AMDIS GC/MS Analysis Report

Data: AKS2298_230228141932.RAW
Library: C:\Program Files (x86)\NISTMS\AMDIS32\libraries\GDM\GMD.MSL
Number of Identifications: 34

RT(min)	Chemical Name
5.7220	M000413_A105003-101-xxx_NA_1031 ,31_TRUE_VAR5_ALK_Pyridine, 2-hydroxy- (1TMS) (ID#:NA)
	RI = 1031.5 RI-RI(lib) = 0.2
7.4010	?? M001233_A114014-101-xxx_NA_1133 ,08_TRUE_VAR5_ALK_Furan-2-carboxylic acid (1TMS) (ID#:NA)
	RI = 1130.9 RI-RI(lib) = -2.2
7.4769	?? M000000_A114002-101-xxx_NA_1131 ,27_TRUE_VAR5_ALK_NA114002 (classified unknown) (ID#:NA)
	RI = 1135.3 RI-RI(lib) = 4.0
7.9387	?? contamination - pyridine/BSTFA (ID#:JCB665-N1022)
	RI = 1161.9 RI-RI(lib) = 2.3
9.7255	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
10.7770	M000000_A136002-101-xxx_NA_1332,55_TRUE_VAR5_ALK_similar to Lumichrome (2MeOX) (ID#:NA)
	RI = 1326.4 RI-RI(lib) = -6.1
13.4984	cis - linalool oxide (furanoid) (ID#:AKS142~1-N1002)
	RI = 1496.8 RI-RI(lib) = 3.1
13.6219	? trans - linalool oxide (furanoid) (ID#:AKS142~1-N1004)
	RI = 1504.8 RI-RI(lib) = 3.7
13.8569	cis - linalool oxide (pyranoid) (ID#:AKS142~1-N1006)
	RI = 1520.0 RI-RI(lib) = 3.3
14.1003	?? M001236_A155002-101-xxx_NA_1536 ,45_TRUE_VAR5_ALK_Benzene-1,2,3-triol (3TMS) (ID#:17864-23-2)
	RI = 1535.8 RI-RI(lib) = -0.7
14.1200	M001212_A155003-101-xxx_NA_1541 ,53_PRED_VAR5_ALK_similar to Ditertbutylphenol (1TMS) (ID#:NA)
	RI = 1537.1 RI-RI(lib) = -4.5

14.1240 M001212_A155003-101-xxx_NA_1541 ,53_PRED_VAR5_ALK_similar to Ditertbutylphenol (1TMS) (ID#:NA)
RI = 1537.3 RI-RI(lib) = -4.2

15.4039 ? M000573_A163003-101-xxx_NA_1620 ,5_TRUE_VAR5_ALK_Triethanolamine (3TMS) (ID#:20836-42-4)
RI = 1621.7 RI-RI(lib) = 1.2

18.0273 ?? contamination_blank (ID#:TAM757-N1008)
RI = 1810.1 RI-RI(lib) = 0.1

18.1109 ? contamination_blank (ID#:TAM757-N1010)
RI = 1816.7 RI-RI(lib) = -0.1

19.3457 ? M000009_A192002-101-xxx_NA_1918 ,78_TRUE_VAR5_ALK_Ferulic acid, cis- (2TMS) (ID#:NA)
RI = 1913.6 RI-RI(lib) = -5.1

19.5385 ? IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1928.8 RI-RI(lib) = 6.2

19.5445 IS - 13C6-Sorbitol (ID#:ARP436-N1002)
RI = 1929.2 RI-RI(lib) = 6.6

19.8146 M000801_A196011-101-xxx_NA_1945,61_TRUE_VAR5_ALK_Gallic acid (4TMS) (ID#:2078-17-3)
RI = 1950.4 RI-RI(lib) = 4.8

20.6883 RI=2020.4, 20.6883 min AKS2298_230228141932 (ID#:AKS229~1-N1010)
RI = 2020.4 RI-RI(lib) = -0.0

20.9513 ? contamination - pyridine/BSTFA - C16:0 acid TMS (ID#:JCB665-N1044)
RI = 2042.5 RI-RI(lib) = -0.4

21.4716 ?? M000009_A192002-101-xxx_NA_1918 ,78_TRUE_VAR5_ALK_Ferulic acid, cis- (2TMS) (ID#:NA)
RI = 2086.3 RI-RI(lib) = 167.5

21.6540 ?? RI=2020.4, 20.6883 min AKS2298_230228141932 (ID#:AKS229~1-N1010)
RI = 2101.7 RI-RI(lib) = 81.3

21.9935 M000649_A214001-101-xxx_NA_2135 ,55_TRUE_VAR5_ALK_Caffeic acid, trans- (3TMS) (ID#:NA)
RI = 2132.1 RI-RI(lib) = -3.5

22.4531 ?? RI=2020.4, 20.6883 min AKS2298_230228141932 (ID#:AKS229~1-N1010)
RI = 2173.2 RI-RI(lib) = 152.8

23.2120 ? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-N1048)
RI = 2241.1 RI-RI(lib) = 1.9

23.2163 ?? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-N1048)
RI = 2241.5 RI-RI(lib) = 2.3

24.6857 ?? M000000_A241003-101-xxx_NA_2386,02_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2379.1 RI-RI(lib) = -6.9

27.1486 ? M000044_A264001-101-xxx_NA_2622 ,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
RI = 2626.8 RI-RI(lib) = 3.9

27.3456 RI=2648.0, 27.3456 min AKS2298_230228141932 (ID#:AKS229~1-N1008)
RI = 2648.0 RI-RI(lib) = 0.0

27.4662 ?? M000000_A267001-101-xxx_NA_2660,62_PRED_VAR5_ALK_NA (ID#:NA)
RI = 2661.0 RI-RI(lib) = 0.4

29.3755 M000832_A289005-101-xxx_NA_2865 ,56_TRUE_VAR5_ALK_Catechin (5TMS) (ID#:NA)
RI = 2871.4 RI-RI(lib) = 5.8

29.7078 ? M000833_A291010-101-xxx_NA_2914 ,99_TRUE_VAR5_ALK_Epigallocatechin (6TMS) (ID#:NA)
RI = 2909.7 RI-RI(lib) = -5.3

32.7677 ?? RI=2960.5, 32.8885 min AKS2164 (ID#:AKS2164-N1008)
RI = 3262.2 RI-RI(lib) = 301.7

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=9.6.
Background (low vs. high retention time):
  median low RT S/N=23, high RT S/N=86
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 5.03 min.
Column Bleed (m/z 207):
  median low RT S/N=2, high RT S/N=10

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