}/\text{Threshold})^{1/2} \text{ if ExpValue} \geq \text{Threshold } (F_i \leq 2 * W_i)$$

$$F_i = W_i * (\text{ExpValue}/\text{Threshold})^{2} \text{ if ExpValue} < \text{Threshold}$$

The total of the filters (ΣF_i) must be greater to or equal to the required score (4 in this example) for a component to be accepted. In the example below, all of the factors are weighted equally; however, if one factor is judged to be more important it can be overweighted.

Table S1: Values used in AMDIS filtering

Filter	Threshold	Weight	Comment
Model Peaks	≥7	1	Must have 7 model ions to get full weight
S/N	≥20	1	S/N must be ≥20 to get full weight
Fraction Good	≥0.75	1	Only 25% of extracted signal can be uncertain
Minimum Abundance	≤0.2	1	Smallest extractable peak must be 0.2% or less of base peak
Required Total Score		4	Total of filters must be 4 or component is not retained

Using these filters, an extracted component with 5 model peaks, a S/N of 20, a fraction good of 0.8 -and a minimum abundance of 0.15 would get weights of 0.51, 1, 1.03, 1.78 from the respective factors for a total of 4.32 and so would pass. This set of filter values reduced the number of unidentified components extracted by AMDIS by 40% to 50%.

Post-AMDIS Filters

A significant number of poor quality spectra remained even after using the above filters within AMDIS. After examining deconvoluted spectra passing those filters which nevertheless appeared to be low quality spectra, additional filters were developed in the following categories to further reduce the number of questionable spectra generated by AMDIS. These included:

- Purity - the fraction of the total ion current at the peak maximum assigned to the component. Components with low purity are more likely to contain contaminant ions and therefore more prone to imperfect deconvolution from nearby components. AMDIS can easily identify low purity components, but if the extracted spectrum is from a low purity component, it is less certain that it is a true component.
- Number of peaks in the extracted spectrum – a common symptom of a poor quality extracted spectrum was its small number of peaks. Therefore all extracted mass spectra were required to contain more than 20 peaks. Most of compounds that were being sought in this analysis were assumed to be reasonably complex (6+ C,N,O,S,P,Si atoms) and for such complex molecules it is rare for there to be as few as 20 m/z values in a spectrum starting at m/z=35. As a point of reference the library of identified compounds used in this work had on average over 120 peaks and the spectrum with the fewest peaks had 24.
- Presence of m/z 73 or 75 – since the present data all arose from TMS derivatization, a peak of either m/z 73 or 75 with greater than 10% of the base peak was required. It should be noted that the 73 ion which is present in essentially all TMS spectra was often one of the most difficult to extract since it was often in adjacent peaks.
- Saturation - any unidentified spectrum with a base peak greater than or equal 7.8×10^6 – which is 95% of saturation (8.2×10^6) - was rejected from further consideration – note that this value is specific to the instruments used in this study.

In addition, when the deconvolution yielded multiple unidentified spectra at the same retention time (RT) due to different model ions chosen at the same retention time, the resulting spectral components were separately filtered and only the “best” one was used. The best spectrum was decided by a voting process that looked at the parameters noted above and the total extracted signal (area). The single spectrum at the retention time that had the best value (e.g. the highest purity or the highest number of peaks) in the most categories was chosen to be used for the final filtering.

The final filtering used a total of 6 thresholds, derived from the 4 above and 3 filters used within AMDIS – fraction good, minimum abundance and signal to noise. For a spectrum to pass through this filter it must satisfy 5 of the 6 conditions (1) fraction good (≥0.8), (2) purity (≥70%), (3) minimum abundance (≤0.5% of base peak), (4) number of peaks(≥20), (5) signal to noise (≥100), and (6) the presence of either m/z 73 or 75 (≥ 10% of base peak). Saturation served as an independent filter - all spectra containing a saturated ion signal were dropped.

The filtering was done with a program written specifically to process large numbers of files. A list of the files of the deconvoluted spectra (the ELU files generated by AMDIS) was used as input, the program then examined each component in the ELU file, determined if it had been identified and if it had not, applied the filters noted above to the component. The same program also compared the extracted spectra to the NIST library to identify components not in the AMDIS library. As noted in the paper, the process was repeated until there were no longer any high quality identifications; at this point the remaining components that did pass the filter were clustered.

Scoring Match Factors in AMDIS

AMDIS initially scores a match based on the comparison between the library and unknown spectra using a mass weighted dot product of the intensities at each mass. The value of the retention index (RI) of the unknown is then compared to the RI of library spectrum. For this analysis, a retention window of 3 RI units with a penalty to the mass spectral match factor of 2 points for each window outside the first was used. Thus for these conditions, if a spectrum had a spectral match factor to the library spectrum of 85 but was 9 RI units off from the library value, the net match factor was 81 (the RI value was 3 retention index unit windows from the library value – with no penalty for the first window and 2 points each for the next two windows, the match factor was reduced by 4). The net match factor threshold for AMDIS identification was set at 70 (out of 100).

Availability of Software

AMDIS can be downloaded at:
http://chemdata.nist.gov/dokuwiki/doku.php?id=chemdata:downloads:start

The post processing software is also available; however, the current version of the software is not designed to be user friendly. It is anticipated that a user friendly version will be available in early 2015 and will be available at the above site. A copy of the current program can be obtained - further questions can be addressed to gary.mallard@nist.gov.

Figure S1

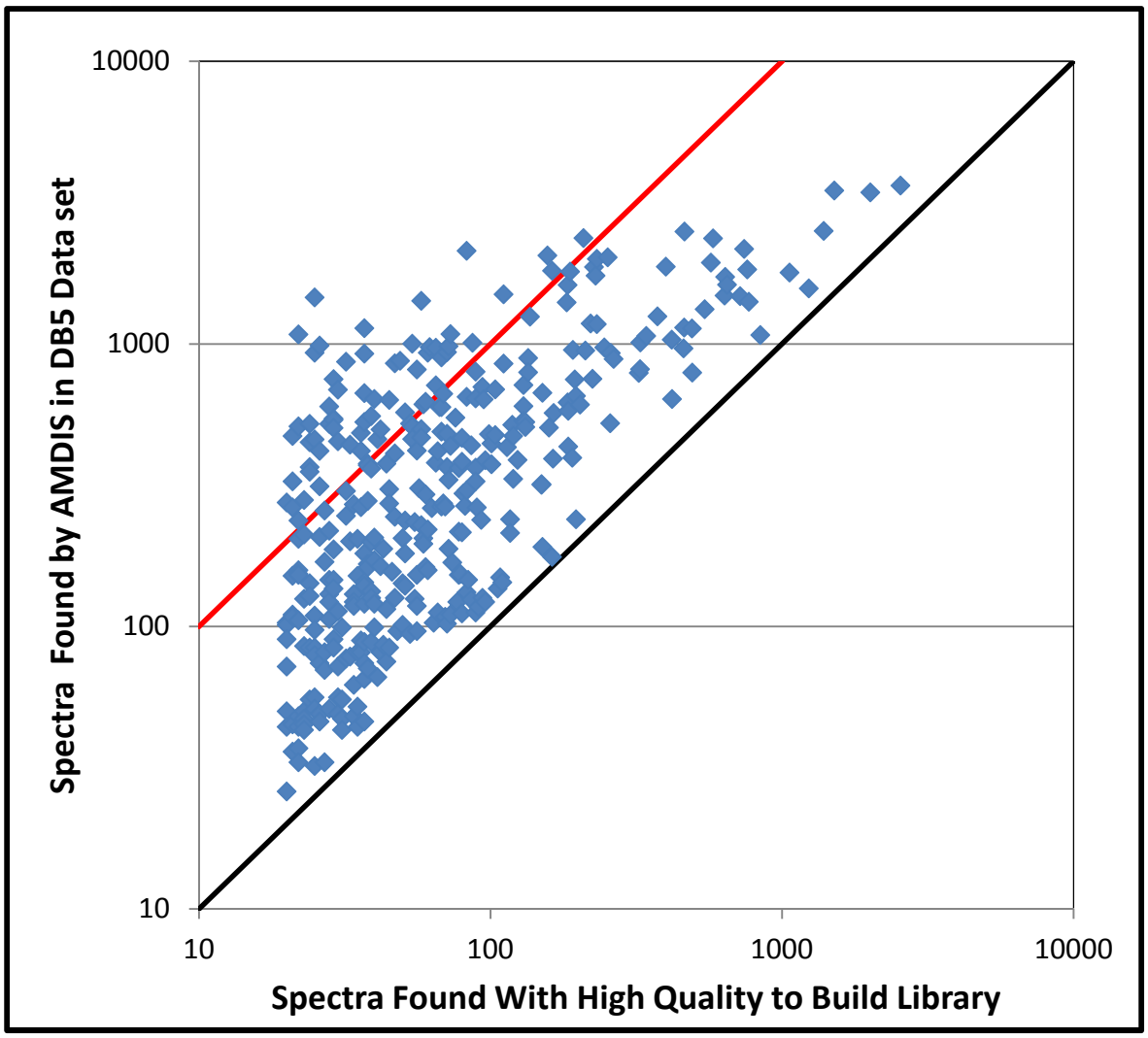

Figure S1
Number of spectra found by AMDIS for Recurrent Unidentified Spectra (RUS) vs the number of RUS found in establishing the library. Note, because only high quality spectra were used to build the library, the number of spectra found in the data set by AMDIS would be expected to be higher. The red line indicates 10x as many spectra found by AMDIS as were used in the original build.

