

Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_X\DATA\VX010320\  
 Data File : VX014404.D  
 Acq On : 03 Jan 2020 16:37  
 Operator : JC/SP  
 Sample : K6476-06  
 Misc : 7.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 WP022SB455\_191227-14-16ME

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M

Title : SW846 8260

Signal : TIC

| 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         | 1.070       | 26            | 30          | 42           | rBV      | 520157         | 667989        | 10.30%          | 0.513%        |
| 2         | 1.631       | 105           | 122         | 123          | rBV      | 78157          | 260858        | 4.02%           | 0.200%        |
| 3         | 5.496       | 743           | 756         | 771          | rBV      | 238656         | 887417        | 13.68%          | 0.681%        |
| 4         | 5.648       | 772           | 781         | 800          | rVB      | 496240         | 1532144       | 23.61%          | 1.176%        |
| 5         | 6.051       | 837           | 847         | 861          | rBV      | 279468         | 809303        | 12.47%          | 0.621%        |
| 6         | 6.849       | 969           | 978         | 994          | rBV      | 726043         | 1826320       | 28.15%          | 1.402%        |
| 7         | 7.453       | 1069          | 1077        | 1084         | rBV      | 155798         | 349081        | 5.38%           | 0.268%        |
| 8         | 8.660       | 1269          | 1275        | 1278         | rBV3     | 146120         | 275790        | 4.25%           | 0.212%        |
| 9         | 8.709       | 1278          | 1283        | 1293         | rVV      | 1554351        | 2623290       | 40.43%          | 2.014%        |
| 10        | 9.440       | 1395          | 1403        | 1413         | rVB      | 151160         | 237841        | 3.67%           | 0.183%        |
| 11        | 9.556       | 1416          | 1422        | 1428         | rBV2     | 165003         | 360222        | 5.55%           | 0.276%        |
| 12        | 9.617       | 1428          | 1432        | 1437         | rVB      | 250262         | 342403        | 5.28%           | 0.263%        |
| 13        | 9.672       | 1437          | 1441        | 1445         | rBV      | 235055         | 353472        | 5.45%           | 0.271%        |
| 14        | 9.873       | 1468          | 1474        | 1479         | rVV3     | 232172         | 559677        | 8.63%           | 0.430%        |
| 15        | 10.062      | 1498          | 1505        | 1508         | rBV      | 406907         | 611539        | 9.43%           | 0.469%        |
| 16        | 10.111      | 1508          | 1513        | 1528         | rVB2     | 1545229        | 3229821       | 49.78%          | 2.479%        |
| 17        | 10.233      | 1528          | 1533        | 1540         | rBV2     | 139822         | 256211        | 3.95%           | 0.197%        |
| 18        | 10.331      | 1540          | 1549        | 1552         | rBV2     | 380930         | 739566        | 11.40%          | 0.568%        |
| 19        | 10.373      | 1552          | 1556        | 1559         | rVV      | 553791         | 792581        | 12.22%          | 0.608%        |
| 20        | 10.404      | 1559          | 1561        | 1573         | rVB3     | 343250         | 695386        | 10.72%          | 0.534%        |
| 21        | 10.507      | 1573          | 1578        | 1583         | rBV2     | 253019         | 383787        | 5.92%           | 0.295%        |
| 22        | 10.635      | 1593          | 1599        | 1607         | rVV3     | 1137823        | 1987634       | 30.63%          | 1.526%        |
| 23        | 10.721      | 1607          | 1613        | 1616         | rVV3     | 646519         | 1058012       | 16.31%          | 0.812%        |
| 24        | 10.763      | 1617          | 1620        | 1623         | rVB2     | 421362         | 523291        | 8.07%           | 0.402%        |
| 25        | 10.830      | 1623          | 1631        | 1635         | rBV      | 3031911        | 4440469       | 68.44%          | 3.408%        |
| 26        | 10.910      | 1635          | 1644        | 1647         | rVV3     | 2358560        | 4332820       | 66.78%          | 3.326%        |
| 27        | 10.946      | 1647          | 1650        | 1655         | rVV      | 1781686        | 2464943       | 37.99%          | 1.892%        |
| 28        | 11.001      | 1655          | 1659        | 1663         | rVB3     | 507027         | 822957        | 12.68%          | 0.632%        |
| 29        | 11.080      | 1668          | 1672        | 1677         | rVB2     | 1715121        | 2496979       | 38.49%          | 1.917%        |
| 30        | 11.135      | 1677          | 1681        | 1685         | rVB2     | 1528828        | 1968398       | 30.34%          | 1.511%        |
| 31        | 11.178      | 1685          | 1688        | 1691         | rBV2     | 366492         | 431511        | 6.65%           | 0.331%        |
| 32        | 11.215      | 1691          | 1694        | 1697         | rBV      | 529549         | 670282        | 10.33%          | 0.514%        |
| 33        | 11.269      | 1697          | 1703        | 1714         | rVB2     | 1984993        | 3244001       | 50.00%          | 2.490%        |
| 34        | 11.391      | 1718          | 1723        | 1727         | rBV2     | 836561         | 1487615       | 22.93%          | 1.142%        |

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 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 WP022SB455\_191227-14-16ME

## Integration Parameters: RTEINT.P

Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
 Title : SW846 8260

|    |        |      |      |      |      |         |         |         |        |
|----|--------|------|------|------|------|---------|---------|---------|--------|
| 35 | 11.440 | 1727 | 1731 | 1734 | rBV3 | 682731  | 863300  | 13.31%  | 0.663% |
| 36 | 11.483 | 1734 | 1738 | 1742 | rBV  | 2553210 | 3346870 | 51.58%  | 2.569% |
| 37 | 11.532 | 1742 | 1746 | 1750 | rVB3 | 1328529 | 2235850 | 34.46%  | 1.716% |
| 38 | 11.574 | 1750 | 1753 | 1758 | rVB5 | 335442  | 464553  | 7.16%   | 0.357% |
| 39 | 11.623 | 1758 | 1761 | 1764 | rBV  | 423576  | 527850  | 8.14%   | 0.405% |
| 40 | 11.653 | 1764 | 1766 | 1767 | rBV  | 457476  | 408818  | 6.30%   | 0.314% |
| 41 | 11.684 | 1767 | 1771 | 1775 | rVB5 | 1014131 | 1602431 | 24.70%  | 1.230% |
| 42 | 11.733 | 1775 | 1779 | 1781 | rBV4 | 500286  | 616099  | 9.50%   | 0.473% |
| 43 | 11.763 | 1781 | 1784 | 1787 | rBV  | 764281  | 788971  | 12.16%  | 0.606% |
| 44 | 11.800 | 1787 | 1790 | 1791 | rBV2 | 557616  | 663107  | 10.22%  | 0.509% |
| 45 | 11.885 | 1800 | 1804 | 1807 | rBV  | 1013989 | 1578938 | 24.34%  | 1.212% |
| 46 | 11.940 | 1807 | 1813 | 1818 | rVV6 | 2169358 | 4977746 | 76.72%  | 3.821% |
| 47 | 11.995 | 1818 | 1822 | 1825 | rVV  | 4614434 | 6155485 | 94.87%  | 4.725% |
| 48 | 12.025 | 1825 | 1827 | 1832 | rVV3 | 1270635 | 1994321 | 30.74%  | 1.531% |
| 49 | 12.074 | 1832 | 1835 | 1841 | rVV2 | 2144395 | 3393936 | 52.31%  | 2.605% |
| 50 | 12.129 | 1841 | 1844 | 1846 | rVB3 | 250961  | 255197  | 3.93%   | 0.196% |
| 51 | 12.166 | 1846 | 1850 | 1851 | rBV3 | 355657  | 466352  | 7.19%   | 0.358% |
| 52 | 12.208 | 1852 | 1857 | 1860 | rVB4 | 620696  | 1098427 | 16.93%  | 0.843% |
| 53 | 12.300 | 1867 | 1872 | 1877 | rBV4 | 841466  | 1561400 | 24.07%  | 1.198% |
| 54 | 12.367 | 1878 | 1883 | 1890 | rVV2 | 3445949 | 6488167 | 100.00% | 4.980% |
| 55 | 12.470 | 1891 | 1900 | 1905 | rVV2 | 1510055 | 3536310 | 54.50%  | 2.714% |
| 56 | 12.519 | 1905 | 1908 | 1913 | rVB4 | 1705483 | 2884262 | 44.45%  | 2.214% |
| 57 | 12.605 | 1916 | 1922 | 1928 | rBV6 | 1511688 | 3525597 | 54.34%  | 2.706% |
| 58 | 12.733 | 1938 | 1943 | 1944 | rBV4 | 198113  | 377521  | 5.82%   | 0.290% |
| 59 | 12.775 | 1947 | 1950 | 1954 | rVV4 | 562923  | 997199  | 15.37%  | 0.765% |
| 60 | 12.812 | 1954 | 1956 | 1961 | rVV4 | 581830  | 991913  | 15.29%  | 0.761% |
| 61 | 12.873 | 1961 | 1966 | 1972 | rVB3 | 3041523 | 4798755 | 73.96%  | 3.683% |
| 62 | 12.940 | 1972 | 1977 | 1980 | rBV2 | 2263075 | 3362206 | 51.82%  | 2.581% |
| 63 | 12.976 | 1980 | 1983 | 1987 | rVB2 | 1607666 | 2076707 | 32.01%  | 1.594% |
| 64 | 13.037 | 1988 | 1993 | 1997 | rBV2 | 2326573 | 2878536 | 44.37%  | 2.209% |
| 65 | 13.074 | 1997 | 1999 | 2007 | rVB4 | 974450  | 1689467 | 26.04%  | 1.297% |
| 66 | 13.147 | 2007 | 2011 | 2016 | rBV2 | 525111  | 1021275 | 15.74%  | 0.784% |
| 67 | 13.263 | 2027 | 2030 | 2033 | rBV2 | 225334  | 247439  | 3.81%   | 0.190% |
| 68 | 13.306 | 2033 | 2037 | 2040 | rVB3 | 243863  | 378317  | 5.83%   | 0.290% |
| 69 | 13.348 | 2040 | 2044 | 2049 | rVB4 | 906795  | 1267975 | 19.54%  | 0.973% |
| 70 | 13.421 | 2053 | 2056 | 2058 | rVB  | 434479  | 410960  | 6.33%   | 0.315% |
| 71 | 13.464 | 2058 | 2063 | 2075 | rVB8 | 770587  | 2204059 | 33.97%  | 1.692% |

