AMDIS GC/MS Analysis Report

Data: AKS2296.RAW
Library: C:\Program Files (x86)\NISTMS\AMDIS32\libraries\GDM\GMD.MSL
Number of Identifications: 43

RT(min)	Chemical Name
5.7389	M000413_A105003-101-xxx_NA_1031 ,31_TRUE_VAR5_ALK_Pyridine, 2-hydroxy- (1TMS) (ID#:NA)
RI = 1032.5	RI-RI(lib) = 1.2
5.7979	RI=1036.0, 5.7979 min AKS2296 (ID#:AKS2296-N1006)
RI = 1036.0	RI-RI(lib) = 0.0
7.4848	?? M000000_A114002-101-xxx_NA_1131 ,27_TRUE_VAR5_ALK_NA114002 (classified unknown) (ID#:NA)
RI = 1135.8	RI-RI(lib) = 4.5
7.9512	? contamination - pyridine/BSTFA (ID#:JCB665-N1022)
RI = 1162.6	RI-RI(lib) = 3.0
9.7313	M000075_A129001-101-xxx_NA_1262 ,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9)
RI = 1265.1	RI-RI(lib) = 2.7
10.7349	? M000073_A135003-101-xxx_NA_1319 ,94_TRUE_VAR5_ALK_Glyceric acid (3TMS) (ID#:38191-87-6)
RI = 1323.9	RI-RI(lib) = 3.9
13.3055	?? RI=1490.7, 13.4205 min AKS2164 (ID#:AKS2164-N1004)
RI = 1484.3	RI-RI(lib) = -6.4
13.9645	? 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
14.1254	M001212_A155003-101-xxx_NA_1541 ,53_PRED_VAR5_ALK_similar to Ditertbutylphenol (1TMS) (ID#:NA)
RI = 1537.4	RI-RI(lib) = -4.1
14.3867	RI=1554.3, 14.3867 min AKS2296 (ID#:AKS2296-N1004)
RI = 1554.3	RI-RI(lib) = 0.0
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

15.8822   ? M000582_A167011-101-xxx_NA_1649
                ,64_TRUE_VAR5_ALK_Ribose (1MEOX) (4TMS) BP (ID#:56196-08-
                8)
        RI = 1654.9   RI-RI(lib) = 5.2

16.6504   ?? M000590_A172002-101-xxx_NA_1707
                ,41_TRUE_VAR5_ALK_Rhamnose (1MEOX) (4TMS) MP (ID#:NA)
        RI = 1708.7   RI-RI(lib) = 1.3

16.9792   ? RI=1731.6, 16.7359 min LMV1405 (ID#:LMV1405-N1006)
        RI = 1732.7   RI-RI(lib) = 1.1

17.2823   ? M000605_A177001-101-xxx_NA_1750
                ,73_TRUE_VAR5_ALK_Ribonic acid (5TMS) (ID#:NA)
        RI = 1754.9   RI-RI(lib) = 4.2

17.4268   ?? M000991_A178005-101-xxx_NA_1759
                ,34_TRUE_VAR5_ALK_Lyxonic acid (5TMS) (ID#:NA)
        RI = 1765.5   RI-RI(lib) = 6.2

17.9315   ?? M000607_A181002-101-xxx_NA_1794
                ,63_TRUE_VAR5_ALK_Shikimic acid (4TMS) (ID#:NA)
        RI = 1802.6   RI-RI(lib) = 8.0

18.0415   ? M000069_A182004-101-xxx_NA_1804
                ,71_TRUE_VAR5_ALK_Citric acid (4TMS) (ID#:NA)
        RI = 1811.3   RI-RI(lib) = 6.5

18.1073   ?? contamination_blank (ID#:TAM757-N1010)
        RI = 1816.4   RI-RI(lib) = -0.4

18.5486   ?? M000007_A185001-101-xxx_NA_1842
                ,69_TRUE_VAR5_ALK_Quinic acid (5TMS) (ID#:NA)
        RI = 1851.1   RI-RI(lib) = 8.4

18.7177   ? M000606_A188004-101-xxx_NA_1863
                ,13_TRUE_VAR5_ALK_Fructose (1MEOX) (5TMS) BP (ID#:NA)
        RI = 1864.3   RI-RI(lib) = 1.2

