GT081
GL Sciences Inc.

GC/MS Metabolites Library

There are several methods with GC to analyze metabolites, such as amino acids, organic acids, fatty acids, sugars, and so on. Methoximation and trimethylsilylation (TMS) is the classical and most widely used derivatization procedure for metebolome analysis with GC.

In this note, the about 400 metabolites widely used TMS derivatized were detected with GC-MS (the column was InertCap 5MS Metabolomics).

Derivatizing procedure

Evaporated sample (～about 10 mg)

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＜Methoximation＞
100 µL of methoxyamine hydrochloride in pyridine (20 mg/mL) Incubation (30 ºC, 90 min)

↓

＜Trimethylsilylation＞ 50 µL of MSTFA (Cat.No. 1022-11061)
Incubation (37 ºC, 30 min)

↓

Derivatized sample

GC/MS Conditions

System	: GC-MS
Column	: InertCap 5MS Metabolomics 0.25 mm I.D. × 30 m df = 0.25 µm (Cat.No. 1010-18952)
Injection Inj. Temp.	: Split
Oven Temp.	: 230 ºC
Carrier gas	: 80 ºC (2 min) - 15 ºC /min - 330 ºC (13 min)
Carrier gas control	: Helium
Septum purge flow	: Constant Pressure 75 kPa
Split ratio Interface	: 5 mL/min
Temp.	: 1:25
Ion source Temp.	: 250 ºC
Ionization Vortage	: 200 ºC
Scan range	: 70 eV
Injection Vol.	: *m/z* 85 - 500 : 1 µL

Compounds	Retention Indices	Retention Time(s)	Cas.No.
C10	1000	257.88	
Propyleneglycol	1002	258.99	57-55-6
n-Propylamine	1026	276.44	107-10-8
2-Hydroxypyridine	1038	284.99	142-08-5
Pyruvate	1049	292.71	127-17-3
Oxalacetic acid	1049	292.86	328-42-7
α-Methylbenzylamine_1	1051	294.78	618-36-0
Lactic acid	1064	303.72	79-33-4
Glycolic acid	1077	313.46	79-14-1
n-Methylethanolamine	1082	317.02	109-83-1
Valine_1	1091	322.90	72-18-4
C11	1100	329.64	
Isobutylamine	1100	329.76	78-81-9
Alanine_1	1106	333.59	56-41-7
n-Butylamine	1111	337.08	109-73-9
Ketovaline_1	1114	339.23	3715-29-5
Glycine_1	1124	346.02	56-40-6
2-Hydroxybutyrate	1132	351.69	5094-24-6
Oxalate	1134	353.38	144-62-7
Ketovaline_2	1140	357.33	
Sarcosine	1143	359.28	107-97-1
2-Aminoisobutyrate	1147	362.05	62-57-7
4-Hydroxypyridine	1154	367.10	626-64-2
3-Hydroxybutyrate	1165	374.70	300-85-6
2-Aminobutyric acid	1177	383.33	1492-24-6
Ketoisoleucine_1	1185	389.00	3715-31-9
C12	1200	399.18	
Norleucine_1	1204	401.51	327-57-1
Ketoisoleucine_2	1206	403.08	
Malonic acid	1208	404.25	141-82-2
Glyceraldehyde_1	1213	407.84	56-82-6
1-Aminocycropropane-1-carboxylic acid	1214	407.99	22059-21-8
α-Methylbenzylamine_2	1224	414.72	
Valine_2	1225	415.49	
Glyceraldehyde_2	1227	416.96	
Urea	1236	422.71	57-13-6
Norvaline	1248	430.04	760-78-1
Benzoic acid	1251	432.56	65-85-0
Dihydroxyacetone	1260	437.88	96-26-4
Oxamic acid	1260	438.09	471-47-6
Serine_1	1264	440.66	56-45-1
n-Caprylic acid	1264	440.72	124-07-2
n-Acetyl-DL-alanine	1264	440.95	1115-69-1
2-Aminoethanol	1275	447.60	141-43-5
Leucine	1280	451.26	61-90-5
Phosphate	1282	452.70	7664-38-2
Glycerol	1283	453.00	56-81-5
Ethylmalonate	1285	454.41	601-75-2
2-Oxobutyrate_1	1289	457.05	600-18-0
Nicotinic acid	1294	460.31	59-67-6
3-Hydroxypyruvate_1	1295	460.79	1113-60-6
C13	1300	464.10	
Threonine_1	1302	465.17	72-19-5
Isoleucine	1303	466.07	73-32-5
Proline	1307	468.20	147-85-3
Maleic acid	1309	469.43	141-82-2
2-Oxobutyrate_2	1315	472.99	
Succinic acid	1317	474.08	110-15-6
Glycine_2	1318	474.76	