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 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 WP022SB455\_191227-14-16ME

## Integration Parameters: RTEINT.P

Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
 Title : SW846 8260

|     |        |      |      |      |      |         |         |        |        |
|-----|--------|------|------|------|------|---------|---------|--------|--------|
| 72  | 13.562 | 2075 | 2079 | 2083 | rBV5 | 268536  | 612979  | 9.45%  | 0.470% |
| 73  | 13.629 | 2087 | 2090 | 2095 | rBV3 | 585990  | 809217  | 12.47% | 0.621% |
| 74  | 13.677 | 2095 | 2098 | 2099 | rVV2 | 192510  | 237082  | 3.65%  | 0.182% |
| 75  | 13.726 | 2103 | 2106 | 2109 | rVB3 | 336970  | 455865  | 7.03%  | 0.350% |
| 76  | 13.806 | 2113 | 2119 | 2124 | rBV3 | 553852  | 948355  | 14.62% | 0.728% |
| 77  | 13.854 | 2124 | 2127 | 2130 | rBV2 | 298380  | 353562  | 5.45%  | 0.271% |
| 78  | 13.903 | 2131 | 2135 | 2141 | rVB5 | 269481  | 432257  | 6.66%  | 0.332% |
| 79  | 13.982 | 2146 | 2148 | 2152 | rVB3 | 238699  | 307125  | 4.73%  | 0.236% |
| 80  | 14.043 | 2152 | 2158 | 2161 | rBV6 | 134389  | 320472  | 4.94%  | 0.246% |
| 81  | 14.123 | 2167 | 2171 | 2174 | rBV4 | 251811  | 386466  | 5.96%  | 0.297% |
| 82  | 14.214 | 2180 | 2186 | 2191 | rBV6 | 198557  | 402852  | 6.21%  | 0.309% |
| 83  | 14.269 | 2191 | 2195 | 2199 | rBV3 | 324474  | 489035  | 7.54%  | 0.375% |
| 84  | 14.354 | 2206 | 2209 | 2216 | rVB2 | 397134  | 734944  | 11.33% | 0.564% |
| 85  | 14.470 | 2225 | 2228 | 2231 | rBV3 | 270302  | 385435  | 5.94%  | 0.296% |
| 86  | 14.537 | 2235 | 2239 | 2243 | rBV5 | 227970  | 421264  | 6.49%  | 0.323% |
| 87  | 14.665 | 2258 | 2260 | 2267 | rVB7 | 217003  | 387535  | 5.97%  | 0.297% |
| 88  | 14.726 | 2267 | 2270 | 2273 | rBV2 | 364028  | 415622  | 6.41%  | 0.319% |
| 89  | 14.781 | 2274 | 2279 | 2281 | rBV4 | 324639  | 520818  | 8.03%  | 0.400% |
| 90  | 14.842 | 2286 | 2289 | 2296 | rVV8 | 246718  | 508213  | 7.83%  | 0.390% |
| 91  | 14.903 | 2296 | 2299 | 2306 | rVV7 | 179388  | 415725  | 6.41%  | 0.319% |
| 92  | 14.964 | 2306 | 2309 | 2311 | rVV  | 212912  | 261232  | 4.03%  | 0.201% |
| 93  | 14.988 | 2311 | 2313 | 2318 | rVB2 | 208438  | 255748  | 3.94%  | 0.196% |
| 94  | 15.116 | 2329 | 2334 | 2335 | rBV4 | 208865  | 339170  | 5.23%  | 0.260% |
| 95  | 15.147 | 2335 | 2339 | 2344 | rVB  | 1308473 | 1708800 | 26.34% | 1.312% |
| 96  | 15.244 | 2350 | 2355 | 2358 | rBV5 | 199722  | 430151  | 6.63%  | 0.330% |
| 97  | 15.281 | 2358 | 2361 | 2366 | rVB  | 572667  | 793169  | 12.22% | 0.609% |
| 98  | 15.683 | 2422 | 2427 | 2431 | rBV  | 390740  | 612440  | 9.44%  | 0.470% |
| 99  | 15.732 | 2431 | 2435 | 2441 | rVB5 | 147185  | 244166  | 3.76%  | 0.187% |
| 100 | 16.067 | 2486 | 2490 | 2498 | rBV5 | 84268   | 233530  | 3.60%  | 0.179% |

