

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061522\  
 Data File : VX029513.D  
 Acq On : 15 Jun 2022 18:18  
 Operator : JC/MD  
 Sample : N3304-06  
 Misc : 5.15g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 WC-14A-1A-6-G

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
 Title : SW846 8260

Signal : TIC: VX029513.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 5.391       | 695           | 706         | 723          | rBV      | 187011         | 625897        | 19.64%          | 0.703%        |
| 2         | 5.550       | 723           | 732         | 753          | rVB      | 298700         | 929079        | 29.15%          | 1.044%        |
| 3         | 5.958       | 790           | 799         | 820          | rVV      | 208681         | 605029        | 18.98%          | 0.680%        |
| 4         | 6.763       | 920           | 931         | 959          | rVB      | 415506         | 1042599       | 32.71%          | 1.172%        |
| 5         | 7.373       | 1019          | 1031        | 1042         | rVB3     | 329169         | 811139        | 25.45%          | 0.912%        |
| 6         | 7.769       | 1087          | 1096        | 1105         | rVB2     | 177757         | 382800        | 12.01%          | 0.430%        |
| 7         | 7.952       | 1116          | 1126        | 1141         | rVB      | 165779         | 341841        | 10.73%          | 0.384%        |
| 8         | 8.598       | 1224          | 1232        | 1236         | rBV2     | 615960         | 1181123       | 37.06%          | 1.328%        |
| 9         | 8.647       | 1236          | 1240        | 1248         | rVB      | 1141692        | 2048665       | 64.28%          | 2.303%        |
| 10        | 8.775       | 1255          | 1261        | 1266         | rBV      | 233142         | 371130        | 11.64%          | 0.417%        |
| 11        | 8.976       | 1288          | 1294        | 1306         | rVB2     | 721504         | 1192524       | 37.41%          | 1.340%        |
| 12        | 9.104       | 1306          | 1315        | 1320         | rBV      | 336285         | 570967        | 17.91%          | 0.642%        |
| 13        | 9.293       | 1339          | 1346        | 1351         | rVB2     | 146883         | 257137        | 8.07%           | 0.289%        |
| 14        | 9.385       | 1351          | 1361        | 1370         | rBV      | 408792         | 743434        | 23.32%          | 0.836%        |
| 15        | 9.500       | 1375          | 1380        | 1386         | rBV3     | 608456         | 1165936       | 36.58%          | 1.310%        |
| 16        | 9.561       | 1386          | 1390        | 1394         | rVB2     | 392232         | 554657        | 17.40%          | 0.623%        |
| 17        | 9.616       | 1394          | 1399        | 1404         | rBV      | 942855         | 1536185       | 48.20%          | 1.727%        |
| 18        | 9.763       | 1416          | 1423        | 1428         | rBV2     | 227510         | 374813        | 11.76%          | 0.421%        |
| 19        | 9.830       | 1428          | 1434        | 1438         | rBV2     | 694031         | 1303309       | 40.89%          | 1.465%        |
| 20        | 10.006      | 1456          | 1463        | 1467         | rBV      | 239771         | 379363        | 11.90%          | 0.426%        |
| 21        | 10.055      | 1467          | 1471        | 1476         | rBV      | 791765         | 1114774       | 34.98%          | 1.253%        |
| 22        | 10.122      | 1476          | 1482        | 1487         | rVB4     | 148208         | 342438        | 10.74%          | 0.385%        |
| 23        | 10.183      | 1487          | 1492        | 1498         | rBV2     | 327579         | 594033        | 18.64%          | 0.668%        |
| 24        | 10.275      | 1503          | 1507        | 1510         | rBV2     | 459420         | 743566        | 23.33%          | 0.836%        |
| 25        | 10.317      | 1510          | 1514        | 1518         | rVB      | 630059         | 892916        | 28.01%          | 1.004%        |
| 26        | 10.354      | 1518          | 1520        | 1532         | rVB2     | 436744         | 800529        | 25.12%          | 0.900%        |
| 27        | 10.458      | 1532          | 1537        | 1545         | rBV2     | 400358         | 638520        | 20.03%          | 0.718%        |
| 28        | 10.592      | 1552          | 1559        | 1566         | rVB3     | 1203071        | 2300200       | 72.17%          | 2.585%        |
| 29        | 10.671      | 1566          | 1572        | 1577         | rBV4     | 547480         | 1042956       | 32.72%          | 1.172%        |
| 30        | 10.714      | 1577          | 1579        | 1582         | rVB3     | 234849         | 252655        | 7.93%           | 0.284%        |
| 31        | 10.781      | 1582          | 1590        | 1594         | rBV2     | 1988923        | 3187289       | 100.00%         | 3.582%        |
| 32        | 10.860      | 1594          | 1603        | 1606         | rBV3     | 1171318        | 2168021       | 68.02%          | 2.437%        |
| 33        | 10.896      | 1606          | 1609        | 1614         | rVB2     | 1165772        | 1565652       | 49.12%          | 1.760%        |
| 34        | 10.951      | 1614          | 1618        | 1622         | rVB2     | 364124         | 552920        | 17.35%          | 0.621%        |
| 35        | 11.006      | 1622          | 1627        | 1628         | rBV3     | 482702         | 652078        | 20.46%          | 0.733%        |
| 36        | 11.031      | 1628          | 1631        | 1635         | rVB2     | 675945         | 863579        | 27.09%          | 0.971%        |

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Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 WC-14A-1A-6-G

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
 Title : SW846 8260

|    |        |      |      |      |      |         |         |        |        |
|----|--------|------|------|------|------|---------|---------|--------|--------|
| 37 | 11.085 | 1635 | 1640 | 1644 | rVB2 | 1165794 | 1565217 | 49.11% | 1.759% |
| 38 | 11.128 | 1644 | 1647 | 1650 | rVB  | 378604  | 426068  | 13.37% | 0.479% |
| 39 | 11.220 | 1655 | 1662 | 1667 | rBV2 | 1377725 | 2086326 | 65.46% | 2.345% |
| 40 | 11.342 | 1677 | 1682 | 1686 | rBV3 | 556842  | 1026078 | 32.19% | 1.153% |
| 41 | 11.390 | 1686 | 1690 | 1694 | rVV3 | 630386  | 932239  | 29.25% | 1.048% |
| 42 | 11.433 | 1694 | 1697 | 1701 | rVV  | 995955  | 1217254 | 38.19% | 1.368% |
| 43 | 11.482 | 1701 | 1705 | 1709 | rVB2 | 681950  | 998888  | 31.34% | 1.123% |
| 44 | 11.524 | 1709 | 1712 | 1718 | rVB5 | 219347  | 269118  | 8.44%  | 0.302% |
| 45 | 11.604 | 1722 | 1725 | 1727 | rBV  | 299961  | 383685  | 12.04% | 0.431% |
| 46 | 11.634 | 1727 | 1730 | 1734 | rVB5 | 633602  | 867464  | 27.22% | 0.975% |
| 47 | 11.683 | 1734 | 1738 | 1741 | rBV4 | 521789  | 718346  | 22.54% | 0.807% |
| 48 | 11.719 | 1741 | 1744 | 1747 | rBV  | 1409382 | 1546583 | 48.52% | 1.738% |
| 49 | 11.841 | 1759 | 1764 | 1766 | rBV2 | 570748  | 846197  | 26.55% | 0.951% |
| 50 | 11.890 | 1769 | 1772 | 1777 | rVV4 | 995892  | 1814213 | 56.92% | 2.039% |
| 51 | 11.945 | 1777 | 1781 | 1784 | rVV  | 1050043 | 1619245 | 50.80% | 1.820% |
| 52 | 11.976 | 1784 | 1786 | 1790 | rVV2 | 644075  | 932334  | 29.25% | 1.048% |
| 53 | 12.030 | 1791 | 1795 | 1801 | rVV3 | 1002639 | 2151753 | 67.51% | 2.418% |
| 54 | 12.110 | 1805 | 1808 | 1811 | rBV3 | 190958  | 287437  | 9.02%  | 0.323% |
| 55 | 12.158 | 1812 | 1816 | 1820 | rVB4 | 387702  | 600566  | 18.84% | 0.675% |
| 56 | 12.256 | 1826 | 1832 | 1836 | rBV6 | 279068  | 735614  | 23.08% | 0.827% |
| 57 | 12.311 | 1837 | 1841 | 1848 | rBV2 | 1227818 | 2166800 | 67.98% | 2.435% |
| 58 | 12.384 | 1848 | 1853 | 1854 | rBV4 | 221783  | 335506  | 10.53% | 0.377% |
| 59 | 12.421 | 1856 | 1859 | 1864 | rBV2 | 418846  | 620141  | 19.46% | 0.697% |
| 60 | 12.469 | 1864 | 1867 | 1873 | rVB3 | 761881  | 1367787 | 42.91% | 1.537% |
| 61 | 12.561 | 1876 | 1882 | 1883 | rBV4 | 677939  | 1139779 | 35.76% | 1.281% |
| 62 | 12.640 | 1891 | 1895 | 1899 | rBV3 | 235548  | 312746  | 9.81%  | 0.352% |
| 63 | 12.689 | 1899 | 1903 | 1906 | rVV2 | 638053  | 797364  | 25.02% | 0.896% |
| 64 | 12.731 | 1906 | 1910 | 1913 | rVV5 | 194004  | 329631  | 10.34% | 0.370% |
| 65 | 12.768 | 1913 | 1916 | 1919 | rVV4 | 234357  | 355775  | 11.16% | 0.400% |
| 66 | 12.823 | 1920 | 1925 | 1930 | rVB3 | 1320806 | 2091088 | 65.61% | 2.350% |
| 67 | 12.890 | 1930 | 1936 | 1944 | rBV3 | 1075192 | 2383421 | 74.78% | 2.679% |
| 68 | 12.988 | 1948 | 1952 | 1956 | rBV  | 1023340 | 1144841 | 35.92% | 1.287% |
| 69 | 13.097 | 1966 | 1970 | 1975 | rBV3 | 331370  | 521714  | 16.37% | 0.586% |
| 70 | 13.298 | 1998 | 2003 | 2008 | rVB2 | 965101  | 1538345 | 48.26% | 1.729% |
| 71 | 13.347 | 2008 | 2011 | 2014 | rBV2 | 337521  | 405586  | 12.73% | 0.456% |
| 72 | 13.390 | 2014 | 2018 | 2020 | rVV  | 836287  | 1156099 | 36.27% | 1.299% |
| 73 | 13.420 | 2020 | 2023 | 2032 | rVB8 | 907748  | 2568470 | 80.58% | 2.887% |
| 74 | 13.506 | 2033 | 2037 | 2040 | rBV4 | 220385  | 408821  | 12.83% | 0.459% |
| 75 | 13.676 | 2062 | 2065 | 2067 | rBV4 | 259350  | 333402  | 10.46% | 0.375% |
| 76 | 13.707 | 2067 | 2070 | 2072 | rVV2 | 485869  | 531766  | 16.68% | 0.598% |

