

## AMDIS GC/MS Analysis Report

Data: AKS2328.RAW

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

Number of Identifications: 148

<u>RT(min)</u>	<u>Chemical Name</u>
5.6994	? reagent artefact_1 (ID#:FAH348-N1002)
5.7156	?? alfa - hydroxyisobutyric acid (ID#:FAH383-N1002)
5.8297	RI=959.7, 14.1197 min FAH388 (ID#:FAH388-N1048)
6.0708	RI=795.7, 11.2931 min OAB4671 (ID#:OAB467~1-N1002)
6.2042	contaminant_silanol (ID#:TVL0020-N1008)
6.2376	? 1,2 - dihydroxyethane (ID#:FAH0040-N1002)
6.3414	? reagent artefact_4 (ID#:FAH360-N1008)
6.3475	? reagent artefact_4 (ID#:FAH360-N1008)
6.4979	? Oxalic acid (ID#:FAH957-N1038)
6.6220	contaminant_silanol (ID#:TVL0020-N1010)
6.7804	? reagent artefact_5 (ID#:FAH360-N1010)
6.8298	? Oxalic acid (ID#:FAH957-N1038)
7.0807	?? Oxalic acid (ID#:FAH957-N1038)
7.0876	?? Oxalic acid (ID#:FAH957-N1038)
7.1531	contaminant_silanol (ID#:TVL0020-N1016)
7.2651	?? Oxalic acid (ID#:FAH957-N1038)
7.4672	?? Oxalic acid (ID#:FAH957-N1038)
7.4937	contaminant_silanol (ID#:TVL0020-N1012)

7.5391	phenol (ID#:TVL0020-N1014)
7.6029	2 - hydroxypropanoic acid (lactic acid) (ID#:FAH0040-N1008)
7.9081	reagent artefact_9 (ID#:FAH360-N1016)
7.9154	? hydroxyacetic acid (glycolic acid) (ID#:FAH0040-N1004)
7.9154	? reagent artefact_9 (ID#:FAH360-N1016)
7.9967	? 2 - hydroxypropenoic acid (pyruvic acid) (ID#:TVL0020-N1018)
8.4173	?? Oxalic acid (ID#:FAH957-N1038)
8.5659	? 2 - hydroxypropenoic acid (pyruvic acid) (ID#:TVL0020-N1018)
8.7253	propanal_artifact (ID#:FAH0040-N1006)
8.9333	RI=1124.1, 7.4028 min AKS1974 (ID#:AKS1974-N1054)
9.0411	?? furan-2-carboxylic acid (ID#:FAH388-N1010)
9.1757	RI=1136.8, 7.6203 min AKS1976 (ID#:AKS1976-N1156)
9.3797	?? C1 - phenol_I3 (ID#:TVL0020-N1024)
9.5560	? reagent artefact_11 (ID#:FAH360-N1020)
9.6122	contaminant (ID#:FAH1384-N1014)
10.0241	?? Threonic acid (ID#:FAH957-N1024)
10.3267	?? contaminant (ID#:FAH1384-N1014)
10.5909	? RI=1214.9, 20.4578 min FAH388 (ID#:FAH388-N1014)
10.6385	RI=1218.7, 9.0147 min AKS1976 (ID#:AKS1976-N1154)
10.7218	guaiacol (ID#:OAB466~1-N1002)
10.9651	? RI=1256.0, 21.1538 min FAH0040 (ID#:FAH0040-N1020)
11.0885	RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
11.4602	RI=1272.7, 9.9318 min AKS1975 (ID#:AKS1975-N1052)
11.4870	?? 2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)
11.5122	? glycerol (ID#:TVL0020-N1040)