Figure S2

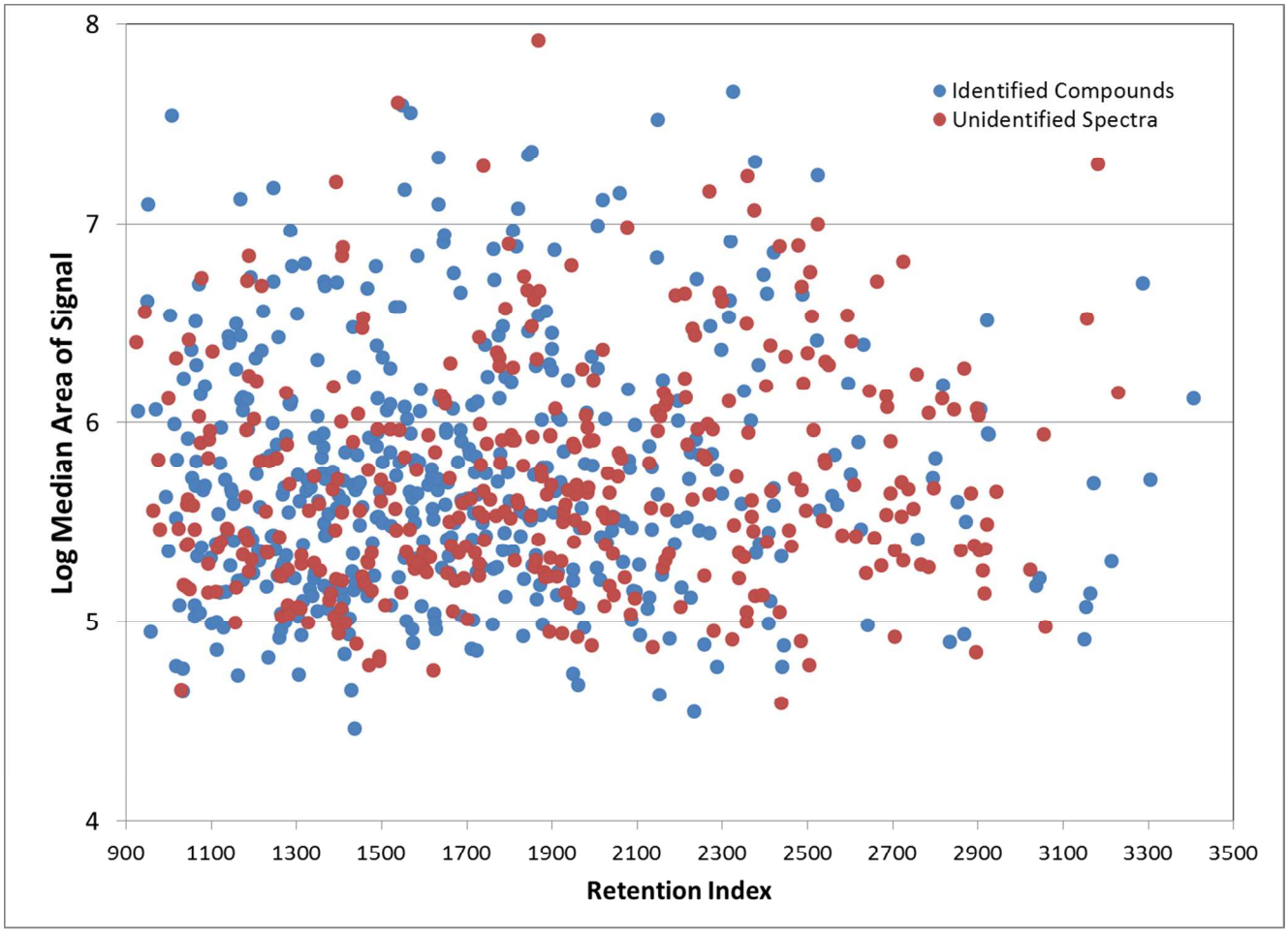

Figure S2
The median signal strength as a function of retention index for both identified and recurrent unidentified spectra – note only cases were a spectrum (identified or RUS) was identified are included. In some cases the number of instances of finding a spectrum is very low but when the compound is found the concentration is high. Zero values are not included in the computation of the median.

The table below contains the identified compounds in the data set, their formulas and the measured retention indices for both the DB5 and DB5MS columns. The number of data files for which a compound was identified in each set is also given. The data set had 3620 files of DB5 data and 2018 files of DB5MS data.

When a compound has "#" as the end of its names, it indicates that the identification is uncertain.

Internal standards are shown with a "†" at the end of the name.

Notes on the names:

In general the compounds are named as the base compound, thus
Pyruvic acid-2TMS rather than Trimethylsilyl 2-[(trimethylsilyl)oxy]acrylate
Citric acid – 3TMS
Citric acid – 4TMS

Where ethyl oximes are formed to block the carbonyl group the abbreviation EO is used, thus
3-Methyl-2-ketobutyric acid-EO-TMS

For most common components of urine, common names have been used, thus
Stearic acid-TMS rather than Octadecanoic acid-TMS

For the glucuronide, the names are given in terms of the compound before the glucuronide is formed rather than the IUPAC name

Note on ID numbers:

When known the ID number is the CAS registry number (CASRN), however for many of these compounds there is not a CASRN assigned. These are given a number that conforms to the CASRN check sum rules but is higher than any current CASRN – these numbers all start with 20600 and are 10 digits. A few of the ID numbers start with N, these numbers are the NIST/NIH/EPA numbers from the NIST database and are used in the NIST database when CASRN are not available. For a few compounds the ID number is a CASRN followed by TMS, the CASRN prior to the TMS is that of the parent compound. If the CASRN is followed by 2TMS or 3TMS it is the corresponding 2 or 3 TMS derivative.

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
1	N333797	3-Hydroxy-2-butanone-TMS	C7H16O2Si	--	--	0	895	1.1	29
2	13435-12-6	Acetamide-TMS	C5H13NOSi	928	2.5	178	942	21.0	666
3	2060000-79-3	Trifluoroacetamidine-2TMS	C8H19F3N2Si2	951	2.4	204	958	15.6	923
4	10416-59-8	Ethanimidic acid-2TMS	C8H21NOSi2	949	2.3	132	972	3.1	159
5	616-02-4	2,5-Furandione, 3-methyl-	C5H4O3	--	--	0	962	--	1
6	15500-60-4	Formamide-2TMS	C7H19NOSi2	957	1.7	80	976	10.8	186
7	1000-70-0	Carbodiimide-2TMS	C7H18N2Si2	970	4.2	208	969	11.1	1960
8	959022-28-7	Ethoxyamine-2TMS (reagent)	C8H23NOSi2	1003	8.1	78	977	9.4	1675
9	7381-30-8	Ethylene glycol-2TMS	C8H22O2Si2	999	9.8	364	985	11.3	1441
10	4325-85-3	Boric acid-3TMS	C9H27BO3Si3	1007	10.5	1024	989	7.0	2002
11	25561-30-2	Trifluoroacetamide-2TMS	C8H18F3NOSi2	992	5.8	144	1004	0.5	3
12	108-67-8	Mesitylene	C9H12	1018	8.3	383	1000	5.4	102
13	17887-27-3	Propylene Glycol-2TMS	C9H24O2Si2	1014	9.4	1402	1005	9.7	1540
14	13871-89-1	Cyclohexanol-TMS	C9H20OSi	1018	8.5	1085	1014	9.9	1686
15	556-67-2	Siloxane-Cyclotetrasiloxane, octamethyl-	C8H24O4Si4	1025	7.9	1594	1013	12.2	780
16	25436-25-3	3-Methylcrotonic acid-TMS	C8H16O2Si	1020	8.7	168	1020	10.4	131
17	7331-84-2	Propylamine-2TMS	C9H25NSi2	1035	11.4	1275	1027	9.4	18
18	41262-38-8	Trichloroethanol-TMS	C5H11Cl3OSi	1034	10.0	89	1028	10.8	74
19	77-73-6	Dicyclopentadiene	C10H12	1034	1.0	783	1033	4.2	250
20	2060000-14-6	3-Hydroxyisovaleric acid-TMS	C8H18O3Si	1045	10.0	869	1041	8.1	642
21	141-62-8	Siloxane-Tetrasiloxane, decamethyl-	C10H30O3Si4	1055	8.3	2849	1045	7.3	1987
22	53274-85-4	2,3-Butanediol-2TMS (meso)	C10H26O2Si2	1062	4.2	739	1053	5.6	338
23	6651-36-1	Cyclohexene-1-ol-TMS	C9H18OSi	1061	5.8	330	1057	7.0	237
24	2060000-73-7	Sulfurous acid-2TMS	C6H18O3SSi2	1060	5.5	377	1058	9.1	41
25	1529-17-5	Phenol-TMS	C9H14OSi	1063	7.8	2456	1057	7.5	1684
26	2060000-69-1	2,3-Butanediol monoacetate-TMS	C9H20O3Si	1066	5.1	369	1055	7.3	69
27	N366749	2-Acetoxyacetic acid-TMS	C7H14O4Si	1068	12.0	111	1058	7.4	32
28	17887-80-8	Propanediol-2TMS	C9H24O2Si2	1067	6.1	325	1059	6.3	123
29	2060000-37-3	Diethylcarbamic acid-2TMS	C8H19NO2Si	1065	7.7	2042	--	--	0
30	17596-96-2	Lactic Acid-2TMS	C9H22O3Si2	1071	6.0	3449	1062	6.4	1992
31	55133-92-1	2-Hydroxyisobutyric acid-2TMS	C10H24O3Si2	1075	6.3	2888	1066	6.4	1535
32	107-51-7	Trisiloxane, octamethyl-	C8H24O2Si3	1080	5.9	2321	1073	6.0	725
33	2060000-47-5	2-Butoxyethanol-TMS	C9H22O2Si	1077	5.3	728	1076	7.4	192

