AMDIS GC/MS Analysis Report

Data: AKS2295_230228090832.RAW
Library: C:\Program Files (x86)\NISTMS\AMDIS32\libraries\GDM\GMD.MSL
Number of Identifications: 38

RT(min)	Chemical Name
5.7202	M000413_A105003-101-xxx_NA_1031 ,31_TRUE_VAR5_ALK_Pyridine, 2-hydroxy- (1TMS) (ID#:NA)
	RI = 1031.4 RI-RI(lib) = 0.1
6.8894	?? M000000_A110007-101-xxx_NA_1095 ,09_PRED_VAR5_ALK_Butylamine_2TMS (ID#:NA)
	RI = 1101.5 RI-RI(lib) = 6.4
7.4680	?? M000000_A114002-101-xxx_NA_1131 ,27_TRUE_VAR5_ALK_NA114002 (classified unknown) (ID#:NA)
	RI = 1134.8 RI-RI(lib) = 3.5
7.9335	?? contamination - pyridine/BSTFA (ID#:JCB665-N1022)
	RI = 1161.6 RI-RI(lib) = 2.0
9.7117	? M000075_A129001-101-xxx_NA_1262 ,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9)
	RI = 1264.0 RI-RI(lib) = 1.6
9.7354	M000075_A129001-101-xxx_NA_1262 ,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9)
	RI = 1265.4 RI-RI(lib) = 2.9
9.7395	M000075_A129001-101-xxx_NA_1262 ,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9)
	RI = 1265.6 RI-RI(lib) = 3.2
10.7305	?? M000073_A135003-101-xxx_NA_1319 ,94_TRUE_VAR5_ALK_Glyceric acid (3TMS) (ID#:38191-87-6)
	RI = 1323.6 RI-RI(lib) = 3.7
13.3060	?? RI=1490.7, 13.4205 min AKS2164 (ID#:AKS2164-N1004)
	RI = 1484.4 RI-RI(lib) = -6.3
13.9653	?? 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

14.1284 M001212_A155003-101-xxx_NA_1541
,53_PRED_VAR5_ALK_similar to Ditertbutylphenol (1TMS) (ID#:NA)
RI = 1537.6 RI-RI(lib) = -3.9

14.3878 RI=1554.3, 14.3867 min AKS2296 (ID#:AKS2296-N1004)
RI = 1554.4 RI-RI(lib) = 0.1

15.8845 ? 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

16.6557 ?? M000590_A172002-101-xxx_NA_1707
,41_TRUE_VAR5_ALK_Rhamnose (1MEOX) (4TMS) MP (ID#:NA)
RI = 1709.1 RI-RI(lib) = 1.6

17.2881 ?? M000991_A178005-101-xxx_NA_1759
,34_TRUE_VAR5_ALK_Lyxonic acid (5TMS) (ID#:NA)
RI = 1755.4 RI-RI(lib) = -4.0

18.0461 ? M000069_A182004-101-xxx_NA_1804
,71_TRUE_VAR5_ALK_Citric acid (4TMS) (ID#:NA)
RI = 1811.6 RI-RI(lib) = 6.9

18.5516 ?? M000007_A185001-101-xxx_NA_1842
,69_TRUE_VAR5_ALK_Quinic acid (5TMS) (ID#:NA)
RI = 1851.3 RI-RI(lib) = 8.6

18.5568 ?? M000007_A185001-101-xxx_NA_1842
,69_TRUE_VAR5_ALK_Quinic acid (5TMS) (ID#:NA)
RI = 1851.7 RI-RI(lib) = 9.0

18.7206 ? M000606_A188004-101-xxx_NA_1863
,13_TRUE_VAR5_ALK_Fructose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1864.6 RI-RI(lib) = 1.4

18.7247 ? M000606_A188004-101-xxx_NA_1863
,13_TRUE_VAR5_ALK_Fructose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1864.9 RI-RI(lib) = 1.8

18.8456 RI=1874.2, 18.8427 min AKS2296 (ID#:AKS2296-N1002)
RI = 1874.4 RI-RI(lib) = 0.2

18.9652 ?? M000637_A189009-101-xxx_NA_1880
,27_TRUE_VAR5_ALK_Altrose (1MEOX) (5TMS) MP (ID#:NA)
RI = 1883.8 RI-RI(lib) = 3.5

19.0469 ?? M000632_A190004-101-xxx_NA_1885
,22_TRUE_VAR5_ALK_Allose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1890.2 RI-RI(lib) = 5.0

19.0469 ?? M000633_A189001-101-xxx_NA_1885
,22_TRUE_VAR5_ALK_Mannose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1890.2 RI-RI(lib) = 5.0

19.2914 ?? M000687_A193002-101-xxx_NA_1913 ,17_TRUE_VAR5_ALK_Mannitol (6TMS) (ID#:NA)
RI = 1909.4 RI-RI(lib) = -3.8

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

19.5480 IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1929.5 RI-RI(lib) = 6.9

19.8192 M000801_A196011-101-xxx_NA_1945,61_TRUE_VAR5_ALK_Gallic acid (4TMS) (ID#:2078-17-3)
RI = 1950.8 RI-RI(lib) = 5.2

20.6700 ? M000000_A203010-101-xxx_NA_2018,15_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2018.8 RI-RI(lib) = 0.7

20.9575 ? contamination - pyridine/BSTFA - C16:0 acid TMS (ID#:JCB665-N1044)
RI = 2043.0 RI-RI(lib) = 0.1

21.4216 M000060_A209002-101-xxx_NA_2080 ,23_TRUE_VAR5_ALK_Inositol, myo- (6TMS) (ID#:NA)
RI = 2082.1 RI-RI(lib) = 1.8

21.4258 M000060_A209002-101-xxx_NA_2080 ,23_TRUE_VAR5_ALK_Inositol, myo- (6TMS) (ID#:NA)
RI = 2082.4 RI-RI(lib) = 2.2

21.6305 ?? M000000_A211001-101-xxx_NA_2098 ,3_PRED_VAR5_ALK_NA211001 (ID#:NA)
RI = 2099.6 RI-RI(lib) = 1.3

23.2182 ? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-N1048)
RI = 2241.7 RI-RI(lib) = 2.5

27.1591 M000044_A264001-101-xxx_NA_2622 ,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
RI = 2627.9 RI-RI(lib) = 5.1

28.2450 ?? M000000_A276007-101-xxx_NA_2752,25_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2744.9 RI-RI(lib) = -7.3

30.2816 RI=2975.8, 30.2817 min AKS2302_230301070748 (ID#:AKS230~1-N1002)
RI = 2975.8 RI-RI(lib) = -0.0

30.2869 RI=2975.8, 30.2817 min AKS2302_230301070748 (ID#:AKS230~1-N1002)
RI = 2976.4 RI-RI(lib) = 0.6

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=5.8.
Background (low vs. high retention time):
  median low RT S/N=29, high RT S/N=93
Solvent Tailing (m/z 84). Run begins at 5.00 min. Solvent falls below:
  S/N=5 before run
  S/N=2 at 5.01 min.
  S/N=1 at 5.25 min.
Column Bleed (m/z 207):
  median low RT S/N=2, high RT S/N=11

This report consists of 4 pages