Compounds	Retention Indices	Retention Time(s)	Cas.No.
2-Phenylpropionate	1322	477.40	492-37-5
2-Picolinate	1324	478.25	98-98-6
Catechol	1326	479.77	120-80-9
Oxamide	1326	480.00	471-46-5
Norleucine_2	1328	480.88	
2-Methyl benzoic acid	1329	481.85	118-90-1
Methylsuccinic acid	1330	482.24	498-21-5
Glyceric acid	1341	488.72	473-81-4
3-Hydroxypyruvate_2	1342	489.32	
Uracil	1345	491.46	66-22-8
Fumaric acid	1349	493.33	110-17-8
Nonanoric acid	1361	500.70	112-05-0
4-Methyl benzoic acid	1368	504.81	99-94-5
Serine_2	1371	506.89	
Alanine_2	1373	508.11	
Pipecolic acid	1374	508.53	535-75-1
n-Acetyl-DL-valine	1380	512.39	3067-19-4
β-Cyano-L-alanine	1381	512.64	6232-19-5
n-Formylglycine	1382	513.65	2491-15-8
3-Pyridylacetic acid	1392	519.19	6419-36-9
Ketoleucine	1393	519.84	816-66-0
Threonine_2	1399	523.50	
C14	1400	524.28	
Allothreonine	1404	526.68	144-98-9
Glutaric acid	1406	527.64	110-94-1
Thymine	1409	529.56	65-71-4
2-Methylglutarate	1419	535.17	18069-17-5
2,3-Bisphospho-glycerate	1420	535.45	102814-02-8
Hydrocinnamate	1425	538.10	501-52-0
3-Methylglutarate	1428	540.18	626-51-7
Phenoxyacetic acid	1430	540.85	122-59-8
Cinnamyl alcohol	1433	542.77	104-54-1
β-Alanine	1438	545.86	107-95-9
n-Acetyl-L-leucine	1444	549.15	1188-21-2
Maleamic acid	1445	549.31	557-24-4
Homoserine	1461	558.55	672-15-1
Nicotinamide	1484	571.66	98-92-0
Citramalic acid	1486	572.84	6236-10-8
Madelic acid	1488	573.61	611-71-2
Malic acid	1498	579.19	6915-15-7
p-Hydroxybenzaldehyde	1499	580.09	123-08-0
C15	1500	580.44	
Homoserine lactone	1504	582.50	6305-38-0
Adipic acid	1509	585.15	124-04-9
4-Hydroxybenzylalcohol	1512	586.59	623-05-2
Threitol	1516	588.70	2418-52-2
Acetylsalicylic acid	1522	592.29	50-78-2
Meso-erythritol	1525	593.47	149-32-6
Methionine	1531	596.79	63-68-3
2-Thiouracil	1531	596.82	141-90-2
Aspartic acid	1531	596.87	56-84-8
α-Phenylglycine	1532	597.54	875-74-1
Cytosine	1533	597.94	71-30-7
Pyroglutamic acid	1535	598.73	149-87-1
trans-4-Hydroxy-L-proline	1540	601.47	51-35-4
4-Aminobutyric acid	1543	602.93	1956-12-2
Pyrogallol	1561	612.56	87-66-1
5-Methylcytosine	1563	613.73	58366-64-6
3-Hydroxybenzoate	1573	619.07	1999-6-9

