AMDIS GC/MS Analysis Report

Data: AKS2300.RAW
Library: C:\Program Files (x86)\NISTMS\AMDIS32\libraries\GDM\GMD.MSL
Number of Identifications: 25

RT(min)	Chemical Name
5.7235	? M000413_A105003-101-xxx_NA_1031 ,31_TRUE_VAR5_ALK_Pyridine, 2-hydroxy- (1TMS) (ID#:NA)
	RI = 1031.6 RI-RI(lib) = 0.3
6.0700	?? contamination - pyridine/BSTFA (ID#:JCB665-N1012)
	RI = 1052.4 RI-RI(lib) = -6.6
7.4758	?? M000000_A114002-101-xxx_NA_1131 ,27_TRUE_VAR5_ALK_NA114002 (classified unknown) (ID#:NA)
	RI = 1135.2 RI-RI(lib) = 4.0
9.7261	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
10.7773	? M000000_A136002-101-xxx_NA_1332 ,55_TRUE_VAR5_ALK_similar to Lumichrome (2MeOX) (ID#:NA)
	RI = 1326.4 RI-RI(lib) = -6.1
13.4964	? cis - linalool oxide (furanoid) (ID#:AKS142~1-N1002)
	RI = 1496.7 RI-RI(lib) = 3.0
13.8517	cis - linalool oxide (pyranoid) (ID#:AKS142~1-N1006)
	RI = 1519.7 RI-RI(lib) = 3.0
14.1218	M001212_A155003-101-xxx_NA_1541 ,53_PRED_VAR5_ALK_similar to Ditertbutylphenol (1TMS) (ID#:NA)
	RI = 1537.2 RI-RI(lib) = -4.3
18.0201	?? contamination_blank (ID#:TAM757-N1008)
	RI = 1809.6 RI-RI(lib) = -0.4
18.1055	?? contamination_blank (ID#:TAM757-N1010)
	RI = 1816.3 RI-RI(lib) = -0.5
18.7104	?? M000606_A188004-101-xxx_NA_1863 ,13_TRUE_VAR5_ALK_Fructose (1MEOX) (5TMS) BP (ID#:NA)
	RI = 1863.8 RI-RI(lib) = 0.6
18.8335	? RI=1874.2, 18.8427 min AKS2296 (ID#:AKS2296-N1002)
	RI = 1873.4 RI-RI(lib) = -0.8

19.0343 ?? M000633_A189001-101-xxx_NA_1885 ,22_TRUE_VAR5_ALK_Mannose (1MEOX) (5TMS) BP (ID#:NA)
RI = 1889.2 RI-RI(lib) = 4.0

19.5386 IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1928.8 RI-RI(lib) = 6.2

19.8047 M000801_A196011-101-xxx_NA_1945,61_TRUE_VAR5_ALK_Gallic acid (4TMS) (ID#:2078-17-3)
RI = 1949.7 RI-RI(lib) = 4.1

19.8089 M000801_A196011-101-xxx_NA_1945,61_TRUE_VAR5_ALK_Gallic acid (4TMS) (ID#:2078-17-3)
RI = 1950.0 RI-RI(lib) = 4.4

20.9469 ? contamination - pyridine/BSTFA - C16:0 acid TMS (ID#:JCB665-N1044)
RI = 2042.1 RI-RI(lib) = -0.8

21.4118 ?? M000060_A209002-101-xxx_NA_2080 ,23_TRUE_VAR5_ALK_Inositol, myo- (6TMS) (ID#:NA)
RI = 2081.2 RI-RI(lib) = 1.0

23.2076 ? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-N1048)
RI = 2240.7 RI-RI(lib) = 1.5

23.2130 ? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-N1048)
RI = 2241.2 RI-RI(lib) = 2.0

27.1469 ?? M000044_A264001-101-xxx_NA_2622 ,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
RI = 2626.6 RI-RI(lib) = 3.7

27.3416 ? RI=2648.0, 27.3456 min AKS2298_230228141932 (ID#:AKS229~1-N1008)
RI = 2647.6 RI-RI(lib) = -0.4

29.3721 ?? M000832_A289005-101-xxx_NA_2865 ,56_TRUE_VAR5_ALK_Catechin (5TMS) (ID#:NA)
RI = 2871.0 RI-RI(lib) = 5.4

31.7158 ?? contamination_blank (ID#:TAM757-N1014)
RI = 3141.0 RI-RI(lib) = 7.4

31.7224 ?? contamination_blank (ID#:TAM757-N1014)
RI = 3141.7 RI-RI(lib) = 8.1

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=5.6.

Background (low vs. high retention time):
  median low RT S/N=34, high RT S/N=107
Solvent Tailing (m/z 84). Run begins at 5.00 min. Solvent falls below:
  S/N=2 before run
  S/N=1 at 5.17 min.
Column Bleed (m/z 207):
  median low RT S/N=3, high RT S/N=13

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