11.6710	4 - vinyl - phenol (ID#:TVL0020-N1042)
11.7659	RI=1282.8, 10.1027 min AKS1976 (ID#:AKS1976-N1148)
12.0283	?? Oxalic acid (ID#:FAH957-N1038)
12.5266	?? RI=1325.4, 22.9173 min TVL0020 (ID#:TVL0020-N1044)
12.9434	?? 2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)
13.0907	? RI=1361.1, 23.4092 min FAH388 (ID#:FAH388-N1012)
13.2091	?? Oxalic acid (ID#:FAH957-N1038)
13.3787	? 1,3 - dihydroxybenzene (resorcinol) (ID#:TVL0017-N1046)
13.4906	4 - methyl - catechol (ID#:TVL0017-N1052)
14.1097	RI=1424.3, 24.8188 min FAH0040 (ID#:FAH0040-N1034)
14.2708	3 - hydroxy - 2 - hydroxymethyl - 2 - cyclopenten - 1 - one (ID#:FAH0040-N1038)
14.3000	4 - vinylguaiacol (ID#:OAB466~1-N1006)
14.3091	2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)
14.4023	RI=1442.2, 12.6794 min AKS1976 (ID#:AKS1976-N1140)
14.5130	? RI=1450.2, 12.8019 min AKS1975 (ID#:AKS1975-N1058)
14.6526	? RI=1454.5, 25.3715 min TVL0017 (ID#:TVL0017-N1060)
14.7285	RI=1464.2, 13.0157 min AKS1975 (ID#:AKS1975-N1060)
14.9078	?? RI=1475.3, 13.1862 min AKS1976 (ID#:AKS1976-N1138)
14.9473	3,5 - dihydroxy - 2 - methyl - 4H - pyran-4-one (ID#:FAH0040-N1042)
15.0457	?? Malic acid (ID#:38166-11-9)
15.2176	RI=1490.9, 26.0371 min TVL0020 (ID#:TVL0020-N1066)
15.4471	? RI=1510.6, 13.7245 min AKS1975 (ID#:AKS1975-N1044)
15.8560	1,2,3 - trihydroxybenzene (ID#:FAH0040-N1050)
16.1637	? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)

16.1678	? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
16.3576	? 4-Hydroxyphenylethanol (ID#:FAH956~1-N1048)
16.4346	RI=1578.7, 27.3745 min FAH388 (ID#:FAH388-N1032)
16.5738	? RI=1578.7, 27.3745 min FAH388 (ID#:FAH388-N1032)
16.6805	2 - hydroxymethyl - 5 - hydroxy - 2,3 - dihydro - (4H) - pyran - 4 - one ( ID#:FAH0040-N1056)
16.7179	4 - vinylsyringol (ID#:P_E_W_S7)
16.7620	1,2,4 - trihydroxybenzene (ID#:FAH0040-N1058)
17.1036	?? 1,6 - anhydro - b - D - glucopyranose (levoglucosane - 2TMS) ( ID#:FAH0040-N1060)
17.1837	? 3 - hydroxy - benzoic acid (ID#:FAH956~1-N1050)
17.3370	RI=1636.6, 15.6135 min AKS1975 (ID#:AKS1975-N1068)
17.3828	RI=1640.3, 15.6669 min AKS1975 (ID#:AKS1975-N1036)
17.4752	? RI=1439.7, 25.0999 min TVL0017 (ID#:TVL0017-N1054)
17.5534	RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)
17.6172	Arabinose (MEOX/TMS) (ID#:FAH957-N1004)
17.6520	RI=1658.1, 15.9216 min AKS1975 (ID#:AKS1975-N1034)
17.8214	? 1,4 - anhydro - b - D - glucopyranose (ID#:FAH0040-N1068)
17.8575	RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)
17.8626	RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)
18.0783	?? RI=1687.4, 16.3403 min AKS1976 (ID#:AKS1976-N1128)
18.2008	1,6 -anhydro - D - galactopyranose (ID#:FAH0040-N1062)
18.2008	? 1,6 - anhydro - b - D - glucopyranose (levoglucosane - 3TMS) ( ID#:FAH0040-N1064)
18.2069	? 1,6 - anhydro - b - D - glucopyranose (levoglucosane - 3TMS) ( ID#:FAH0040-N1064)
18.2129	2,3,5 - trihyddroxy - 4H - pyran - 4 - one (ID#:OAB467~1-N1066)

