

## AMDIS GC/MS Analysis Report

Data: AKS2303.RAW

Library: C:\Program Files (x86)\NISTMS\AMDIS32\libraries\GDM\GMD.MSL

Number of Identifications: 78

<u>RT(min)</u>	<u>Chemical Name</u>
5.7107	M000413_A105003-101-xxx_NA_1031 ,31_TRUE_VAR5_ALK_Pyridine, 2-hydroxy- (1TMS) (ID#:NA) RI = 1030.8 RI-RI (lib) = -0.5
6.3453	?? M000886_A106002-101-xxx_NA_1062 ,88_TRUE_VAR5_ALK_Glycolic acid (2TMS) (ID#:33581-77-0) RI = 1068.9 RI-RI (lib) = 6.0
7.3927	M001233_A114014-101-xxx_NA_1133,08_TRUE_VAR5_ALK_Furan- 2-carboxylic acid (1TMS) (ID#:NA) RI = 1130.4 RI-RI (lib) = -2.6
7.4690	? M000000_A114002-101-xxx_NA_1131 ,27_TRUE_VAR5_ALK_NA114002 (classified unknown) (ID#:NA) RI = 1134.8 RI-RI (lib) = 3.6
7.5403	? 3-Hydroxypropanoic acid (ID#:ARP433-N1002) RI = 1138.9 RI-RI (lib) = -1.3
7.9292	? contamination - pyridine/BSTFA (ID#:JCB665-N1022) RI = 1161.3 RI-RI (lib) = 1.7
9.7192	M000075_A129001-101-xxx_NA_1262 ,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9) RI = 1264.4 RI-RI (lib) = 2.0
9.7253	M000075_A129001-101-xxx_NA_1262 ,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9) RI = 1264.8 RI-RI (lib) = 2.4
9.7800	?? contamination - pyridine/BSTFA (ID#:JCB665-N1036) RI = 1267.9 RI-RI (lib) = 2.1
10.4877	?? M000074_A134001-101-xxx_NA_1310 ,36_TRUE_VAR5_ALK_Succinic acid (2TMS) (ID#:40309-57-7) RI = 1309.0 RI-RI (lib) = -1.3
10.7292	? M000073_A135003-101-xxx_NA_1319 ,94_TRUE_VAR5_ALK_Glyceric acid (3TMS) (ID#:38191-87-6) RI = 1323.5 RI-RI (lib) = 3.6

10.7739 ? M000000\_A136002-101-xxx\_NA\_1332  
,55\_TRUE\_VAR5\_ALK similar to Lumichrome (2MeOX) (ID#:NA)  
RI = 1326.2 RI-RI(lib) = -6.3

13.3025 ?? RI=1490.7, 13.4205 min AKS2164 (ID#:AKS2164-N1004)  
RI = 1484.1 RI-RI(lib) = -6.6

13.4950 cis - linalool oxide (furanoid) (ID#:AKS142~1-N1002)  
RI = 1496.6 RI-RI(lib) = 2.9

13.5069 ?? cis - linalool oxide (furanoid) (ID#:AKS142~1-N1002)  
RI = 1497.4 RI-RI(lib) = 3.7

13.6197 ? trans - linalool oxide (furanoid) (ID#:AKS142~1-N1004)  
RI = 1504.7 RI-RI(lib) = 3.6

13.8547 cis - linalool oxide (pyranoid) (ID#:AKS142~1-N1006)  
RI = 1519.9 RI-RI(lib) = 3.2

13.9620 ? M000114\_A153003-101-xxx\_NA\_1526  
,01\_TRUE\_VAR5\_ALK Butanoic acid, 4-amino- (3TMS) (ID#:39508-23-1)  
RI = 1526.8 RI-RI(lib) = 0.8

14.0997 ? 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

14.1229 M001212\_A155003-101-xxx\_NA\_1541  
,53\_PRED\_VAR5\_ALK similar to Diterbutylphenol (1TMS) (ID#:NA)  
RI = 1537.3 RI-RI(lib) = -4.3

14.4211 ? M000000\_A155014-101-xxx\_NA\_1554  
,13\_TRUE\_VAR5\_ALK D155405 (ID#:NA)  
RI = 1556.6 RI-RI(lib) = 2.4

15.4623 ?? M000582\_A167011-101-xxx\_NA\_1649  
,64\_TRUE\_VAR5\_ALK\_Ribose (1MeOX) (4TMS) BP (ID#:56196-08-8)  
RI = 1625.7 RI-RI(lib) = -23.9