Compounds	Retention Indices	Retention Time(s)	Cas.No.
Creatinine	1576	620.27	60-27-5
Threonic acid	1577	620.99	70753-61-6
Acetoacetic acid	1579	622.02	3483-11-2
6-Hydroxynicotinic acid	1579	622.09	5006-66-6
2-Hydroxyphenylacetic acid	1580	622.62	614-75-5
1-Hydroxyphenethyl alcohol	1580	622.71	501-94-0
1-Methyluracil	1582	623.81	615-77-0
α-Ketoglutaric acid	1582	623.84	328-50-7
3-Amino-2,3-dihydrobenzoic acid	1589	627.13	59556-17-1
Ethionine	1594	630.00	67-21-0
2-Isopropylmalic acid	1595	630.32	3237-44-3
Prephenate	1597	631.52	2931-08-0
3-Phenyllactic acid	1599	632.60	103-82-2
C16	1600	633.12	
Heptanedioate	1606	635.95	111-16-0
Phosphoenolpyruvic acid	1612	639.01	138-08-9
3-Hydroxy-3-methylglutarate	1614	639.94	503-49-1
3-Hydroxyphenylacetic acid	1618	641.83	621-37-4
Hypotaurine	1618	641.90	300-84-5
β-Glutamic acid	1623	644.66	1948-48-7
Anthranilic acid	1625	645.40	118-92-3
Glutamic acid	1630	647.97	56-86-0
4-Hydroxybenzoic acid	1636	650.88	99-96-7
5-Aminovaleric acid	1641	653.41	660-88-8
Phenylalanine	1643	654.48	63-91-2
Paeonol_1	1644	654.78	552-41-0
4-Hydroxyphenylacetic acid	1648	657.00	156-38-7
Lauric acid	1653	659.37	143-07-7
Tartrate	1657	661.20	87-69-4
Paeonol_2	1664	664.97	
1,3-Propanediamine	1669	667.14	109-76-2
Prolinamide	1669	667.19	7531-52-4
Xylose_1	1673	669.08	58-86-6
Lyxose_1	1673	669.50	1949-78-6
threo-3-Hydroxy-L-aspartic acid	1676	670.79	4294-45-5
Homocysteine	1678	671.64	454-29-5
Xylose_2	1679	672.27	
5-Hydroxymethyluracil	1680	672.75	4433-40-3
Lyxose_2	1683	674.49	
Asparagine	1684	674.70	70-47-3
Arabionose	1685	675.45	147-81-9
Kojic acid	1686	675.54	501-30-4
Taurine	1686	675.95	107-35-7
N-Formyl methionine_1	1689	677.44	4289-98-9
Cysteine sulfinic acid	1695	680.03	207121-48-0
Methyl jasmonate_1	1698	681.48	39924-52-2
Bicine	1699	682.05	150-25-4
Xylulose	1700	682.63	551-84-8
C17	1700	682.73	
Ribulose	1700	682.82	488-84-6
Suberic acid	1700	682.90	505-48-6
Ribose	1701	683.13	50-69-1
n-Formyl methionine_2	1705	684.81	
Phthalic acid	1706	685.69	88-99-3
1,6-Anhydroglucose	1726	694.88	498-07-7
2-Aminoadipic acid	1727	695.32	1118-90-7
Xylitol	1734	698.70	88-99-0
Methyl jasmonate_2	1738	700.63	
Quinolinic acid	1742	702.54	89-00-9