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 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 WC-14A-1A-6-G

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
 Title : SW846 8260

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 77  | 13.744 | 2072 | 2076 | 2082 | rVB3 | 594364 | 1155370 | 36.25% | 1.299% |
| 78  | 13.804 | 2082 | 2086 | 2089 | rBV3 | 704936 | 883811  | 27.73% | 0.993% |
| 79  | 13.847 | 2089 | 2093 | 2096 | rBV  | 755421 | 910113  | 28.55% | 1.023% |
| 80  | 13.908 | 2099 | 2103 | 2111 | rVB8 | 456114 | 1082399 | 33.96% | 1.217% |
| 81  | 13.993 | 2112 | 2117 | 2119 | rBV3 | 297253 | 544615  | 17.09% | 0.612% |
| 82  | 14.073 | 2126 | 2130 | 2132 | rBV3 | 276541 | 363585  | 11.41% | 0.409% |
| 83  | 14.103 | 2132 | 2135 | 2138 | rVB2 | 335949 | 344723  | 10.82% | 0.387% |
| 84  | 14.140 | 2138 | 2141 | 2143 | rBV3 | 280164 | 271409  | 8.52%  | 0.305% |
| 85  | 14.219 | 2151 | 2154 | 2157 | rVB2 | 423866 | 541074  | 16.98% | 0.608% |
| 86  | 14.420 | 2184 | 2187 | 2193 | rVB5 | 357953 | 730936  | 22.93% | 0.822% |
| 87  | 14.493 | 2194 | 2199 | 2201 | rBV3 | 315592 | 576356  | 18.08% | 0.648% |
| 88  | 14.615 | 2216 | 2219 | 2222 | rBV2 | 622354 | 738915  | 23.18% | 0.830% |
| 89  | 14.676 | 2226 | 2229 | 2233 | rVB2 | 385724 | 469753  | 14.74% | 0.528% |
| 90  | 14.725 | 2234 | 2237 | 2240 | rBV3 | 278169 | 433013  | 13.59% | 0.487% |
| 91  | 14.792 | 2245 | 2248 | 2254 | rVB6 | 313437 | 490849  | 15.40% | 0.552% |
| 92  | 14.853 | 2255 | 2258 | 2261 | rVB3 | 361051 | 401941  | 12.61% | 0.452% |
| 93  | 15.182 | 2308 | 2312 | 2315 | rBV3 | 262092 | 445594  | 13.98% | 0.501% |
| 94  | 15.213 | 2315 | 2317 | 2320 | rVB2 | 298345 | 293135  | 9.20%  | 0.329% |
| 95  | 15.377 | 2341 | 2344 | 2348 | rBV3 | 354322 | 473172  | 14.85% | 0.532% |
| 96  | 15.420 | 2348 | 2351 | 2354 | rVV3 | 228586 | 335264  | 10.52% | 0.377% |
| 97  | 15.481 | 2358 | 2361 | 2367 | rVB2 | 338107 | 503975  | 15.81% | 0.566% |
| 98  | 15.615 | 2380 | 2383 | 2385 | rBV  | 192205 | 260573  | 8.18%  | 0.293% |
| 99  | 15.652 | 2386 | 2389 | 2397 | rVB5 | 370247 | 773687  | 24.27% | 0.870% |
| 100 | 16.274 | 2487 | 2491 | 2494 | rBV2 | 143635 | 285300  | 8.95%  | 0.321% |