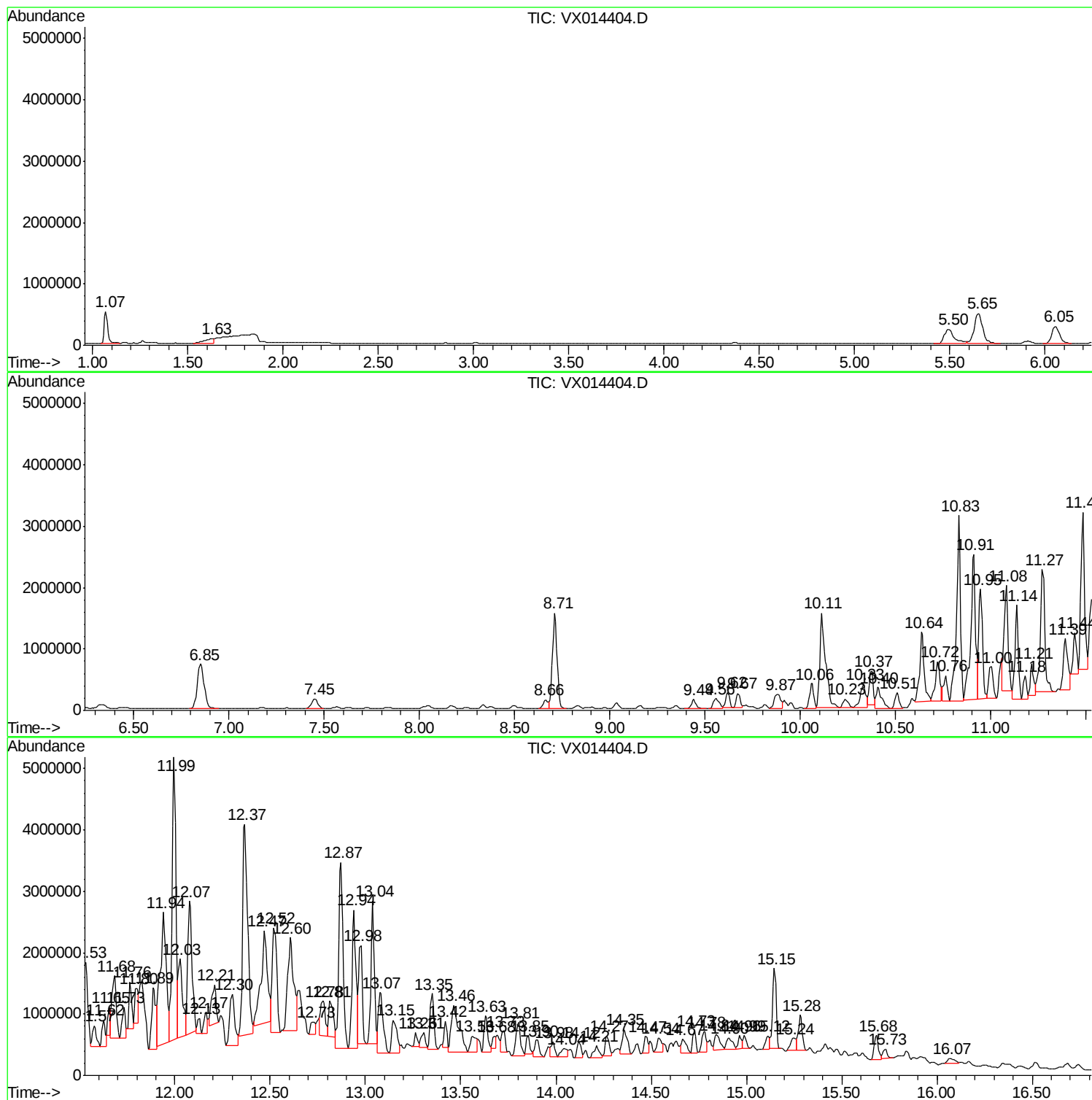
Sum of corrected areas: 130283155

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Instrument :  
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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WP022SB455\_191227-14-16ME

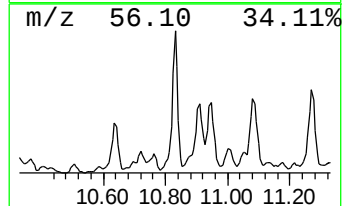
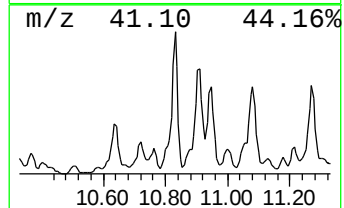
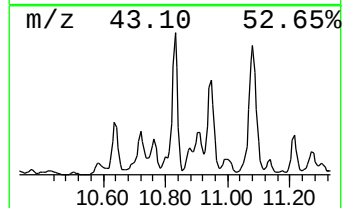
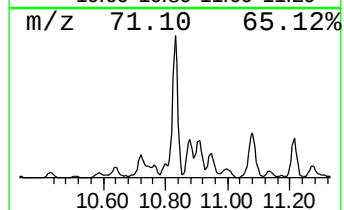
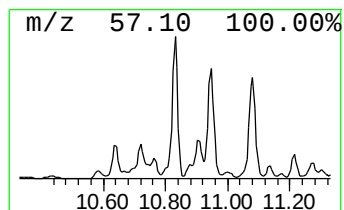
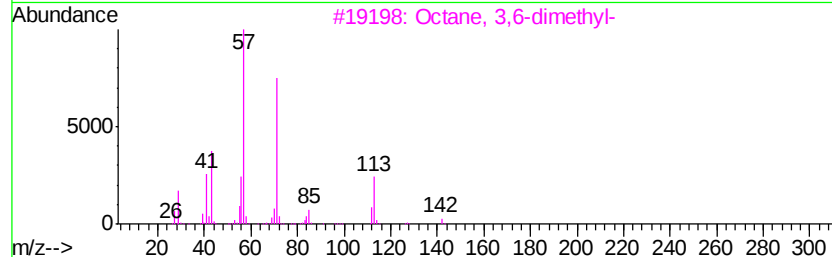
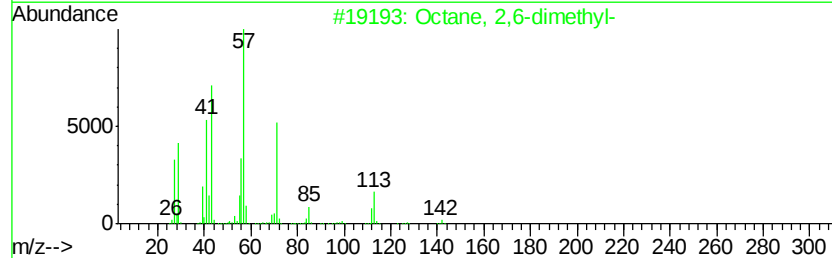
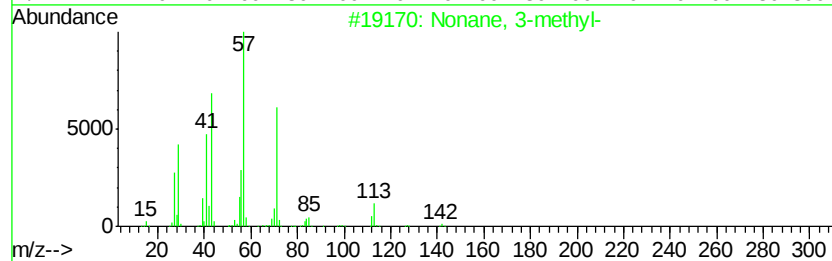
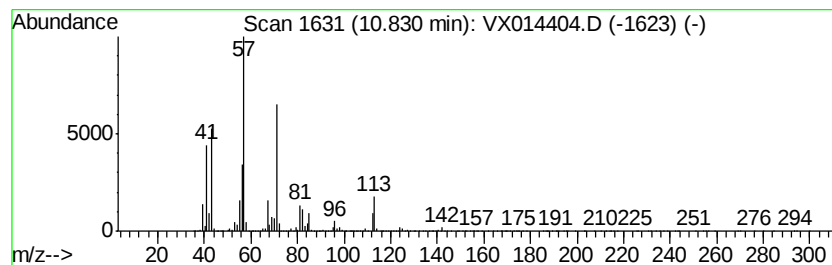
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Nonane, 3-methyl- Concentration Rank 3

| R.T.  | EstConc    | Area    | Relative to ISTD | R.T.  |
|-------|------------|---------|------------------|-------|
| 10.83 | 68.74 ug/l | 4440470 | Chlorobenzene-d5 | 10.11 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | Nonane, 3-methyl-                   | 142 | C10H22    | 005911-04-6  | 87   |
| 2    |    | Octane, 2,6-dimethyl-               | 142 | C10H22    | 002051-30-1  | 87   |
| 3    |    | Octane, 3,6-dimethyl-               | 142 | C10H22    | 015869-94-0  | 81   |
| 4    |    | Sulfurous acid, butyl 2-ethylhex... | 250 | C12H26O3S | 1000309-18-8 | 59   |
| 5    |    | Undecane, 4,5-dimethyl-             | 184 | C13H28    | 017312-79-7  | 53   |



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ALS Vial : 15 Sample Multiplier: 1

