

## AMDIS GC/MS Analysis Report

Data: AKS2329.RAW

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

Number of Identifications: 114

<u>RT(min)</u>	<u>Chemical Name</u>
5.7219	?? Oxalic acid (ID#:FAH957-N1038)
5.8399	RI=959.7, 14.1197 min FAH388 (ID#:FAH388-N1048)
6.0911	?? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)
6.2511	?? Oxalic acid (ID#:FAH957-N1038)
6.3542	? reagent artefact_4 (ID#:FAH360-N1008)
6.3641	? reagent artefact_4 (ID#:FAH360-N1008)
6.5086	? Oxalic acid (ID#:FAH957-N1038)
6.7982	? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)
7.2644	?? Oxalic acid (ID#:FAH957-N1038)
7.2743	?? Oxalic acid (ID#:FAH957-N1038)
7.2803	?? Oxalic acid (ID#:FAH957-N1038)
7.5534	? phenol (ID#:TVL0020-N1014)
7.5534	?? 3 - hydroxy - (4H) - pyran - 4 - one (ID#:FAH0040-N1014)
7.6143	2 - hydroxypropanoic acid (lactic acid) (ID#:FAH0040-N1008)
7.9312	? hydroxyacetic acid (glycolic acid) (ID#:FAH0040-N1004)
8.0154	? 2 - hydroxypropenoic acid (pyruvic acid) (ID#:TVL0020-N1018)
8.4198	? Oxalic acid (ID#:FAH957-N1038)
8.5774	? 2 - hydroxypropenoic acid (pyruvic acid) (ID#:TVL0020-N1018)

8.9392	RI=1124.1, 7.4028 min AKS1974 (ID#:AKS1974-N1054)
9.1121	? 3 - hydroxy - pyridine (ID#:FAH388-N1008)
9.1873	RI=1136.8, 7.6203 min AKS1976 (ID#:AKS1976-N1156)
9.3906	?? C1 - phenol_l3 (ID#:TVL0020-N1024)
9.5010	?? Oxalic acid (ID#:FAH957-N1038)
9.5010	?? 4-Hydroxybutanoic acid (GHB) (ID#:FAH956~1-N1046)
9.6218	contaminant (ID#:FAH1384-N1014)
10.2615	? phenol (ID#:TVL0020-N1014)
10.6476	RI=1218.7, 9.0147 min AKS1976 (ID#:AKS1976-N1154)
10.7313	guaiacol (ID#:OAB466~1-N1002)
11.4728	RI=1272.7, 9.9318 min AKS1975 (ID#:AKS1975-N1052)
11.5200	?? glycerol (ID#:TVL0020-N1040)
11.6810	4 - vinyl - phenol (ID#:TVL0020-N1042)
12.2802	? 1,2 - dihydroxybenzene (catechol) (ID#:OAB467~1-N1028)
12.9473	?? 2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)
13.0980	? RI=1361.1, 23.4092 min FAH388 (ID#:FAH388-N1012)
13.3831	? 1,4 - dihydroxybenzene (hydroquinone) (ID#:TVL0020-N1048)
13.4974	?? 4 - methyl - catechol (ID#:TVL0017-N1052)
13.7193	? RI=1399.2, 12.0214 min AKS1975 (ID#:AKS1975-N1056)
14.2763	3 - hydroxy - 2 - hydroxymethyl - 2 - cyclopenten - 1 - one (ID#:FAH0040-N1038)
14.3048	4 - vinylguaiacol (ID#:OAB466~1-N1006)
14.4068	RI=1442.2, 12.6794 min AKS1976 (ID#:AKS1976-N1140)
14.5177	? RI=1450.2, 12.8019 min AKS1975 (ID#:AKS1975-N1058)
14.6724	?? 1,3 - dihydroxybenzene (resorcinol) (ID#:TVL0017-N1046)

14.7346	?? RI=1464.2, 13.0157 min AKS1975 (ID#:AKS1975-N1060)
14.9127	? RI=1475.3, 13.1862 min AKS1976 (ID#:AKS1976-N1138)
14.9502	3,5 - dihydroxy - 2 - methyl - 4H - pyran-4-one (ID#:FAH0040-N1042)
15.0535	?? Malic acid (ID#:38166-11-9)
15.4617	?? 1,3 - dihydroxybenzene (resorcinol) (ID#:TVL0017-N1046)
15.8580	1,2,3 - trihydroxybenzene (ID#:FAH0040-N1050)
16.1685	?? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)
16.4042	? 1,6 - anhydro - D - galactopyranose (2TMS) (ID#:FAH0040-N1054)
16.4391	RI=1578.7, 27.3745 min FAH388 (ID#:FAH388-N1032)
16.4799	? RI=1576.1, 27.3294 min FAH388 (ID#:FAH388-N1030)
16.6852	? 2 - hydroxymethyl - 5 - hydroxy - 2,3 - dihydro - (4H) - pyran - 4 - one (ID#:FAH0040-N1056)
16.7191	4 - vinylsyringol (ID#:P_E_W_S7)
16.7623	1,2,4 - trihydroxybenzene (ID#:FAH0040-N1058)
16.9685	? RI=1399.2, 12.0214 min AKS1975 (ID#:AKS1975-N1056)
17.1091	? 1,6 - anhydro - b - D - glucopyranose (levoglucosane - 2TMS) (ID#:FAH0040-N1060)
17.1855	? 3 - hydroxy - benzoic acid (ID#:FAH956~1-N1050)
17.3393	RI=1636.6, 15.6135 min AKS1975 (ID#:AKS1975-N1068)
17.3865	RI=1640.3, 15.6669 min AKS1975 (ID#:AKS1975-N1036)
17.4792	? RI=1439.7, 25.0999 min TVL0017 (ID#:TVL0017-N1054)
17.6208	Arabinose (MEOX/TMS) (ID#:FAH957-N1004)
17.6552	RI=1658.1, 15.9216 min AKS1975 (ID#:AKS1975-N1034)
17.8237	? 1,4 - anhydro - b - D - glucopyranose (ID#:FAH0040-N1068)
17.8636	RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)
18.0818	?? RI=1687.4, 16.3403 min AKS1976 (ID#:AKS1976-N1128)

