

## AMDIS GC/MS Analysis Report

Data: AKS2327.RAW

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

Number of Identifications: 144

| <u>RT(min)</u> | <u>Chemical Name</u>   |
|----------------|--|
| 5.7277         | reagent artefact_1 (ID#:FAH348-N1002)                          |
| 5.8591         | RI=959.7, 14.1197 min FAH388 (ID#:FAH388-N1048)                |
| 6.1031         | RI=795.7, 11.2931 min OAB4671 (ID#:OAB467~1-N1002)             |
| 6.2289         | contaminant_silanol (ID#:TVL0020-N1008)                        |
| 6.3717         | ? reagent artefact_4 (ID#:FAH360-N1008)                        |
| 6.3756         | ? reagent artefact_4 (ID#:FAH360-N1008)                        |
| 6.6521         | contaminant_silanol (ID#:TVL0020-N1010)                        |
| 6.8036         | ?? reagent artefact_5 (ID#:FAH360-N1010)                       |
| 6.9673         | ?? reagent artefact_5 (ID#:FAH360-N1010)                       |
| 7.1085         | ?? Oxalic acid (ID#:FAH957-N1038)                              |
| 7.1813         | contaminant_silanol (ID#:TVL0020-N1016)                        |
| 7.5243         | contaminant_silanol (ID#:TVL0020-N1012)                        |
| 7.5682         | phenol (ID#:TVL0020-N1014)                                     |
| 7.6315         | 2 - hydroxypropanoic acid (lactic acid) (ID#:FAH0040-N1008)    |
| 7.9407         | ? hydroxyacetic acid (glycolic acid) (ID#:FAH0040-N1004)       |
| 8.0286         | ? 2 - hydroxypropenoic acid (pyruvic acid) (ID#:TVL0020-N1018) |
| 8.1602         | ?? Oxalic acid (ID#:FAH957-N1038)                              |
| 8.4471         | ?? Oxalic acid (ID#:FAH957-N1038)                              |

8.5937 ? Oxalic acid (ID#:FAH957-N1038)

8.7552 propanal\_artifact (ID#:FAH0040-N1006)

8.9588 RI=1124.1, 7.4028 min AKS1974 (ID#:AKS1974-N1054)

9.0696 ?? furan-2-carboxylic acid (ID#:FAH388-N1010)

9.1291 ? 3 - hydroxy - pyridine (ID#:FAH388-N1008)

9.2055 RI=1136.8, 7.6203 min AKS1976 (ID#:AKS1976-N1156)

9.4084 ? C1 - phenol\_I3 (ID#:TVL0020-N1024)

9.6422 contaminant (ID#:FAH1384-N1014)

10.0554 ?? Glyceric acid (ID#:38191-87-6)

10.2702 ?? 3 - hydroxy - (4H) - pyran - 4 - one (ID#:FAH0040-N1014)

10.3562 ? contaminant (ID#:FAH1384-N1014)

10.6198 RI=1214.9, 20.4578 min FAH388 (ID#:FAH388-N1014)

10.6685 ? RI=1218.7, 9.0147 min AKS1976 (ID#:AKS1976-N1154)

10.7519 guaiacol (ID#:OAB466~1-N1002)

10.9970 ? RI=1256.0, 21.1538 min FAH0040 (ID#:FAH0040-N1020)

11.1201 RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)

11.1417 ?? Benzoic acid (ID#:FAH1388-N1004)

11.4920 RI=1272.7, 9.9318 min AKS1975 (ID#:AKS1975-N1052)

11.5433 ? glycerol (ID#:TVL0020-N1040)

11.7043 4 - vinyl - phenol (ID#:TVL0020-N1042)

11.7953 RI=1282.8, 10.1027 min AKS1976 (ID#:AKS1976-N1148)

12.0591 ? RI=1296.4, 10.3341 min AKS1976 (ID#:AKS1976-N1146)

12.2622 ? Succinic acid (ID#:40309-57-7)

12.5032 ?? Glyceric acid (ID#:38191-87-6)

12.5571 ?? RI=1325.4, 22.9173 min TVL0020 (ID#:TVL0020-N1044)