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
34	14246-15-2	Hexanoic acid-TMS	C9H20O2Si	1084	5.7	339	1075	5.5	337
35	33581-77-0	Glycolic Acid-2TMS	C8H20O3Si2	1085	6.1	3561	1077	6.2	1969
36	55816-59-6	3-Hydroxybutyric acid ethyl ester-TMS	C9H20O3Si	1098	4.8	53	1089	5.2	25
37	55191-13-4	Pyruvic acid-2TMS	C9H20O3Si2	1100	5.1	1737	1093	5.8	793
38	7480-78-6	Valine-TMS	C8H19NO2Si	1106	--	1	--	--	0
39	823-22-3	2H-Pyran-2-one, tetrahydro-6-methyl-	C6H10O2	1110	3.2	271	1105	5.2	271
40	18023-53-5	2-Ethylhexyl alcohol-TMS	C11H26OSi	1114	4.5	594	1110	5.2	151
41	18394-04-2	Butylamine-2TMS	C10H27NSi2	1112	3.5	1032	--	--	0
42	27844-07-1	Alanine-2TMS	C9H23NO2Si2	1117	4.7	133	1109	9.6	19
43	2060000-89-5	Pyruvic acid-EO-TMS	C8H17NO3Si	1120	3.2	2916	1109	5.6	1864
44	N332856	3-Methyl-2-oxovaleric acid-TMS	C9H18O3Si	1120	3.5	9	1114	5.1	49
45	74367-71-8	2-Ketoisocaproic acid-TMS	C9H18O3Si	1122	5.9	2	1118	4.5	26
46	88239-46-7	trans-2-Hexenoic acid-TMS	C9H18O2Si	1129	3.5	636	1127	5.0	274
47	72101-11-2	Levulinic acid-2TMS	C11H24O3Si2	1135	1.7	707	1124	2.4	540
48	7364-42-3	Glycine-2TMS	C8H21NO2Si2	1133	2.7	145	1129	8.9	21
49	55133-93-2	2-Hydroxybutyric acid-2TMS	C10H24O3Si2	1137	2.6	1346	1127	4.5	939
50	18294-04-7	Oxalic acid-2TMS	C8H18O4Si2	1141	2.3	3412	1132	4.2	1990
51	55557-18-1	2-Methyl-2-hydroxybutanoic acid-2TMS	C11H26O3Si2	1146	3.6	1431	1135	3.6	944
52	55887-53-1	2-Furoic acid-TMS	C8H12O3Si	1145	2.6	144	1136	4.5	202
53	2060000-24-8	5-methylpyrrolidin-2-one-TMS	C8H17NOSi	1142	3.0	680	1140	5.2	700
54	41571-88-4	3-Hydroxypyridine-TMS	C8H13NOSi	1148	2.2	359	1147	7.5	2
55	55162-32-8	3-Hydroxypropionic acid-2TMS	C9H22O3Si2	1152	2.5	3253	1145	3.9	1795
56	140-29-4	Benzyl nitrile	C8H7N	1151	3.1	23	1151	1.9	44
57	541-02-6	Siloxane-Cyclopentasiloxane, decamethyl-	C10H30O5Si5	1162	7.1	1980	1146	8.5	880
58	2060000-44-2	Valproic acid-TMS	C11H24O2Si	1158	3.2	128	1150	2.8	61
59	17902-32-8	p-Cresol-TMS	C10H16OSi	1158	3.5	2268	1153	4.5	1582
60	14642-79-6	Benzyl alcohol-TMS	C10H16OSi	1162	3.0	639	1157	3.6	129
61	55133-94-3	3-Hydroxybutanoic acid-2TMS	C10H24O3Si2	1169	2.7	450	1160	2.9	209
62	55530-42-2	3-Hydroxyisobutyric acid-2TMS	C10H24O3Si2	1169	2.1	3389	1160	3.0	1852
63	2060001-01-4	Leucine-TMS	C9H21NO2Si	1166	--	1	--	--	0
64	209981-27-1	2-Ethylhexanoic acid-TMS	C11H24O2Si	1170	2.6	1579	1166	3.4	293
65	55124-92-0	2-Hydroxyisovaleric acid-2TMS	C11H26O3Si2	1174	2.2	1225	1165	4.9	515
66	18306-29-1	Sulfuric acid-2TMS	C6H18O4SSi2	1174	2.8	545	1167	5.7	192

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
67	2060000-78-2	Heptanoic acid-TMS	C10H22O2Si	1175	1.6	260	1171	2.8	247
68	2060000-90-8	Acetoacetic acid-EO-TMS-PK1	C9H19NO3Si	1184	1.9	516	1175	3.8	395
69	141-63-9	Siloxane-Pentasiloxane, dodecamethyl-	C12H36O4Si5	1186	4.1	3368	1176	6.0	1894
70	60615-84-1	Urea-3TMS	C10H28N2OSi3	1192	1.2	1415	1178	2.3	252
71	2060001-00-3	Isoleucine-TMS	C9H21NO2Si	1185	--	1	--	--	0
72	14246-16-3	Octanol-TMS	C11H26OSi	1186	1.1	76	--	--	0
73	N332246	3-Methyl-2-ketobutyric acid EO-TMS	C10H21NO3Si	1193	11.3	47	1185	4.2	42
74	42411-50-7	Pantoyl lactone-TMS	C9H18O3Si	1197	1.8	371	1189	4.0	601
75	2060000-91-9	Acetoacetic acid-EO-TMS-PK2	C9H19NO3Si	1204	1.7	507	1195	3.6	247
76	55557-17-0	2-Methyl-3-hydroxybutyric acid-2TMS	C11H26O3Si2	1206	2.0	2687	1195	3.7	1806
77	2060001-99-0	Carbamic acid-3TMS	C10H27NO2Si3	1210	1.1	1176	1198	0.7	21
78	18457-04-0	Malonic acid-2TMS	C9H20O4Si2	1212	3.1	714	1203	2.5	776
79	2060001-14-9	Acetoacetic acid-2TMS-PK1	C10H22O3Si2	1215	2.6	347	1206	2.7	341
80	55124-90-8	3-Hydroxyisovaleric acid-2TMS	C11H26O3Si2	1217	1.4	3001	1209	4.5	1741
81	2060001-02-5	d3-Methylmalonic Acid-2TMS†	C10H19D3O4Si2	1222	1.7	155	1212	4.4	1924
82	40333-07-1	Methylmalonic acid-2TMS	C10H22O4Si2	1223	1.5	2673	1213	2.8	399
83	59523-07-8	Uracil-TMS	C7H12N2O2Si	1231	2.1	165	1225	2.6	188
84	6689-37-8	Guaiacol-TMS	C10H16O2Si	1233	1.4	403	1225	1.8	431
85	2060000-39-5	2-Ethyl-3-hydroxypropionic acid-2TMS	C11H26O3Si2	1237	1.0	3388	1227	3.6	1887
86	2060000-71-5	2-Keto-3-methylvaleric acid-EO-2TMS PK1	C11H23NO3Si	1243	1.2	261	1231	3.4	639
87	55133-95-4	4-Hydroxybutyric acid-2TMS	C10H24O3Si2	1242	1.4	72	1236	2.8	314
88	54890-08-3	Pentanoic acid, 4-methyl-2-hydroxy-2TMS	C12H28O3Si2	1246	2.0	261	1234	3.1	155
89	79628-62-9	3-Hydroxyvaleric acid-2TMS	C11H26O3Si2	1245	2.0	25	1235	4.1	84
90	54890-09-4	2-Hydroxy-3-methylvaleric acid-2TMS	C12H28O3Si2	1250	2.3	278	1236	4.6	385
91	18297-63-7	Urea-2TMS	C7H20N2OSi2	1245	2.6	3189	1242	4.2	1521
92	2060001-15-0	Acetoacetic acid-2TMS-PK2	C10H22O3Si2	1255	1.1	959	1246	2.8	314
93	2078-12-8	Benzoic acid-TMS	C10H14O2Si	1253	1.8	2853	1248	3.4	1785
94	2060000-62-4	2-Keto-3-methylvaleric acid-EO-2TMS PK2	C11H23NO3Si	1259	1.1	151	1247	3.5	30
95	2060001-89-8	cis-1,2-cyclohexandiol-2TMS	C12H28O2Si2	1260	--	1	1252	2.0	257
96	105-60-2	Caprolactam	C6H11NO	1258	3.6	4	1261	3.2	40
97	72101-10-1	4-Hydroxyvaleric acid-2TMS	C11H26O3Si2	1266	1.0	149	1258	2.0	165
98	55517-38-9	Dihydroxy acetic acid-3TMS	C11H28O4Si3	1263	1.1	270	--	--	0
99	29753-64-8	trans-1,3-Cyclohexanediol-2TMS	C12H28O2Si2	1269	1.0	558	1260	3.5	381

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
100	55494-06-9	Octanoic acid-TMS	C11H24O2Si	1267	1.2	1204	1264	2.5	603
101	2060001-64-9	2,4-Diene-valproic acid-TMS	C11H20O2Si	1272	1.3	109	1263	2.3	37
102	2060000-68-0	2-Ketoisocaproic acid-EO-TMS-PK2	C11H23NO3Si	1274	1.4	551	1263	2.2	300
103	54890-07-2	2-Hydroxyhexanoic acid-2TMS	C12H28O3Si2	1305	0.3	11	1235	2.9	11
104	39789-21-4	trans-1,2-Cyclohexanediol-2TMS	C12H28O2Si2	1276	1.1	703	1264	2.8	506
105	2060001-19-4	Glyceraldehyde-EO-2TMS-PK1	C11H27NO3Si2	1277	0.9	598	1264	1.8	218
106	5630-81-9	Ethanolamine-3TMS	C11H31NOSi3	1276	1.3	205	1267	6.5	50
107	25436-37-7	Nicotinic acid-TMS	C9H13NO2Si	1276	2.2	300	--	--	0
108	7364-46-7	Leucine-2TMS	C12H29NO2Si2	1282	0.9	174	1271	1.3	33
109	98779-02-3	2-Methylacetoacetic acid-2TMS	C11H24O3Si2	1277	7.3	12	1279	4.4	6
110	2060000-31-7	Glutaric acid, methyl-TMS	C9H18O4Si	1283	1.4	3	1275	1.0	2
111	6787-10-6	Glycerol-3TMS	C12H32O3Si3	1286	0.8	410	1273	2.7	287
112	10497-05-9	Phosphoric Acid-3TMS	C9H27O4PSi3	1286	1.3	3522	1273	4.2	1977
113	18187-06-9	Sulfamic acid-2TMS	C6H19NO3SSi2	1289	5.3	4	1277	1.9	20
114	55557-24-9	Ethylmalonic acid-2TMS	C11H24O4Si2	1288	0.9	3363	1278	3.0	1973
115	2060001-27-4	Glyceraldehyde-EO-2TMS-PK2	C11H27NO3Si2	1296	1.0	2214	1284	2.7	1396
116	2060001-23-0	Ethosuximide-TMS	C10H19NO2Si	1296	1.1	11	--	--	0
117	7483-92-3	Isoleucine-2TMS	C12H29NO2Si2	1303	0.8	17	1291	1.3	16
118	2078-18-4	Phenylacetic acid-TMS	C11H16O2Si	1303	2.0	892	1297	2.4	600
119	629-50-5	Tridecane	C13H28	1301	0.6	106	1301	2.5	374
120	2060001-63-8	2-Propyl-4-oxopentanoic acid-TMS	C11H22O3Si	1308	1.9	75	1298	2.0	35
121	23508-82-9	Maleic-2TMS	C10H20O4Si2	1312	1.2	788	1301	1.8	542
122	136788-82-4	3-hydroxyhexanoic acid-2TMS	C12H28O3Si2	1315	0.9	1747	1303	2.4	931
123	5630-82-0	Glycine-3TMS	C11H29NO2Si3	1316	0.8	329	1305	4.3	42
124	29753-62-6	trans-1,4-Cyclohexanediol-2TMS	C12H28O2Si2	1322	0.8	512	1310	2.5	383
125	40309-57-7	Succinic acid-2TMS	C10H22O4Si2	1320	1.3	3610	1312	2.7	2000
126	5075-52-5	Pyrocatechol-2TMS	C12H22O2Si2	1326	0.9	1182	1313	2.2	838
127	2060000-63-5	p-Chlorocresol-TMS	C10H15ClOSi	1331	1.5	56	1325	4.4	24
128	55557-26-1	Methyl succinic acid-2TMS	C11H24O4Si2	1333	1.2	3455	1324	2.5	1874
129	2060000-48-6	5-Hydroxyvaleric acid-2TMS	C11H26O3Si2	1338	1.3	1248	1330	1.9	543
130	55012-80-1	Thymol-TMS	C13H22OSi	1337	3.5	63	1334	11.1	52
131	38191-87-6	Glyceric acid-3TMS	C12H30O4Si3	1344	1.1	2120	1329	2.7	1030
132	N352107	2-(2-Butoxyethoxy)ethanol-TMS	C11H26O3Si	1343	3.2	29	1336	1.4	68