Compounds	Retention Indices	Retention Time(s)	Cas.No.
Glycerol-2-phosphate	1745	703.87	819-93-0
Rhamnose_1	1746	704.15	10485-94-6
Arabitol	1746	704.48	488-82-4
Ribitol	1752	707.15	488-81-3
Aconitate	1754	707.91	585-84-2
Rhamnose_2	1755	708.47	
Orotic acid	1756	709.17	65-86-1
Fucose_1	1756	709.19	2438-80-4
Putrescine	1758	709.97	333-93-7
2,3-Dihydroxybenzoate	1760	711.08	303-38-8
Ciliatine	1764	712.57	2041-14-7
1,3-Benzenedicarboxylic acid	1766	713.57	121-91-5
2,6-Pyridinedicarboxylic acid	1768	714.47	499-83-2
Fucose_2	1770	715.42	
n-Acetyl-L-Glutamate_1	1771	716.19	1188-37-0
1-Methylhistamine	1776	718.23	6481-48-7
5-Amino-levulinate_1	1778	719.28	5451-9-2
Theanine_1	1778	719.54	3081-61-6
3-Methoxy-4-hydroxyphenylacetate	1783	721.89	306-08-1
Glutamine	1786	723.18	5959-95-5
Gentisic acid	1789	724.56	490-79-9
n-Acetyl-L-glutamate_2	1790	724.87	
Dihydroorotate	1792	725.83	5988-19-2
Theanine_2	1792	726.03	
4-Hydroxymandelate	1792	726.11	184901-84-6
Xylonic acid	1794	726.70	526-91-0
C18	1800	729.66	
1,4-Benzenedicarboxylic acid	1802	730.70	100-21-0
O-Phosphoethanolamine	1804	731.60	1071-23-4
5-Amino-levulinate_2	1805	731.70	
Indole-3-acetaldehyde_1	1809	733.67	20095-27-6
2-Deoxy-D-glucose	1816	736.83	154-17-6
Phenanthrene	1818	737.79	1985-1-8
Hippurate_1	1819	738.03	495-69-2
Hypoxanthine	1820	738.53	68-94-0
Shikimic acid	1820	738.71	138-59-0
2-Aminopimelic acid	1822	739.40	627-76-9
1-Methyl histidine_1	1825	740.88	332-80-9
Anthracene	1829	742.66	120-12-7
Dimethylbenzimidazole	1829	742.72	582-60-5
3,4-Dihydrophenylacetic acid	1834	744.74	102-32-9
3,4-Dihydroxybenzoate	1834	744.76	99-50-3
Glycyl-glycine_1	1835	745.13	556-50-3
Citrulline	1836	745.93	372-75-8
Ornithine	1838	746.54	3184-13-2
Isocitric acid	1838	746.72	320-77-4
Glycyl-glycine_2	1838	746.81	
Citric acid	1840	747.34	77-92-9
Methionine sulfone	1846	750.13	7314-32-1
Hippurate_2	1849	751.45	
Homogentisate	1849	751.58	451-13-8
2-Methylhippurate_1	1851	752.47	42013-20-7
Alanyl-alanine_1	1852	752.90	2867-20-1
o-Phospho-L-serine	1857	755.35	407-41-0
Cadaverine	1858	755.70	462-94-2
Caffeine	1867	759.79	1958-8-2
Lysine_2	1868	760.10	
Histidinol	1870	760.97	
5-Hydroxyanthranilic acid	1871	761.50	394-31-0