15.7846 ? M000582\_A167011-101-xxx\_NA\_1649  
,64\_TRUE\_VAR5\_ALK\_Ribose (1MeOX) (4TMS) BP (ID#:56196-08-8)  
RI = 1648.1 RI-RI(lib) = -1.5

15.8828 ? M000582\_A167011-101-xxx\_NA\_1649  
,64\_TRUE\_VAR5\_ALK\_Ribose (1MeOX) (4TMS) BP (ID#:56196-08-8)  
RI = 1654.9 RI-RI(lib) = 5.3

16.6500 ?? M000590\_A172002-101-xxx\_NA\_1707  
,41\_TRUE\_VAR5\_ALK\_Rhamnose (1MeOX) (4TMS) MP (ID#:NA)  
RI = 1708.6 RI-RI(lib) = 1.2

16.6564            ?? M000590\_A172002-101-xxx\_NA\_1707  
                  ,41\_TRUE\_VAR5\_ALK\_Rhamnose (1MEOX) (4TMS) MP (ID#:NA)  
                  RI = 1709.1                            RI-RI(lib) = 1.7

16.7628            ?? M000155\_A173001-101-xxx\_NA\_1712  
                  ,74\_TRUE\_VAR5\_ALK\_Ribitol (5TMS) (ID#:32381-53-6)  
                  RI = 1716.9                            RI-RI(lib) = 4.2

16.9828            RI=1731.6, 16.7359 min LMV1405 (ID#:LMV1405-N1006)  
                  RI = 1733.0                            RI-RI(lib) = 1.4

17.2873            ? M000605\_A177001-101-xxx\_NA\_1750  
                  ,73\_TRUE\_VAR5\_ALK\_Ribonic acid (5TMS) (ID#:NA)  
                  RI = 1755.3                            RI-RI(lib) = 4.6

17.3612            ? M000040\_A177004-101-xxx\_NA\_1755  
                  ,94\_TRUE\_VAR5\_ALK\_Glucopyranose [-H2O] (4TMS) (ID#:NA)  
                  RI = 1760.7                            RI-RI(lib) = 4.8

17.4260            ?? M000994\_A179001-101-xxx\_NA\_1764  
                  ,84\_TRUE\_VAR5\_ALK\_Arabinonic acid (5TMS) (ID#:NA)  
                  RI = 1765.4                            RI-RI(lib) = 0.6

17.5741            ?? M000000\_A179010-101-xxx\_NA\_1781,65\_PRED\_VAR5\_ALK\_NA  
                  (ID#:NA)  
                  RI = 1776.3                            RI-RI(lib) = -5.4

17.9352            ?? RI=1813.5, 18.0471 min AKS2164 (ID#:AKS2164-N1016)  
                  RI = 1802.9                            RI-RI(lib) = -10.6

18.0427            ? M000069\_A182004-101-xxx\_NA\_1804  
                  ,71\_TRUE\_VAR5\_ALK\_Citric acid (4TMS) (ID#:NA)  
                  RI = 1811.4                            RI-RI(lib) = 6.6

18.5552            ?? M000007\_A185001-101-xxx\_NA\_1842  
                  ,69\_TRUE\_VAR5\_ALK\_Quinic acid (5TMS) (ID#:NA)  
                  RI = 1851.6                            RI-RI(lib) = 8.9

18.5594            ?? M000007\_A185001-101-xxx\_NA\_1842  
                  ,69\_TRUE\_VAR5\_ALK\_Quinic acid (5TMS) (ID#:NA)  
                  RI = 1851.9                            RI-RI(lib) = 9.2

18.7313            ? M000606\_A188004-101-xxx\_NA\_1863  
                  ,13\_TRUE\_VAR5\_ALK\_Fructose (1MEOX) (5TMS) BP (ID#:NA)  
                  RI = 1865.4                            RI-RI(lib) = 2.3

18.8541            ?? RI=1883.8, 18.9557 min AKS2164 (ID#:AKS2164-N1006)  
                  RI = 1875.0                            RI-RI(lib) = -8.8

18.9686            ?? M000040\_A189002-101-xxx\_NA\_1880  
                  ,5\_TRUE\_VAR5\_ALK\_Glucose (1MEOX) (5TMS) MP (ID#:NA)  
                  RI = 1884.0                            RI-RI(lib) = 3.5

19.0573            ?? M000637\_A190005-101-xxx\_NA\_1887  
                  ,55\_TRUE\_VAR5\_ALK\_Altrose (1MEOX) (5TMS) BP (ID#:NA)  
                  RI = 1891.0                            RI-RI(lib) = 3.4