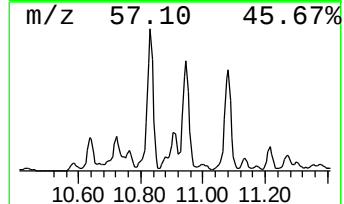
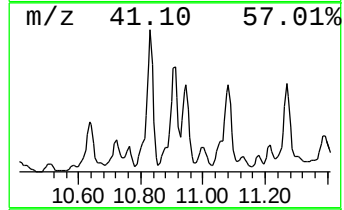
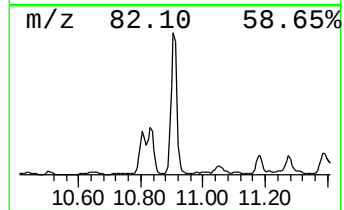
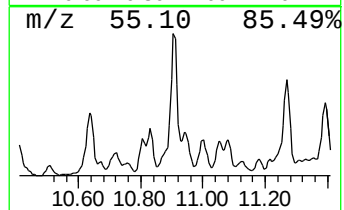
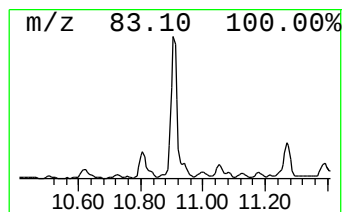
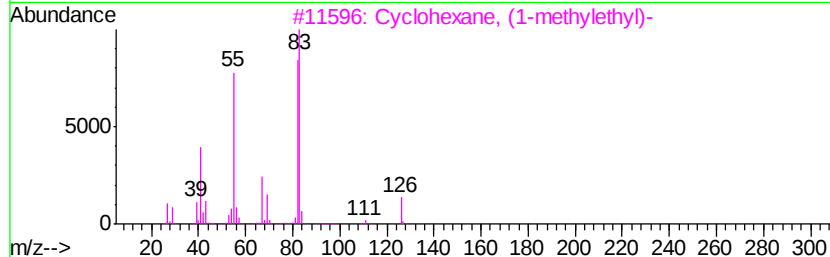
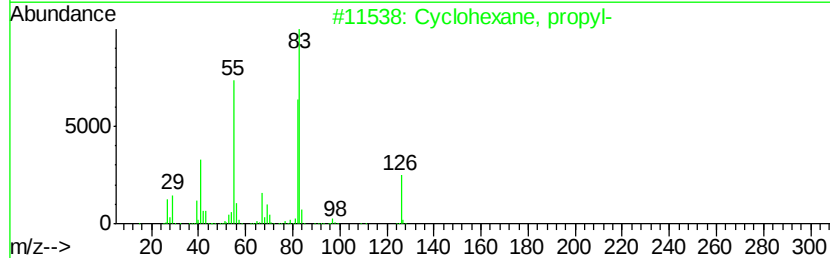
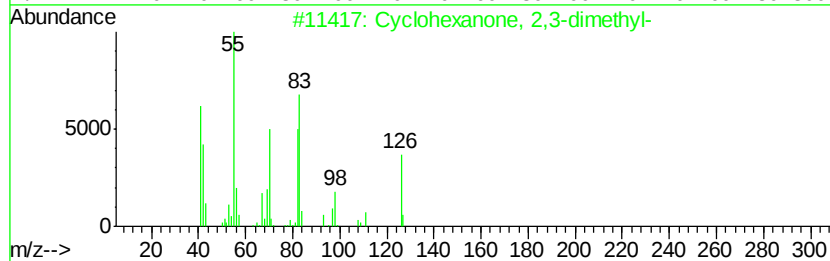
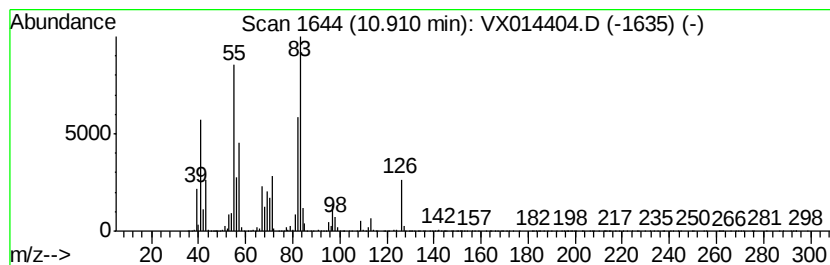
Instrument :  
MSVOA\_X  
ClientSampleId :  
WP022SB455\_191227-14-16ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Cyclohexanone, 2,3-dimethyl- Concentration Rank 4

| R.T.    | EstConc    | Area                          | Relative to ISTD | R.T.           |
|---------|------------|-------------------------------|------------------|----------------|
| 10.91   | 67.08 ug/l | 4332820                       | Chlorobenzene-d5 | 10.11          |
| Hit# of | 5          | Tentative ID                  | MW MolForm       | CAS# Qual      |
| 1       |            | Cyclohexanone, 2,3-dimethyl-  | 126 C8H14O       | 013395-76-1 83 |
| 2       |            | Cyclohexane, propyl-          | 126 C9H18        | 001678-92-8 68 |
| 3       |            | Cyclohexane, (1-methylethyl)- | 126 C9H18        | 000696-29-7 64 |
| 4       |            | Cyclohexane, butyl-           | 140 C10H20       | 001678-93-9 59 |
| 5       |            | Ethanone, 1-cyclohexyl-       | 126 C8H14O       | 000823-76-7 46 |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_X\DATA\VX010320\  
Data File : VX014404.D  
Acq On : 03 Jan 2020 16:37  
Operator : JC/SP  
Sample : K6476-06  
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WP022SB455\_191227-14-16ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
Quant Title : SW846 8260

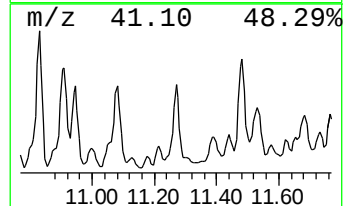
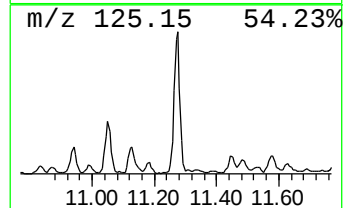
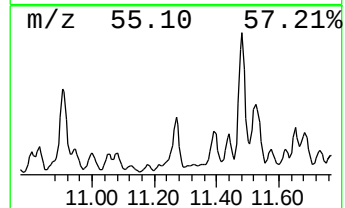
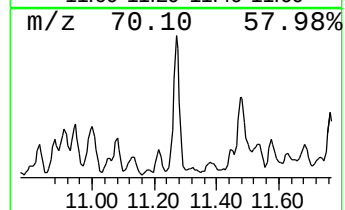
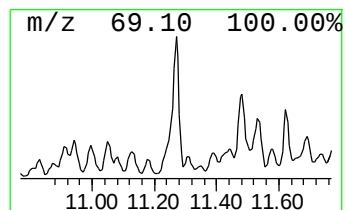
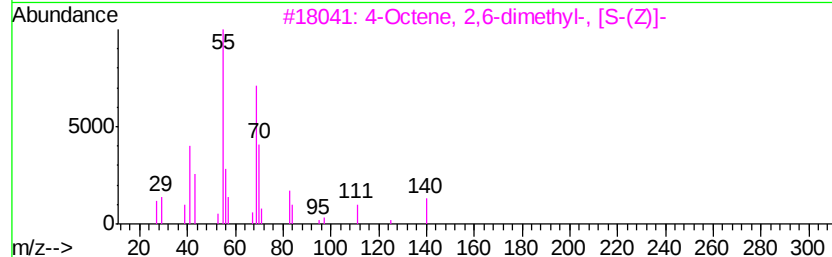
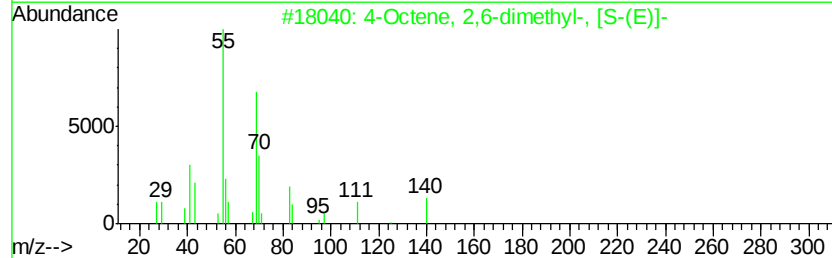
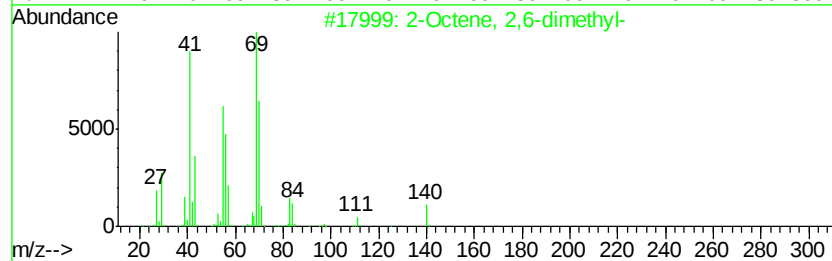
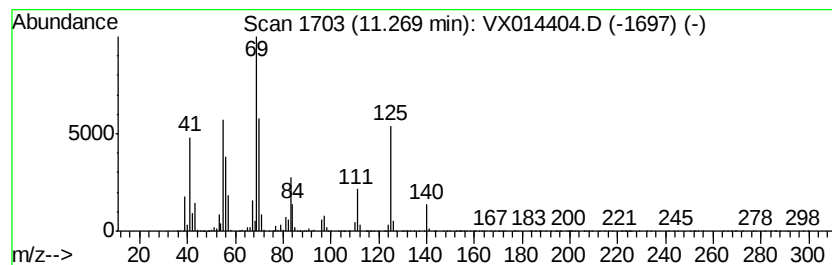
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 2-Octene, 2,6-dimethyl- Concentration Rank 9

| R.T.  | EstConc    | Area    | Relative to ISTD       | R.T.  |
|-------|------------|---------|------------------------|-------|
| 11.27 | 47.79 ug/l | 3244000 | 1,4-Dichlorobenzene-d4 | 12.07 |

| Hit# | of | Tentative ID                      | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Octene, 2,6-dimethyl-           | 140 | C10H20  | 004057-42-5 | 70   |
| 2    |    | 4-Octene, 2,6-dimethyl-, [S-(E)]- | 140 | C10H20  | 062960-76-3 | 59   |
| 3    |    | 4-Octene, 2,6-dimethyl-, [S-(Z)]- | 140 | C10H20  | 062960-77-4 | 58   |
| 4    |    | 3-Ethyl-4-octene                  | 140 | C10H20  | 019781-32-9 | 55   |
| 5    |    | 3-Nonene, 3-methyl-, (E)-         | 140 | C10H20  | 069405-42-1 | 50   |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_X\DATA\VX010320\  
Data File : VX014404.D  
Acq On : 03 Jan 2020 16:37  
Operator : JC/SP  
Sample : K6476-06  
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WP022SB455\_191227-14-16ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
Quant Title : SW846 8260