Compounds	Retention Indices	Retention Time(s)	Cas.No.
Alanyl-alanine_2	1874	762.80	
1,5-Anhydeo-D-glucitol	1877	763.94	154-58-5
Homocysteic acid	1877	764.27	50433-6
Tagatose_1	1881	766.07	87-81-0
Adenine	1886	767.94	73-24-5
3-Hydroxyanthranilic acid	1886	768.13	548-93-6
Psicose_1	1888	769.18	551-68-8
6-Amino-1-methyluracil	1889	769.33	2434-53-9
Quinic acid	1891	770.56	77-95-2
Histamine	1892	770.79	51-45-6
3-Methoxy-4-hydroxymandelate	1893	771.29	1955-10-7
Sebacic acid	1895	772.14	111-20-6
2-Methylhippurate_2	1897	773.16	
C19	1900	774.36	
Psicose_2	1900	774.41	
Tagatose_2	1901	774.86	
Imidazole-4-acetate	1902	775.32	14403-45-3
Fructose_1	1905	776.40	57-48-7
Sorbose_1	1906	776.84	87-79-6
2-Dehydro-D-gluconate_1	1907	777.27	3470-37-9
Glucono-1,5-lactone_1	1910	778.81	4253-68-3
Gluconic acid_1	1911	778.86	526-95-4
Sorbose_2	1911	779.00	
5-Dehydroquinic acid	1911	779.12	494211-79-9
Allantoin_1	1912	779.55	97-59-6
Allose_1	1913	779.96	2595-97-3
Fructose_2	1915	780.60	
Indole-3-acetaldehyde_2	1916	781.12	
4-Hydroxyphenyl pyruvate	1918	781.80	156-39-8
Pyridoxine	1919	782.44	65-23-6
Allantoin_2	1920	782.91	
Mannose_1	1921	783.11	31103-86-3
2-Dehydro-D-gluconate_2	1924	784.35	
Glucono-1,5-lactone_2	1925	784.87	
Gluconic acid_2	1925	784.98	
Galactose_1	1927	785.92	26566-61-0
Homocitrulline	1928	786.20	1190-49-4
Glucose_1	1932	788.03	921-60-8
Indole-3-acetaldehyde_3	1933	788.17	
Tyramine	1934	788.72	51-67-2
Allose_2	1939	791.06	
Mannose_2	1940	791.15	
Lysine_1	1941	791.61	56-87-1
Histidine	1942	792.01	71-00-1
n-Carbamoyl-L-aspartate	1942	792.14	923-37-5
3,4-Dihydroxymandelic acid_1	1944	793.06	775-01-9
n-Acetyl-L-glutamine	1946	793.97	2490-97-3
Glucosamine_1	1947	794.35	3416-24-8
Coniferyl alcohol	1949	795.35	458-35-5
Galactose_2	1951	795.82	
p-Coumaric acid	1951	796.11	501-98-4
Glucose_2	1953	796.82	
Coniferyl aldehyde_1	1955	797.71	458-36-6
Tyrosine	1958	798.80	60-18-4
1-Hexadecanol	1961	800.39	36653-82-4
Coniferyl aldehyde_2	1962	800.59	
Pyridoxamine_1	1963	801.23	524-36-7
Pyridoxine_2	1963	801.23	
Mannitol	1969	803.78	69-65-8

Compounds	Retention Indices	Retention Time(s)	Cas.No.
Galactosamine_1	1971	804.43	1772-03-8
Gallic acid	1974	805.83	149-91-7
Glucuronate_1	1975	806.37	6556-12-3
5-Keto-D-gluconate_1	1976	806.50	91446-96-7
Cysteric acid	1976	806.62	23537-25-9
Ascorbic acid	1976	806.64	50-81-7
Sorbitol	1976	806.70	50-70-4
Glucosamine_2	1977	807.25	
Glucarate_1	1981	808.56	87-73-0
Galactitol	1981	808.76	608-66-2
Galactosamine_2	1981	808.88	
5-Keto-D-gluconate_2	1982	809.20	
Paraxanthine	1982	809.22	611-59-6
Galacturonic acid_1	1982	809.33	91510-62-2
Epinephrine	1990	812.65	51-43-4
Glucuronate_2	1993	814.05	
n-Acetyl-L-ornithine_1	1998	816.15	6205-8-9
C20	2000	816.82	
Glucarate_2	2001	817.42	501-98-4
Galacturonic acid_2	2003	817.98	
Diaminopimelate	2005	818.95	
Urocanate	2013	821.97	104-98-3
S-Benzyl-L-cysteine_1	2013	821.98	3054-1-1
Pantothenate	2014	822.55	137-08-6
n-Acetyl-L-ornithine_2	2018	824.20	
Palmitoleate	2029	828.70	373-49-9
3-Methyladenine	2031	829.19	5142-23-4
Xanthine	2039	832.73	69-89-6
Glucono-1,5-lactone_3	2044	834.71	
Gluconic acid_3	2044	834.73	
2-Deoxyribose-5-phosphate	2053	838.23	102916-66-5
o-Succinyl-L-homoserine	2059	840.63	1492-23-5
Glucarate_3	2060	840.93	
1-Methyl histidine_2	2074	846.76	
Allantoin_3	2086	851.69	
Kynurenate	2089	853.02	492-27-3
n-Acetyl-L-lysine_1	2093	854.54	1946-82-3
C21	2100	857.31	
Allantoin_4	2102	857.99	
Ferulic acid	2105	859.14	537-98-4
Dopamine	2106	859.50	51-61-6
Sinapyl aldehyde	2116	863.50	4206-58-0
n-Acetyl-D-glucosamine	2119	864.65	7512-17-6
Lanthionine	2122	865.81	496-98-0
Dopa	2125	866.91	59-92-7
Uric acid	2126	867.31	69-93-2
n-Acetyl-L-lysine_2	2126	867.55	
Flavanone	2126	867.57	487-26-3
Cystathionine_1	2131	869.15	535-34-2
Inositol	2134	870.50	87-89-8
Arabinose 5-phosphate_1	2136	871.37	89927-09-3
Pydroxamine	2139	872.43	85-87-0
Ribulose 5-phosphate_1	2139	872.57	108321-99-9
Dethiobiotin_1	2143	873.88	533-48-2
Arabinose 5-phosphate_2	2144	874.55	
Hexadecanoate	2146	875.24	506-12-7
Cafferic acid	2151	877.10	331-39-5
Guanine	2154	878.22	73-40-5
Ribulose 5-phosphate_2	2155	878.52	