|         |   |
|---------|---|
| 12.6864 | ? RI=1337.2, 11.0052 min AKS1975 (ID#:AKS1975-N1054)                            |
| 12.8553 | ?? Oxalic acid (ID#:FAH957-N1038)   |
| 12.9729 | ?? 2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)             |
| 13.1233 | RI=1361.1, 23.4092 min FAH388 (ID#:FAH388-N1012)                                |
| 13.2373 | ?? Oxalic acid (ID#:FAH957-N1038)   |
| 13.3573 | ? 4 - hydroxy - benzaldehyde (ID#:FAH375-N1042)                                 |
| 13.4117 | ? 1,4 - dihydroxybenzene (hydroquinone) (ID#:TVL0020-N1048)                     |
| 13.5219 | 4 - methyl - catechol (ID#:TVL0017-N1052)                                       |
| 13.5815 | ? 2 - hydroxypropanoic acid (lactic acid) (ID#:FAH0040-N1008)                   |
| 13.6945 | ? RI=1394.6, 11.9462 min AKS1976 (ID#:AKS1976-N1142)                            |
| 13.7463 | RI=1399.2, 12.0214 min AKS1975 (ID#:AKS1975-N1056)                              |
| 14.0755 | ? reagent artefact_15_?_GOLM (ID#:FAH360-N1026)                                 |
| 14.3023 | 3 - hydroxy - 2 - hydroxymethyl - 2 - cyclopenten - 1 - one (ID#:FAH0040-N1038) |
| 14.3326 | 4 - vinylguaiaicol (ID#:OAB466~1-N1006)   |
| 14.3417 | 2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040)                |
| 14.4318 | ? RI=1442.2, 12.6794 min AKS1976 (ID#:AKS1976-N1140)                            |
| 14.5463 | RI=1450.2, 12.8019 min AKS1975 (ID#:AKS1975-N1058)                              |
| 14.6817 | RI=1454.5, 25.3715 min TVL0017 (ID#:TVL0017-N1060)                              |
| 14.7575 | RI=1464.2, 13.0157 min AKS1975 (ID#:AKS1975-N1060)                              |
| 14.9382 | ? RI=1475.3, 13.1862 min AKS1976 (ID#:AKS1976-N1138)                            |
| 14.9779 | 3,5 - dihydroxy - 2 - methyl - 4H - pyran-4-one (ID#:FAH0040-N1042)             |
| 15.0759 | Malic acid (ID#:38166-11-9)   |
| 15.2506 | RI=1490.9, 26.0371 min TVL0020 (ID#:TVL0020-N1066)                              |
| 15.4783 | RI=1510.6, 13.7245 min AKS1975 (ID#:AKS1975-N1044)                              |

|         |  |
|---------|--|
| 15.5637 | ? 4 - hydroxyphenyl - acetonitrile (ID#:FAH388-N1020)  |
| 15.8825 | ? 1,2,4 - trihydroxybenzene (ID#:FAH0040-N1058)  |
| 15.8879 | 1,2,3 - trihydroxybenzene (ID#:FAH0040-N1050)  |
| 16.1958 | ? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)  |
| 16.3910 | ? 4-Hydroxyphenylethanol (ID#:FAH956~1-N1048)  |
| 16.4656 | RI=1578.7, 27.3745 min FAH388 (ID#:FAH388-N1032)   |
| 16.7169 | 2 - hydroxymethyl - 5 - hydroxy - 2,3 - dihydro - (4H) - pyran - 4 - one (ID#:FAH0040-N1056) |
| 16.7499 | 4 - vinylsyringol (ID#:P_E_W_S7)   |
| 16.7937 | 1,2,4 - trihydroxybenzene (ID#:FAH0040-N1058)  |
| 16.9207 | ? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)  |
| 16.9976 | RI=1399.2, 12.0214 min AKS1975 (ID#:AKS1975-N1056)   |
| 17.1359 | ? 1,6 - anhydro - b - D - glucopyranose (levoglucosane - 2TMS) (ID#:FAH0040-N1060)           |
| 17.2145 | ? 3 - hydroxy - benzoic acid (ID#:FAH956~1-N1050)  |
| 17.2823 | ?? RI=1635.7, 15.5076 min FAH1972 (ID#:FAH197~1-N1002)                                       |
| 17.3672 | RI=1636.6, 15.6135 min AKS1975 (ID#:AKS1975-N1068)   |
| 17.4088 | RI=1640.3, 15.6669 min AKS1975 (ID#:AKS1975-N1036)   |
| 17.4139 | RI=1640.3, 15.6669 min AKS1975 (ID#:AKS1975-N1036)   |
| 17.5825 | RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)   |
| 17.6505 | Arabinose (MEOX/TMS) (ID#:FAH957-N1004)  |
| 17.6819 | RI=1658.1, 15.9216 min AKS1975 (ID#:AKS1975-N1034)   |
| 17.8502 | ?? 1,4 - anhydro - b - D - glucopyranose (ID#:FAH0040-N1068)                                 |
| 17.8562 | ?? 1,4 - anhydro - b - D - glucopyranose (ID#:FAH0040-N1068)                                 |
| 17.8916 | RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)   |
| 17.8956 | RI=1645.8, 28.4907 min FAH388 (ID#:FAH388-N1036)   |

17.9504 1,6 - anhydro - b - D - glucopyranose (levoglucosane - 3TMS) (ID#:FAH0040-N1064)

18.1055 ?? RI=1687.4, 16.3403 min AKS1976 (ID#:AKS1976-N1128)

18.2270 ? 1,6 -anhydro - D - galactopyranose (ID#:FAH0040-N1062)

18.2321 1,6 - anhydro - b - D - glucopyranose (levoglucosane - 3TMS) (ID#:FAH0040-N1064)

18.2422 ?? 2,3,5 - trihyddroxy - 4H - pyran - 4 - one (ID#:OAB467~1-N1066)