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
133	10457-14-4	Uracil-2TMS	C10H20N2O2Si2	1349	1.1	1294	1334	1.9	644
134	55494-04-7	Itaconic acid-2TMS	C11H22O4Si2	1349	1.8	660	1340	1.9	546
135	2060000-32-8	Glutaric acid, ethyl ester-TMS	C10H20O4Si	1350	1.2	10	1343	0.4	2
136	17962-03-7	Fumaric acid-2TMS	C10H20O4Si2	1352	1.3	3080	1347	2.1	1569
137	38165-91-2	(R*,S*)-2,3-Dihydroxybutanoic acid-3TMS	C13H32O4Si3	1361	3.8	1385	1340	1.9	909
138	77220-12-3	Methylmaleic acid-2TMS	C11H22O4Si2	1360	1.2	660	1346	2.1	544
139	2060000-45-3	Pyrrole-2-carboxylic acid-2TMS	C11H21NO2Si2	1364	1.3	48	1346	2.1	49
140	2060000-43-1	(R*,R*)-2,3-Dihydroxybutanoic acid-3TMS	C13H32O4Si3	1366	4.1	2691	1345	3.5	1709
141	79628-63-0	5-Hydroxyhexanoic acid-2TMS	C12H28O3Si2	1364	1.1	696	1354	2.0	537
142	2060000-05-5	2-Hydroxyglutaric lactone-TMS	C8H14O4Si	1363	4.6	88	1355	3.4	142
143	82326-11-2	Nonanoic acid-TMS	C12H26O2Si	1362	1.7	737	1359	1.8	1187
144	55836-38-9	Propionylglycine-TMS	C8H17NO3Si	1365	5.9	5	1359	2.6	6
145	2060000-01-1	PenicillinFamilyMetabolite-TMS	C9H17NO2SSi	1368	2.1	246	1362	3.1	210
146	64625-17-8	Serine-3TMS	C12H31NO3Si3	1373	0.9	149	1360	3.6	7
147	107-52-8	Siloxane-Hexasiloxane, tetradecamethyl-	C14H42O5Si6	1375	6.1	1056	1358	7.8	538
148	16654-47-0	2-Phenoxyethanol-TMS	C11H18O2Si	1372	3.0	188	1363	1.6	530
149	102146-02-1	Mevalonolactone-TMS	C9H18O3Si	1378	4.4	12	1367	2.2	4
150	1012-12-0	Benzaldehyde, 4-hydroxy-TMS	C10H14O2Si	1369	23.9	23	1377	3.8	48
151	55220-79-6	Threonic acid-1,4-lactone-2TMS	C10H22O4Si2	1385	1.8	1627	1371	2.0	718
152	2060001-65-0	3-Hydroxyvalproic acid-2TMS	C14H32O3Si2	1394	1.4	150	1377	2.4	66
153	2060001-69-4	3-Methylcatechol-2TMS	C13H24O2Si2	1399	1.1	1508	1385	1.5	780
154	343224-19-1	Lactic acid dimer-2TMS	C12H26O5Si2	1401	1.9	280	1384	2.1	142
155	55836-41-4	Isobutyrylglycine-TMS	C9H19NO3Si	1396	3.8	63	1389	1.5	283
156	7537-02-2	Threonine-3TMS	C13H33NO3Si3	1401	1.0	81	1386	0.5	2
157	38165-93-4	Tartronic acid-3TMS	C12H28O5Si3	1404	0.9	327	1385	2.1	350
158	103-81-1	Benzeneacetamide	C8H9NO	1400	7.9	33	1399	8.0	26
159	N352398	1,1,1-Tris(hydroxymethyl)propane-3TMS	C15H38O3Si3	1410	1.8	6	1391	1.7	46
160	2117-24-0	Hydroquinone-2TMS	C12H22O2Si2	1408	5.2	1526	1397	4.8	1345
161	7288-28-0	Thymine-2TMS	C11H22N2O2Si2	1413	1.1	152	1395	0.8	54
162	2060001-36-5	Parabanic acid-2TMS	C9H18N2O3Si2	1413	1.4	433	1398	0.8	39
163	55494-07-0	Glutaric acid-2TMS	C11H24O4Si2	1410	1.7	2774	1403	1.8	1744
164	2060000-61-3	Sulfamic acid-3TMS	C9H27NO3SSi3	1414	0.7	36	1401	0.2	5
165	2060001-29-6	Methylmalonic acid-3TMS	C13H30O4Si3	1428	0.7	60	1405	1.6	6

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
166	55191-52-1	2,4-Dihydroxybutanoic acid-3TMS	C13H32O4Si3	1425	1.3	2473	1410	2.1	1380
167	55530-53-5	2-Methylglutaric acid-2TMS	C12H26O4Si2	1422	1.4	1052	1413	1.7	694
168	2060001-33-2	2-Propyl-3-ketovaleric acid-2TMS	C14H30O3Si2	1432	6.9	95	1407	2.7	40
169	55557-16-9	Propionylglycine-2TMS	C11H25NO3Si2	1434	0.8	5	1416	0.7	4
170	55530-55-7	Isobutrylglycine-2TMS	C12H27NO3Si2	1434	0.7	71	1417	1.1	3
171	55517-41-4	3-Methylpentanedioic acid-2TMS	C12H26O4Si2	1431	1.6	1925	1423	1.6	1019
172	21273-08-5	Phenoxyacetic acid-TMS	C11H16O3Si	1432	3.3	1394	1423	2.2	936
173	74742-33-9	2,3-Dihydroxy-5-deoxypentonic acid, .gamma.-lactone-2TMS	C11H24O4Si2	1439	1.6	952	1418	3.1	483
174	150367-75-2	6-Hydroxyhexanoic acid-2TMS	C12H28O3Si2	1433	1.6	138	1425	1.6	50
175	15667-21-7-2TMS	D-Erythronic acid .gamma.-lactone-2TMS	C10H22O4Si2	1442	2.5	361	1425	1.8	195
176	1011-57-0	Benzamide-TMS	C10H15NOSi	1439	3.0	100	1432	1.8	58
177	55255-77-1	.beta.-alanine-3TMS	C12H31NO2Si3	1437	0.9	34	--	--	0
178	55191-53-2	(R*,S*)-3,4-Dihydroxybutanoic acid-3TMS	C13H32O4Si3	1445	1.3	3289	1429	2.0	1791
179	2060001-70-7	N-Acetylleucine-TMS	C11H23NO3Si	1448	1.6	9	1434	1.2	118
180	55125-08-1	3-Methylglutaconic acid-2TMS (E)	C12H24O4Si2	1448	1.8	3418	1437	1.8	1953
181	55255-43-1	Glutaconic acid-2TMS	C11H22O4Si2	1455	2.5	27	1448	1.4	28
182	2060000-60-2	2-Ketoglutaric acid-2TMS PK1	C11H22O5Si2	1462	0.6	69	1442	1.2	52
183	55494-15-0	Decanoic acid-TMS	C13H28O2Si	1459	1.9	758	1456	1.6	538
184	2060001-44-5	2-Ketooctanoic acid-2TMS	C14H30O3Si2	1466	1.4	124	1450	1.9	39
185	2060001-72-9	Benzeneacetamide-TMS	C11H17NOSi	1467	2.9	85	1457	1.5	61
186	2060001-66-1	4-Hydroxyvalproic acid-2TMS	C14H32O3Si2	1471	2.5	142	1458	4.2	59
187	55493-99-7	2-Methylbutyrylglycine-TMS	C10H21NO3Si	1479	3.5	113	1471	2.5	57
188	136788-83-5	3-Hydroxyoctanoic acid-2TMS	C14H32O3Si2	1482	1.3	792	1469	1.8	42
189	2060000-49-7	Citramalic acid-3TMS	C14H32O5Si3	1488	0.9	2295	1469	2.1	1754
190	2078-19-5	Mandelic acid-2TMS	C14H24O3Si2	1489	1.2	228	1471	1.7	250
191	2060001-67-2	5-Hydroxyvalproic acid-2TMS	C14H32O3Si2	1487	1.5	139	1475	1.9	61
192	2060000-08-8	3-Hydroxy-3-methylglutaric acid-2TMS	C12H26O5Si2	1489	1.1	1975	1479	1.5	763
193	55125-09-2	3-Methylglutaconic acid-2TMS (Z)	C12H24O4Si2	1489	1.7	1366	1480	1.7	1379
194	2060000-07-7	3-Hydroxyadipic lactone-TMS	C9H16O4Si	1491	4.5	1063	1482	2.6	633
195	2060001-87-6	2-Ketoglutaric acid-2TMS PK2	C11H22O5Si2	1496	0.8	72	1484	1.3	47
196	55494-00-3	Isovalerylglycine-TMS	C10H21NO3Si	1493	4.0	169	1487	2.1	236
197	38166-11-9	Malic acid-3TMS	C13H30O5Si3	1502	1.3	2355	1484	1.8	1218

