AMDIS GC/MS Analysis Report

Data: AKS2302_230301070748.RAW
Library: C:\Program Files (x86)\NISTMS\AMDIS32\libraries\GDM\GMD.MSL
Number of Identifications: 86

RT(min)	Chemical Name
5.7039	M000413_A105003-101-xxx_NA_1031 ,31_TRUE_VAR5_ALK_Pyridine, 2-hydroxy- (1TMS) (ID#:NA)
	RI = 1030.4 RI-RI(lib) = -0.9
6.0523	?? M000100_A105001-101-xxx_NA_1044 ,47_TRUE_VAR5_ALK_Lactic acid (2TMS) (ID#:17596-96-2)
	RI = 1051.3 RI-RI(lib) = 6.8
6.3381	? M000886_A106002-101-xxx_NA_1062 ,88_TRUE_VAR5_ALK_Glycolic acid (2TMS) (ID#:33581-77-0)
	RI = 1068.4 RI-RI(lib) = 5.6
7.3855	M001233_A114014-101-xxx_NA_1133,08_TRUE_VAR5_ALK_Furan-2-carboxylic acid (1TMS) (ID#:NA)
	RI = 1130.0 RI-RI(lib) = -3.0
7.4626	? M000000_A114002-101-xxx_NA_1131 ,27_TRUE_VAR5_ALK_NA114002 (classified unknown) (ID#:NA)
	RI = 1134.5 RI-RI(lib) = 3.2
7.5346	? 3-Hydroxypropanoic acid (ID#:ARP433-N1002)
	RI = 1138.6 RI-RI(lib) = -1.6
7.9260	? contamination - pyridine/BSTFA (ID#:JCB665-N1022)
	RI = 1161.2 RI-RI(lib) = 1.6
9.7207	M000075_A129001-101-xxx_NA_1262 ,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9)
	RI = 1264.5 RI-RI(lib) = 2.1
9.7766	?? contamination - pyridine/BSTFA (ID#:JCB665-N1036)
	RI = 1267.7 RI-RI(lib) = 1.9
10.3419	? M000031_A133001-101-xxx_NA_1303 ,64_TRUE_VAR5_ALK_Glycine (3TMS) (ID#:5630-82-0)
	RI = 1300.3 RI-RI(lib) = -3.3
10.4861	?? M000074_A134001-101-xxx_NA_1310 ,36_TRUE_VAR5_ALK_Succinic acid (2TMS) (ID#:40309-57-7)
	RI = 1309.0 RI-RI(lib) = -1.4

10.7294 M000073_A135003-101-xxx_NA_1319
,94_TRUE_VAR5_ALK_Glyceric acid (3TMS) (ID#:38191-87-6)
RI = 1323.6 RI-RI(lib) = 3.6

10.7716 ? M000000_A136002-101-xxx_NA_1332
,55_TRUE_VAR5_ALK_similar to Lumichrome (2MeOX) (ID#:NA)
RI = 1326.1 RI-RI(lib) = -6.5

11.2331 ?? M000026_A138002-101-xxx_NA_1360
,5_PRED_VAR5_ALK_Alanine (3TMS) (ID#:NA)
RI = 1353.8 RI-RI(lib) = -6.7

13.3034 ?? RI=1490.7, 13.4205 min AKS2164 (ID#:AKS2164-N1004)
RI = 1484.2 RI-RI(lib) = -6.5

13.4976 cis - linalool oxide (furanoid) (ID#:AKS142~1-N1002)
RI = 1496.8 RI-RI(lib) = 3.1

13.6203 ? trans - linalool oxide (furanoid) (ID#:AKS142~1-N1004)
RI = 1504.7 RI-RI(lib) = 3.6

13.8560 cis - linalool oxide (pyranoid) (ID#:AKS142~1-N1006)
RI = 1520.0 RI-RI(lib) = 3.3

13.9640 ? M000114_A153003-101-xxx_NA_1526
,01_TRUE_VAR5_ALK_Butanoic acid, 4-amino- (3TMS) (ID#:39508-23-1)
RI = 1527.0 RI-RI(lib) = 1.0

14.1003 ? M001236_A155002-101-xxx_NA_1536
,45_TRUE_VAR5_ALK_Benzene-1,2,3-triol (3TMS) (ID#:17864-23-2)
RI = 1535.8 RI-RI(lib) = -0.7