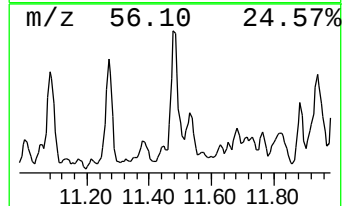
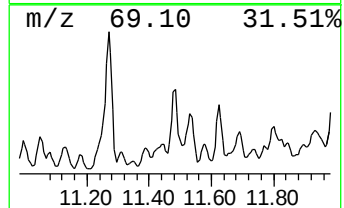
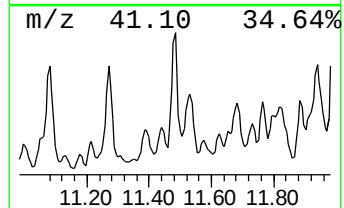
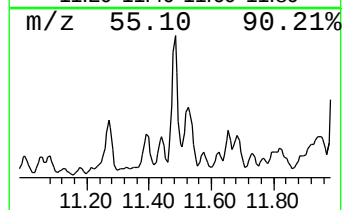
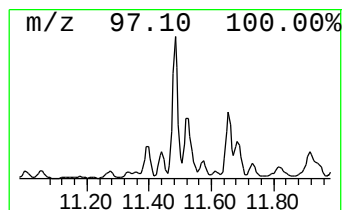
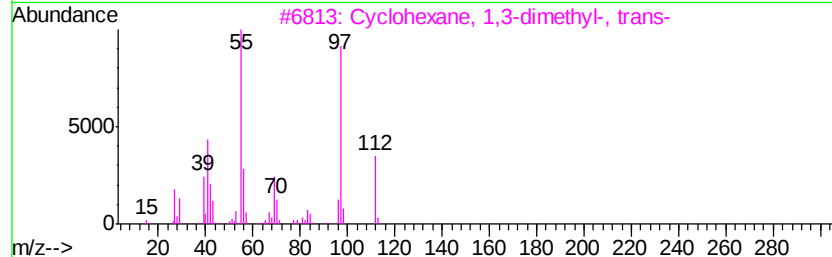
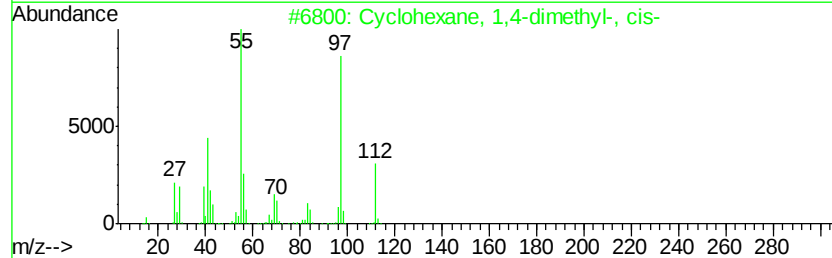
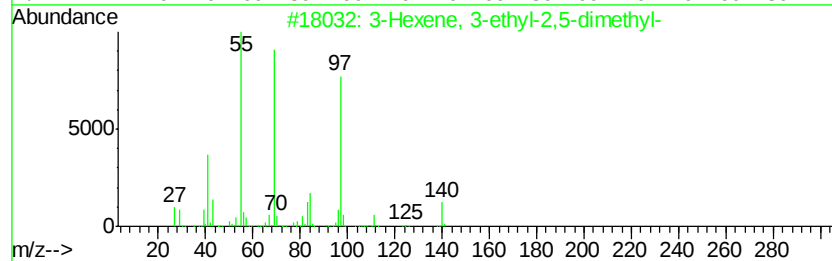
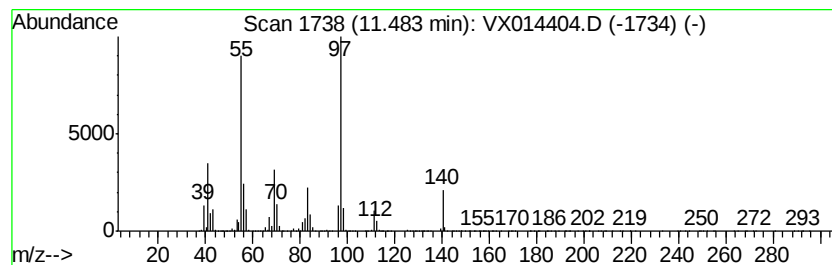
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 3-Hexene, 3-ethyl-2,5-dimet... Concentration Rank 8

| R.T.  | EstConc    | Area    | Relative to ISTD       | R.T.  |
|-------|------------|---------|------------------------|-------|
| 11.48 | 49.31 ug/l | 3346870 | 1,4-Dichlorobenzene-d4 | 12.07 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Hexene, 3-ethyl-2,5-dimethyl-     | 140 | C10H20    | 062338-08-3  | 64   |
| 2    |    | Cyclohexane, 1,4-dimethyl-, cis-    | 112 | C8H16     | 000624-29-3  | 59   |
| 3    |    | Cyclohexane, 1,3-dimethyl-, trans-  | 112 | C8H16     | 002207-03-6  | 59   |
| 4    |    | Sulfurous acid, cyclohexylmethyl... | 262 | C13H26O3S | 1000309-21-6 | 53   |
| 5    |    | Cyclohexane, 1-methyl-3-propyl-     | 140 | C10H20    | 004291-80-9  | 53   |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_X\DATA\VX010320\  
Data File : VX014404.D  
Acq On : 03 Jan 2020 16:37  
Operator : JC/SP  
Sample : K6476-06  
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WP022SB455\_191227-14-16ME