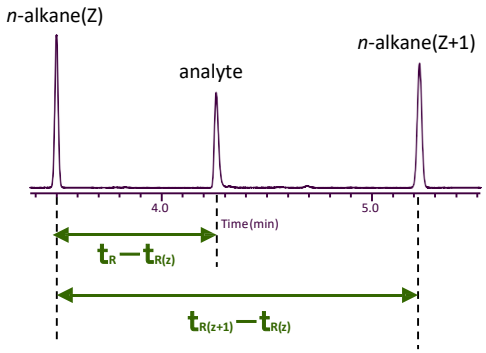
Compounds	Retention Indices	Retention Time(s)	Cas.No.
Methyldopa	2172	885.29	41372-08-1
5-Sulfosalicylate	2194	893.64	5965-83
C22	2200	896.11	
2,6-Diamonopurine	2209	899.56	1904-98-9
Kynurenine	2217	902.52	2922-83-0
5-Hydroxyindoleactate_1	2227	906.06	54-16-0
Elaidic acid	2228	906.48	112-79-8
Cystathionine_2	2235	908.94	
5-Hydroxyindoleactate_2	2237	909.78	
Tryptamine_1	2237	909.84	61-54-1
Cystamine	2238	910.38	56-17-7
Octadecanoate	2244	912.60	1957-11-4
Tryptophan	2251	915.18	73-22-3
Sinapic acid	2256	916.81	530-59-6
Dethiobiotin_2	2259	917.94	
Spermidine	2288	928.92	124-20-9
Xanthurernate	2290	929.58	59-00-7
C23	2300	933.23	
Cysteine	2323	941.58	52-90-4
Cystine	2324	941.82	56-89-3
Sinigrin	2348	950.14	3952-98-5
2-Deoxyuridine_1	2377	960.48	951-78-0
C24	2400	968.79	
Sorbitol 6-phosphate	2422	976.40	108392-12-7
Dehydroisoandrosterone-3-sulfate	2432	979.58	78590-17-7
Icosanoic acid	2443	983.41	506-30-9
p-Aminohippuric acid	2457	988.13	61-78-9
3-Hydroxy-kynurenine	2460	989.21	2147-61-7
2-Deoxyuridine_2	2465	991.11	
5-Hydroxy-L-tryptophan_1	2468	991.87	4350-9-8
Biopterin	2468	992.07	22150-76-1
5-Hydroxy-L-tryptophan_2	2473	993.79	
Saccharopine_1	2475	994.36	997-68-2
Uridine_1	2480	996.03	58-96-8
Uridine_2	2484	997.38	
Serotonin_1	2493	1000.45	153-98-0
C25	2500	1002.98	
Biotin	2507	1005.29	58-85-5
Serotonin_2	2521	1009.87	
n-Acetyl-D-glucosamine 6-phosphate_1	2541	1016.60	102029-88-9
Salicyl alcohol-β-glucoside	2552	1020.18	
Homocystine	2557	1021.93	870-93-9
Saccharopine_2	2563	1023.98	
n-Acetyl-D-glucosamine 6-phosphate_2	2569	1025.90	
2-Deoxyinosine	2575	1027.76	890-38-0
Ribulose 1,5-bisphosphate_1	2582	1030.11	14689-84-0
Ribulose 1,5-bisphosphate_2	2593	1033.72	
C26	2600	1036.15	
Inosine	2605	1037.87	58-63-9
S-Benzyl-L-Cysteine_2	2631	1045.98	
Behenic acid	2640	1048.95	112-85-6
Adenosine	2670	1058.16	58-61-7
Spermine_1	2693	1065.64	71-44-3
C27	2700	1067.80	
Sucrose	2705	1069.26	57-50-1
Xanthosine	2713	1071.88	5968-90-1
Spermine_2	2757	1085.12	
β-Lactose_1	2767	1088.28	5965-66-2
β-Lactose_2	2786	1093.92	