18.2417	RI=1705.8, 16.4992 min FAH1972 (ID#:FAH197~1-N1010)
18.3620	? 1,4 - anhydro - b - D - glucopyranose (ID#:FAH0040-N1068)
18.3884	RI=1710.3, 16.6591 min AKS1975 (ID#:AKS1975-N1032)
18.4272	? RI=1716.8, 16.7466 min AKS1974 (ID#:AKS1974-N1042)
18.4880	RI=1716.8, 16.7466 min AKS1974 (ID#:AKS1974-N1042)
18.7026	? 1,6 - anhydro - b - D - glucofuranose (ID#:FAH0040-N1070)
18.9725	?? RI=1710.1, 16.6563 min AKS1976 (ID#:AKS1976-N1126)
19.0857	?? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
19.4327	? contaminant - terephthalic acid (ID#:FAH348-N1030)
19.4805	?? RI=1777.9, 17.5729 min FAH1972 (ID#:FAH1972-N1004)
19.6622	? RI=1796.1, 17.8199 min AKS1976 (ID#:AKS1976-N1110)
19.7188	? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
19.7802	dihydroconiferyl alcohol (ID#:OAB466~1-N1025)
19.7983	3,4 - dihydroxy - benzoic acid, (ID#:NA)
20.2657	RI=1851.2, 18.5346 min AKS1976 (ID#:AKS1976-N1102)
20.4034	RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)
20.7950	syringic acid (ID#:Py_E_W_S4)
21.0633	Ferulic acid (trans) (ID#:MMA670-N1022)
21.3575	p - coumaric acid (ID#:MMA670-N1024)
21.5219	RI=1951.1, 19.8270 min AKS1975 (ID#:AKS1975-N1002)
21.5292	? RI=1951.1, 19.8270 min AKS1975 (ID#:AKS1975-N1002)
21.5969	?? RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)
21.7624	? RI=1685.6, 16.3146 min AKS1974 (ID#:AKS1974-N1044)
21.9339	?? RI=1980.9, 20.2130 min AKS1975 (ID#:AKS1975-N1030)
22.0086	RI=2005.9, 20.5364 min AKS1975 (ID#:AKS1975-N1026)

22.2666	RI=2005.9, 20.5364 min AKS1975 (ID#:AKS1975-N1026)
22.3836	? RI=1394.6, 11.9462 min AKS1976 (ID#:AKS1976-N1142)
22.4569	RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)
22.6159	? RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)
22.6242	RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)
22.6494	? palmitic acid (ID#:MMA671-N1042)
22.6555	palmitic acid (ID#:MMA671-N1042)
22.7293	RI=2041.4, 20.9961 min AKS1975 (ID#:AKS1975-N1020)
22.8709	RI=2052.4, 21.1375 min AKS1975 (ID#:AKS1975-N1018)
23.0654	? synapyl alcohol (trans) (ID#:Py_E_W_S1)
23.1750	Ferulic acid (trans) (ID#:MMA670-N1022)
23.3434	? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)
23.5968	? RI=2108.4, 21.8630 min AKS1975 (ID#:AKS1975-N1012)
23.6886	Caffeic acid (ID#:FAH383-N1028)
24.0362	RI=2142.6, 22.3047 min AKS1975 (ID#:AKS1975-N1006)
24.1340	? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)
24.8982	RI=2208.9, 23.1630 min AKS1975 (ID#:AKS1975-N1004)
24.9062	?? RI=2208.9, 23.1630 min AKS1975 (ID#:AKS1975-N1004)
25.5497	?? Heneicosane (IS) (ID#:629-94-7)
26.3596	? RI=1636.1, 28.5242 min TVL0020 (ID#:TVL0020-N1076)
26.4843	dehydroabietic acid (ID#:MMA671-N1038)
26.5946	? Heneicosane (IS) (ID#:629-94-7)
27.5997	? Heneicosane (IS) (ID#:629-94-7)
27.8992	?? RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)
28.5678	? Heneicosane (IS) (ID#:629-94-7)

28.8095	RI=2510.2, 27.0619 min AKS1976 (ID#:AKS1976-N1076)
29.5018	Heneicosane (IS) (ID#:629-94-7)
30.4049	? Heneicosane (IS) (ID#:629-94-7)
31.2828	Heneicosane (IS) (ID#:629-94-7)
31.2871	? Heneicosane (IS) (ID#:629-94-7)
32.1341	Heneicosane (IS) (ID#:629-94-7)
32.9592	?? Heneicosane (IS) (ID#:629-94-7)
32.9634	?? 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=4.4.

Background (low vs. high retention time):

median low RT S/N=44, high RT S/N=90

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

S/N=1 before run

Column Bleed (m/z 207):

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

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