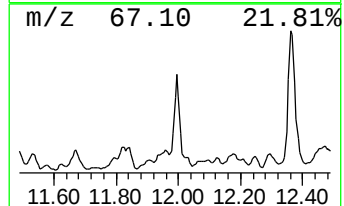
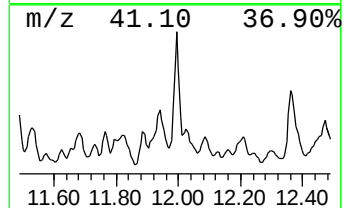
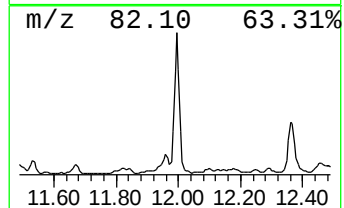
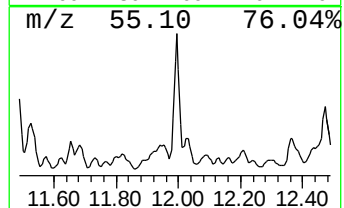
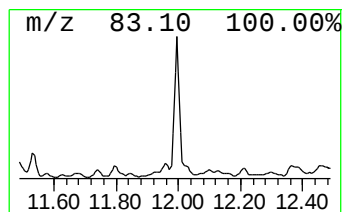
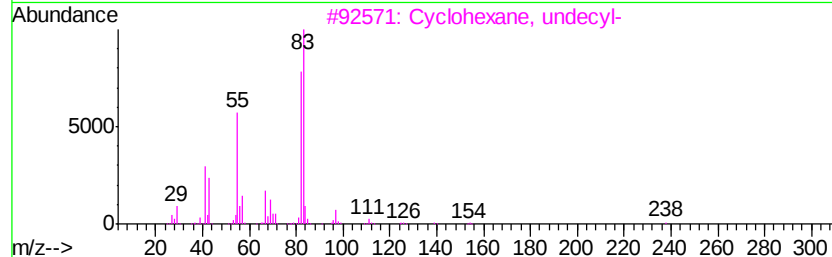
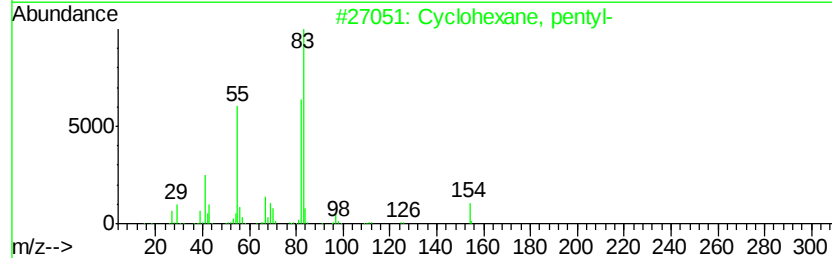
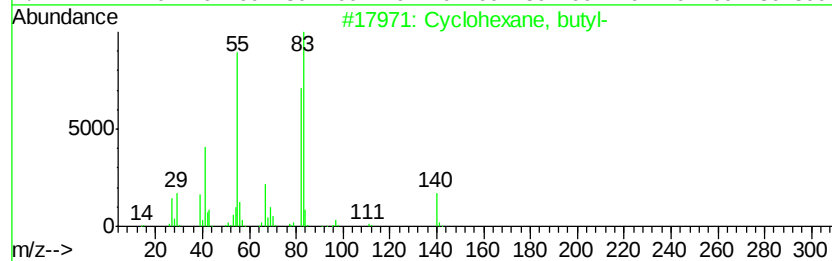
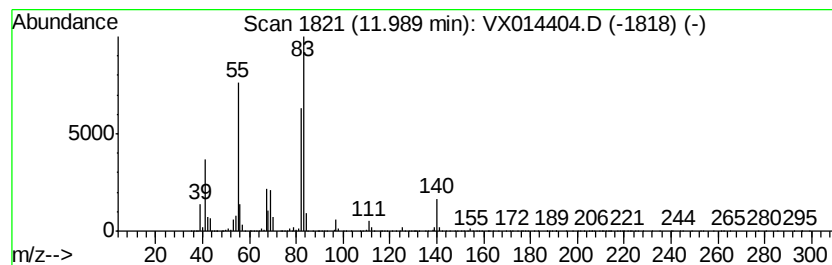
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Cyclohexane, butyl- Concentration Rank 1

| R.T.  | EstConc    | Area    | Relative to ISTD       | R.T.  |
|-------|------------|---------|------------------------|-------|
| 11.99 | 90.68 ug/l | 6155490 | 1,4-Dichlorobenzene-d4 | 12.07 |

| Hit# | of | Tentative ID                  | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------|-----|---------|-------------|------|
| 1    | 5  | Cyclohexane, butyl-           | 140 | C10H20  | 001678-93-9 | 91   |
| 2    |    | Cyclohexane, pentyl-          | 154 | C11H22  | 004292-92-6 | 87   |
| 3    |    | Cyclohexane, undecyl-         | 238 | C17H34  | 054105-66-7 | 72   |
| 4    |    | Cyclohexane, propyl-          | 126 | C9H18   | 001678-92-8 | 72   |
| 5    |    | Cyclohexane, (1-methylethyl)- | 126 | C9H18   | 000696-29-7 | 72   |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_X\DATA\VX010320\  
Data File : VX014404.D  
Acq On : 03 Jan 2020 16:37  
Operator : JC/SP  
Sample : K6476-06  
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 15 Sample Multiplier: 1

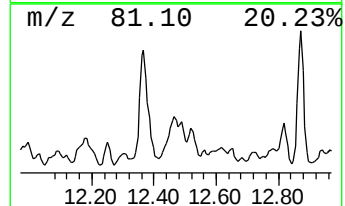
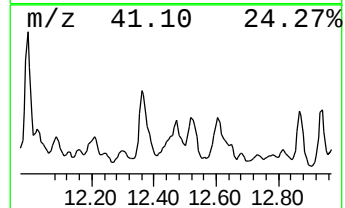
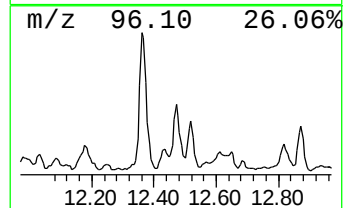
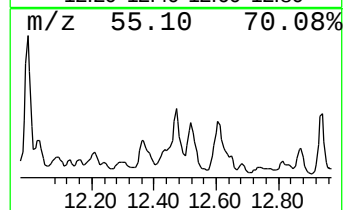
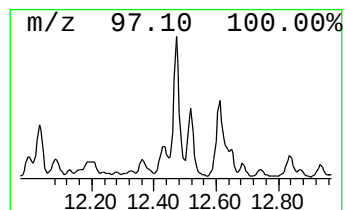
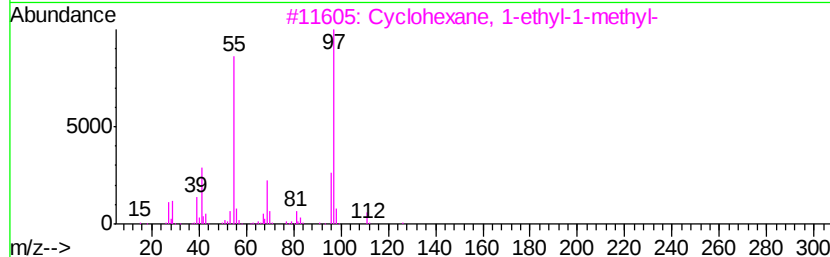
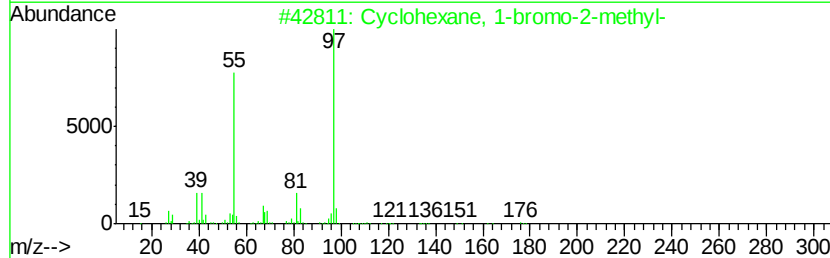
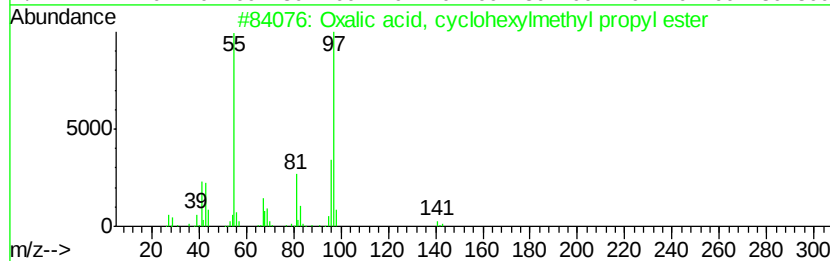
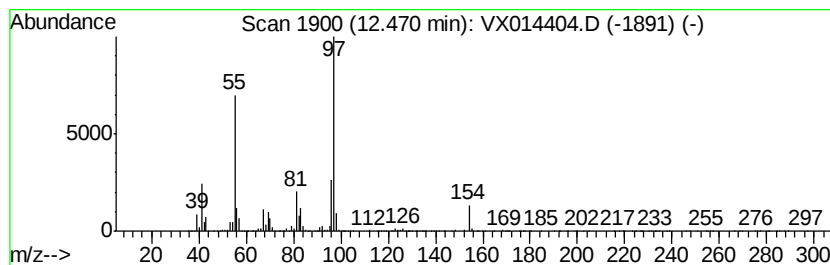
Instrument :  
MSVOA\_X  
ClientSampleId :  
WP022SB455\_191227-14-16ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Oxalic acid, cyclohexylmeth... Concentration Rank 5

| R.T.    | EstConc    | Area                                | Relative to ISTD       | R.T.            |
|---------|------------|-------------------------------------|------------------------|-----------------|
| 12.47   | 52.10 ug/l | 3536310                             | 1,4-Dichlorobenzene-d4 | 12.07           |
| Hit# of | 5          | Tentative ID                        | MW MolForm             | CAS# Qual       |
| 1       |            | Oxalic acid, cyclohexylmethyl pr... | 228 C12H20O4           | 1000309-68-1 78 |
| 2       |            | Cyclohexane, 1-bromo-2-methyl-      | 176 C7H13Br            | 006294-39-9 74  |
| 3       |            | Cyclohexane, 1-ethyl-1-methyl-      | 126 C9H18              | 004926-90-3 72  |
| 4       |            | Sulfurous acid, cyclohexylmethyl... | 262 C13H26O3S          | 1000309-21-5 64 |
| 5       |            | Cyclohexanone, 3-butyl-             | 154 C10H18O            | 039178-69-3 64  |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_X\DATA\VX010320\  
Data File : VX014404.D  
Acq On : 03 Jan 2020 16:37  
Operator : JC/SP  
Sample : K6476-06  
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 15 Sample Multiplier: 1