18.8427   RI=1874.2, 18.8427 min AKS2296 (ID#:AKS2296-N1002)
        RI = 1874.2   RI-RI(lib) = -0.0

18.9591   ?? M000637_A189009-101-xxx_NA_1880
                ,27_TRUE_VAR5_ALK_Altrose (1MEOX) (5TMS) MP (ID#:NA)
        RI = 1883.3   RI-RI(lib) = 3.0

19.0352   ?? M000637_A190005-101-xxx_NA_1887
                ,55_TRUE_VAR5_ALK_Altrose (1MEOX) (5TMS) BP (ID#:NA)
        RI = 1889.3   RI-RI(lib) = 1.7

19.0413   ?? M000633_A189001-101-xxx_NA_1885
                ,22_TRUE_VAR5_ALK_Mannose (1MEOX) (5TMS) BP (ID#:NA)
        RI = 1889.7   RI-RI(lib) = 4.5

19.2873   ?? M000043_A191002-101-xxx_NA_1902
                 ,42_PRED_VAR5_ALK_Galactose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1909.1   RI-RI(lib) = 6.6

19.5330   ?? IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1928.3   RI-RI(lib) = 5.7

19.5391   IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1928.8   RI-RI(lib) = 6.2

19.5462   ? IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1929.4   RI-RI(lib) = 6.8

19.8115   M000801_A196011-101-xxx_NA_1945,61_TRUE_VAR5_ALK_Gallic
                 acid (4TMS) (ID#:2078-17-3)
RI = 1950.2   RI-RI(lib) = 4.6

20.6641   ? M000000_A203010-101-xxx_NA_2018,15_PRED_VAR5_ALK_NA (
                 ID#:NA)
RI = 2018.3   RI-RI(lib) = 0.2

20.9518   ?? contamination - pyridine/BSTFA - C16:0 acid TMS (ID#:JCB665-
                 N1044)
RI = 2042.5   RI-RI(lib) = -0.4

21.4161   M000060_A209002-101-xxx_NA_2080
                 ,23_TRUE_VAR5_ALK_Inositol, myo- (6TMS) (ID#:NA)
RI = 2081.6   RI-RI(lib) = 1.4

21.4212   ? M000060_A209002-101-xxx_NA_2080
                 ,23_TRUE_VAR5_ALK_Inositol, myo- (6TMS) (ID#:NA)
RI = 2082.0   RI-RI(lib) = 1.8

21.6208   ? M000000_A211001-101-xxx_NA_2098
                 ,3_PRED_VAR5_ALK_NA211001 (ID#:NA)
RI = 2098.8   RI-RI(lib) = 0.5

23.2107   ? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-
                 N1048)
RI = 2241.0   RI-RI(lib) = 1.8

24.5385   ?? M000000_A237001-101-xxx_NA_2361,83_PRED_VAR5_ALK_NA
                 (ID#:NA)
RI = 2364.8   RI-RI(lib) = 3.0

27.1464   M000044_A264001-101-xxx_NA_2622
                 ,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
RI = 2626.5   RI-RI(lib) = 3.7

27.1516   M000044_A264001-101-xxx_NA_2622
                 ,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
RI = 2627.1   RI-RI(lib) = 4.2

29.2337   ?? M000000_A286005-101-xxx_NA_2856,98_PRED_VAR5_ALK_NA
                 (ID#:NA)
RI = 2855.0   RI-RI(lib) = -1.9

29.9584   ?? M000000_A295008-101-xxx_NA_2934,06_PRED_VAR5_ALK_NA (ID#:NA)

    RI = 2938.5   RI-RI(lib) = 4.5

30.2677   ? RI=2975.8, 30.2817 min AKS2302_230301070748 (ID#:AKS230~1-N1002)

    RI = 2974.2   RI-RI(lib) = -1.6

30.2760   RI=2975.8, 30.2817 min AKS2302_230301070748 (ID#:AKS230~1-N1002)

    RI = 2975.1   RI-RI(lib) = -0.7

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=5.1.

Background (low vs. high retention time):

  median low RT S/N=31, high RT S/N=96

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

  S/N=20 before run

  S/N=10 at 5.01 min.

  S/N=5 at 5.02 min.

  S/N=2 at 5.02 min.

  S/N=1 at 5.09 min.

Column Bleed (m/z 207):

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

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