

AMDIS GC/MS Analysis Report

Data: AKS2301_230228171553.RAW

Library: C:\Program Files (x86)\NISTMS\AMDIS32\libraries\GDM\GMD.MSL

Number of Identifications: 28

<u>RT(min)</u>	<u>Chemical Name</u>
5.7213	M000413_A105003-101-xxx_NA_1031 ,31_TRUE_VAR5_ALK_Pyridine, 2-hydroxy- (1TMS) (ID#:NA) RI = 1031.4 RI-RI (lib) = 0.1
6.0675	?? contamination - pyridine/BSTFA (ID#:JCB665-N1012) RI = 1052.2 RI-RI (lib) = -6.8
7.4727	?? M000000_A114002-101-xxx_NA_1131 ,27_TRUE_VAR5_ALK_NA114002 (classified unknown) (ID#:NA) RI = 1135.1 RI-RI (lib) = 3.8
7.9393	? contamination - pyridine/BSTFA (ID#:JCB665-N1022) RI = 1161.9 RI-RI (lib) = 2.3
9.7224	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
10.7729	? M000000_A136002-101-xxx_NA_1332 ,55_TRUE_VAR5_ALK similar to Lumichrome (2MeOX) (ID#:NA) RI = 1326.2 RI-RI (lib) = -6.4
13.4929	cis - linalool oxide (furanoid) (ID#:AKS142~1-N1002) RI = 1496.5 RI-RI (lib) = 2.8
13.6169	?? trans - linalool oxide (furanoid) (ID#:AKS142~1-N1004) RI = 1504.5 RI-RI (lib) = 3.4
13.8495	cis - linalool oxide (pyranoid) (ID#:AKS142~1-N1006) RI = 1519.6 RI-RI (lib) = 2.9
14.0960	?? M001236_A155002-101-xxx_NA_1536 ,45_TRUE_VAR5_ALK_Benzene-1,2,3-triol (3TMS) (ID#:17864-23-2) RI = 1535.5 RI-RI (lib) = -0.9
14.1195	M001212_A155003-101-xxx_NA_1541 ,53_PRED_VAR5_ALK similar to Diterbutylphenol (1TMS) (ID#:NA) RI = 1537.0 RI-RI (lib) = -4.5
18.0169	?? contamination_blank (ID#:TAM757-N1008) RI = 1809.3 RI-RI (lib) = -0.7

18.1034 ?? contamination_blank (ID#:TAM757-N1010)
 RI = 1816.1 RI-RI(lib) = -0.7

19.5344 IS - 13C6-Sorbitol (ID#:ARP436-N1002)
 RI = 1928.4 RI-RI(lib) = 5.8

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

19.8026 ?? M000801_A196011-101-xxx_NA_1945
 ,61_TRUE_VAR5_ALK_Gallic acid (4TMS) (ID#:2078-17-3)
 RI = 1949.5 RI-RI(lib) = 3.9

19.8067 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

20.6785 RI=2020.4, 20.6883 min AKS2298_230228141932 (ID#:AKS229~1-
 N1010)
 RI = 2019.6 RI-RI(lib) = -0.8

20.9438 ? contamination - pyridine/BSTFA - C16:0 acid TMS (ID#:JCB665-
 N1044)
 RI = 2041.9 RI-RI(lib) = -1.0

21.9866 ? M000649_A214001-101-xxx_NA_2135
 ,55_TRUE_VAR5_ALK_Caffeic acid, trans- (3TMS) (ID#:NA)
 RI = 2131.5 RI-RI(lib) = -4.1

23.2055 ? contamination - pyridine/BSTFA - C18:0 acid TMS (ID#:JCB665-
 N1048)
 RI = 2240.5 RI-RI(lib) = 1.3

27.1425 ? M000044_A264001-101-xxx_NA_2622
 ,87_TRUE_VAR5_ALK_Sucrose (8TMS) (ID#:NA)
 RI = 2626.1 RI-RI(lib) = 3.3

27.3373 RI=2648.0, 27.3456 min AKS2298_230228141932 (ID#:AKS229~1-
 N1008)
 RI = 2647.1 RI-RI(lib) = -0.9

27.4592 ?? M000000_A267001-101-xxx_NA_2660,62_PRED_VAR5_ALK_NA
 (ID#:NA)
 RI = 2660.3 RI-RI(lib) = -0.4

29.3665 ? M000832_A289005-101-xxx_NA_2865
 ,56_TRUE_VAR5_ALK_Catechin (5TMS) (ID#:NA)
 RI = 2870.3 RI-RI(lib) = 4.8

29.7036 ? M000833_A291010-101-xxx_NA_2914
 ,99_TRUE_VAR5_ALK_Epigallocatechin (6TMS) (ID#:NA)
 RI = 2909.2 RI-RI(lib) = -5.8

31.7096 ?? contamination_blank (ID#:TAM757-N1014)
 RI = 3140.3 RI-RI(lib) = 6.7

32.7605 ?? RI=2960.5, 32.8885 min AKS2164 (ID#:AKS2164-N1008)
RI = 3261.3 RI-RI(lib) = 300.8

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=6.7.

Background (low vs. high retention time):

median low RT S/N=30, high RT S/N=99

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 5.01 min.

Column Bleed (m/z 207):

median low RT S/N=3, high RT S/N=12

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