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
198	27739-17-9	4-Hydroxybenzoic acid methyl ester-TMS	C11H16O3Si	1502	3.7	1456	1493	1.9	998
199	2060000-65-7	Pyroglutamic acid-TMS	C8H15NO3Si	1502	4.1	108	1498	1.6	78
200	18105-31-2	Adipic acid-2TMS	C12H26O4Si2	1512	1.9	3465	1503	1.6	1775
201	2060000-26-0	Pentonic acid, 2-deoxy-3,5-dihydroxy-, .gamma.-lactone-2TMS	C11H24O4Si2	1521	2.0	1137	1503	2.0	248
202	128-37-0	Butylated Hydroxytoluene	C15H24O	1520	1.4	2495	1506	1.5	1699
203	3789-85-3	Salicylic acid-2TMS	C13H22O3Si2	1522	1.9	324	1505	1.2	97
204	55520-90-6	Isovalerylglycine-2TMS	C13H29NO3Si2	1522	1.4	40	1505	1.0	5
205	2060001-74-1	4-Hydroxycyclohexanecarboxylic acid-2TMS	C13H28O3Si2	1520	1.6	518	1509	1.5	527
206	111-82-0	Dodecanoic acid, methyl ester	C13H26O2	1520	--	1	--	--	0
207	30274-77-2	Pyroglutamic acid-2TMS	C11H23NO3Si2	1535	1.8	2845	1517	1.2	1184
208	27844-10-6	Methionine-2TMS	C11H27NO2SSi2	1527	--	1	--	--	0
209	2060000-15-7	Acesulfame-TMS	C7H13NO4SSi	1541	3.0	230	1518	2.7	202
210	21273-16-5	4-Phenyl-butyric acid-TMS	C13H20O2Si	1532	2.1	4	--	--	0
211	2060000-58-8	Thiodiglycolic acid-2TMS	C10H22O4SSi2	1539	1.6	325	1528	1.7	519
212	55520-93-9	3-Methyladipic acid-2TMS	C13H28O4Si2	1543	1.7	2324	1533	1.6	1650
213	10416-73-6	2,6-Di-tert-butyl-phenol-TMS	C17H30OSi	1553	0.8	734	1537	1.6	750
214	17864-23-2	1,2,3-Trihydroxybenzene-3TMS	C15H30O3Si3	1558	1.3	879	1537	1.4	261
215	2060000-76-0	7-Hydroxyoctanoic acid-2TMS	C14H32O3Si2	1554	1.3	93	1542	1.4	64
216	2060001-25-2	2-Ethyl-3-hydroxy-2-methylsuccinimide-2TMS	C13H27NO3Si2	1549	6.1	8	--	--	0
217	2899-42-5	Phenylalanine-TMS	C12H19NO2Si	1549	--	1	--	--	0
218	2060000-46-4	2-Propylpentanedioic acid-2TMS	C14H30O4Si2	1555	1.8	154	1543	1.8	66
219	55517-40-3	5-Hydroxymethyl-2-furan carboxylic acid-2TMS	C12H22O4Si2	1559	2.3	2576	1547	1.6	1418
220	2060001-17-2	2-Ketosuccinic acid-3TMS	C13H28O5Si3	1566	2.2	4	1549	1.5	12
221	55517-45-8	Tiglylglycine-2TMS	C13H27NO3Si2	1568	1.4	32	1549	0.7	4
222	2060001-09-2	Phenylpyruvic acid-2TMS (cis enol)#	C15H24O3Si2	--	--	0	1561	--	1
223	2060000-70-4	Creatinine-3TMS	C13H31N3OSi3	1571	0.9	122	1552	0.5	3
224	2060001-59-2	Keppra Metabolite	C11H21NO3Si	1569	2.9	9	1556	1.3	14
225	2060000-50-0	Threonic acid-3TMS	C16H40O5Si4	1578	7.3	2176	1551	7.3	1349
226	3782-84-1	3-Hydroxybenzoic acid-2TMS	C13H22O3Si2	1573	2.1	1535	1563	1.3	234
227	54824-02-1	3-Methylcrotonylglycine-TMS	C10H19NO3Si	1573	3.2	29	1563	2.3	36
228	2060000-59-9	tert-Butylhydroquinone-2TMS	C16H30O2Si2	1579	1.9	141	1558	1.6	162

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
229	6221-88-1	Decanol-TMS	C15H34OSi	1571	1.1	475	1566	1.5	249
230	27750-52-3	2-Hydroxyphenylacetic acid-2TMS	C14H24O3Si2	1579	1.7	2466	1563	1.4	1128
231	55517-35-6	Tiglylglycine-TMS	C10H19NO3Si	1578	3.6	240	1568	2.0	424
232	55649-86-0	3-Methylcrotonylglycine-2TMS	C13H27NO3Si2	1584	1.4	8	1564	1.9	3
233	2060001-57-0	Benzocaine-TMS	C12H19NO2Si	1579	2.6	102	1571	2.0	130
234	102767-28-2	Levetiracetam	C8H14N2O2	1584	8.4	4	1573	2.8	13
235	55530-62-6	2-Hydroxyglutaric acid-3TMS	C14H32O5Si3	1588	1.6	3440	1571	1.8	1866
236	2060001-05-8	3-Hydroxyglutaric acid-3TMS	C14H32O5Si3	1589	1.6	83	1571	1.9	72
237	2060000-81-7	2-Isopropylmalic acid-3TMS	C16H36O5Si3	1594	1.0	907	1571	2.0	116
238	2060001-48-9	Heptenedioic acid-2TMS	C13H26O4Si2	1591	1.8	2871	1580	1.5	1638
239	27750-45-4	2-Hydroxy-3-phenylpropanoic acid-2TMS	C15H26O3Si2	1598	1.2	1098	1580	1.8	474
240	2060000-77-1	3-Hydroxy-3-phenylpropanic acid-2TMS	C15H26O3Si2	1604	2.3	70	1586	1.4	27
241	55530-58-0	Heptanedioic acid-2TMS	C13H28O4Si2	1610	2.0	2488	1600	1.5	988
242	55590-95-9	3-Hydroxy-3-methylglutaric acid-3TMS	C15H34O5Si3	1617	1.3	3042	1598	1.9	1845
243	72361-20-7	3-Oxoglutaric acid-3TMS	C14H30O5Si3	1621	4.4	9	1598	1.6	10
244	60739-94-8	Cyanuric acid-3TMS	C12H27N3O3Si3	1624	0.8	71	1599	0.3	4
245	27750-55-6	3-Hydroxyphenylacetic acid-2TMS	C14H24O3Si2	1618	1.8	2388	1605	1.5	1729
246	2060001-06-9	2-Ketoglutaric acid-3TMS PK1	C14H30O5Si3	1620	1.6	103	1603	1.4	122
247	18406-07-0	Anthranilic acid-2TMS	C13H23NO2Si2	1625	0.8	1178	1608	1.3	302
248	2060000-67-9	4-Hydroxycyclohexylacetic acid-2TMS	C14H30O3Si2	1623	1.5	977	1612	1.3	243
249	2060001-07-0	2-Ketoglutaric acid-3TMS PK2	C14H30O5Si3	1631	0.3	8	1610	8.4	2
250	55517-43-6	(E,E)-2,4-Hexadienedioic acid-2TMS	C12H22O4Si2	1627	1.9	205	1619	1.2	100
251	2060000-34-0	2-Ketoglutaric acid-EO-2TMS	C13H27NO5Si2	1633	2.2	3457	1615	1.8	1961
252	102767-28-2-TMS	Levetiracetam-TMS	C11H22N2O2Si	1633	0.7	2	1618	1.7	8
253	74810-89-2	Ibuprofen-TMS	C16H26O2Si	1631	1.8	78	1621	0.8	39
254	2078-13-9	4-Hydroxybenzoic acid-2TMS	C13H22O3Si2	1635	1.8	3525	1624	1.5	1954
255	7364-51-4	Phenylalanine-2TMS	C15H27NO2Si2	1641	0.8	72	1622	0.4	12
256	55530-61-5	Paracetamol-2TMS	C14H25NO2Si2	1645	1.0	345	1627	1.4	82
257	2060001-20-7	4-Hydroxypropofol-2TMS	C18H34O2Si2	1650	1.4	56	1627	0.9	22
258	2060001-08-1	Phenylpyruvic acid-EO-TMS	C14H21NO3Si	1650	--	1	1631	1.9	84
259	2060000-75-9	3-Hydroxy-4-methoxybenzyl alcohol-2TMS	C14H26O3Si2	1650	1.7	62	1633	1.3	39
260	27750-57-8	4-Hydroxyphenylacetic acid-2TMS	C14H24O3Si2	1648	1.9	3591	1636	1.5	2008
261	2060000-55-5	Tartaric acid-4TMS	C16H38O6Si4	1662	1.6	419	1633	2.0	268