14.1224 M001212_A155003-101-xxx_NA_1541
,53_PRED_VAR5_ALK_similar to Ditertbutylphenol (1TMS) (ID#:NA)
RI = 1537.2 RI-RI(lib) = -4.3

15.2253 ?? M000000_A161011-101-xxx_NA_1610
,66_TRUE_VAR5_ALK_NA161011 (ID#:NA)
RI = 1609.3 RI-RI(lib) = -1.4

15.7833 ? M000582_A167011-101-xxx_NA_1649
,64_TRUE_VAR5_ALK_Ribose (1MEOX) (4TMS) BP (ID#:56196-08-8)
RI = 1648.0 RI-RI(lib) = -1.6

15.8789 ? M000576_A165006-101-xxx_NA_1650
,36_TRUE_VAR5_ALK_Lyxose (1MEOX) (4TMS) MP (ID#:NA)
RI = 1654.6 RI-RI(lib) = 4.3

15.8843 ?? M000582_A167011-101-xxx_NA_1649
,64_TRUE_VAR5_ALK_Ribose (1MEOX) (4TMS) BP (ID#:56196-08-8)
RI = 1655.0 RI-RI(lib) = 5.4

15.8843 ? M000576_A165006-101-xxx_NA_1650
,36_TRUE_VAR5_ALK_Lyxose (1MEOX) (4TMS) MP (ID#:NA)
RI = 1655.0 RI-RI(lib) = 4.7

16.0953 ?? M000582_A168002-101-xxx_NA_1665
,99_TRUE_VAR5_ALK_Ribose (1MEOX) (4TMS) MP (ID#:NA)
RI = 1669.7 RI-RI(lib) = 3.7

16.6531 ?? M000590_A172002-101-xxx_NA_1707
,41_TRUE_VAR5_ALK_Rhamnose (1MEOX) (4TMS) MP (ID#:NA)
RI = 1708.9 RI-RI(lib) = 1.5

16.7602 ?? M000155_A173001-101-xxx_NA_1712
,74_TRUE_VAR5_ALK_Ribitol (5TMS) (ID#:32381-53-6)
RI = 1716.7 RI-RI(lib) = 4.0

16.9758 ? RI=1731.6, 16.7359 min LMV1405 (ID#:LMV1405-N1006)
RI = 1732.5 RI-RI(lib) = 0.9

16.9834 ? RI=1731.6, 16.7359 min LMV1405 (ID#:LMV1405-N1006)
RI = 1733.0 RI-RI(lib) = 1.4

17.2857 ? M000605_A177001-101-xxx_NA_1750
,73_TRUE_VAR5_ALK_Ribonic acid (5TMS) (ID#:NA)
RI = 1755.2 RI-RI(lib) = 4.4

17.3617 ? M000040_A177004-101-xxx_NA_1755
,94_TRUE_VAR5_ALK_Glucopyranose [-H20] (4TMS) (ID#:NA)
RI = 1760.7 RI-RI(lib) = 4.8

17.4266 ?? M000994_A179001-101-xxx_NA_1764
,84_TRUE_VAR5_ALK_Arabinonic acid (5TMS) (ID#:NA)
RI = 1765.5 RI-RI(lib) = 0.6

17.4329 ?? M000991_A178005-101-xxx_NA_1759
,34_TRUE_VAR5_ALK_Lyxonic acid (5TMS) (ID#:NA)
RI = 1766.0 RI-RI(lib) = 6.6

17.5748 ?? M000000_A179010-101-xxx_NA_1781,65_PRED_VAR5_ALK_NA
(ID#:NA)
RI = 1776.3 RI-RI(lib) = -5.3

17.9349 ?? M000607_A181002-101-xxx_NA_1794
,63_TRUE_VAR5_ALK_Shikimic acid (4TMS) (ID#:NA)
RI = 1802.9 RI-RI(lib) = 8.3

18.0409 ? M000069_A182004-101-xxx_NA_1804
,71_TRUE_VAR5_ALK_Citric acid (4TMS) (ID#:NA)
RI = 1811.2 RI-RI(lib) = 6.5

18.0448 ? M000069_A182004-101-xxx_NA_1804
,71_TRUE_VAR5_ALK_Citric acid (4TMS) (ID#:NA)
RI = 1811.5 RI-RI(lib) = 6.8

18.0490 ?? M000069_A182004-101-xxx_NA_1804
,71_TRUE_VAR5_ALK_Citric acid (4TMS) (ID#:NA)
RI = 1811.8 RI-RI(lib) = 7.1

