AMDIS GC/MS Analysis Report

Data: AKS2299.RAW
Library: C:\Program Files (x86)\NISTMS\AMDIS32\libraries\GDM\GMD.MSL
Number of Identifications: 60

RT(min)	Chemical Name
5.7079	? M000413_A105003-101-xxx_NA_1031 ,31_TRUE_VAR5_ALK_Pyridine, 2-hydroxy- (1TMS) (ID#:NA)
	RI = 1030.6 RI-RI(lib) = -0.7
7.3899	? M001233_A114014-101-xxx_NA_1133,08_TRUE_VAR5_ALK_Furan-2-carboxylic acid (1TMS) (ID#:NA)
	RI = 1130.3 RI-RI(lib) = -2.8
7.4686	? M000000_A114002-101-xxx_NA_1131 ,27_TRUE_VAR5_ALK_NA114002 (classified unknown) (ID#:NA)
	RI = 1134.8 RI-RI(lib) = 3.5
7.9320	? contamination - pyridine/BSTFA (ID#:JCB665-N1022)
	RI = 1161.5 RI-RI(lib) = 1.9
9.7219	M000075_A129001-101-xxx_NA_1262 ,42_TRUE_VAR5_ALK_Phosphoric acid (3TMS) (ID#:10497-05-9)
	RI = 1264.6 RI-RI(lib) = 2.2
9.7262	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
9.7810	?? contamination - pyridine/BSTFA (ID#:JCB665-N1036)
	RI = 1268.0 RI-RI(lib) = 2.2
10.7303	? 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
10.7733	?? M000000_A136002-101-xxx_NA_1332 ,55_TRUE_VAR5_ALK_similar to Lumichrome (2MeOX) (ID#:NA)
	RI = 1326.2 RI-RI(lib) = -6.4
13.3023	?? RI=1490.7, 13.4205 min AKS2164 (ID#:AKS2164-N1004)
	RI = 1484.1 RI-RI(lib) = -6.6
13.9612	? 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

14.1226 M001212_A155003-101-xxx_NA_1541
,53_PRED_VAR5_ALK_similar to Ditertbutylphenol (1TMS) (ID#:NA)
RI = 1537.2 RI-RI(lib) = -4.3

14.3833 RI=1554.3, 14.3867 min AKS2296 (ID#:AKS2296-N1004)
RI = 1554.1 RI-RI(lib) = -0.2

15.7797 ? M000582_A167011-101-xxx_NA_1649
,64_TRUE_VAR5_ALK_Ribose (1MEOX) (4TMS) BP (ID#:56196-08-8)
RI = 1647.8 RI-RI(lib) = -1.9

15.8815 ? M000576_A165006-101-xxx_NA_1650
,36_TRUE_VAR5_ALK_Lyxose (1MEOX) (4TMS) MP (ID#:NA)
RI = 1654.8 RI-RI(lib) = 4.5

16.6497 ?? M000590_A172002-101-xxx_NA_1707
,41_TRUE_VAR5_ALK_Rhamnose (1MEOX) (4TMS) MP (ID#:NA)
RI = 1708.6 RI-RI(lib) = 1.2

16.9784 ? RI=1731.6, 16.7359 min LMV1405 (ID#:LMV1405-N1006)
RI = 1732.7 RI-RI(lib) = 1.1

17.2796 ? M000605_A177001-101-xxx_NA_1750
,73_TRUE_VAR5_ALK_Ribonic acid (5TMS) (ID#:NA)
RI = 1754.7 RI-RI(lib) = 4.0

17.2836 ? M000605_A177001-101-xxx_NA_1750
,73_TRUE_VAR5_ALK_Ribonic acid (5TMS) (ID#:NA)
RI = 1755.0 RI-RI(lib) = 4.3

17.4180 ?? M000991_A178005-101-xxx_NA_1759
,34_TRUE_VAR5_ALK_Lyxonic acid (5TMS) (ID#:NA)
RI = 1764.9 RI-RI(lib) = 5.5

17.4253 ?? M000991_A178005-101-xxx_NA_1759
,34_TRUE_VAR5_ALK_Lyxonic acid (5TMS) (ID#:NA)
RI = 1765.4 RI-RI(lib) = 6.1

17.9253 ?? M000607_A181002-101-xxx_NA_1794
,63_TRUE_VAR5_ALK_Shikimic acid (4TMS) (ID#:NA)
RI = 1802.1 RI-RI(lib) = 7.5

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

18.0401 ? M000069_A182004-101-xxx_NA_1804
,71_TRUE_VAR5_ALK_Citric acid (4TMS) (ID#:NA)
RI = 1811.2 RI-RI(lib) = 6.4

18.1055 ?? contamination_blank (ID#:TAM757-N1010)
RI = 1816.3 RI-RI(lib) = -0.5

18.5218 ?? M000007_A185001-101-xxx_NA_1842
,69_TRUE_VAR5_ALK_Quinic acid (5TMS) (ID#:NA)
RI = 1849.0 RI-RI(lib) = 6.3

18.5524 ?? M000007_A185001-101-xxx_NA_1842
,69_TRUE_VAR5_ALK_Quinic acid (5TMS) (ID#:NA)
RI = 1851.4 RI-RI(lib) = 8.7

18.7221 ? M000606_A188004-101-xxx_NA_1863
,13_TRUE_VAR5_ALK_Fructose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1864.7 RI-RI(lib) = 1.6

