

AMDIS GC/MS Analysis Report

Data: AKS2320.RAW

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

Number of Identifications: 128

<u>RT(min)</u>	<u>Chemical Name</u>
5.7784	reagent artefact_1 (ID#:FAH348-N1002)
5.8656	hydrogen sulfide (ID#:TVL0020-N1002)
5.9177	RI=959.7, 14.1197 min FAH388 (ID#:FAH388-N1048)
6.1455	RI=795.7, 11.2931 min OAB4671 (ID#:OAB467~1-N1002)
6.1526	?? RI=795.7, 11.2931 min OAB4671 (ID#:OAB467~1-N1002)
6.2396	?? contaminant_silanol (ID#:TVL0020-N1010)
6.2849	contaminant_silanol (ID#:TVL0020-N1008)
6.3141	1,2 - dihydroxyethane (ID#:FAH0040-N1002)
6.3141	?? Oxalic acid (ID#:FAH957-N1038)
6.4282	? reagent artefact_4 (ID#:FAH360-N1008)
6.8467	reagent artefact_5 (ID#:FAH360-N1010)
7.0683	reagent artefact_7 (ID#:FAH360-N1012)
7.1533	?? Oxalic acid (ID#:FAH957-N1038)
7.2190	contaminant_silanol (ID#:TVL0020-N1016)
7.3333	?? Oxalic acid (ID#:FAH957-N1038)
7.5243	? Oxalic acid (ID#:FAH957-N1038)
7.5583	? contaminant_silanol (ID#:TVL0020-N1016)
7.5943	reagent artefact_8 (ID#:FAH360-N1014)

7.6606	2 - hydroxypropanoic acid (lactic acid) (ID#:FAH0040-N1008)
7.6645	2 - hydroxypropanoic acid (lactic acid) (ID#:FAH0040-N1008)
7.9678	? reagent artefact_9 (ID#:FAH360-N1016)
7.9719	? hydroxyacetic acid (glycolic acid) (ID#:FAH0040-N1004)
7.9719	? reagent artefact_9 (ID#:FAH360-N1016)
8.4706	?? Oxalic acid (ID#:FAH957-N1038)
8.6394	?? reagent artefact_10 (ID#:FAH360-N1018)
8.7450	? RI=1112.0, 7.1969 min AKS1974 (ID#:AKS1974-N1056)
8.7784	? propanal_artifact (ID#:FAH0040-N1006)
8.9854	RI=1124.1, 7.4028 min AKS1974 (ID#:AKS1974-N1054)
9.2323	RI=1136.8, 7.6203 min AKS1976 (ID#:AKS1976-N1156)
9.6133	? reagent artefact_11 (ID#:FAH360-N1020)
9.6695	contaminant (ID#:FAH1384-N1014)
10.1932	? reagent artefact_12 (ID#:FAH360-N1022)
10.2973	? 3 - hydroxy - (4H) - pyran - 4 - one (ID#:FAH0040-N1014)
10.3832	? contaminant (ID#:FAH1384-N1014)
10.6491	? RI=1214.9, 20.4578 min FAH388 (ID#:FAH388-N1014)
10.6958	? RI=1218.7, 9.0147 min AKS1976 (ID#:AKS1976-N1154)
10.7797	?? guaiacol (ID#:OAB466~1-N1002)
11.0198	? RI=1256.0, 21.1538 min FAH0040 (ID#:FAH0040-N1020)
11.1700	Benzoic acid (ID#:FAH1388-N1004)
11.5151	RI=1272.7, 9.9318 min AKS1975 (ID#:AKS1975-N1052)
11.5693	glycerol (ID#:TVL0020-N1040)
11.7325	4 - vinyl - phenol (ID#:TVL0020-N1042)
11.8219	RI=1282.8, 10.1027 min AKS1976 (ID#:AKS1976-N1148)