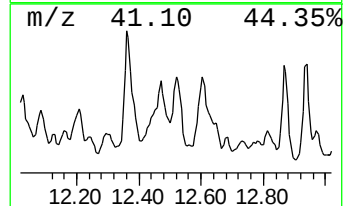
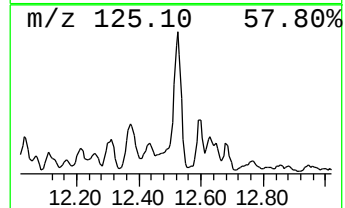
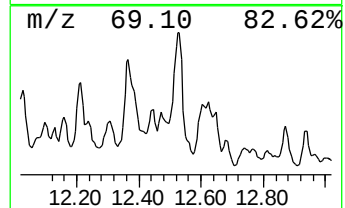
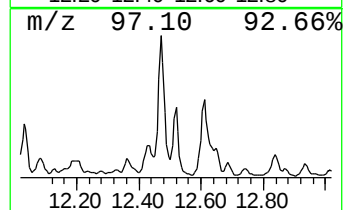
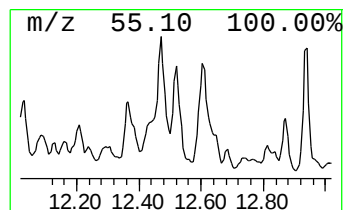
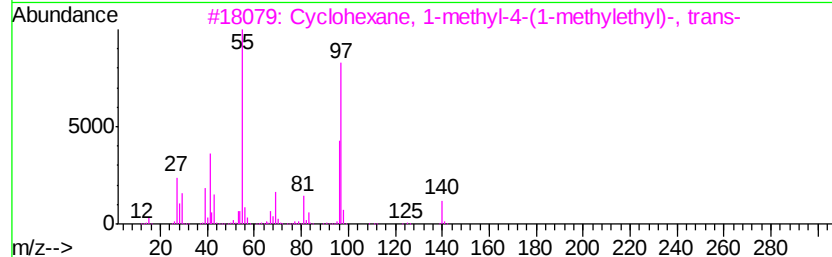
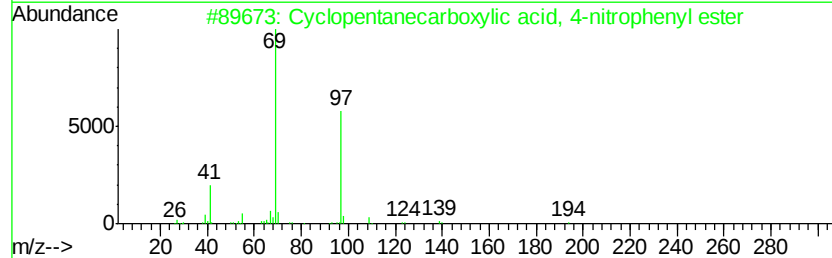
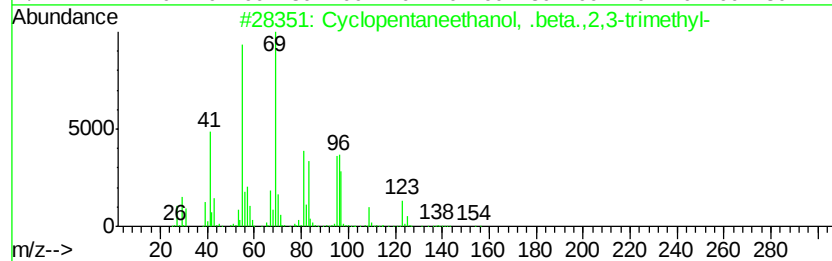
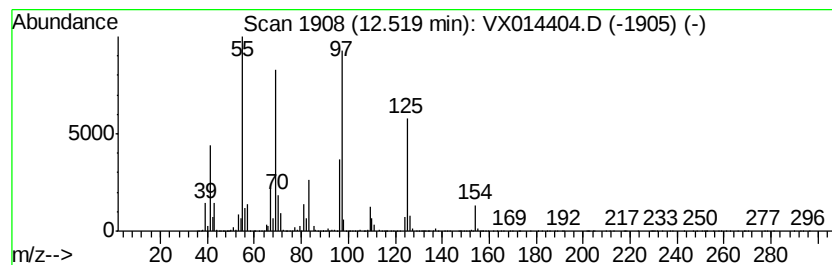
Instrument :  
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ClientSampleId :  
WP022SB455\_191227-14-16ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 unknown12.52 Concentration Rank 10

| R.T.    | EstConc    | Area                                | Relative to ISTD       | R.T.            |
|---------|------------|-------------------------------------|------------------------|-----------------|
| 12.52   | 42.49 ug/l | 2884260                             | 1,4-Dichlorobenzene-d4 | 12.07           |
| Hit# of | 5          | Tentative ID                        | MW MolForm             | CAS# Qual       |
| 1       |            | Cyclopentaneethanol, .beta.,2,3-... | 156 C10H20O            | 021721-18-6 47  |
| 2       |            | Cyclopentanecarboxylic acid, 4-n... | 235 C12H13NO4          | 1000307-58-0 47 |
| 3       |            | Cyclohexane, 1-methyl-4-(1-methy... | 140 C10H20             | 001678-82-6 35  |
| 4       |            | Cyclohexane, 1-ethyl-4-methyl-, ... | 126 C9H18              | 004926-78-7 35  |
| 5       |            | Oxalic acid, di(cyclohexylmethyl... | 282 C16H26O4           | 1000309-68-5 35 |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_X\DATA\VX010320\  
Data File : VX014404.D  
Acq On : 03 Jan 2020 16:37  
Operator : JC/SP  
Sample : K6476-06  
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 15 Sample Multiplier: 1

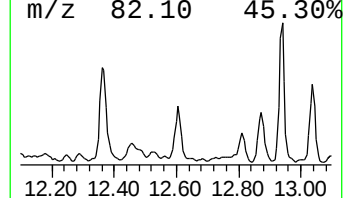
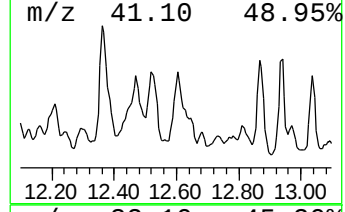
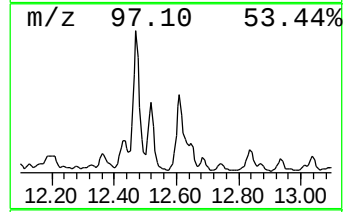
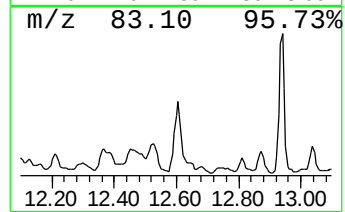
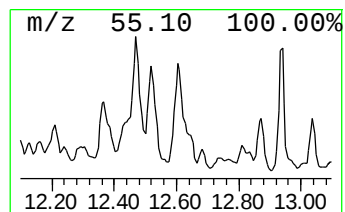
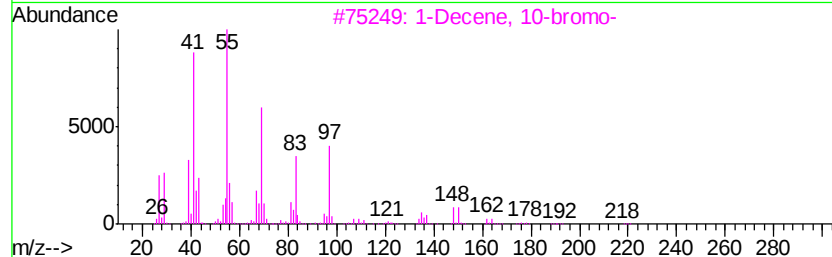
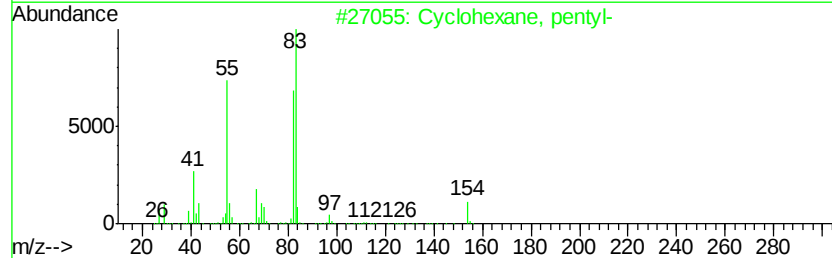
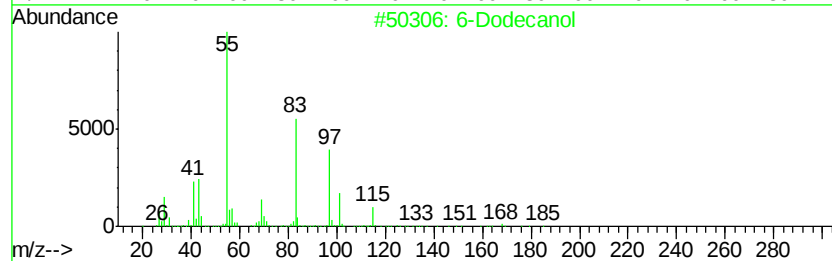
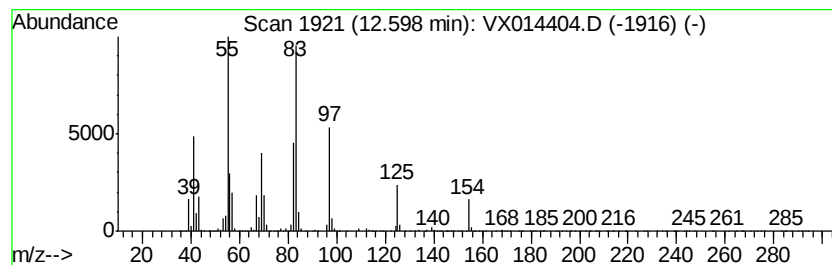
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WP022SB455\_191227-14-16ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 8 6-Dodecanol Concentration Rank 6