19.0624            ?? M000637\_A190005-101-xxx\_NA\_1887  
                  ,55\_TRUE\_VAR5\_ALK\_Altrose (1MEOX) (5TMS) BP (ID#:NA)  
                  RI = 1891.4                            RI-RI(lib) = 3.8

19.2900            ?? M000043\_A191002-101-xxx\_NA\_1902  
                  ,42\_PRED\_VAR5\_ALK\_Galactose (1MEOX) (5TMS) BP (ID#:NA)  
                  RI = 1909.3                            RI-RI(lib) = 6.8

19.5417            ? IS - 13C6-Sorbitol (ID#:ARP436-N1002)  
                  RI = 1929.0                            RI-RI(lib) = 6.4

19.5477            IS - 13C6-Sorbitol (ID#:ARP436-N1002)  
                  RI = 1929.5                            RI-RI(lib) = 6.9

19.5714            ? IS - 13C6-Sorbitol (ID#:ARP436-N1002)  
                  RI = 1931.3                            RI-RI(lib) = 8.7

19.8016            ? M000801\_A196011-101-xxx\_NA\_1945  
                  ,61\_TRUE\_VAR5\_ALK\_Gallic acid (4TMS) (ID#:2078-17-3)  
                  RI = 1949.4                            RI-RI(lib) = 3.8

19.8183            M000801\_A196011-101-xxx\_NA\_1945,61\_TRUE\_VAR5\_ALK\_Gallic  
                  acid (4TMS) (ID#:2078-17-3)  
                  RI = 1950.7                            RI-RI(lib) = 5.1

19.8489            ?? M000801\_A196011-101-xxx\_NA\_1945  
                  ,61\_TRUE\_VAR5\_ALK\_Gallic acid (4TMS) (ID#:2078-17-3)  
                  RI = 1953.1                            RI-RI(lib) = 7.5

20.2761            ?? M000508\_A200001-101-xxx\_NA\_1984  
                  ,83\_TRUE\_VAR5\_ALK\_Gluconic acid (6TMS) (ID#:NA)  
                  RI = 1986.7                            RI-RI(lib) = 1.8

20.3278            ?? M000508\_A200001-101-xxx\_NA\_1984  
                  ,83\_TRUE\_VAR5\_ALK\_Gluconic acid (6TMS) (ID#:NA)  
                  RI = 1990.7                            RI-RI(lib) = 5.9

20.6682            ? M000000\_A203010-101-xxx\_NA\_2018,15\_PRED\_VAR5\_ALK\_NA (  
                  ID#:NA)  
                  RI = 2018.7                            RI-RI(lib) = 0.5

20.8473            ?? M000594\_A204001-101-xxx\_NA\_2030  
                  ,47\_TRUE\_VAR5\_ALK\_Galactaric acid (6TMS) (ID#:NA)  
                  RI = 2033.7                            RI-RI(lib) = 3.3

20.9544            ? contamination - pyridine/BSTFA - C16:0 acid TMS (ID#:JCB665-  
                  N1044)  
                  RI = 2042.8                            RI-RI(lib) = -0.1

20.9596            ?? contamination - pyridine/BSTFA - C16:0 acid TMS (ID#:JCB665-  
                  N1044)  
                  RI = 2043.2                            RI-RI(lib) = 0.3

21.4253            M000060\_A209002-101-xxx\_NA\_2080  
                  ,23\_TRUE\_VAR5\_ALK\_Inositol, myo- (6TMS) (ID#:NA)  
                  RI = 2082.4                            RI-RI(lib) = 2.1

21.6258        ?? M000000\_A211001-101-xxx\_NA\_2098  
              ,3\_PRED\_VAR5\_ALK\_NA211001 (ID#:NA)  
RI = 2099.2                      RI-RI(lib) = 0.9

21.8971        ?? M000000\_A214003-101-xxx\_NA\_2127,28\_PRED\_VAR5\_ALK\_NA  
              (ID#:NA)  
RI = 2123.5                      RI-RI(lib) = -3.8

21.9649        ?? M000000\_A214003-101-xxx\_NA\_2127,28\_PRED\_VAR5\_ALK\_NA  
              (ID#:NA)  
RI = 2129.5                      RI-RI(lib) = 2.2

22.4556        ?? RI=2175.5, 22.6111 min LFF858 (ID#:LFF858-N1006)  
RI = 2173.4                      RI-RI(lib) = -2.1