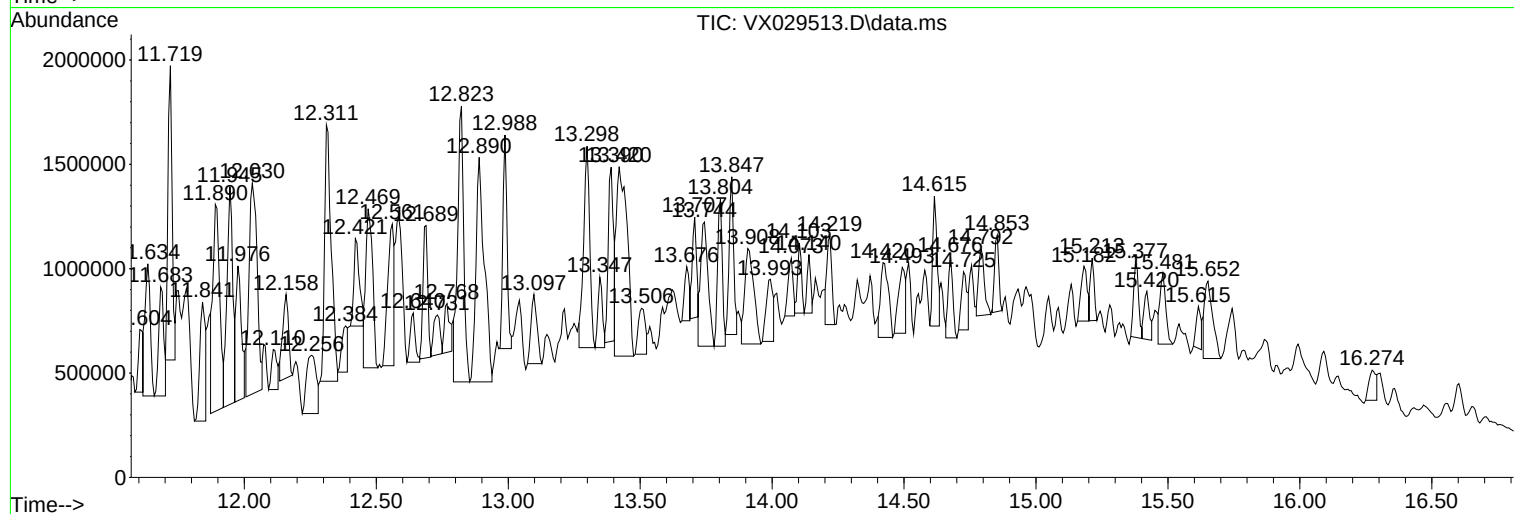
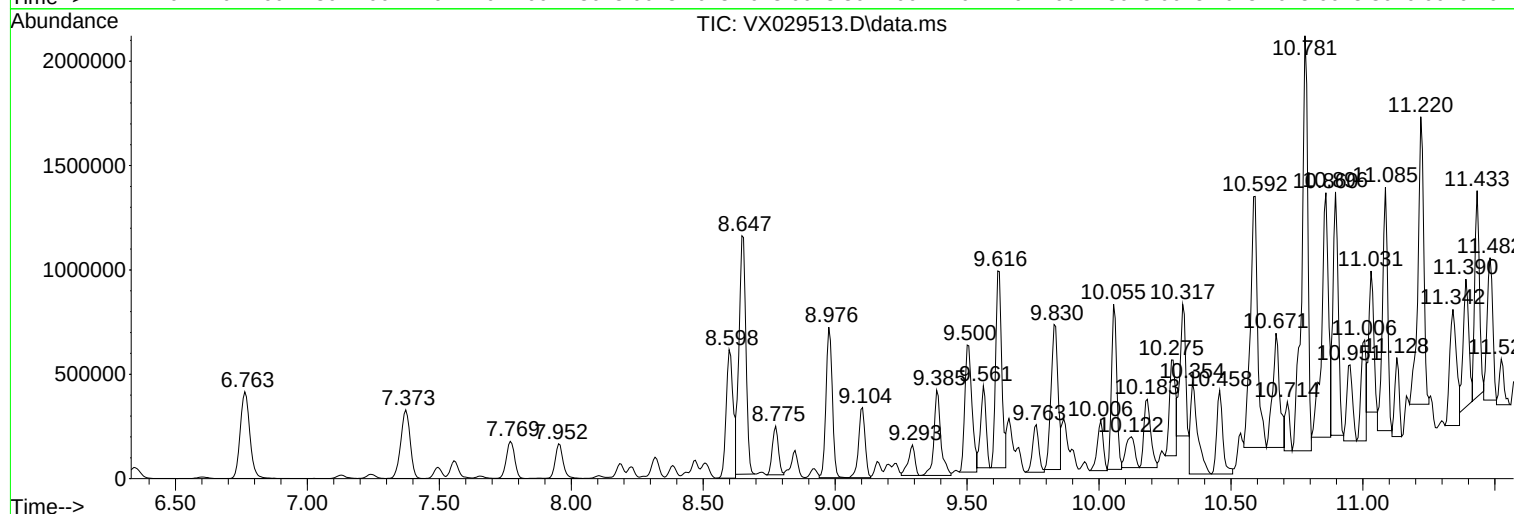
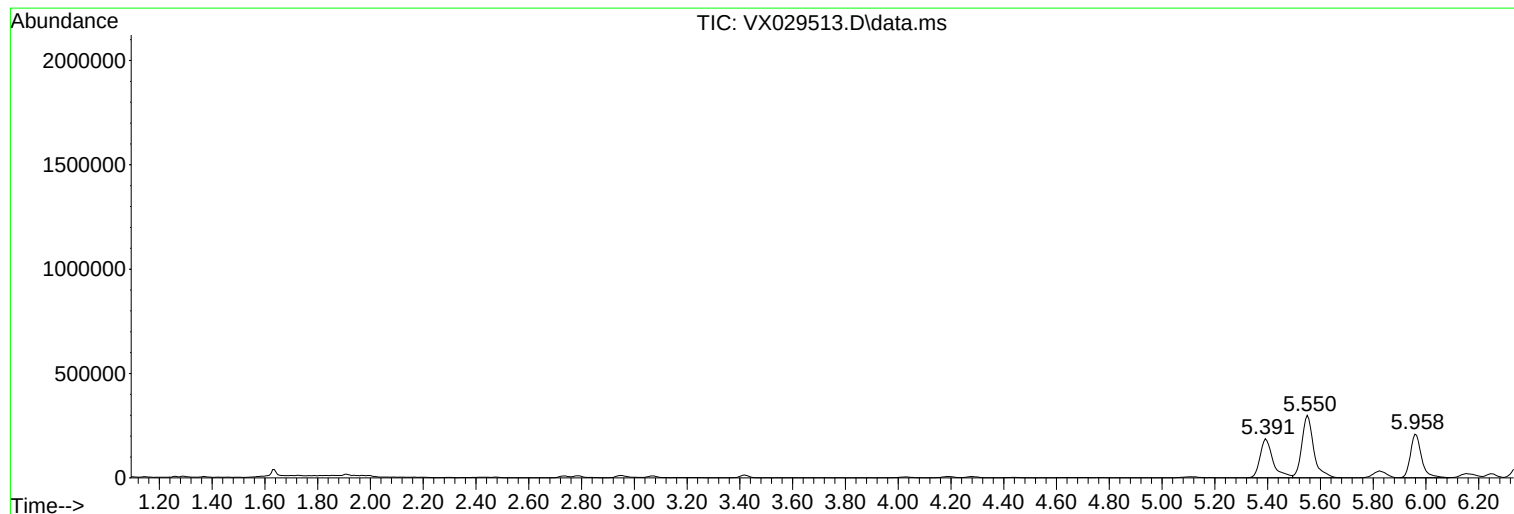
Sum of corrected areas: 88973022

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
Quant Title : SW846 8260

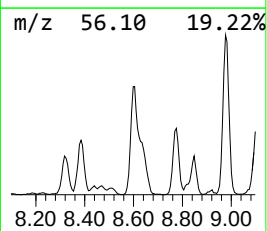
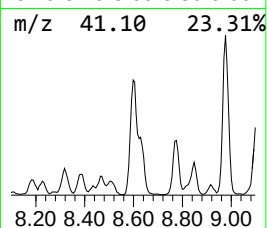
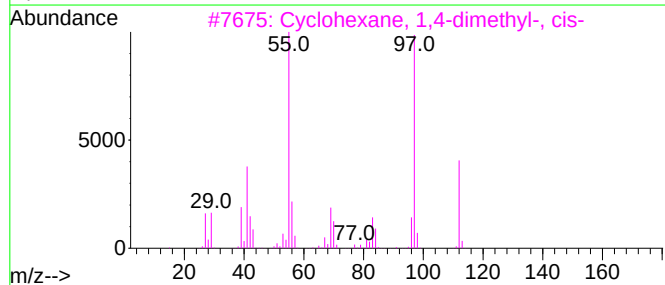
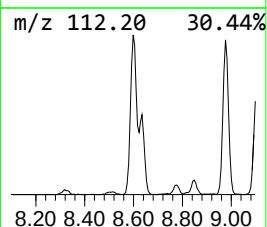
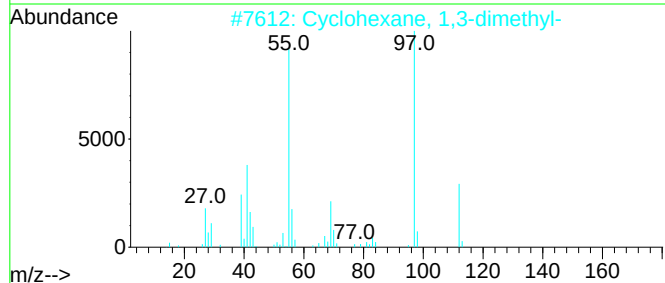
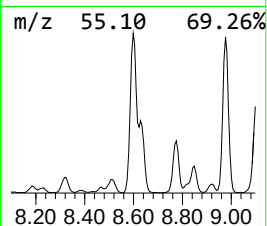
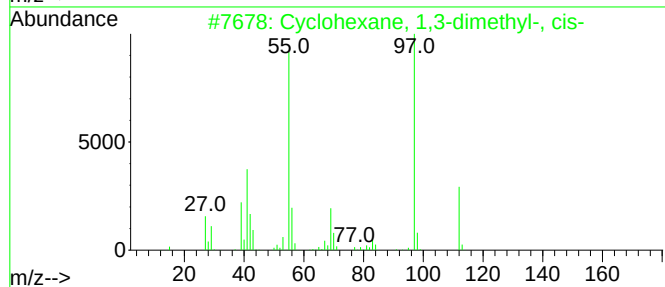
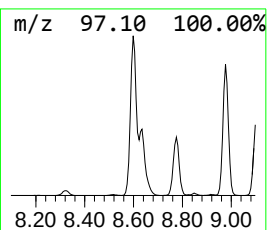
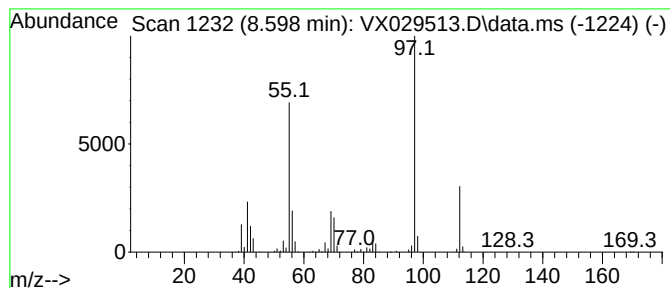
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 10

| R.T.  | EstConc    | Area    | Relative to ISTD | R.T.   |
|-------|------------|---------|------------------|--------|
| 8.598 | 52.98 ug/l | 1181120 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexane, 1,3-dimethyl-, cis-   | 112 | C8H16   | 000638-04-0 | 94   |
| 2    |    |   | Cyclohexane, 1,3-dimethyl-         | 112 | C8H16   | 000591-21-9 | 91   |
| 3    |    |   | Cyclohexane, 1,4-dimethyl-, cis-   | 112 | C8H16   | 000624-29-3 | 91   |
| 4    |    |   | Cyclohexane, 1,4-dimethyl-         | 112 | C8H16   | 000589-90-2 | 90   |
| 5    |    |   | Cyclohexane, 1,3-dimethyl-, trans- | 112 | C8H16   | 002207-03-6 | 90   |



