

AMDIS GC/MS Analysis Report

Data: AKS2326.RAW

Library: C:\Program Files (x86)\NISTMS\AMDIS32\libraries\TMS\LIB_THS.MSL

Number of Identifications: 153

<u>RT(min)</u>	<u>Chemical Name</u>
5.7486	?? alfa - hydroxyisobutyric acid (ID#:FAH383-N1002)
5.7535	?? alfa - hydroxyisobutyric acid (ID#:FAH383-N1002)
5.8628	RI=959.7, 14.1197 min FAH388 (ID#:FAH388-N1048)
6.1068	RI=795.7, 11.2931 min OAB4671 (ID#:OAB467~1-N1002)
6.2328	? contaminant_silanol (ID#:TVL0020-N1008)
6.2693	? 1,2 - dihydroxyethane (ID#:FAH0040-N1002)
6.2693	?? Oxalic acid (ID#:FAH957-N1038)
6.3766	? reagent artefact_4 (ID#:FAH360-N1008)
6.3816	? reagent artefact_4 (ID#:FAH360-N1008)
6.5231	?? Oxalic acid (ID#:FAH957-N1038)
6.6513	contaminant_silanol (ID#:TVL0020-N1010)
7.1138	? Oxalic acid (ID#:FAH957-N1038)
7.1828	contaminant_silanol (ID#:TVL0020-N1016)
7.2953	? Oxalic acid (ID#:FAH957-N1038)
7.5232	contaminant_silanol (ID#:TVL0020-N1016)
7.5727	phenol (ID#:TVL0020-N1014)
7.6362	2 - hydroxypropanoic acid (lactic acid) (ID#:FAH0040-N1008)
7.9458	hydroxyacetic acid (glycolic acid) (ID#:FAH0040-N1004)

8.0292	? 2 - hydroxypropenoic acid (pyruvic acid) (ID#:TVL0020-N1018)
8.1671	? 2 - hydroxypropenoic acid (pyruvic acid) (ID#:TVL0020-N1018)
8.4487	? Oxalic acid (ID#:FAH957-N1038)
8.5927	? 2 - hydroxypropenoic acid (pyruvic acid) (ID#:TVL0020-N1018)
8.7610	? propanal_artifact (ID#:FAH0040-N1006)
8.9675	RI=1124.1, 7.4028 min AKS1974 (ID#:AKS1974-N1054)
9.0247	? C1 - phenol_l1 (ID#:TVL0020-N1020)
9.0763	?? furan-2-carboxylic acid (ID#:FAH388-N1010)
9.2084	RI=1136.8, 7.6203 min AKS1976 (ID#:AKS1976-N1156)
9.6450	contaminant (ID#:FAH1384-N1014)
10.0593	?? Glyceric acid (ID#:38191-87-6)
10.2793	? 3 - hydroxy - (4H) - pyran - 4 - one (ID#:FAH0040-N1014)
10.3608	? contaminant (ID#:FAH1384-N1014)
10.6258	RI=1214.9, 20.4578 min FAH388 (ID#:FAH388-N1014)
10.6768	RI=1218.7, 9.0147 min AKS1976 (ID#:AKS1976-N1154)
10.7584	guaiacol (ID#:OAB466~1-N1002)
11.0035	? RI=1256.0, 21.1538 min FAH0040 (ID#:FAH0040-N1020)
11.1268	RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
11.1498	?? Benzoic acid (ID#:FAH1388-N1004)
11.5000	RI=1272.7, 9.9318 min AKS1975 (ID#:AKS1975-N1052)
11.5517	? glycerol (ID#:TVL0020-N1040)
11.7100	4 - vinyl - phenol (ID#:TVL0020-N1042)
11.8070	RI=1282.8, 10.1027 min AKS1976 (ID#:AKS1976-N1148)
12.0625	?? RI=1296.4, 10.3341 min AKS1976 (ID#:AKS1976-N1146)
12.3138	?? RI=1296.4, 10.3341 min AKS1976 (ID#:AKS1976-N1146)