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
262	55530-57-9	1,2-Benzenedicarboxylic acid ethyl ester-TMS	C13H18O4Si	1657	2.3	146	1640	1.4	45
263	55494-09-2	2,5-Furandicarboxylic acid-2TMS	C12H20O5Si2	1655	2.2	2078	1642	1.6	1512
264	2060001-98-9	3-(Methylthio)benzoic acid-TMS	C11H16O2SSi	1652	2.7	36	1645	2.5	2
265	2060000-17-9	Hexanoylglycine-2TMS	C14H31NO3Si2	1659	0.3	5	1640	--	1
266	55520-95-1	Dodecanoic acid-TMS	C15H32O2Si	1654	2.2	393	1650	1.5	185
267	2060001-03-6	N-Acetylaspartic acid-2TMS	C12H25NO5Si2	1671	2.4	1433	1652	1.8	1419
268	71428-92-7	Furoylglycine-TMS	C10H15NO4Si	1667	4.2	893	1656	2.4	1082
269	2060001-38-7	Topiramate metabolite-TMS	C15H28O6Si	1669	1.7	27	1655	0.8	19
270	55556-83-7	2-Furoylglycine-2TMS	C13H23NO4Si2	1679	1.2	168	1657	2.0	20
271	2060001-39-8	Succinylacetone-2EO-TMS-PK1	C14H28N2O4Si	1683	--	1	1660	--	1
272	2060001-04-7	N-Acetylaspartic acid-3TMS	C15H33NO5Si3	1687	0.7	199	1662	2.1	35
273	2060000-28-2	Cyclamate-2TMS	C12H29NO3SSi2	1685	1.0	94	1666	0.8	36
274	2060000-80-6	2-Hydroxyadipic acid-3TMS	C15H34O5Si3	1686	1.2	2068	1666	1.8	1282
275	2060001-22-9	Thiosalicylic acid-2TMS	C13H22O2SSi2	1686	1.9	18	1670	1.1	9
276	2060000-09-9	Octenedioic acid-2TMS	C14H28O4Si2	1688	1.7	2953	1676	1.7	1439
277	2060001-85-4	Succinylacetone-EO(1)-2TMS-PK2	C15H31NO4Si2	--	--	0	1684	1.1	2
278	73105-00-7	3-Hydroxyadipic acid-3TMS	C15H34O5Si3	1696	1.5	1591	1678	1.8	550
279	2060001-86-5	Succinylacetone-EO(1)-2TMS-PK1	C15H31NO4Si2	1700	0.7	4	1678	1.0	4
280	2060001-42-3	Succinylacetone-2EO-TMS-PK2	C14H28N2O4Si	1700	--	1	1680	1.0	6
281	2078-22-0	Phthalic acid-2TMS	C14H22O4Si2	1706	2.2	835	1686	1.7	861
282	2060001-41-2	Succinylacetone-2EO-TMS-PK3	C14H28N2O4Si	1707	--	1	1687	--	1
283	18510-49-1	3,5-Di-tert-butyl-4-hydroxytoluene-TMS	C18H32OSi	1710	1.1	1071	1687	1.1	116
284	43199-48-0	Suberic acid-2TMS	C14H30O4Si2	1705	1.8	3124	1694	1.5	1680
285	2060001-13-8	2-Hydroxy-3-methoxybenzoic acid-2TMS	C14H24O4Si2	1716	8.4	72	1687	0.6	35
286	55334-16-2	2-Ketoadipic acid-3TMS PK1	C15H32O5Si3	1713	0.6	20	1691	1.6	5
287	2060001-40-1	Succinylacetone-2EO-TMS-PK4	C14H28N2O4Si	1716	--	1	1692	--	1
288	2060001-95-6	Succinyl acetone-EO(1)-2TMS-PK3	C15H31NO4Si2	1714	0.6	5	1697	1.1	3
289	2060001-30-9	2-Ketoadipic acid-EO-2TMS-PK1	C14H29NO5Si2	1713	2.5	93	1700	1.3	13
290	2060001-31-0	2-Ketoadipic acid-EO-2TMS-PK2	C14H29NO5Si2	1719	1.5	1505	1700	1.5	1281
291	7449-14-1	Levoglucosan-3TMS	C15H34O5Si3	1726	2.1	410	1697	1.4	153
292	2060000-03-3	Phenylpyruvic acid-2TMS (trans enol)#	C15H24O3Si2	1722	0.2	3	1701	0.8	4
293	2060000-16-8	5-Hydroxyindole-2TMS	C14H23NOSi2	1723	2.5	770	1703	1.4	287
294	65143-62-6	Isocitric lactone-2TMS	C12H22O6Si2	1721	1.7	1499	1706	1.5	1029

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
295	2060000-21-5	2-[2-hydroxy-3-(propan-2-yl)phenyl]propanoic acid-2TMS	C18H32O3Si2	1724	0.3	2	--	--	0
296	27798-58-9	Benzoic acid, 3,4-dihydroxy-, methyl ester-2TMS	C14H24O4Si2	1735	1.5	247	1715	1.8	116
297	55887-87-1	(3-Hydroxyphenyl)propionic acid-2TMS	C15H26O3Si2	1737	1.7	949	1725	1.4	652
298	2060000-54-4	Quinolinic acid-2TMS	C13H21NO4Si2	1745	1.8	773	1721	1.7	837
299	2060001-84-3	Succinyl acetone-EO(1)-2TMS-PK4	C15H31NO4Si2	1745	--	1	1724	--	1
300	2060000-40-8	Tricarballylic acid - 3TMS	C15H32O6Si3	1745	1.2	746	1727	1.7	586
301	2060000-35-1	Heptanoylglycine- TMS†	C12H25NO3Si	1742	3.3	3133	1732	2.2	1896
302	2060000-18-0	Heptanoylglycine-2TMS†	C15H33NO3Si2	1748	1.2	1310	1728	1.5	222
303	3618-19-7	2,3-Dihydroxybenzoic acid-3TMS	C16H30O4Si3	1760	0.7	230	1734	1.3	192
304	31111-36-1	Orotic acid-3TMS	C14H28N2O4Si3	1763	1.3	269	1739	1.2	402
305	55530-71-7	cis-Aconitic acid-3TMS (585-84-2)	C15H30O6Si3	1762	1.8	3532	1744	1.7	2012
306	41571-82-8	Paracetamol-TMS	C11H17NO2Si	1764	6.6	255	1749	3.0	245
307	2060000-42-0	trans-Aconitic acid-3TMS (4023-65-8)	C15H30O6Si3	1772	0.8	1795	1751	1.7	8
308	27750-62-5	4-Hydroxyhydrocinnamic acid-2TMS	C15H26O3Si2	1771	1.1	279	1757	0.9	73
309	68595-68-6	Benzoic acid, 4-methoxy-3-hydroxy-2TMS	C14H24O4Si2	1772	2.6	158	1758	3.4	60
310	2078-15-1	Vanillic acid-2TMS	C14H24O4Si2	1775	1.8	1645	1760	1.5	1601
311	3782-85-2	2,6-Dihydroxybenzoic acid-3TMS	C16H30O4Si3	1783	2.5	120	1753	1.6	555
312	31038-11-6	2-Glycerophosphoric acid-4TMS	C15H41O6PSi4	1788	1.6	125	1757	1.7	68
313	37148-61-1	Homovanillic acid-2TMS	C15H26O4Si2	1784	2.1	3620	1767	1.6	2018
314	3618-20-0	2,5-Dihydroxybenzoic acid-3TMS	C16H30O4Si3	1791	2.3	1631	1769	2.6	836
315	2060000-83-9	Citric acid-3TMS	C15H32O7Si3	1791	2.3	282	1772	1.3	172
316	2060000-51-1	4-Hydroxymandelic acid-3TMS	C17H32O4Si3	1797	1.6	3400	1774	1.7	1941
317	4147-84-6	Terephthalic acid-2TMS	C14H22O4Si2	1800	2.1	327	1785	1.5	989
318	2060000-82-8	Citric acid ethyl ester-3TMS	C17H36O7Si3	1807	1.0	1005	1779	1.6	611
319	17906-08-0	Azelaic acid-2TMS	C15H32O4Si2	1803	2.0	2059	1792	1.6	1689
320	2060000-29-3	1H-Indole-2,3-dione, 5-methoxy-1-hydroxy-EO-TMS# (EO on 3-carbonyl)	C14H20N2O3Si	1809	0.6	32	1790	0.8	15
321	495-69-2	Hippuric acid	C9H9NO3	1818	23.9	93	1799	44.8	3
322	55133-85-2	Hippuric acid-2TMS	C15H25NO3Si2	1821	1.5	829	1799	1.8	210
323	2060001-47-8	N-Acetylphenylalanine-TMS	C14H21NO3Si	1826	1.5	40	1804	1.2	98
324	2060000-84-0	3-Ethoxy-4-hydroxybenzoic acid-2TMS	C15H26O4Si2	1827	1.7	210	1810	1.0	80

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
325	10586-16-0	2,4-Dihydroxybenzoic acid-3TMS	C16H30O4Si3	1832	2.0	5	1806	6.3	10
326	79314-27-5	3,5-dihydroxybenzoic acid-3TMS	C16H30O4Si3	1831	2.0	1750	1814	1.7	426
327	2347-40-2	3,4-Dihydroxybenzoic acid-3TMS	C16H30O4Si3	1835	1.3	546	1814	1.5	99
328	14330-97-3	Citric acid-4TMS	C18H40O7Si4	1845	1.6	3364	1814	2.0	1908
329	55517-57-2	Isocitric acid-4TMS	C18H40O7Si4	1845	2.5	238	1816	2.3	293
330	37148-62-2	3,4-Dihydroxyphenylacetic acid-3TMS	C17H32O4Si3	1847	1.5	2365	1824	1.8	1748
331	55334-62-8	Homogentisic acid-3TMS	C17H32O4Si3	1853	1.1	97	1830	1.1	44
332	55556-97-3	D-Glucuronic acid, 2,4,5-trihydroxy-, lactone-3TMS	C15H32O6Si3	1857	2.5	228	1829	1.5	179
333	2078-24-2	Hippuric acid-TMS	C12H17NO3Si	1852	4.0	3119	1842	3.2	1827
334	2060000-93-1	(2S,3S)-Methylcitric acid-4TMS	C19H42O7Si4	1864	1.0	2045	1832	2.2	1120
335	18603-17-3	Tetradecanoic acid-TMS	C17H36O2Si	1850	2.3	411	1846	1.8	466
336	2060000-94-2	(2R,3S)Methylcitric acid-4TMS	C19H42O7Si4	1872	0.8	1687	1838	1.5	824
337	2060000-36-2	3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS#	C18H34O4Si3	1867	1.9	2000	1844	1.6	981
338	58-08-2	Caffeine	C8H10N4O2	1861	5.6	47	1851	5.9	26
339	2060001-56-9	2,6-bis(1-hydroxy-2-propyl)phenol-3TMS	C21H42O3Si3	1874	1.4	38	1844	1.1	7
340	2060001-16-1	2-Ketoglutaric Acid-4TMS	C17H38O5Si4	1863	0.9	93	--	--	0
341	2060001-75-2	cis-4-Decene-1,10-dioic acid-2TMS	C16H32O4Si2	1877	4.6	247	1859	1.9	133
342	84-69-5	Isobutyl phthalate	C16H22O4	1876	3.5	1574	1862	1.7	1616
343	2060001-78-5	Guaifenesin-2TMS	C16H28O5Si2	1885	1.9	24	1862	0.9	2
344	32342-01-1	m-Hydroxycinnamic acid-2TMS	C15H24O3Si2	1878	2.1	426	1871	0.4	72
345	2060000-12-4	3-Hydroxyhexanedioic acid-3TMS	C17H38O5Si3	1888	1.4	1172	1868	1.6	355
346	55268-66-1	Vanillylmandelic acid-3TMS	C18H34O5Si3	1900	2.0	3423	1871	1.8	2003
347	2060000-20-4	Phenylacetylglycine-TMS	C13H19NO4Si	1895	3.0	403	1881	2.2	382
348	2060001-43-4	2-O-methyl ascorbic acid-3TMS	C16H34O6Si3	1904	1.9	591	1873	1.4	82
349	2060000-19-1	Hydroxy-Ibuprofen-2TMS	C19H34O3Si2	1899	1.3	192	1880	0.8	134
350	18408-42-9	Sebacic acid-2TMS	C16H34O4Si2	1900	2.8	158	1889	1.5	605
351	55515-33-8	Gluconic acid-lactone-4TMS-PK1	C18H42O6Si4	1913	1.9	99	1879	1.6	66
352	56051-49-1	3-Methoxy-4-hydroxybenzenepropionic acid-2TMS	C16H28O4Si2	1908	2.4	1078	1888	3.0	428
353	2060000-06-6	2-(2'-Octenyl)succinic acid-2TMS	C18H36O4Si2	1906	1.5	65	1890	2.4	56
354	2060001-21-8	beta-4-Hydroxyphenylhydracrylic acid-3TMS	C18H34O4Si3	1913	1.9	582	1888	1.4	237