18.1111 ?? contamination_blank (ID#:TAM757-N1010)
RI = 1816.7 RI-RI(lib) = -0.1

18.5281 ?? M000007_A185001-101-xxx_NA_1842
,69_TRUE_VAR5_ALK_Quinic acid (5TMS) (ID#:NA)
RI = 1849.5 RI-RI(lib) = 6.8

18.5583 ?? M000007_A185001-101-xxx_NA_1842
,69_TRUE_VAR5_ALK_Quinic acid (5TMS) (ID#:NA)
RI = 1851.8 RI-RI(lib) = 9.1

18.7076 ?? M000606_A188004-101-xxx_NA_1863
,13_TRUE_VAR5_ALK_Fructose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1863.5 RI-RI(lib) = 0.4

18.7308 M000606_A188004-101-xxx_NA_1863
,13_TRUE_VAR5_ALK_Fructose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1865.4 RI-RI(lib) = 2.2

18.8526 ?? RI=1883.8, 18.9557 min AKS2164 (ID#:AKS2164-N1006)
RI = 1874.9 RI-RI(lib) = -8.9

18.9675 ?? M000040_A189002-101-xxx_NA_1880
,5_TRUE_VAR5_ALK_Glucose (1MEOX) (5TMS) MP (ID#:NA)
RI = 1883.9 RI-RI(lib) = 3.4

19.0521 ?? M000633_A189001-101-xxx_NA_1885
,22_TRUE_VAR5_ALK_Mannose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1890.6 RI-RI(lib) = 5.4

19.0574 ?? M000637_A190005-101-xxx_NA_1887
,55_TRUE_VAR5_ALK_Altrose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1891.0 RI-RI(lib) = 3.5

19.2930 ?? M000043_A191002-101-xxx_NA_1902
,42_PRED_VAR5_ALK_Galactose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1909.5 RI-RI(lib) = 7.1

19.5388 IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1928.8 RI-RI(lib) = 6.2

19.5451 IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1929.3 RI-RI(lib) = 6.7

19.5675 ?? IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1931.0 RI-RI(lib) = 8.4

19.6507 ? M000801_A196011-101-xxx_NA_1945
,61_TRUE_VAR5_ALK_Gallic acid (4TMS) (ID#:2078-17-3)
RI = 1937.6 RI-RI(lib) = -8.0

19.8154 M000801_A196011-101-xxx_NA_1945,61_TRUE_VAR5_ALK_Gallic acid (4TMS) (ID#:2078-17-3)
RI = 1950.5 RI-RI(lib) = 4.9

19.8683 ?? M000801_A196011-101-xxx_NA_1945 ,61_TRUE_VAR5_ALK_Gallic acid (4TMS) (ID#:2078-17-3)
RI = 1954.7 RI-RI(lib) = 9.0

20.2707 ?? M000508_A200001-101-xxx_NA_1984 ,83_TRUE_VAR5_ALK_Gluconic acid (6TMS) (ID#:NA)
RI = 1986.2 RI-RI(lib) = 1.4

20.3256 ? M000508_A200001-101-xxx_NA_1984 ,83_TRUE_VAR5_ALK_Gluconic acid (6TMS) (ID#:NA)
RI = 1990.6 RI-RI(lib) = 5.7

20.4641 ?? M000093_A201001-101-xxx_NA_1999 ,87_TRUE_VAR5_ALK_Saccharic acid (6TMS) (ID#:NA)
RI = 2001.5 RI-RI(lib) = 1.7

20.6693 ? M000000_A203010-101-xxx_NA_2018,15_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2018.8 RI-RI(lib) = 0.6

20.8438 ?? M000594_A204001-101-xxx_NA_2030 ,47_TRUE_VAR5_ALK_Galactaric acid (6TMS) (ID#:NA)
RI = 2033.5 RI-RI(lib) = 3.0

20.9523 ? contamination - pyridine/BSTFA - C16:0 acid TMS (ID#:JCB665-N1044)
RI = 2042.6 RI-RI(lib) = -0.3

21.4235 M000060_A209002-101-xxx_NA_2080 ,23_TRUE_VAR5_ALK_Inositol, myo- (6TMS) (ID#:NA)
RI = 2082.2 RI-RI(lib) = 2.0

21.6255 ?? M000000_A211001-101-xxx_NA_2098 ,3_PRED_VAR5_ALK_NA211001 (ID#:NA)
RI = 2099.2 RI-RI(lib) = 0.9

21.8944 ?? M000000_A214003-101-xxx_NA_2127,28_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2123.2 RI-RI(lib) = -4.1