18.8425 RI=1874.2, 18.8427 min AKS2296 (ID#:AKS2296-N1002)
RI = 1874.1 RI-RI(lib) = -0.1

18.8469 RI=1874.2, 18.8427 min AKS2296 (ID#:AKS2296-N1002)
RI = 1874.5 RI-RI(lib) = 0.3

18.9611 ?? M000637_A189009-101-xxx_NA_1880
,27_TRUE_VAR5_ALK_Altrose (1MEOX) (5TMS) MP (ID#:NA)
RI = 1883.4 RI-RI(lib) = 3.2

18.9611 ?? M000040_A189002-101-xxx_NA_1880
,5_TRUE_VAR5_ALK_Glucose (1MEOX) (5TMS) MP (ID#:NA)
RI = 1883.4 RI-RI(lib) = 2.9

19.0401 ?? M000637_A190005-101-xxx_NA_1887
,55_TRUE_VAR5_ALK_Altrose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1889.6 RI-RI(lib) = 2.1

19.0452 ?? M000632_A190004-101-xxx_NA_1885
,22_TRUE_VAR5_ALK_Allose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1890.0 RI-RI(lib) = 4.8

19.0452 ?? M000633_A189001-101-xxx_NA_1885
,22_TRUE_VAR5_ALK_Mannose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1890.0 RI-RI(lib) = 4.8

19.2831 ?? M000043_A191002-101-xxx_NA_1902
,42_PRED_VAR5_ALK_Galactose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1908.7 RI-RI(lib) = 6.3

19.5396 IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1928.9 RI-RI(lib) = 6.3

19.5470 ? IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1929.4 RI-RI(lib) = 6.8

19.8099 M000801_A196011-101-xxx_NA_1945,61_TRUE_VAR5_ALK_Gallic acid (4TMS) (ID#:2078-17-3)
RI = 1950.1 RI-RI(lib) = 4.5

20.3236 ?? M000508_A200001-101-xxx_NA_1984
,83_TRUE_VAR5_ALK_Gluconic acid (6TMS) (ID#:NA)
RI = 1990.4 RI-RI(lib) = 5.6

20.6656 ? M000000_A203010-101-xxx_NA_2018,15_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2018.5 RI-RI(lib) = 0.3

20.8409 ?? M000594_A204001-101-xxx_NA_2030 ,47_TRUE_VAR5_ALK_Galactaric acid (6TMS) (ID#:NA)
RI = 2033.2 RI-RI(lib) = 2.7

20.9484 ?? contamination - pyridine/BSTFA - C16:0 acid TMS (ID#:JCB665-N1044)
RI = 2042.3 RI-RI(lib) = -0.6

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

21.4148 M000060_A209002-101-xxx_NA_2080 ,23_TRUE_VAR5_ALK_Inositol, myo- (6TMS) (ID#:NA)
RI = 2081.5 RI-RI(lib) = 1.3

21.4191 M000060_A209002-101-xxx_NA_2080 ,23_TRUE_VAR5_ALK_Inositol, myo- (6TMS) (ID#:NA)
RI = 2081.8 RI-RI(lib) = 1.6

21.6226 ?? M000000_A211001-101-xxx_NA_2098 ,3_PRED_VAR5_ALK_NA211001 (ID#:NA)
RI = 2099.0 RI-RI(lib) = 0.7

21.9580 ?? M000000_A214003-101-xxx_NA_2127,28_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2128.9 RI-RI(lib) = 1.6

22.5010 ? RI=2175.5, 22.6111 min LFF858 (ID#:LFF858-N1006)
RI = 2177.5 RI-RI(lib) = 2.0

23.2081 ? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-N1048)
RI = 2240.8 RI-RI(lib) = 1.6

24.5396 ?? M000000_A237001-101-xxx_NA_2361,83_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2364.9 RI-RI(lib) = 3.1

25.8152 ?? M000000_A250001-101-xxx_NA_2484,98_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2488.6 RI-RI(lib) = 3.6

27.1505 M000044_A264001-101-xxx_NA_2622 ,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
RI = 2627.0 RI-RI(lib) = 4.1

27.1557 M000044_A264001-101-xxx_NA_2622 ,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
RI = 2627.6 RI-RI(lib) = 4.7

28.5052 ?? M000000_A277012-101-xxx_NA_2768,8_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2773.0 RI-RI(lib) = 4.2

29.2315 ?? M000107_A287001-101-xxx_NA_2846 ,96_TRUE_VAR5_ALK_Isomaltose (1MEOX) (8TMS) MP (ID#:NA)
RI = 2854.8 RI-RI(lib) = 7.8

29.2315 ?? M000000_A286005-101-xxx_NA_2856,98_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2854.8 RI-RI(lib) = -2.2

29.4896 ?? M000107_A291002-101-xxx_NA_2881 ,28_TRUE_VAR5_ALK_Isomaltose (1MEOX) (8TMS) BP (ID#:NA)
RI = 2884.5 RI-RI(lib) = 3.2

29.9580 ?? M000000_A295008-101-xxx_NA_2934,06_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2938.5 RI-RI(lib) = 4.4

30.2708 RI=2975.8, 30.2817 min AKS2302_230301070748 (ID#:AKS230~1-N1002)
RI = 2974.5 RI-RI(lib) = -1.3

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=7.5.
Background (low vs. high retention time):
  median low RT S/N=33, high RT S/N=97
Solvent Tailing (m/z 84). Run begins at 5.00 min. Solvent falls below:
  S/N=2 before run
  S/N=1 at 5.12 min.
Column Bleed (m/z 207):
  median low RT S/N=3, high RT S/N=12

This report consists of 5 pages