22.5083        RI=2175.5, 22.6111 min LFF858 (ID#:LFF858-N1006)  
RI = 2178.1                      RI-RI(lib) = 2.6

23.2172        ? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-  
              N1048)  
RI = 2241.6                      RI-RI(lib) = 2.4

23.9082        ?? M000000\_A231002-101-xxx\_NA\_2298  
              ,8\_PRED\_VAR5\_ALK\_similar to Glycerolaldopyranosid (6TMS) (  
              ID#:NA)  
RI = 2303.7                      RI-RI(lib) = 4.9

24.5484        ?? M000000\_A237001-101-xxx\_NA\_2361,83\_PRED\_VAR5\_ALK\_NA  
              (ID#:NA)  
RI = 2365.8                      RI-RI(lib) = 3.9

25.8229        ?? M000000\_A250001-101-xxx\_NA\_2484,98\_PRED\_VAR5\_ALK\_NA  
              (ID#:NA)  
RI = 2489.3                      RI-RI(lib) = 4.3

27.1524        ?? M000044\_A264001-101-xxx\_NA\_2622  
              ,87\_TRUE\_VAR5\_ALK\_Sucrose (8TMS) (ID#:NA)  
RI = 2627.2                      RI-RI(lib) = 4.3

27.1606        M000044\_A264001-101-xxx\_NA\_2622  
              ,87\_TRUE\_VAR5\_ALK\_Sucrose (8TMS) (ID#:NA)  
RI = 2628.1                      RI-RI(lib) = 5.2

27.1667        M000044\_A264001-101-xxx\_NA\_2622  
              ,87\_TRUE\_VAR5\_ALK\_Sucrose (8TMS) (ID#:NA)  
RI = 2628.7                      RI-RI(lib) = 5.9

28.0550        ?? M000671\_A274002-101-xxx\_NA\_2726  
              ,3\_TRUE\_VAR5\_ALK\_Trehalose, alpha,alpha'-, D- (8TMS) (ID#:NA)  
RI = 2724.5                      RI-RI(lib) = -1.8

28.1039        ?? M000671\_A274002-101-xxx\_NA\_2726  
              ,3\_TRUE\_VAR5\_ALK\_Trehalose, alpha,alpha'-, D- (8TMS) (ID#:NA)  
RI = 2729.7                      RI-RI(lib) = 3.4

29.2432            ?? M000000\_A286005-101-xxx\_NA\_2856,98\_PRED\_VAR5\_ALK\_NA  
                  (ID#:NA)  
                  RI = 2856.1                    RI-RI(lib) = -0.8

29.3846            ? M000832\_A289005-101-xxx\_NA\_2865  
                  ,56\_TRUE\_VAR5\_ALK\_Catechin (5TMS) (ID#:NA)  
                  RI = 2872.4                    RI-RI(lib) = 6.9

29.5057            ?? M000107\_A291002-101-xxx\_NA\_2881  
                  ,28\_TRUE\_VAR5\_ALK\_Isomaltose (1MEOX) (8TMS) BP (ID#:NA)  
                  RI = 2886.4                    RI-RI(lib) = 5.1

29.7260            M000833\_A291010-101-xxx\_NA\_2914  
                  ,99\_TRUE\_VAR5\_ALK\_Epigallocatechin (6TMS) (ID#:NA)  
                  RI = 2911.7                    RI-RI(lib) = -3.2

30.2841            ?? RI=2975.8, 30.2817 min AKS2302\_230301070748 (  
                  ID#:AKS230~1-N1002)  
                  RI = 2976.1                    RI-RI(lib) = 0.3

30.2904            RI=2975.8, 30.2817 min AKS2302\_230301070748 (ID#:AKS230~1-  
                  N1002)  
                  RI = 2976.8                    RI-RI(lib) = 1.0

31.9180            ? M000526\_A319004-101-xxx\_NA\_3169  
                  ,3\_TRUE\_VAR5\_ALK\_Quercetin (5TMS) (ID#:NA)  
                  RI = 3164.3                    RI-RI(lib) = -5.0

32.7930            ?? RI=2960.5, 32.8885 min AKS2164 (ID#:AKS2164-N1008)  
                  RI = 3265.1                    RI-RI(lib) = 304.6

33.7550            ? M000815\_A341001-101-xxx\_NA\_3381  
                  ,36\_PRED\_VAR5\_ALK\_Kestose, 6- (11TMS) (ID#:NA)  
                  RI = 3375.9                    RI-RI(lib) = -5.4

**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=28, high RT S/N=81

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=12

This report consists of 6 pages