18.2708 RI=1705.8, 16.4992 min FAH1972 (ID#:FAH197~1-N1010)

18.3919 ?? 1,4 - anhydro - b - D - glucopyranose (ID#:FAH0040-N1068)

18.4175 RI=1710.3, 16.6591 min AKS1975 (ID#:AKS1975-N1032)

18.4560 ? RI=1716.8, 16.7466 min AKS1974 (ID#:AKS1974-N1042)

18.7284 1,6 - anhydro - b - D - glucofuranose (ID#:FAH0040-N1070)

19.5857 RI=1796.1, 17.8199 min AKS1976 (ID#:AKS1976-N1110)

19.6890 RI=1796.1, 17.8199 min AKS1976 (ID#:AKS1976-N1110)

19.7463 ?? RI=1245.3, 9.4662 min AKS1975 (ID#:AKS1975-N1050)

19.8083 ? dihydroconiferyl alcohol (ID#:OAB466~1-N1025)

19.8242 3,4 - dihydroxy - benzoic acid, (ID#:NA)

20.2937 RI=1851.2, 18.5346 min AKS1976 (ID#:AKS1976-N1102)

20.4309 RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)

20.7349 ? RI=1884.7, 18.9674 min AKS1976 (ID#:AKS1976-N1162)

20.8224 syringic acid (ID#:Py\_E\_W\_S4)

21.0927 Ferulic acid (trans) (ID#:MMA670-N1022)

21.1900 ?? Mannose (MEOX/TMS) (ID#:FAH957-N1006)

21.3803 p - coumaric acid (ID#:MMA670-N1024)

21.5508 RI=1951.1, 19.8270 min AKS1975 (ID#:AKS1975-N1002)

21.7875 RI=1966.6, 20.0279 min AKS1976 (ID#:AKS1976-N1092)

|         |  |
|---------|--|
| 22.0305 | RI=2005.9, 20.5364 min AKS1975 (ID#:AKS1975-N1026)                 |
| 22.0378 | RI=2005.9, 20.5364 min AKS1975 (ID#:AKS1975-N1026)                 |
| 22.2930 | RI=2005.9, 20.5364 min AKS1975 (ID#:AKS1975-N1026)                 |
| 22.4098 | ? RI=1394.6, 11.9462 min AKS1976 (ID#:AKS1976-N1142)               |
| 22.4829 | RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)                 |
| 22.6474 | RI=2034.1, 20.9016 min AKS1975 (ID#:AKS1975-N1022)                 |
| 22.6806 | palmitic acid (ID#:MMA671-N1042)                                   |
| 22.7508 | RI=2041.4, 20.9961 min AKS1975 (ID#:AKS1975-N1020)                 |
| 22.8925 | ? RI=2052.4, 21.1375 min AKS1975 (ID#:AKS1975-N1018)               |
| 22.9318 | ?? RI=1862.0, 18.6745 min AKS1974 (ID#:AKS1974-N1036)              |
| 23.0914 | synapyl alcohol (cis) (ID#:Py_E_W_S3)                              |
| 23.1460 | ? RI=2070.2, 21.3687 min AKS1974 (ID#:AKS1974-N1022)               |
| 23.2010 | Ferulic acid (trans) (ID#:MMA670-N1022)                            |
| 23.3688 | ? 1,2 - dihydroxyethene (ID#:TVL0020-N1006)                        |
| 23.6218 | RI=2108.4, 21.8630 min AKS1975 (ID#:AKS1975-N1012)                 |
| 23.6682 | RI=2096.3, 21.7057 min AKS1975 (ID#:AKS1975-N1014)                 |
| 23.7141 | ? Caffeic acid (ID#:FAH383-N1028)                                  |
| 24.0611 | RI=2142.6, 22.3047 min AKS1975 (ID#:AKS1975-N1006)                 |
| 24.9182 | ? RI=2208.9, 23.1630 min AKS1975 (ID#:AKS1975-N1004)               |
| 24.9246 | RI=2208.9, 23.1630 min AKS1975 (ID#:AKS1975-N1004)                 |
| 26.3633 | ? 2,3 - dihydroxy - 2 - cyclopenten - 1 - one (ID#:OAB467~1-N1040) |
| 26.5116 | dehydroabietic acid (ID#:MMA671-N1038)                             |
| 28.5928 | ? Heneicosane (IS) (ID#:629-94-7)                                  |
| 28.8323 | RI=2510.2, 27.0619 min AKS1976 (ID#:AKS1976-N1076)                 |
| 29.5276 | ? Heneicosane (IS) (ID#:629-94-7)                                  |

30.4292           ? Heneicosane (IS) (ID#:629-94-7)  
 31.3003           ? Heneicosane (IS) (ID#:629-94-7)  
 32.1524           ? Heneicosane (IS) (ID#:629-94-7)  
 32.9824           ? 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=3.7.

Background (low vs. high retention time):

    median low RT S/N=49, high RT S/N=91

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

    S/N=2 before run

    S/N=1 at 5.01 min.

Column Bleed (m/z 207):

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

This report consists of 7 pages