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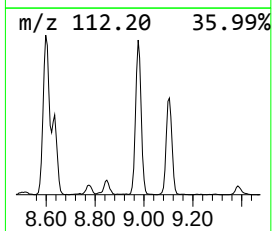
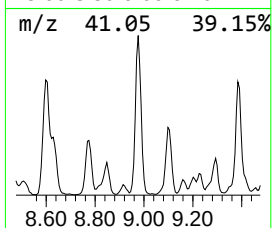
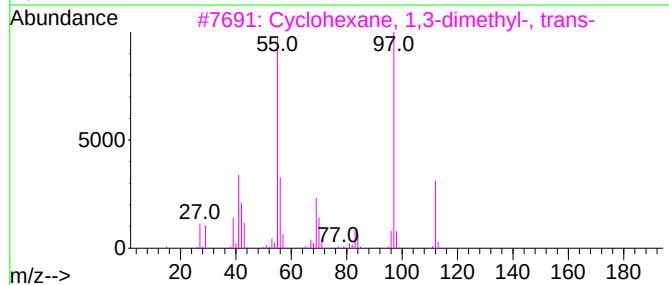
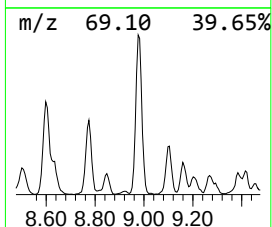
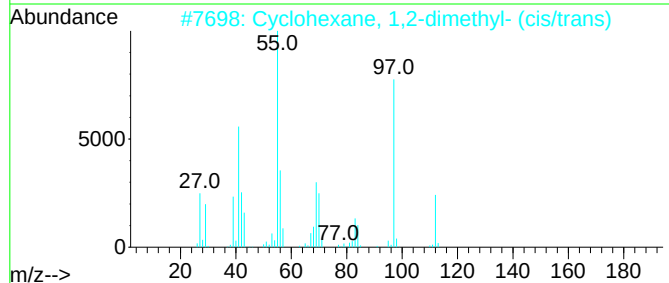
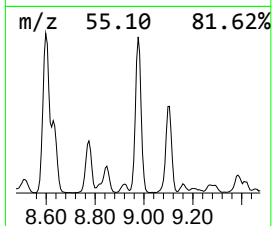
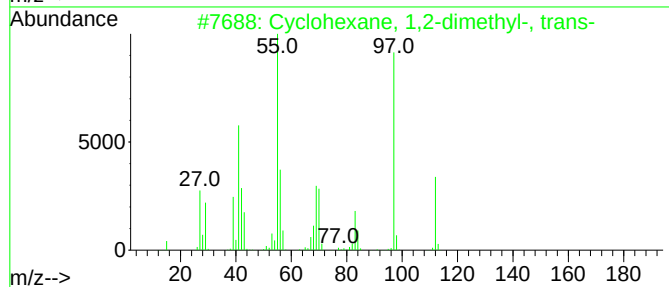
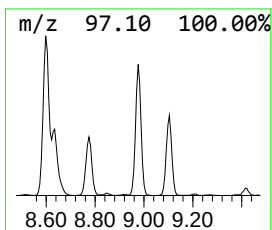
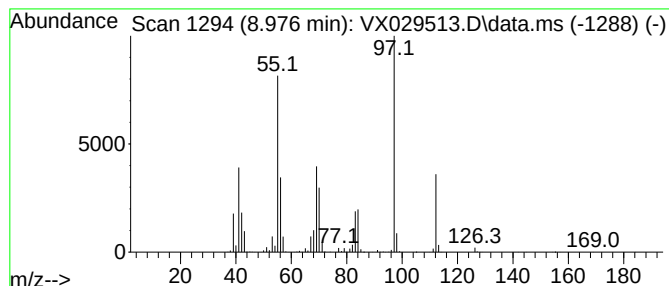
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 9

| R.T.  | EstConc    | Area    | Relative to ISTD | R.T.   |
|-------|------------|---------|------------------|--------|
| 8.976 | 53.49 ug/l | 1192520 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexane, 1,2-dimethyl-, trans-  | 112 | C8H16   | 006876-23-9 | 93   |
| 2    |    |   | Cyclohexane, 1,2-dimethyl- (cis/... | 112 | C8H16   | 000583-57-3 | 90   |
| 3    |    |   | Cyclohexane, 1,3-dimethyl-, trans-  | 112 | C8H16   | 002207-03-6 | 74   |
| 4    |    |   | Cyclohexane, 1,4-dimethyl-, cis-    | 112 | C8H16   | 000624-29-3 | 72   |
| 5    |    |   | Cyclohexane, 1,4-dimethyl-, trans-  | 112 | C8H16   | 002207-04-7 | 72   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061522\  
Data File : VX029513.D  
Acq On : 15 Jun 2022 18:18  
Operator : JC/MD  
Sample : N3304-06  
Misc : 5.15g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WC-14A-1A-6-G

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
Quant Title : SW846 8260

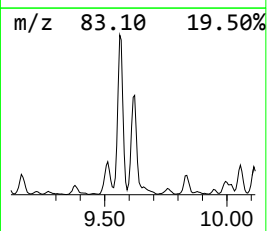
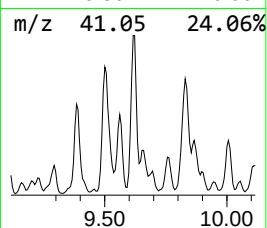
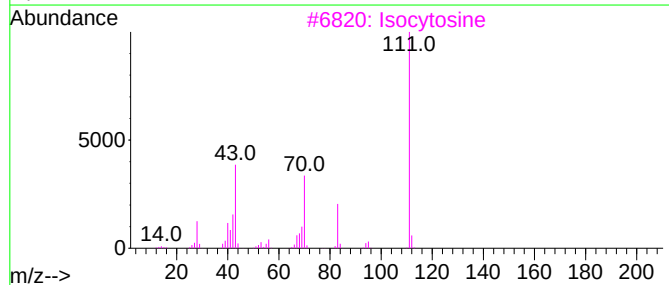
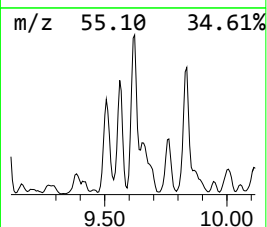
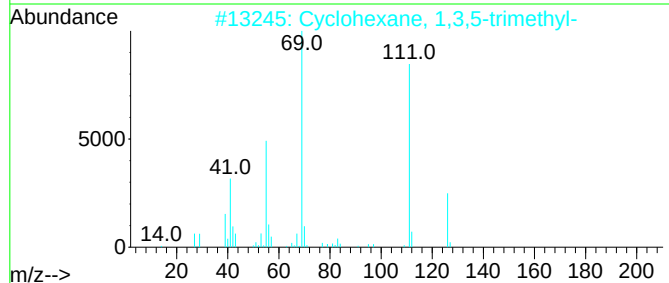
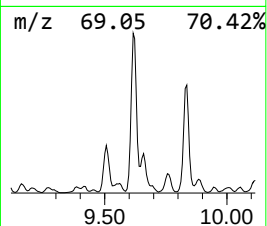
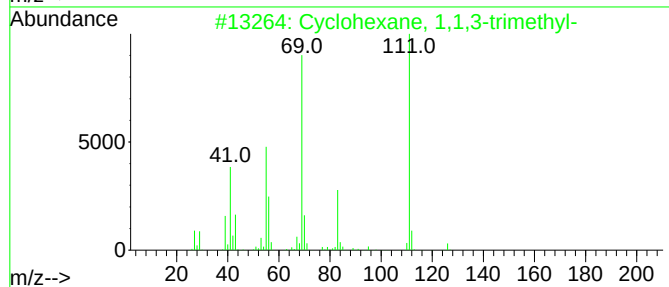
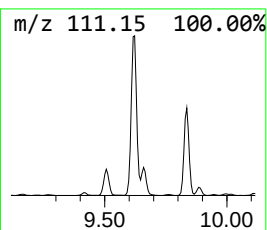
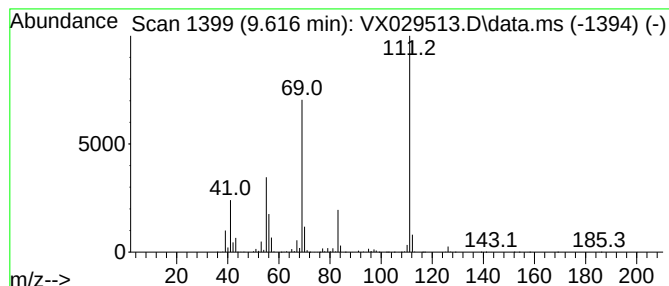
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 5

| R.T.  | EstConc    | Area    | Relative to ISTD | R.T.   |
|-------|------------|---------|------------------|--------|
| 9.616 | 68.90 ug/l | 1536190 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                  | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexane, 1,1,3-trimethyl- | 126 | C9H18   | 003073-66-3 | 95   |
| 2    |    |   | Cyclohexane, 1,3,5-trimethyl- | 126 | C9H18   | 001839-63-0 | 64   |
| 3    |    |   | Isocytosine                   | 111 | C4H5N3O | 000108-53-2 | 64   |
| 4    |    |   | 1,1,4-Trimethylcyclohexane    | 126 | C9H18   | 007094-27-1 | 59   |
| 5    |    |   | Cyclooctane, butyl-           | 168 | C12H24  | 016538-93-5 | 56   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061522\  
Data File : VX029513.D  
Acq On : 15 Jun 2022 18:18  
Operator : JC/MD  
Sample : N3304-06  
Misc : 5.15g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WC-14A-1A-6-G