Compounds	Retention Indices	Retention Time(s)	Cas.No.
1-Methyladenosine	2793	1095.98	15763-06-1
Spermine_3	2796	1096.99	
C28	2800	1098.19	
Guanosine	2809	1100.84	118-00-3
2-Deoxyguanosine	2812	1101.86	961-07-9
Trehalose	2819	1103.85	99-20-7
Maltose_1	2822	1104.88	69-79-4
Turanose_1	2825	1105.71	547-25-1
5-Methylthioadenosine	2833	1108.15	2457-80-9
lignoceric acid	2839	1109.81	557-59-5
Lactitol	2851	1113.42	585-86-4
Turanose_2	2852	1113.75	
Maltose_2	2853	1113.84	
Acetoaminophen glucronide	2872	1119.53	120595-80-4
Epicatechin	2894	1126.15	
C29	2900	1127.98	
Sakuranetin_1	2904	1129.26	2957-21-3
Naringenin_1	2907	1130.24	93602-28-9
Maltitol	2929	1136.95	585-88-6
Melibiose_1	2944	1141.35	5340-95-4
Epigallocatechin	2976	1151.39	
Melibiose_2	2977	1151.69	
Daidzein	2979	1152.32	488-66-8
Genistein	2991	1155.79	446-72-0
Sakuranetin_2	2992	1156.35	
Naringenin_2	2994	1156.91	
C30	3000	1158.67	
Apigenine_1	3031	1168.65	520-36-5
Chlorogenic acid_1	3045	1173.14	327-97-9
C31	3100	1191.04	
Kaempferol	3117	1196.78	
Apigenin_2	3138	1204.24	
Chlorogenic acid_2	3168	1214.54	
Apigenin_3	3189	1222.07	
C32	3200	1225.75	
Octacosanoic acid	3234	1238.91	506-48-9
C33	3300	1263.94	
C34	3400	1306.80	
Podophyllotoxin	3423	1317.97	518-28-5
C35	3500	1355.23	
Raffinose	3504	1357.55	17629-30-0
1-Kestose	3514	1363.29	470-69-9
Melezitose	3596	1408.87	10030-67-8
C36	3600	1411.28	
Albiflorin	3631	1431.60	39011-90-0
Maltotriose_1	3689	1469.04	1109-28-0
C37	3700	1476.02	
Maltotriose_2	3721	1491.62	
Panose_1	3776	1533.28	33401-87-5
Panose_2	3789	1542.83	
C38	3800	1551.37	

Calculating retention indices

Retention indices were able to calculate with *n*-alkane.

$$\text{Retention index I} = 100 \times \frac{t_R - t_{R(Z)}}{t_{R(Z+1)} - t_{R(Z)}} + 100 \times Z$$



t_R = Retention time of analyte

$t_{R(Z)}$ = Retention time of *n*-alkane before the analyte

$t_{R(Z+1)}$ = Retention time of *n*-alkane after the analyte Z

= Carbon number of $t_{R(Z)}$

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