12.8629	? Oxalic acid (ID#:FAH957-N1038)
12.9074	?? 1,3 - dihydroxybenzene (resorcinol) (ID#:TVL0017-N1046)
12.9820	?? 2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)
13.1315	RI=1361.1, 23.4092 min FAH388 (ID#:FAH388-N1012)
13.3121	?? RI=1450.2, 12.8019 min AKS1975 (ID#:AKS1975-N1058)
13.3658	? 4 - hydroxy - benzaldehyde (ID#:FAH375-N1042)
13.4209	? 1,4 - dihydroxybenzene (hydroquinone) (ID#:TVL0020-N1048)
13.5308	4 - methyl - catechol (ID#:TVL0017-N1052)
13.5914	? 2 - hydroxypropanoic acid (lactic acid) (ID#:FAH0040-N1008)
13.7011	?? Oxalic acid (ID#:FAH957-N1038)
13.7531	RI=1399.2, 12.0214 min AKS1975 (ID#:AKS1975-N1056)
14.1500	? RI=1424.3, 24.8188 min FAH0040 (ID#:FAH0040-N1034)
14.3111	3 - hydroxy - 2 - hydroxymethyl - 2 - cyclopenten - 1 - one (ID#:FAH0040-N1038)
14.3409	4 - vinylguaiacol (ID#:OAB466~1-N1006)
14.3492	2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)
14.4448	? RI=1442.2, 12.6794 min AKS1976 (ID#:AKS1976-N1140)
14.5534	? RI=1450.2, 12.8019 min AKS1975 (ID#:AKS1975-N1058)
14.6923	RI=1454.5, 25.3715 min TVL0017 (ID#:TVL0017-N1060)
14.7678	? RI=1464.2, 13.0157 min AKS1975 (ID#:AKS1975-N1060)
14.9477	? RI=1475.3, 13.1862 min AKS1976 (ID#:AKS1976-N1138)
14.9887	3,5 - dihydroxy - 2 - methyl - 4H - pyran-4-one (ID#:FAH0040-N1042)
15.0855	? Oxalic acid (ID#:FAH957-N1038)
15.2582	RI=1490.9, 26.0371 min TVL0020 (ID#:TVL0020-N1066)
15.4876	? RI=1510.6, 13.7245 min AKS1975 (ID#:AKS1975-N1044)

15.8996	1,2,3 - trihydroxybenzene (ID#:FAH0040-N1050)
16.2079	? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
16.4035	?? 4-Hydroxyphenylethanol (ID#:FAH956~1-N1048)
16.4787	RI=1578.7, 27.3745 min FAH388 (ID#:FAH388-N1032)
16.7281	2 - hydroxymethyl - 5 - hydroxy - 2,3 - dihydro - (4H) - pyran - 4 - one (ID#:FAH0040-N1056)
16.7619	? 4 - vinylsyringol (ID#:P_E_W_S7)
16.8052	1,2,4 - trihydroxybenzene (ID#:FAH0040-N1058)
16.9325	?? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
17.1496	1,6 - anhydro - b - D - glucopyranose (levoglucosane - 2TMS) (ID#:FAH0040-N1060)
17.2274	? 3 - hydroxy - benzoic acid (ID#:FAH956~1-N1050)
17.2498	?? RI=1626.4, 15.4682 min AKS1975 (ID#:AKS1975-N1038)
17.2917	?? 2 - hydroxypropenoic acid (pyruvic acid) (ID#:TVL0020-N1018)
17.3333	?? RI=1687.4, 16.3403 min AKS1976 (ID#:AKS1976-N1128)
17.3805	RI=1636.6, 15.6135 min AKS1975 (ID#:AKS1975-N1068)
17.4274	RI=1640.3, 15.6669 min AKS1975 (ID#:AKS1975-N1036)
17.5194	? RI=1439.7, 25.0999 min TVL0017 (ID#:TVL0017-N1054)
17.5977	RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)
17.6630	Arabinose (MEOX/TMS) (ID#:FAH957-N1004)
17.6956	RI=1658.1, 15.9216 min AKS1975 (ID#:AKS1975-N1034)
17.8685	? 1,4 - anhydro - b - D - glucopyranose (ID#:FAH0040-N1068)
17.9026	RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)
17.9079	? RI=1667.9, 28.8525 min FAH388 (ID#:FAH388-N1040)
17.9079	RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)
18.1229	?? RI=1687.4, 16.3403 min AKS1976 (ID#:AKS1976-N1128)