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
Quant Title : SW846 8260

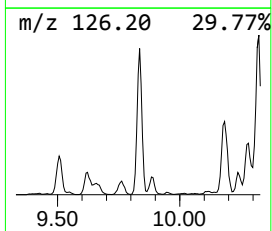
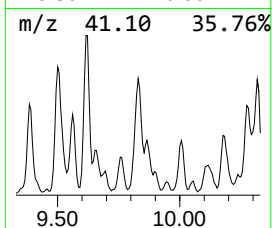
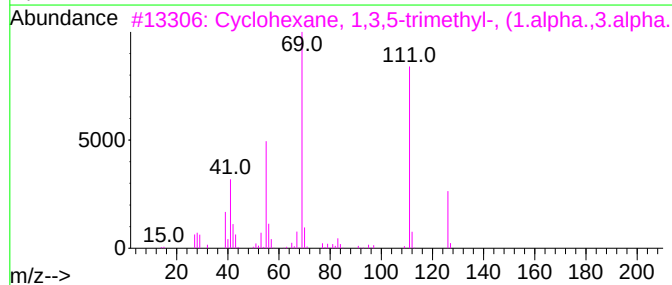
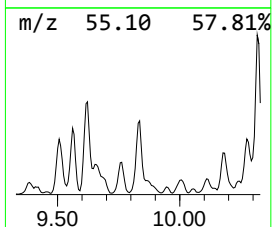
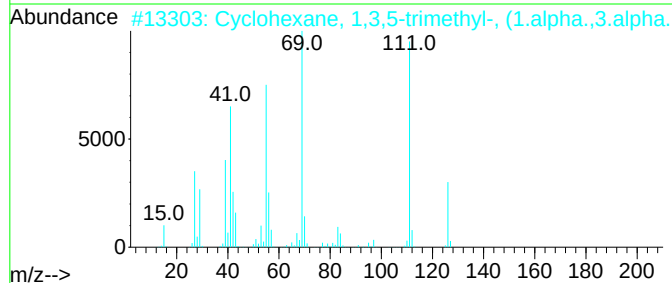
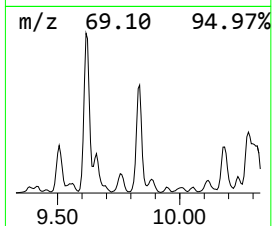
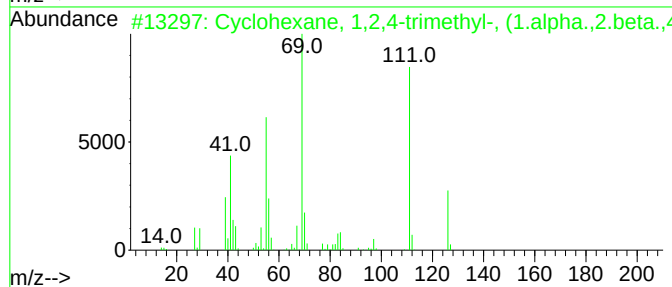
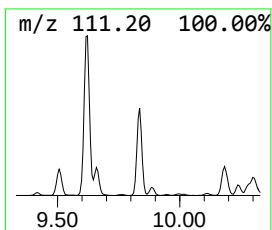
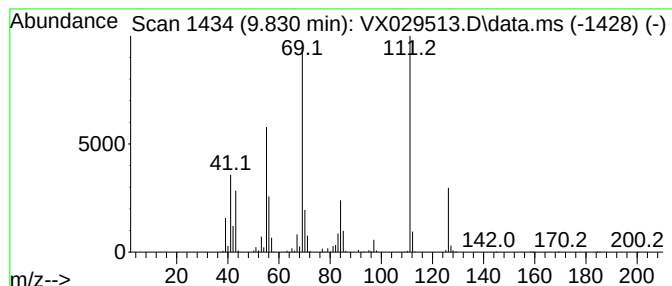
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Cyclohexane, 1,2,4-trimethyl... Concentration Rank 7

| R.T.  | EstConc    | Area    | Relative to ISTD | R.T.   |
|-------|------------|---------|------------------|--------|
| 9.830 | 58.46 ug/l | 1303310 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexane, 1,2,4-trimethyl-, (... | 126 | C9H18   | 007667-60-9 | 90   |
| 2    |    |   | Cyclohexane, 1,3,5-trimethyl-, (... | 126 | C9H18   | 001795-26-2 | 83   |
| 3    |    |   | Cyclohexane, 1,3,5-trimethyl-, (... | 126 | C9H18   | 001795-27-3 | 81   |
| 4    |    |   | Cyclohexane, 1,2,4-trimethyl-       | 126 | C9H18   | 002234-75-5 | 76   |
| 5    |    |   | Cyclohexane, 1,3,5-trimethyl-       | 126 | C9H18   | 001839-63-0 | 74   |





Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061522\  
Data File : VX029513.D  
Acq On : 15 Jun 2022 18:18  
Operator : JC/MD  
Sample : N3304-06  
Misc : 5.15g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WC-14A-1A-6-G

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
Quant Title : SW846 8260

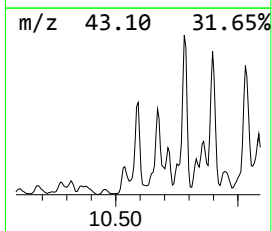
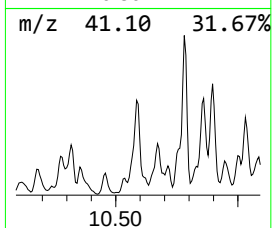
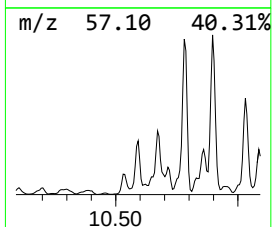
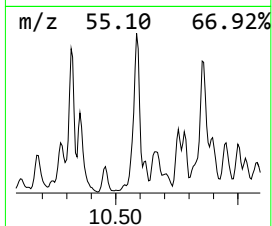
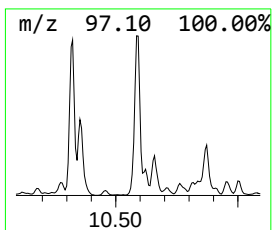
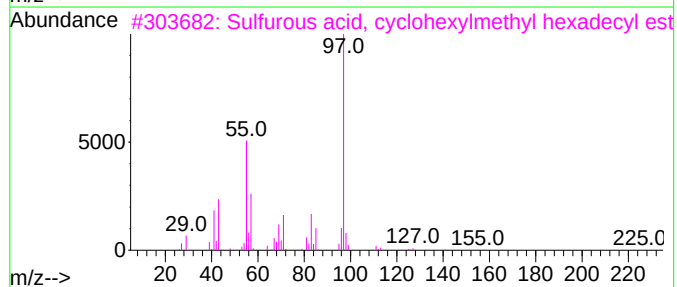
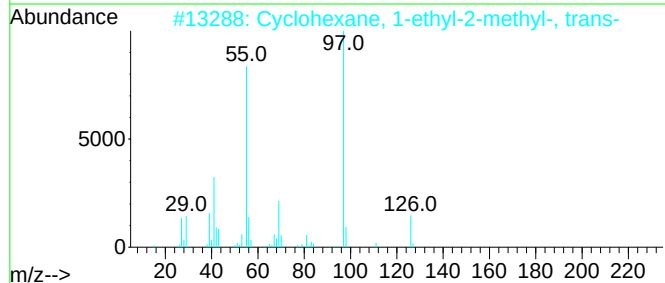
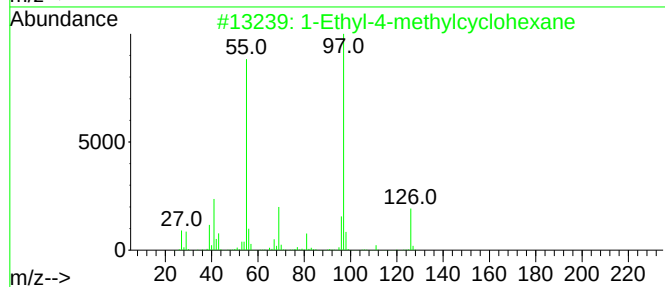
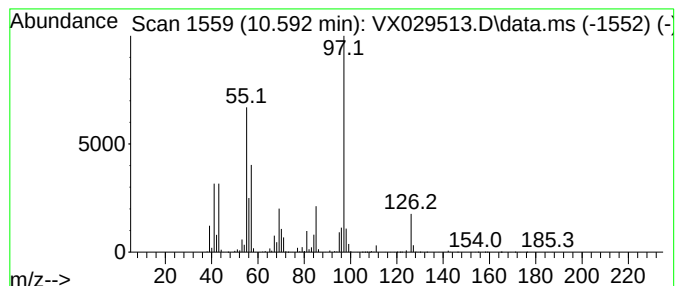
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 1-Ethyl-4-methylcyclohexane Concentration Rank 2

