AMDIS GC/MS Analysis Report

Data: AKS2294.RAW
Library: C:\Program Files (x86)\NISTMS\AMDIS32\libraries\GDM\GMD.MSL
Number of Identifications: 37

RT(min)	Chemical Name
5.7482	?? M000413_A105003-101-xxx_NA_1031,31_TRUE_VAR5_ALK_Pyridine, 2-hydroxy- (1TMS) (ID#:NA)
	RI = 1033.1 RI-RI(lib) = 1.8
6.9141	? M000000_A110007-101-xxx_NA_1095,09_PRED_VAR5_ALK_Butylamine_2TMS (ID#:NA)
	RI = 1102.9 RI-RI(lib) = 7.8
7.9505	?? contamination - pyridine/BSTFA (ID#:JCB665-N1022)
	RI = 1162.6 RI-RI(lib) = 3.0
9.7379	M000075_A129001-101-xxx_NA_1262,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9)
	RI = 1265.5 RI-RI(lib) = 3.1
9.7529	M000075_A129001-101-xxx_NA_1262,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9)
	RI = 1266.4 RI-RI(lib) = 3.9
9.7582	M000075_A129001-101-xxx_NA_1262,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9)
	RI = 1266.7 RI-RI(lib) = 4.2
10.7351	? M000073_A135003-101-xxx_NA_1319,94_TRUE_VAR5_ALK_Glyceric acid (3TMS) (ID#:38191-87-6)
	RI = 1323.9 RI-RI(lib) = 4.0
12.2953	?? M000000_A144004-101-xxx_NA_1415,51_PRED_VAR5_ALK_NA (ID#:NA)
	RI = 1418.9 RI-RI(lib) = 3.4
13.3021	?? RI=1490.7, 13.4205 min AKS2164 (ID#:AKS2164-N1004)
	RI = 1484.1 RI-RI(lib) = -6.6
13.9610	? 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

14.1216 M001212_A155003-101-xxx_NA_1541
,53_PRED_VAR5_ALK_similar to Ditertbutylphenol (1TMS) (ID#:NA)
RI = 1537.2 RI-RI(lib) = -4.4

14.3807 RI=1554.3, 14.3867 min AKS2296 (ID#:AKS2296-N1004)
RI = 1553.9 RI-RI(lib) = -0.4

15.7766 ? M000582_A167011-101-xxx_NA_1649
,64_TRUE_VAR5_ALK_Ribose (1MEOX) (4TMS) BP (ID#:56196-08-8)
RI = 1647.5 RI-RI(lib) = -2.1

15.8799 ? M000582_A167011-101-xxx_NA_1649
,64_TRUE_VAR5_ALK_Ribose (1MEOX) (4TMS) BP (ID#:56196-08-8)
RI = 1654.7 RI-RI(lib) = 5.1

16.6451 ?? M000590_A172002-101-xxx_NA_1707
,41_TRUE_VAR5_ALK_Rhamnose (1MEOX) (4TMS) MP (ID#:NA)
RI = 1708.3 RI-RI(lib) = 0.9

17.9268 ?? M000607_A181002-101-xxx_NA_1794
,63_TRUE_VAR5_ALK_Shikimic acid (4TMS) (ID#:NA)
RI = 1802.3 RI-RI(lib) = 7.6

18.0320 ?? M000069_A182004-101-xxx_NA_1804
,71_TRUE_VAR5_ALK_Citric acid (4TMS) (ID#:NA)
RI = 1810.5 RI-RI(lib) = 5.8

18.0391 ? M000069_A182004-101-xxx_NA_1804
,71_TRUE_VAR5_ALK_Citric acid (4TMS) (ID#:NA)
RI = 1811.1 RI-RI(lib) = 6.4

18.5482 ?? M000007_A185001-101-xxx_NA_1842
,69_TRUE_VAR5_ALK_Quinic acid (5TMS) (ID#:NA)
RI = 1851.0 RI-RI(lib) = 8.3

18.7125 ? M000606_A188004-101-xxx_NA_1863
,13_TRUE_VAR5_ALK_Fructose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1863.9 RI-RI(lib) = 0.8

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

18.8362 RI=1874.2, 18.8427 min AKS2296 (ID#:AKS2296-N1002)
RI = 1873.6 RI-RI(lib) = -0.6

18.9521 ?? M000040_A189002-101-xxx_NA_1880
,5_TRUE_VAR5_ALK_Glucose (1MEOX) (5TMS) MP (ID#:NA)
RI = 1882.7 RI-RI(lib) = 2.2

19.0365 ?? M000633_A189001-101-xxx_NA_1885
,22_TRUE_VAR5_ALK_Mannose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1889.4 RI-RI(lib) = 4.1

19.2807 ?? M000043_A191002-101-xxx_NA_1902 ,42_PRED_VAR5_ALK_Galactose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1908.5 RI-RI(lib) = 6.1

19.5367 IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1928.6 RI-RI(lib) = 6.0

19.5410 IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1929.0 RI-RI(lib) = 6.4

19.8063 M000801_A196011-101-xxx_NA_1945,61_TRUE_VAR5_ALK_Gallic acid (4TMS) (ID#:2078-17-3)
RI = 1949.8 RI-RI(lib) = 4.2

20.6595 ? M000000_A203010-101-xxx_NA_2018,15_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2018.0 RI-RI(lib) = -0.2

20.6638 ?? M000000_A203003-101-xxx_NA_2014,18_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2018.3 RI-RI(lib) = 4.1

20.9466 ?? contamination - pyridine/BSTFA - C16:0 acid TMS (ID#:JCB665-N1044)
RI = 2042.1 RI-RI(lib) = -0.8

21.4117 M000060_A209002-101-xxx_NA_2080 ,23_TRUE_VAR5_ALK_Inositol, myo- (6TMS) (ID#:NA)
RI = 2081.2 RI-RI(lib) = 1.0

21.6165 ?? M000000_A211001-101-xxx_NA_2098 ,3_PRED_VAR5_ALK_NA211001 (ID#:NA)
RI = 2098.4 RI-RI(lib) = 0.1

23.2079 ? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-N1048)
RI = 2240.8 RI-RI(lib) = 1.6

27.1461 M000044_A264001-101-xxx_NA_2622 ,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
RI = 2626.5 RI-RI(lib) = 3.6

29.2209 ?? M000107_A287001-101-xxx_NA_2846 ,96_TRUE_VAR5_ALK_Isomaltose (1MEOX) (8TMS) MP (ID#:NA)
RI = 2853.6 RI-RI(lib) = 6.6

30.2643 RI=2975.8, 30.2817 min AKS2302_230301070748 (ID#:AKS230~1-N1002)
RI = 2973.8 RI-RI(lib) = -2.0

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=7.1.
Background (low vs. high retention time):
  median low RT S/N=36, high RT S/N=92
Solvent Tailing (m/z 84). Run begins at 5.00 min. Solvent falls below:
  S/N=20 before run
  S/N=10 at 5.02 min.
  S/N=5 at 5.03 min.
  S/N=2 at 5.05 min.
  S/N=1 at 5.25 min.
Column Bleed (m/z 207):
  median low RT S/N=2, high RT S/N=8

This report consists of 4 pages