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
355	10517-29-0	Syringic acid-2TMS	C15H26O5Si2	1912	2.0	500	1891	1.4	291
356	2060001-94-5	2-(2'-Octenyl)succinic acid-2TMS-PK2	C18H36O4Si2	1915	--	1	1891	0.7	18
357	2060001-93-4	Gluconic acid-lactone-4TMS-PK2	C18H42O6Si4	1921	7.0	213	1890	2.7	93
358	27750-67-0	3-(4-hydroxyphenyl)-lactic acid-3TMS	C18H34O4Si3	1919	1.6	3345	1893	1.7	1934
359	62374-32-7	Theophyline-TMS	C10H16N4O2Si	1928	--	1	1906	--	1
360	74367-45-6	1H-Indole-2-carboxylic acid, 5-ethyl-1-hydroxy-2TMS	C17H27NO2Si2	1937	2.3	59	1907	0.7	64
361	2060000-72-6	3-Indoleacetic acid-TMS	C13H17NO2Si	1927	5.0	211	1918	3.0	209
362	112-39-0	Hexadecanoic acid, methyl ester	C17H34O2	1923	--	1	--	--	0
363	37148-65-5	Mandelic acid, 3,4-dihydroxy-4TMS	C20H40O5Si4	1950	2.6	233	1917	2.1	342
364	10517-30-3	p-Hydroxycinnamic acid-2TMS	C15H24O3Si2	1950	2.2	294	1935	1.7	244
365	74367-22-9	Pentanedecanoic acid-TMS	C18H38O2Si	1948	2.3	110	1944	0.7	69
366	27750-68-1	3,4-Dihydroxyhydrocinnamic acid-3TMS	C18H34O4Si3	1962	1.4	761	1939	1.8	572
367	2060000-41-9	4-Hydroxyphenylpyruvic acid-EO-2TMS	C17H29NO4Si2	1966	1.6	2149	1945	1.8	1360
368	55517-56-1	Ascorbic acid-4TMS	C18H40O6Si4	1978	1.5	596	1941	1.6	374
369	2060001-24-1	Salicyluric acid-3TMS	C18H33NO4Si3	1975	1.0	65	1944	3.1	7
370	6221-90-5	Hexadecanol-TMS	C19H42OSi	1962	1.8	1018	1957	2.2	98
371	84-74-2	Dibutyl phthalate	C16H22O4	1970	4.2	1307	1956	2.2	203
372	56114-66-0	Indole-3-acetic acid-2TMS	C16H25NO2Si2	1981	2.4	2955	1957	1.7	1867
373	2060000-00-0	Phenobarbital-2TMS – 1#	C18H28N2O3Si2	2007	1.0	67	1979	0.9	48
374	628-97-7	Ethyl hexadecanoate	C18H36O2	1995	0.9	149	--	--	0
375	256-96-2	Iminostilbene	C14H11N	1994	0.6	3	1999	0.9	2
376	2060000-38-4	Vanillylhydracrylic acid-3TMS	C19H36O5Si3	2013	3.2	1504	1986	3.0	923
377	2060000-25-9	Pantothenic acid-3TMS	C18H41NO5Si3	2016	1.3	2536	1986	1.9	1436
378	50-06-6	Phenobarbital	C12H12N2O3	2007	6.8	96	2001	4.2	126
379	2060001-35-4	3-Phenylpropionylglycine-2TMS	C17H29NO3Si2	2006	--	1	--	--	0
380	55530-80-8	D-Glucuronic acid-5TMS	C21H50O7Si5	2005	2.3	507	2012	2.7	121
381	52937-73-2	Phenobarbital-2TMS-2#	C18H28N2O3Si2	2020	3.1	35	2005	1.9	11
382	2060000-13-5	Carboxyibuprofen-2TMS	C19H32O4Si2	2024	1.7	241	2003	1.1	174
383	2060000-88-4	cis-9-Hexadecenoic acid-TMS	C19H38O2Si	2028	2.7	110	2020	2.9	105
384	55887-61-1	Vanillactic acid-3TMS	C19H36O5Si3	2042	1.1	818	2010	1.7	628
385	55255-79-3	#1H-Indole-5-carboxylic acid-2TMS	C15H23NO2Si2	2040	2.4	1332	2020	1.8	1414
386	55520-89-3	Hexadecanoic acid-TMS	C19H40O2Si	2048	1.9	3138	2042	1.8	1910

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
387	27750-74-9	4-Hydroxyphenylpyruvic acid-3TMS	C18H32O4Si3	2067	0.9	126	2040	1.0	158
388	2060001-11-6	trans-Traumatic acid-2TMS	C18H36O4Si2	--	--	0	2054	--	1
389	2060000-57-7	2-Hydroxysebacic acid-3TMS	C19H42O5Si3	2066	1.2	1704	2044	1.7	1069
390	506-12-7	Heptadecanoic acid	C17H34O2	2059	2.2	327	2062	1.9	5
391	55517-54-9	3-Hydroxyhippuric acid-3TMS	C18H33NO4Si3	2078	1.7	81	2050	0.6	19
392	76735-13-2	3-Hydroxysebacic acid-3TMS	C19H42O5Si3	2080	1.4	2460	2058	1.8	1319
393	68595-72-2	Catechollactic acid-4TMS	C21H42O5Si4	2091	0.7	153	2056	3.3	121
394	71428-95-0	Salicyluric acid-2TMS	C15H25NO4Si2	2087	1.8	1122	2062	1.9	849
395	36972-84-6	Kynurenic acid-2TMS	C16H23NO3Si2	2087	1.2	250	2062	1.7	187
396	112-91-4	Oleanitrile	C18H33N	2083	3.3	200	2081	0.6	50
397	74793-83-2	Naproxen-TMS	C17H22O3Si	2096	4.2	2	2084	0.7	3
398	74381-41-2	2,5-Dihydroxyindole-3TMS	C17H31NO2Si3	2106	1.6	563	2079	1.5	220
399	14010-23-2	Heptadecanoic acid, ethyl ester	C19H38O2	2095	1.5	287	2091	1.2	254
400	112-63-0	Linoleic acid, methyl ester	C19H34O2	2094	--	1	2092	--	1
401	10517-09-6	3-Hydroxy-4-methoxycinnamic acid-2TMS	C16H26O4Si2	2105	2.3	1668	2087	1.8	1005
402	112-62-9	Oleic acid, methyl ester	C19H36O2	2100	--	1	2099	--	1
403	2060001-50-3	Carbamazepine Metabolite (-CONH2)-10,11-diOH-2TMS	C20H29NO2Si2	2124	2.4	40	2087	1.0	11
404	2582-79-8	Myo-Inositol-6TMS	C24H60O6Si6	2129	0.9	224	2085	1.9	27
405	2060000-52-2	Uric acid-4TMS	C17H36N4O3Si4	2134	1.4	1117	2091	1.4	404
406	2060000-66-8	2-Ethylhexyl phthalate-TMS	C19H30O4Si	2129	2.5	524	2105	1.5	210
407	2060001-97-8	Carbamazepine Metabolite -CONH2+10OH-TMS	C17H21NOSi	2135	--	1	2113	--	1
408	78695-25-7	Octadec-9(Z)-en-ol-TMS	C21H44OSi	2134	1.5	45	2127	0.7	12
409	55517-55-0	4-Hydroxyhippuric acid-3TMS	C18H33NO4Si3	2146	3.0	32	2120	1.9	22
410	2060000-56-6	N-Acetyltyrosine-2TMS	C17H29NO4Si2	2148	2.6	445	2121	2.3	908
411	10586-03-5	3,4-Dihydroxycinnamic acid-3TMS	C18H32O4Si3	2152	1.2	808	2132	1.5	424
412	55517-58-3	Margaric acid-TMS†	C20H42O2Si	2147	2.1	3559	2141	1.7	1987
413	2060000-53-3	3-Hydroxyhippuric acid-2TMS	C15H25NO4Si2	2160	3.6	1473	2143	3.0	754
414	18748-98-6	Octadecanol-TMS	C21H46OSi	2158	2.0	1052	2153	1.9	671
415	2060001-58-1	Naproxen metabolite-2TMS	C19H28O3Si2	2176	1.6	14	2158	0.8	6
416	2060000-30-6	1H-Indole-2,3-dione, -6-hydroxy-, EO-2TMS (EO on 3-carbonyl)	C16H26N2O3Si2	2195	1.7	392	2169	1.1	115