| R.T.   | EstConc     | Area    | Relative to ISTD | R.T.   |
|--------|-------------|---------|------------------|--------|
| 10.592 | 103.17 ug/l | 2300200 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | 1-Ethyl-4-methylcyclohexane         | 126 | C9H18     | 003728-56-1  | 70   |
| 2    |    |   | Cyclohexane, 1-ethyl-2-methyl-, ... | 126 | C9H18     | 004923-78-8  | 64   |
| 3    |    |   | Sulfurous acid, cyclohexylmethyl... | 402 | C23H46O3S | 1000309-22-4 | 59   |
| 4    |    |   | Cyclohexane, 1-ethyl-2-methyl-, ... | 126 | C9H18     | 004923-77-7  | 58   |
| 5    |    |   | Sulfurous acid, butyl cyclohexyl... | 234 | C11H22O3S | 1000309-21-4 | 53   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061522\  
Data File : VX029513.D  
Acq On : 15 Jun 2022 18:18  
Operator : JC/MD  
Sample : N3304-06  
Misc : 5.15g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WC-14A-1A-6-G

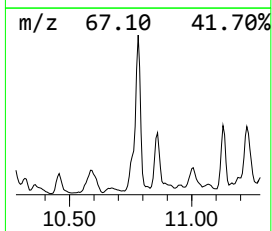
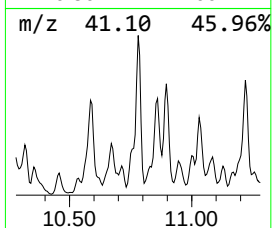
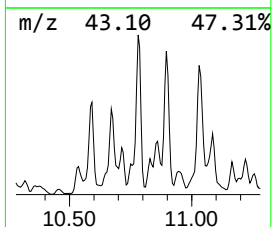
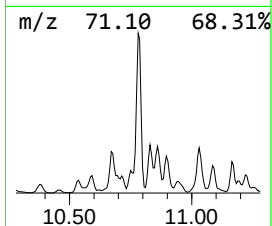
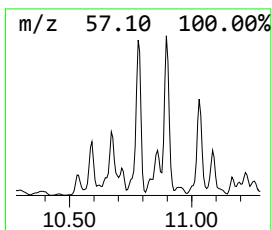
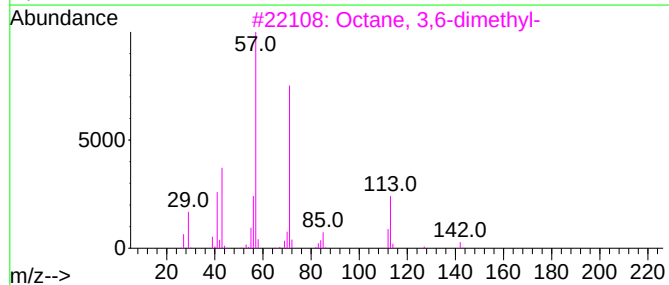
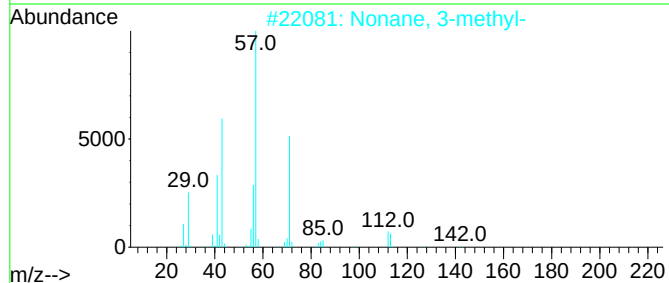
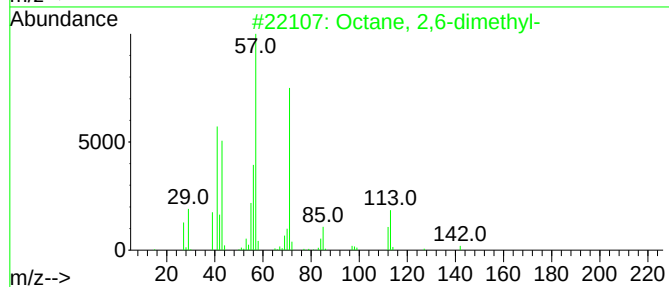
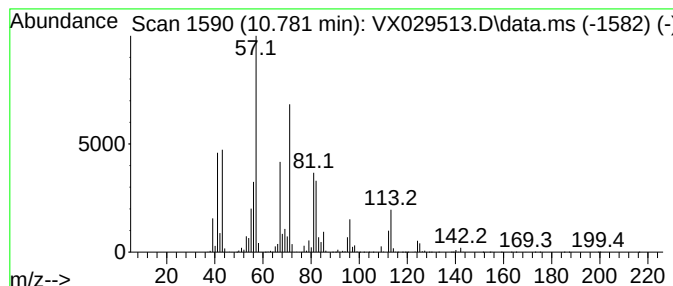
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Octane, 2,6-dimethyl- Concentration Rank 1

| R.T.   | EstConc     | Area    | Relative to ISTD | R.T.   |
|--------|-------------|---------|------------------|--------|
| 10.781 | 142.96 ug/l | 3187290 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm   | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Octane, 2,6-dimethyl-                | 142 | C10H22    | 002051-30-1  | 60   |
| 2    |    |   | Nonane, 3-methyl-                    | 142 | C10H22    | 005911-04-6  | 55   |
| 3    |    |   | Octane, 3,6-dimethyl-                | 142 | C10H22    | 015869-94-0  | 55   |
| 4    |    |   | Undecane, 2,6-dimethyl-              | 184 | C13H28    | 017301-23-4  | 38   |
| 5    |    |   | Sulfurous acid, di(2-ethylhexyl)-... | 306 | C16H34O3S | 1000309-19-1 | 38   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061522\  
Data File : VX029513.D  
Acq On : 15 Jun 2022 18:18  
Operator : JC/MD  
Sample : N3304-06  
Misc : 5.15g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WC-14A-1A-6-G

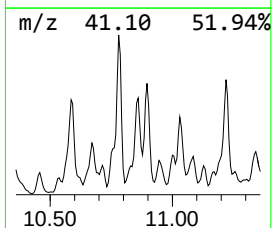
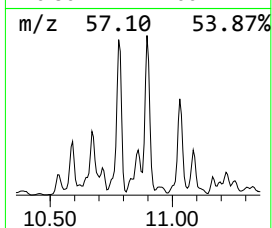
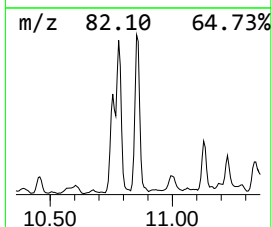
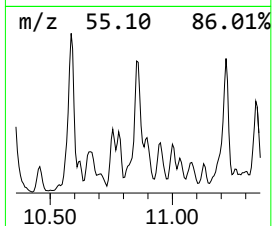
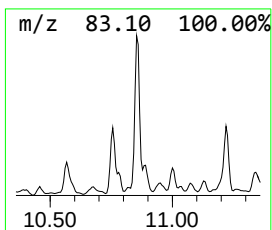
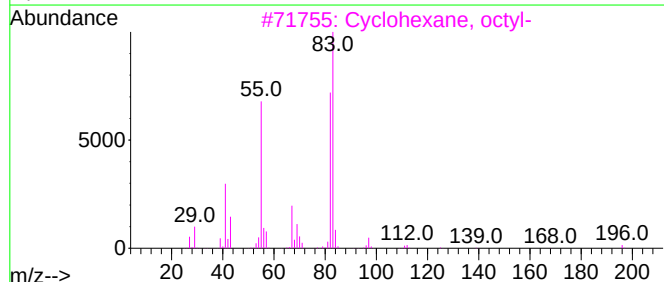
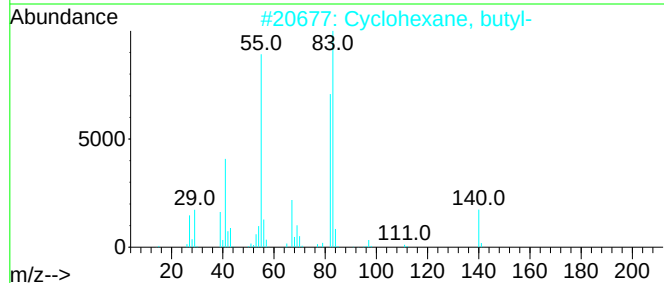
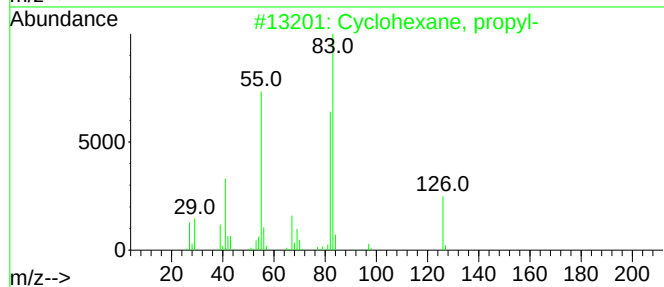
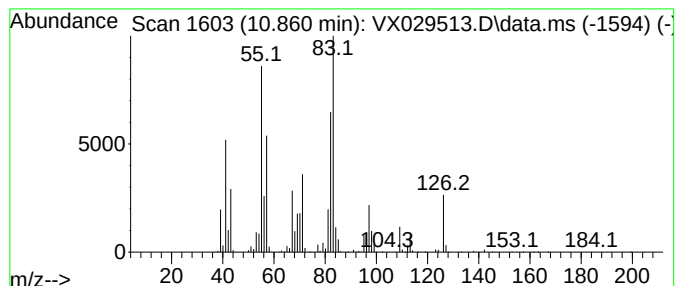
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Cyclohexane, propyl- Concentration Rank 3