12.2906	? Succinic acid (ID#:40309-57-7)
12.5322	?? Glyceric acid (ID#:38191-87-6)
12.5834	?? RI=1325.4, 22.9173 min TVL0020 (ID#:TVL0020-N1044)
12.7130	RI=1337.2, 11.0052 min AKS1975 (ID#:AKS1975-N1054)
13.1475	? RI=1361.1, 23.4092 min FAH388 (ID#:FAH388-N1012)
13.2731	?? 2 - hydroxypropenoic acid (pyruvic acid) (ID#:TVL0020-N1018)
13.6106	? 2 - hydroxypropanoic acid (lactic acid) (ID#:FAH0040-N1008)
13.7173	?? RI=1394.6, 11.9462 min AKS1976 (ID#:AKS1976-N1142)
13.8133	?? 4-Hydroxybutanoic acid (GHB) (ID#:FAH956~1-N1046)
13.9351	?? Succinic acid (ID#:40309-57-7)
14.1034	? reagent artefact_15_?_GOLM (ID#:FAH360-N1026)
14.2140	? RI=1427.6, 24.8786 min FAH0040 (ID#:FAH0040-N1036)
14.3268	3 - hydroxy - 2 - hydroxymethyl - 2 - cyclopenten - 1 - one (ID#:FAH0040-N1038)
14.3681	2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)
14.5499	?? RI=1445.0, 25.0173 min FAH388 (ID#:FAH388-N1018)
14.7081	? RI=1454.5, 25.3715 min TVL0017 (ID#:TVL0017-N1060)
14.7851	RI=1464.2, 13.0157 min AKS1975 (ID#:AKS1975-N1060)
14.9638	? RI=1475.3, 13.1862 min AKS1976 (ID#:AKS1976-N1138)
15.0058	3,5 - dihydroxy - 2 - methyl - 4H - pyran-4-one (ID#:FAH0040-N1042)
15.1043	Malic acid (ID#:38166-11-9)
15.5926	? 4 - hydroxyphenyl - acetonitrile (ID#:FAH388-N1020)
15.9151	1,2,3 - trihydroxybenzene (ID#:FAH0040-N1050)
16.1828	? RI=1554.5, 14.3961 min AKS1976 (ID#:AKS1976-N1136)
16.8221	1,2,4 - trihydroxybenzene (ID#:FAH0040-N1058)

17.0255 ? RI=1399.2, 12.0214 min AKS1975 (ID#:AKS1975-N1056)

17.4075 ?? RI=1424.3, 24.8188 min FAH0040 (ID#:FAH0040-N1034)

17.4417 ? RI=1640.3, 15.6669 min AKS1975 (ID#:AKS1975-N1036)

17.9216 ? RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)

18.2272 ? 2 - hydroxy - 1 methyl - 1 - cyclopentan - 3 - one (ID#:FAH0040-N1016)

18.2712 2,3,5 - trihyddroxy - 4H - pyran - 4 - one (ID#:OAB467~1-N1066)

18.4970 ?? RI=1713.1, 16.6971 min AKS1976 (ID#:AKS1976-N1124)

18.5456 ? RI=1716.8, 16.7466 min AKS1974 (ID#:AKS1974-N1042)

18.7267 ?? RI=1730.5, 16.9318 min AKS1976 (ID#:AKS1976-N1120)

19.1302 vanillic acid (ID#:TVL0020-N1082)

19.4903 contaminant - terephthalic acid (ID#:FAH348-N1030)

19.5711 ? RI=1793.3, 17.7820 min AKS1976 (ID#:AKS1976-N1112)

19.6112 ? RI=1804.1, 17.9255 min AKS1976 (ID#:AKS1976-N1106)

19.6183 RI=1804.1, 17.9255 min AKS1976 (ID#:AKS1976-N1106)

19.7248 RI=1804.1, 17.9255 min AKS1976 (ID#:AKS1976-N1106)

19.7885 ? RI=1808.8, 17.9859 min AKS1976 (ID#:AKS1976-N1104)