18.2036        ?? 1,6 -anhydro - D - galactopyranose (ID#:FAH0040-N1062)

18.2036        1,6 - anhydro - b - D - glucopyranose (levoglucosane - 3TMS) (ID#:FAH0040-N1064)

18.2077        1,6 -anhydro - D - galactopyranose (ID#:FAH0040-N1062)

18.3628        ? 1,4 - anhydro - b - D - glucopyranose (ID#:FAH0040-N1068)

18.3924        RI=1710.3, 16.6591 min AKS1975 (ID#:AKS1975-N1032)

18.7066        1,6 - anhydro - b - D - glucofuranose (ID#:FAH0040-N1070)

18.8262        ?? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)

18.9779        ? RI=1710.1, 16.6563 min AKS1976 (ID#:AKS1976-N1126)

19.0849        ?? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)

19.4172        p - coumaric acid (ID#:MMA670-N1024)

19.5596        RI=1796.1, 17.8199 min AKS1976 (ID#:AKS1976-N1110)

19.6672        ? RI=1804.1, 17.9255 min AKS1976 (ID#:AKS1976-N1106)

19.7246        RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)

19.7827        dihydroconiferyl alcohol (ID#:OAB466~1-N1025)

20.0935        ?? 1,6 - anhydro - b - D - glucopyranose (levoglucosane - 2TMS) (ID#:FAH0040-N1060)

20.0935        ? RI=1793.3, 17.7820 min AKS1976 (ID#:AKS1976-N1112)

20.2682        RI=1851.2, 18.5346 min AKS1976 (ID#:AKS1976-N1102)

20.4069        RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)

20.7130        ? RI=1685.6, 16.3146 min AKS1974 (ID#:AKS1974-N1044)

20.8992        RI=1636.1, 28.5242 min TVL0020 (ID#:TVL0020-N1076)

21.5255        RI=1951.1, 19.8270 min AKS1975 (ID#:AKS1975-N1002)

21.7658        ? RI=1966.6, 20.0279 min AKS1976 (ID#:AKS1976-N1092)

22.0117        RI=1985.9, 20.2770 min AKS1975 (ID#:AKS1975-N1028)

22.2687        RI=1985.9, 20.2770 min AKS1975 (ID#:AKS1975-N1028)

22.3866        ?? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)

22.4573        RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)

22.6258        RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)

22.6565        palmitic acid (ID#:MMA671-N1042)

22.7309        RI=2041.4, 20.9961 min AKS1975 (ID#:AKS1975-N1020)

22.9091        ?? RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)

23.0677        ? synapyl alcohol (cis) (ID#:Py\_E\_W\_S3)

23.1201        ?? RI=2070.2, 21.3687 min AKS1974 (ID#:AKS1974-N1022)

23.1767        Ferulic acid (trans) (ID#:MMA670-N1022)

23.3458        ? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)

23.6915        ? Caffeic acid (ID#:FAH383-N1028)

24.9018        RI=2208.9, 23.1630 min AKS1975 (ID#:AKS1975-N1004)

26.3640        ?? RI=1702.7, 29.6148 min TVL0020 (ID#:TVL0020-N1078)

26.4891        ? dehydroabietic acid (ID#:MMA671-N1038)

26.5980        ? Heneicosane (IS) (ID#:629-94-7)

27.6056        ?? Heneicosane (IS) (ID#:629-94-7)

27.9027        ?? RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)

28.5715        ? Heneicosane (IS) (ID#:629-94-7)

28.8152        RI=2510.2, 27.0619 min AKS1976 (ID#:AKS1976-N1076)

29.5061        ? Heneicosane (IS) (ID#:629-94-7)

30.4063        Heneicosane (IS) (ID#:629-94-7)

31.2855        Heneicosane (IS) (ID#:629-94-7)

32.1347        ? Heneicosane (IS) (ID#:629-94-7)

32.9630        ?? 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=3.5.

Background (low vs. high retention time):

median low RT S/N=43, high RT S/N=101

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

S/N=2 before run

S/N=1 at 5.06 min.

Column Bleed (m/z 207):

median low RT S/N=5, high RT S/N=25

This report consists of 6 pages