| R.T.   | EstConc    | Area    | Relative to ISTD | R.T.   |
|--------|------------|---------|------------------|--------|
| 10.860 | 97.24 ug/l | 2168020 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexane, propyl-                | 126 | C9H18   | 001678-92-8 | 58   |
| 2    |    |   | Cyclohexane, butyl-                 | 140 | C10H20  | 001678-93-9 | 50   |
| 3    |    |   | Cyclohexane, octyl-                 | 196 | C14H28  | 001795-15-9 | 50   |
| 4    |    |   | Cyclohexane, (1-methylethyl)-       | 126 | C9H18   | 000696-29-7 | 49   |
| 5    |    |   | Cyclohexane, 1,1'-(1,4-butanediyl)- | 222 | C16H30  | 006165-44-2 | 47   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061522\  
Data File : VX029513.D  
Acq On : 15 Jun 2022 18:18  
Operator : JC/MD  
Sample : N3304-06  
Misc : 5.15g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WC-14A-1A-6-G

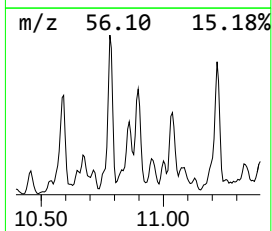
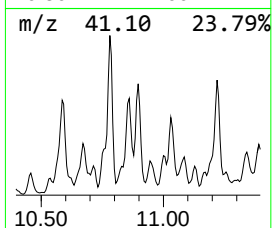
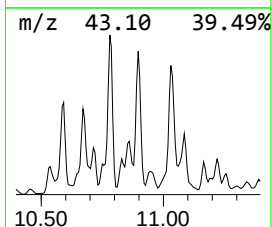
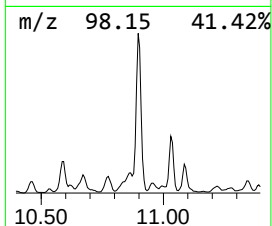
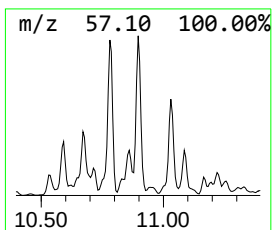
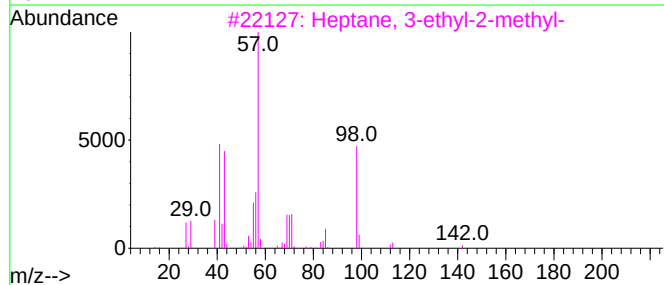
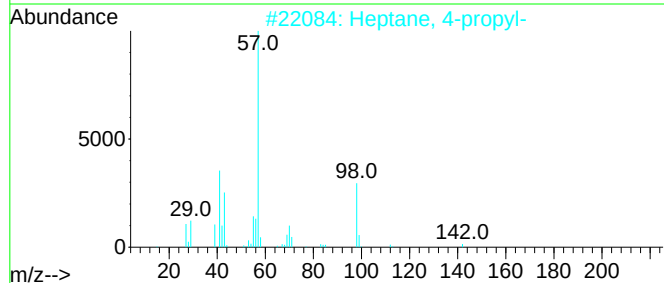
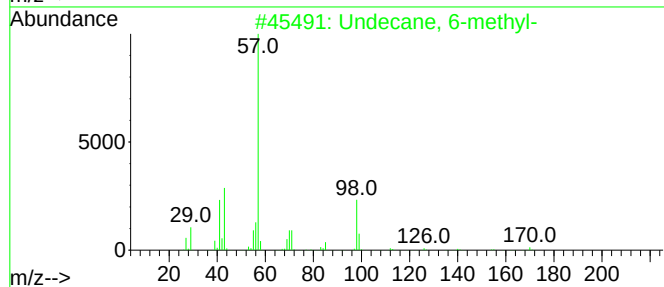
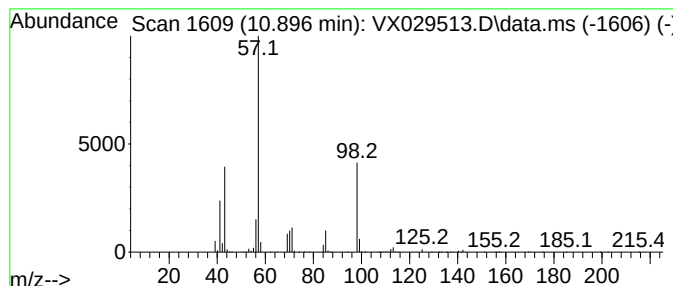
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 Undecane, 6-methyl- Concentration Rank 4

| R.T.   | EstConc    | Area    | Relative to ISTD | R.T.   |
|--------|------------|---------|------------------|--------|
| 10.897 | 70.22 ug/l | 1565650 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID               | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------|-----|---------|-------------|------|
| 1    |    |   | Undecane, 6-methyl-        | 170 | C12H26  | 017302-33-9 | 72   |
| 2    |    |   | Heptane, 4-propyl-         | 142 | C10H22  | 003178-29-8 | 72   |
| 3    |    |   | Heptane, 3-ethyl-2-methyl- | 142 | C10H22  | 014676-29-0 | 62   |
| 4    |    |   | Decane, 2,5-dimethyl-      | 170 | C12H26  | 017312-50-4 | 53   |
| 5    |    |   | Octane, 2,3-dimethyl-      | 142 | C10H22  | 007146-60-3 | 43   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061522\  
Data File : VX029513.D  
Acq On : 15 Jun 2022 18:18  
Operator : JC/MD  
Sample : N3304-06  
Misc : 5.15g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WC-14A-1A-6-G

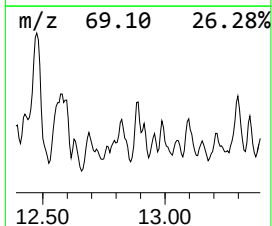
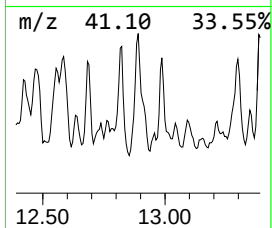
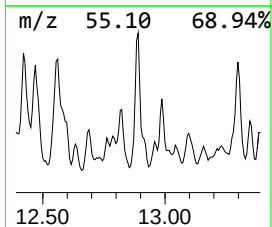
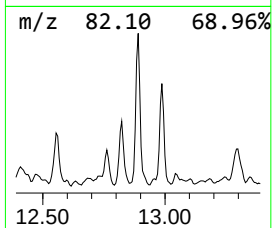
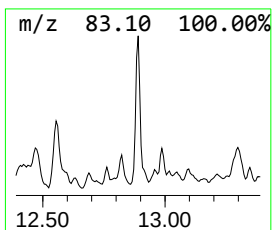
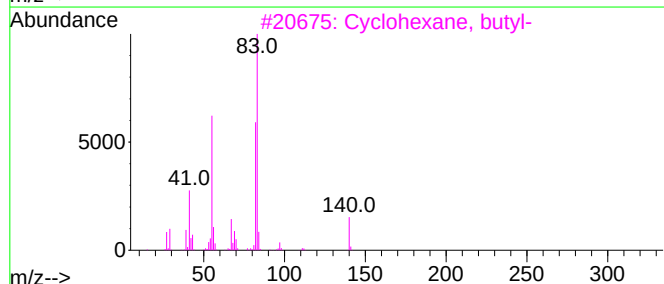
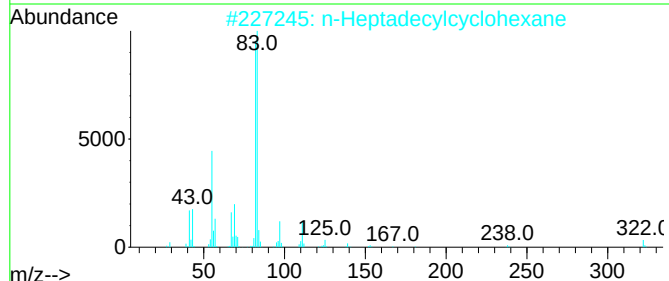
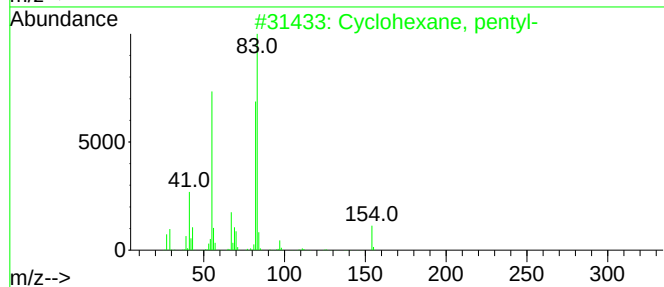
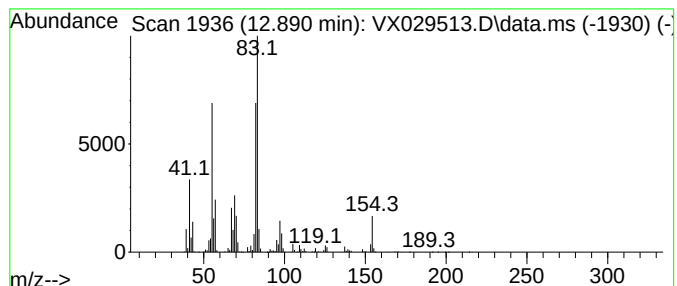
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 9 Cyclohexane, pentyl- Concentration Rank 8