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
417	55319-91-0	Indole-3-lactic acid-3TMS	C20H35NO3Si3	2204	1.3	1576	2167	2.0	886
418	111-06-8	Hexadecanoic acid, butyl ester	C20H40O2	2187	2.6	225	2184	1.0	199
419	2060000-02-2	Penicillin Family Metabolite-II-2TMS #	C14H30N2O4SSi2	2203	2.9	42	2169	1.3	78
420	111-61-5	Octadecanoic acid, ethyl ester	C20H40O2	2196	1.2	186	2191	--	1
421	56259-07-5	Linoleic acid-TMS	C21H40O2Si	2217	1.3	255	2207	0.9	94
422	2060000-64-6	Benzyl phthalate-TMS	C18H20O4Si	2226	2.6	79	2203	1.5	24
423	69937-41-3	5-Hydroxyindole-3-acetic acid-2TMS	C16H25NO3Si2	2226	3.0	1476	2205	2.9	896
424	21556-26-3	Oleic acid-TMS	C21H42O2Si	2221	2.3	512	2213	2.1	439
425	55268-67-2	5-Hydroxyindole-3-acetic acid-3TMS	C19H33NO3Si3	2238	5.1	2602	2208	2.2	1890
426	4387-16-0	Bisphenol A-2TMS	C21H32O2Si2	2234	1.2	974	2215	1.3	630
427	55622-53-2	4-Hydroxyhippuric acid-2TMS	C15H25NO4Si2	2239	3.2	2473	2223	3.0	1846
428	2060000-11-3	3-Hydroxydodecenedioic acid-3TMS	C21H44O5Si3	2247	1.1	156	2223	1.0	50
429	18748-91-9	Stearic acid-TMS	C21H44O2Si	2246	1.5	3185	2240	1.9	1947
430	27750-80-7	3,5-Dimethoxy-4-hydroxycinnamic acid-2TMS	C17H28O5Si2	2258	1.4	784	2237	1.6	444
431	2060000-27-1	Topiramate-TMS	C15H29NO8SSi	2270	1.9	15	2241	1.3	12
432	2060000-10-2	3-hydroxydodecanedioic acid-3TMS	C21H46O5Si3	2270	1.4	679	2247	1.4	381
433	2060001-10-5	Suberylglycine-2TMS	C16H33NO5Si2	2275	2.3	9	2256	1.8	14
434	63435-72-3	Phenytoin-2TMS	C21H28N2O2Si2	2286	1.4	41	2250	0.9	14
435	55319-89-6	Xanthurenic acid-3TMS	C19H31NO4Si3	2287	1.1	1034	2251	1.9	562
436	2060001-26-3	Flucloxacillin Metabolite-TMS #	C14H16ClFN2O3Si	2297	3.5	25	2265	2.4	20
437	139432-41-0	Tetradecandioic acid-2TMS	C20H42O4Si2	2292	--	1	2277	0.4	6
438	959264-31-4	Carbamazepine-TMS	C18H20N2OSi	2299	1.6	18	2272	1.3	5
439	2060001-60-5	Trichloroethanol glucuronide-4TMS	C20H43Cl3O7Si4	2325	1.8	155	2276	1.4	88
440	2060001-82-1	3-(2-chloro-6-fluorophenyl)-5-formyl-N-[(3S)-2-oxoazetidin-3-yl]-2,3-dihydro-1,2-oxazole-4-carboxamide #	C14H11ClFN3O4	2316	3.5	41	2286	2.2	22
441	2060001-28-5	Non-4-ene-1,2,9-tricarboxylic acid-3TMS	C21H42O6Si3	2319	1.8	74	2296	1.5	81
442	21414-46-0	Pimaric acid-TMS	C23H38O2Si	--	--	0	2311	2.0	53
443	74367-35-4	Nonadecanoic acid-TMS	C22H46O2Si	2345	1.4	213	2338	1.8	467
444	2060001-81-0	4-Hydroxy-phenobarbital-2TMS	C18H28N2O4Si2	2350	4.1	124	2339	3.1	120
445	301-02-0	9-Octadecenamide, (Z)-	C18H35NO	2366	2.1	128	2361	--	1
446	2060001-45-6	Vanillylglycine-2TMS	C16H27NO5Si2	2379	2.7	1448	2355	3.1	1012

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
447	2060001-80-9	9-Hydroxy-9-methylacridine-10(9H)-carboxamide-2TMS	C21H30N2O2Si2	2394	--	1	2354	3.3	2
448	298-46-4	Carbamazepine	C15H12N2O	2385	1.6	3	2366	5.4	4
449	2060001-73-0	Valproic acid glucronide-4TMS	C26H56O8Si4	2402	6.6	240	2351	6.5	133
450	113516-18-0	Arachidonic acid-TMS	C23H40O2Si	2377	1.5	3	--	--	0
451	123-95-5	Octadecanoic acid, butyl ester	C22H44O2	2387	2.8	178	2385	1.2	151
452	2060001-54-7	Carbamazepine-10,11-dihydro-11-ol-2TMS	C21H30N2O2Si2	2413	0.9	26	2377	1.2	8
453	2060001-76-3	cis-5,8,11-Eicosatrienoic acid-TMS	C23H42O2Si	2397	2.4	4	--	--	0
454	1188-73-4	Myristic acid-2,3-dihydroxypropyl ester-2TMS	C23H50O4Si2	2409	1.0	418	2388	--	1
455	21414-49-3	Dehydroabietic acid-TMS	C23H36O2Si	2409	2.1	1285	2390	1.8	719
456	150367-80-9	Ricinoleic acid-2TMS	C24H50O3Si2	2420	1.2	73	2400	1.1	106
457	2060000-86-2	Oleamide-TMS	C21H43NOSi	2420	0.8	54	2410	3.0	28
458	2060000-99-7	cis-11-Eicosenoic acid-TMS	C23H46O2Si	2420	2.3	5	2412	0.6	7
459	2060000-33-9	3-Hydroxytetradecendioic acid-3TMS	C23H48O5Si3	2438	1.8	100	2412	1.0	49
460	21414-50-6	Abietic acid-TMS	C23H38O2Si	2441	0.7	13	2426	2.2	138
461	55530-70-6	Eicosanoic acid-TMS	C23H48O2Si	2445	1.7	415	2437	1.3	169
462	2060001-52-5	Carbamazepine-10 OH-TMS	C18H22N2O2Si	2464	--	1	2436	1.6	2
463	2060000-23-7	Cloxacillin Metabolite-2TMS #	C19H27ClN2O5Si2	2488	1.3	21	2445	1.6	8
464	2060001-12-7	Hexadecandioic acid-2TMS	C22H46O4Si2	--	--	0	2473	0.5	5
465	2060001-55-8	Carbamazepine-10,11-dihydrodiol-3TMS	C24H38N2O3Si3	2524	1.3	51	2473	1.4	17
466	2060001-92-3	Valproic acid glucuronide-4TMS (second peak)	C26H56O8Si4	2528	1.7	444	2478	2.4	206
467	2060001-49-0	Phenylacetylglutamine-2TMS	C19H32N2O4Si2	2522	2.1	715	2493	2.4	239
468	27554-26-3	Diisooctyl phthalate	C24H38O4	2557	3.7	3368	2532	2.8	1943
479	63435-71-2	5-(p-Hydroxyphenyl)-5-phenylhydantoin-3TMS	C24H36N2O3Si3	2564	1.4	51	2526	1.9	23
470	53212-97-8	2-Monopalmitin-2TMS	C25H54O4Si2	2569	1.4	361	2547	1.0	11
471	2060001-51-4	Carbamazepine metabolite-(10,11-diOH)-2TMS	C21H30N2O3Si2	2596	2.4	45	2546	1.8	19
472	1188-74-5	1-Monopalmitin-2TMS	C25H54O4Si2	2602	1.6	2541	2580	2.3	397
473	2060001-79-6	Steroid - 2 double bonds, 2OH (TMS) - struct unclear#	C25H44O2Si2	2626	2.2	677	2585	2.5	426
474	2060000-22-6	Flucloxacillin Metabolite-2TMS #	C19H26ClFN2O5Si2	2631	2.3	48	2589	1.7	27
475	2060000-96-4	cis-13-Docosenoic acid-TMS	C25H50O2Si	2619	3.0	6	2609	0.9	11
476	74367-36-5	Docosanoic acid-TMS	C25H52O2Si	2641	2.1	76	2631	1.8	59

Index	ID Number	Name	Formula	DB5 Data			DB5MS Data		
				RI	SD	Files	RI	SD	Files
477	22316-47-8	Clobazam	C16H13ClN2O2	2642	--	1	--	--	0
478	53336-13-3	2-Monostearin-2TMS	C27H58O4Si2	2758	1.8	313	2732	1.5	14
479	13111-28-9	Androst-5-en-17-one, 3,16-dihydroxy-2TMS	C25H44O3Si2	2799	2.7	67	2754	2.7	110
480	1188-75-6	Monostearin-2TMS	C27H58O4Si2	2795	1.9	2239	2770	2.9	509
481	2060000-97-5	cis-15-Tetracosenoic acid-TMS	C27H54O2Si	2818	4.1	5	2807	--	1
482	74367-37-6	Tetracosanoic acid-TMS	C27H56O2Si	2833	5.0	49	2823	3.3	42
483	2060001-61-6	Androst-5-en-17-one, 3,16-dihydroxy-EO-2TMS	C27H49NO3Si2	2851	7.9	700	2809	3.6	436
484	33287-32-0	3.beta.,16.alpha.,17.beta.-trihydroxy-androst-5-ene-3TMS	C28H54O3Si3	2871	11.2	479	2817	4.4	321
485	55836-51-6	Paracetamol glucuronide-5TMS	C29H57NO8Si5	2867	8.1	7	--	--	0
486	18888-17-0	Estratriol-3TMS	C27H48O3Si3	2925	14.9	33	2858	1.8	25
487	40822-79-5	Pregn-5-en-20-one, 3,16-dihydroxy-, (3.beta.,16.alpha.)-2TMS	C27H48O3Si2	2924	14.5	254	2868	6.5	146
488	2060000-92-0	Furosemide-2TMS	C18H27ClN2O5SSi2	2917	12.2	18	2880	8.7	35
489	747-90-0	Cholesta-3,5-diene	C27H44	2907	12.5	11	--	--	0
490	72088-06-3	Paracetamol glucuronide-4TMS	C26H49NO8Si4	3043	13.7	58	2960	1.3	32
491	2060000-98-6	Hexacosanoic acid-TMS	C29H60O2Si	3034	0.4	5	2992	1.8	3
492	57305-40-5	(3.beta.,20S)-pregn-5-ene-3,20,21-trihydroxy-3TMS	C30H58O3Si3	3154	4.4	189	3078	9.9	93
493	52760-33-5	.alpha.-Tocopherol-TMS	C32H58O2Si	3150	4.9	23	3101	0.3	6
494	1856-05-9	Cholesterol-TMS	C30H54OSi	3164	4.6	1291	3108	6.6	784
495	2060000-85-1	Ursodeoxycholic acid-3TMS	C33H64O4Si3	3172	3.5	25	3122	4.2	60
496	18880-60-9	Desmosterol-TMS	C30H52OSi	3214	3.5	10	--	--	0
497	2060001-62-7	Flucloxacillin-TMS	C22H25ClFN3O5SSi	3288	7.5	21	3200	4.2	8
498	55429-62-4	Campesterol-TMS	C31H56OSi	3306	16.0	14	3246	0.7	4
499	2625-46-9	.beta.-Sitosterol-TMS	C32H58OSi	3408	23.7	27	--	--	0