18.2453	1,6 - anhydro - b - D - glucopyranose (levoglucosane - 3TMS) (ID#:FAH0040-N1064)
18.2506	1,6 -anhydro - D - galactopyranose (ID#:FAH0040-N1062)
18.2537	?? 2,3,5 - trihyddroxy - 4H - pyran - 4 - one (ID#:OAB467~1-N1066)
18.2855	RI=1705.8, 16.4992 min FAH1972 (ID#:FAH197~1-N1010)
18.4081	? 1,4 - anhydro - b - D - glucopyranose (ID#:FAH0040-N1068)
18.4333	RI=1710.3, 16.6591 min AKS1975 (ID#:AKS1975-N1032)
18.4758	? RI=1716.8, 16.7466 min AKS1974 (ID#:AKS1974-N1042)
18.7506	?? 1,6 - anhydro - b - D - glucofuranose (ID#:FAH0040-N1070)
19.1279	?? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
19.7132	?? RI=1796.1, 17.8199 min AKS1976 (ID#:AKS1976-N1110)
19.7674	? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
19.8445	3,4 - dihydroxy - benzoic acid, (ID#:NA)
20.3128	? RI=1851.2, 18.5346 min AKS1976 (ID#:AKS1976-N1102)
20.4519	RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)
20.7568	?? RI=1685.6, 16.3146 min AKS1974 (ID#:AKS1974-N1044)
20.7883	? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
20.8419	syringic acid (ID#:Py_E_W_S4)
21.1111	Ferulic acid (trans) (ID#:MMA670-N1022)
21.2830	?? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)
21.5675	? RI=1951.1, 19.8270 min AKS1975 (ID#:AKS1975-N1002)
21.5738	RI=1951.1, 19.8270 min AKS1975 (ID#:AKS1975-N1002)
21.6487	? RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)
21.8104	? RI=1636.1, 28.5242 min TVL0020 (ID#:TVL0020-N1076)
21.8894	?? RI=1808.3, 17.8578 min FAH1972 (ID#:FAH197~1-N1016)

21.9838	?? RI=1980.9, 20.2130 min AKS1975 (ID#:AKS1975-N1030)
22.0552	RI=1985.9, 20.2770 min AKS1975 (ID#:AKS1975-N1028)
22.0628	RI=2005.9, 20.5364 min AKS1975 (ID#:AKS1975-N1026)
22.3175	RI=2005.9, 20.5364 min AKS1975 (ID#:AKS1975-N1026)
22.4352	?? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)
22.5045	RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)
22.6721	RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)
22.6784	RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)
22.7021	palmitic acid (ID#:MMA671-N1042)
22.7094	? palmitic acid (ID#:MMA671-N1042)
22.7798	RI=2041.4, 20.9961 min AKS1975 (ID#:AKS1975-N1020)
22.9178	RI=2052.4, 21.1375 min AKS1975 (ID#:AKS1975-N1018)
22.9583	?? RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)
23.2269	Ferulic acid (trans) (ID#:MMA670-N1022)
23.3961	? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)
23.6994	RI=2096.3, 21.7057 min AKS1975 (ID#:AKS1975-N1014)
23.7383	Caffeic acid (ID#:FAH383-N1028)
24.0890	RI=2142.6, 22.3047 min AKS1975 (ID#:AKS1975-N1006)
24.1879	?? RI=1966.6, 20.0279 min AKS1976 (ID#:AKS1976-N1092)
24.3440	?? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)
24.5184	?? Heneicosane (IS) (ID#:629-94-7)
24.9529	RI=2208.9, 23.1630 min AKS1975 (ID#:AKS1975-N1004)
25.6070	?? Heneicosane (IS) (ID#:629-94-7)
26.2056	? 2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)
26.3952	? 2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)

26.5399	dehydroabietic acid (ID#:MMA671-N1038)
26.6508	?? Heneicosane (IS) (ID#:629-94-7)
27.6545	? Heneicosane (IS) (ID#:629-94-7)
28.6273	? Heneicosane (IS) (ID#:629-94-7)
28.8672	RI=2510.2, 27.0619 min AKS1976 (ID#:AKS1976-N1076)
29.5620	? Heneicosane (IS) (ID#:629-94-7)
30.4667	Heneicosane (IS) (ID#:629-94-7)
30.4718	? Heneicosane (IS) (ID#:629-94-7)
31.3422	? Heneicosane (IS) (ID#:629-94-7)
31.3474	? Heneicosane (IS) (ID#:629-94-7)
32.1878	?? Heneicosane (IS) (ID#:629-94-7)
32.1932	? Heneicosane (IS) (ID#:629-94-7)
33.0156	?? Heneicosane (IS) (ID#:629-94-7)

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=4.1.

Background (low vs. high retention time):

median low RT S/N=47, high RT S/N=92

Solvent Tailing (m/z 84). Run begins at 5.00 min. Solvent falls below:

S/N=2 before run

S/N=1 at 5.07 min.

Column Bleed (m/z 207):

median low RT S/N=5, high RT S/N=22

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