21.9631 ?? M000000_A214003-101-xxx_NA_2127,28_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2129.4 RI-RI(lib) = 2.1

21.9943 ? M000649_A214001-101-xxx_NA_2135 ,55_TRUE_VAR5_ALK_Caffeic acid, trans- (3TMS) (ID#:NA)
RI = 2132.1 RI-RI(lib) = -3.4

22.5032 ? RI=2175.5, 22.6111 min LFF858 (ID#:LFF858-N1006)
RI = 2177.7 RI-RI(lib) = 2.2

23.2122 ?? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-N1048)
RI = 2241.1 RI-RI(lib) = 1.9

23.2175 ? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-N1048)
RI = 2241.6 RI-RI(lib) = 2.4

23.9005 ?? M000000_A231002-101-xxx_NA_2298,8_PRED_VAR5_ALK_similar to Glycerolaldopyranosid (6TMS) (ID#:NA)
RI = 2303.0 RI-RI(lib) = 4.2

24.5445 ?? M000000_A237001-101-xxx_NA_2361,83_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2365.4 RI-RI(lib) = 3.6

24.6902 ?? M000000_A241003-101-xxx_NA_2386,02_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2379.5 RI-RI(lib) = -6.5

27.1541 M000044_A264001-101-xxx_NA_2622,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
RI = 2627.4 RI-RI(lib) = 4.5

27.1581 M000044_A264001-101-xxx_NA_2622,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
RI = 2627.8 RI-RI(lib) = 4.9

27.4703 ? M000000_A267001-101-xxx_NA_2660,62_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2661.4 RI-RI(lib) = 0.8

28.0472 ?? M000671_A274002-101-xxx_NA_2726,3_TRUE_VAR5_ALK_Trehalose, alpha,alpha'-, D- (8TMS) (ID#:NA)
RI = 2723.6 RI-RI(lib) = -2.7

28.0912 ?? M000671_A274002-101-xxx_NA_2726,3_TRUE_VAR5_ALK_Trehalose, alpha,alpha'-, D- (8TMS) (ID#:NA)
RI = 2728.4 RI-RI(lib) = 2.1

29.2368 ?? M000107_A287001-101-xxx_NA_2846,96_TRUE_VAR5_ALK_Isomaltose (1MEOX) (8TMS) MP (ID#:NA)
RI = 2855.4 RI-RI(lib) = 8.4

29.3784 ? M000832_A289005-101-xxx_NA_2865,56_TRUE_VAR5_ALK_Catechin (5TMS) (ID#:NA)
RI = 2871.7 RI-RI(lib) = 6.1

29.3861 ? M000832_A289005-101-xxx_NA_2865,56_TRUE_VAR5_ALK_Catechin (5TMS) (ID#:NA)
RI = 2872.6 RI-RI(lib) = 7.0

29.4984 ?? M000107_A291002-101-xxx_NA_2881 ,28_TRUE_VAR5_ALK_Isomaltose (1MEOX) (8TMS) BP (ID#:NA)
RI = 2885.5 RI-RI(lib) = 4.2

29.7142 ? M000833_A291010-101-xxx_NA_2914 ,99_TRUE_VAR5_ALK_Epigallocatechin (6TMS) (ID#:NA)
RI = 2910.4 RI-RI(lib) = -4.6

29.7176 ? M000833_A291010-101-xxx_NA_2914 ,99_TRUE_VAR5_ALK_Epigallocatechin (6TMS) (ID#:NA)
RI = 2910.8 RI-RI(lib) = -4.2

30.2817 RI=2975.8, 30.2817 min AKS2302_230301070748 (ID#:AKS230~1-N1002)
RI = 2975.8 RI-RI(lib) = -0.0

32.7763 ?? RI=2960.5, 32.8885 min AKS2164 (ID#:AKS2164-N1008)
RI = 3263.2 RI-RI(lib) = 302.7

QA/QC:

Instrument type: Ion Trap

Scan Direction None

Highest m/z detected = 799, high m/z setting = 800

High noise level. Median Signal(Noise Level)/Threshold=10.9.

Background (low vs. high retention time):

median low RT S/N=26, high RT S/N=79

Solvent Tailing (m/z 84). Run begins at 5.00 min. Solvent falls below:

S/N=1 before run

Column Bleed (m/z 207):

median low RT S/N=2, high RT S/N=11

This report consists of 7 pages