19.7885 ? RI=1796.1, 17.8199 min AKS1976 (ID#:AKS1976-N1110)

19.8571 3,4 - dihydroxy - benzoic acid, (ID#:NA)

20.1196 ?? 1,6 - anhydro - b - D - glucofuranose (ID#:FAH0040-N1070)

20.1513 ? RI=1793.3, 17.7820 min AKS1976 (ID#:AKS1976-N1112)

20.3226 RI=1851.2, 18.5346 min AKS1976 (ID#:AKS1976-N1102)

20.3279 RI=1851.2, 18.5346 min AKS1976 (ID#:AKS1976-N1102)

20.4652 RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)

20.7029 ? RI=1879.9, 18.9057 min AKS1976 (ID#:AKS1976-N1098)

20.7693 ? RI=1966.6, 20.0279 min AKS1976 (ID#:AKS1976-N1092)

20.8553 syringic acid (ID#:Py_E_W_S4)

20.9560 ? RI=1636.1, 28.5242 min TVL0020 (ID#:TVL0020-N1076)

21.3145 ? Glucose (MEOX/TMS) (ID#:FAH957-N1010)

21.5831 RI=1951.1, 19.8270 min AKS1975 (ID#:AKS1975-N1002)

21.7374 ?? RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)

21.8195 RI=1966.6, 20.0279 min AKS1976 (ID#:AKS1976-N1092)

21.8237 ?? RI=1884.7, 18.9674 min AKS1976 (ID#:AKS1976-N1162)

21.8237 RI=1966.6, 20.0279 min AKS1976 (ID#:AKS1976-N1092)

21.9481 ? RI=1975.6, 20.1437 min AKS1976 (ID#:AKS1976-N1088)

22.3269 RI=1985.9, 20.2770 min AKS1975 (ID#:AKS1975-N1028)

22.6840 ? RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)

22.7168 palmitic acid (ID#:MMA671-N1042)

22.7219 palmitic acid (ID#:MMA671-N1042)

22.8533 ?? RI=1955.3, 19.8813 min AKS1974 (ID#:AKS1974-N1028)

22.9708 ?? RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)

23.1327 ? synapyl alcohol (cis) (ID#:Py_E_W_S3)

23.1849 ? RI=2070.2, 21.3687 min AKS1974 (ID#:AKS1974-N1022)

24.9652 RI=2208.9, 23.1630 min AKS1975 (ID#:AKS1975-N1004)

26.6608 ? Heneicosane (IS) (ID#:629-94-7)

27.6674 Heneicosane (IS) (ID#:629-94-7)

27.6758 ?? Heneicosane (IS) (ID#:629-94-7)

27.7523 RI=2510.2, 27.0619 min AKS1976 (ID#:AKS1976-N1076)

27.9680 ?? RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)

28.4003 RI=2510.2, 27.0619 min AKS1976 (ID#:AKS1976-N1076)

28.6388	Heneicosane (IS) (ID#:629-94-7)
28.8778	RI=2510.2, 27.0619 min AKS1976 (ID#:AKS1976-N1076)
28.9576	? RI=2510.2, 27.0619 min AKS1976 (ID#:AKS1976-N1076)
29.5698	Heneicosane (IS) (ID#:629-94-7)
29.5761	? Heneicosane (IS) (ID#:629-94-7)
30.4754	Heneicosane (IS) (ID#:629-94-7)
30.4815	? Heneicosane (IS) (ID#:629-94-7)
31.3483	? Heneicosane (IS) (ID#:629-94-7)
31.3534	Heneicosane (IS) (ID#:629-94-7)
32.1999	? Heneicosane (IS) (ID#:629-94-7)
33.0209	? Heneicosane (IS) (ID#:629-94-7)
33.0272	?? 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=3.9.

Background (low vs. high retention time):

median low RT S/N=39, high RT S/N=103

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 5.44 min.

Column Bleed (m/z 207):

median low RT S/N=5, high RT S/N=23

This report consists of 6 pages