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 12.890 | 55.38 ug/l | 2383420 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexane, pentyl-           | 154 | C11H22  | 004292-92-6 | 83   |
| 2    |    |   | n-Heptadecylcyclohexane        | 322 | C23H46  | 019781-73-8 | 72   |
| 3    |    |   | Cyclohexane, butyl-            | 140 | C10H20  | 001678-93-9 | 64   |
| 4    |    |   | Cyclohexane, (1-methylethyl)-  | 126 | C9H18   | 000696-29-7 | 64   |
| 5    |    |   | Cyclohexane, (4-methylpentyl)- | 168 | C12H24  | 061142-20-9 | 59   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061522\  
Data File : VX029513.D  
Acq On : 15 Jun 2022 18:18  
Operator : JC/MD  
Sample : N3304-06  
Misc : 5.15g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WC-14A-1A-6-G

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
Quant Title : SW846 8260

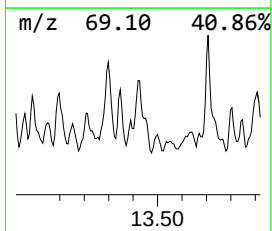
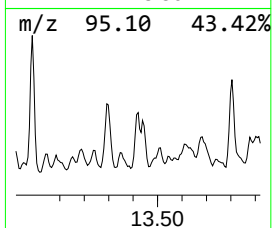
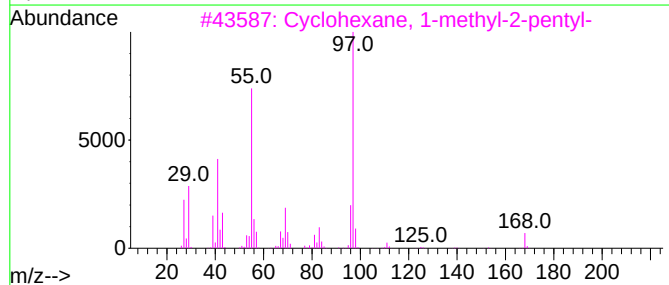
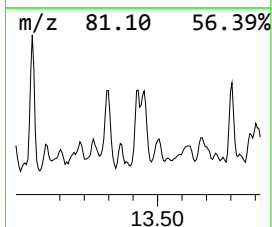
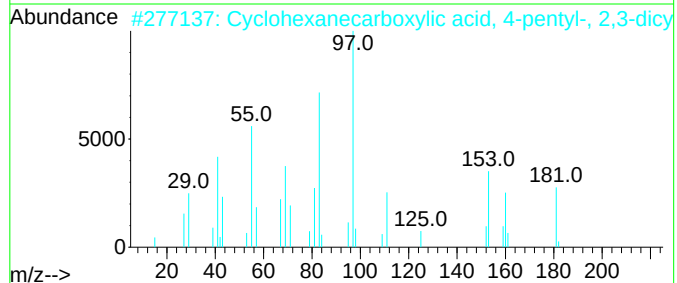
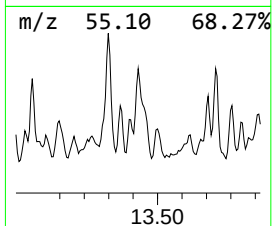
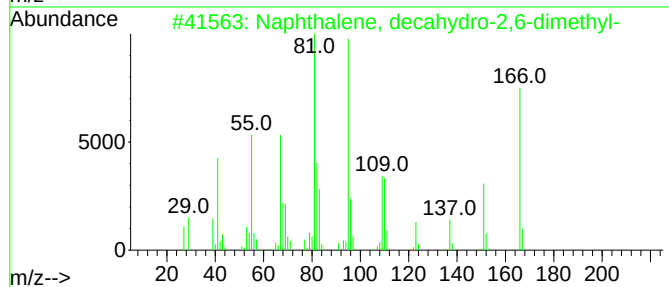
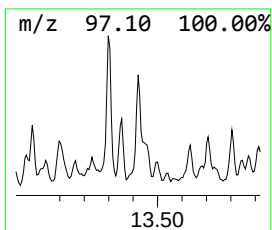
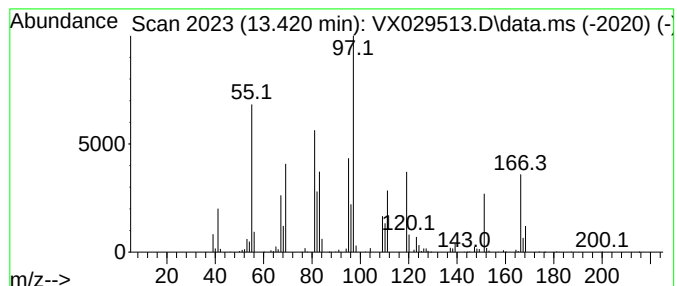
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 10 unknown13.420 Concentration Rank 6

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 13.420 | 59.68 ug/l | 2568470 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Naphthalene, decahydro-2,6-dimet... | 166 | C12H22     | 001618-22-0 | 42   |
| 2    |    |   | Cyclohexanecarboxylic acid, 4-pe... | 368 | C22H28N2O3 | 133856-87-8 | 35   |
| 3    |    |   | Cyclohexane, 1-methyl-2-pentyl-     | 168 | C12H24     | 054411-01-7 | 35   |
| 4    |    |   | Methylphosphonic acid, mono-(2,2... | 206 | C9H19O3P   | 959027-86-2 | 32   |
| 5    |    |   | Cyclohexane, 1-ethyl-1-methyl-      | 126 | C9H18      | 004926-90-3 | 27   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX061522\  
Data File : VX029513.D  
Acq On : 15 Jun 2022 18:18  
Operator : JC/MD  
Sample : N3304-06  
Misc : 5.15g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WC-14A-1A-6-G

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X060722W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Cyclohexane, 1,... | 8.598  | 53.0    | ug/l  | 1181120  | 3                     | 10.055 | 1114770 | 50.0 |
| Cyclohexane, 1,... | 8.976  | 53.5    | ug/l  | 1192520  | 3                     | 10.055 | 1114770 | 50.0 |
| Cyclohexane, 1,... | 9.616  | 68.9    | ug/l  | 1536190  | 3                     | 10.055 | 1114770 | 50.0 |
| Cyclohexane, 1,... | 9.830  | 58.5    | ug/l  | 1303310  | 3                     | 10.055 | 1114770 | 50.0 |
| 1-Ethyl-4-methy... | 10.592 | 103.2   | ug/l  | 2300200  | 3                     | 10.055 | 1114770 | 50.0 |
| Octane, 2,6-dim... | 10.781 | 143.0   | ug/l  | 3187290  | 3                     | 10.055 | 1114770 | 50.0 |
| Cyclohexane, pr... | 10.860 | 97.2    | ug/l  | 2168020  | 3                     | 10.055 | 1114770 | 50.0 |
| Undecane, 6-met... | 10.897 | 70.2    | ug/l  | 1565650  | 3                     | 10.055 | 1114770 | 50.0 |
| Cyclohexane, pe... | 12.890 | 55.4    | ug/l  | 2383420  | 4                     | 12.024 | 2151750 | 50.0 |
| unknown13.420      | 13.420 | 59.7    | ug/l  | 2568470  | 4                     | 12.024 | 2151750 | 50.0 |