| R.T.    | EstConc                            | Area         | Relative to ISTD       | R.T.      |
|---------|------------------------------------|--------------|------------------------|-----------|
| 12.60   | 51.94 ug/l                         | 3525600      | 1,4-Dichlorobenzene-d4 | 12.07     |
| Hit# of | 5                                  | Tentative ID | MW MolForm             | CAS# Qual |
| 1       | 6-Dodecanol                        | 186 C12H26O  | 006836-38-0            | 53        |
| 2       | Cyclohexane, pentyl-               | 154 C11H22   | 004292-92-6            | 47        |
| 3       | 1-Decene, 10-bromo-                | 218 C10H19Br | 062871-09-4            | 47        |
| 4       | Cyclohexane, 1,3-dimethyl-, trans- | 112 C8H16    | 002207-03-6            | 43        |
| 5       | Cyclohexane, propyl-               | 126 C9H18    | 001678-92-8            | 43        |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_X\DATA\VX010320\  
Data File : VX014404.D  
Acq On : 03 Jan 2020 16:37  
Operator : JC/SP  
Sample : K6476-06  
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WP022SB455\_191227-14-16ME

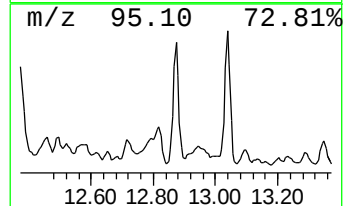
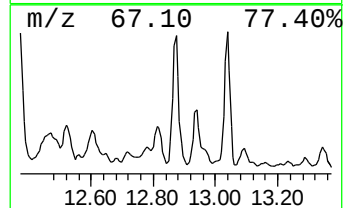
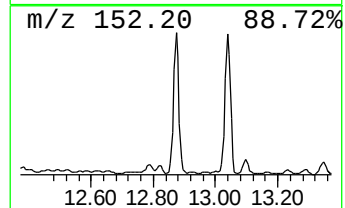
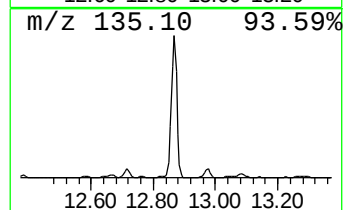
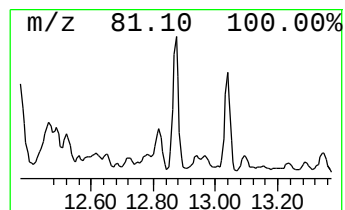
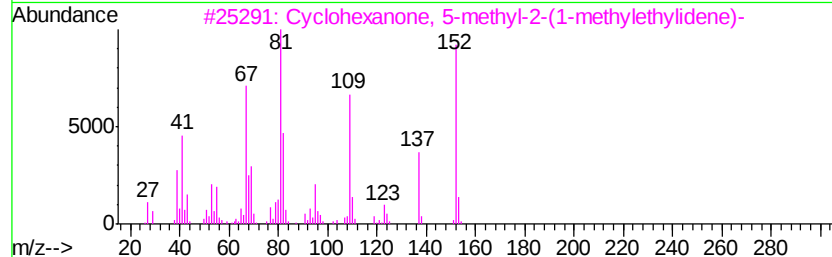
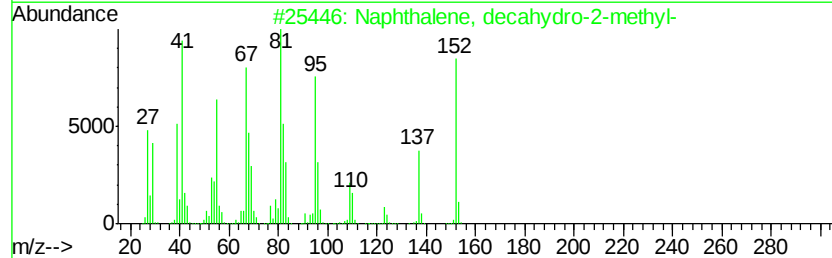
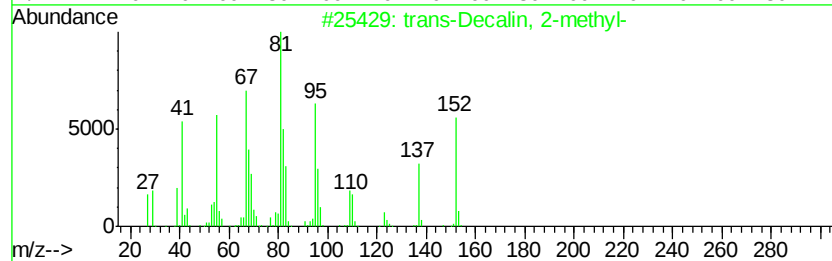
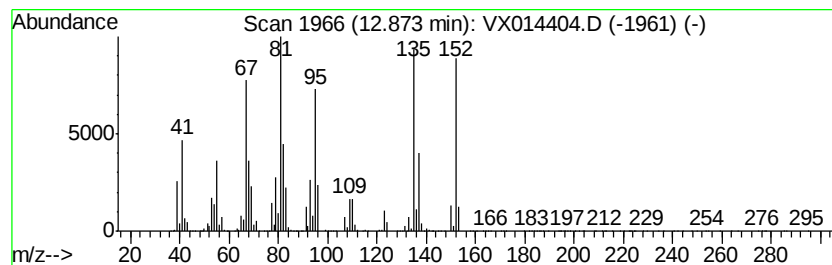
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 9 trans-Decalin, 2-methyl- Concentration Rank 2

| R.T.  | EstConc    | Area    | Relative to ISTD       | R.T.  |
|-------|------------|---------|------------------------|-------|
| 12.87 | 70.70 ug/l | 4798760 | 1,4-Dichlorobenzene-d4 | 12.07 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|-------------------------------------|-----|---------|--------------|------|
| 1    | 5  | trans-Decalin, 2-methyl-            | 152 | C11H20  | 1000152-47-3 | 95   |
| 2    |    | Naphthalene, decahydro-2-methyl-    | 152 | C11H20  | 002958-76-1  | 93   |
| 3    |    | Cyclohexanone, 5-methyl-2-(1-met... | 152 | C10H16O | 015932-80-6  | 86   |
| 4    |    | Pulegone                            | 152 | C10H16O | 000089-82-7  | 64   |
| 5    |    | 9-Methylbicyclo[3.3.1]nonane        | 138 | C10H18  | 025107-01-1  | 45   |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_X\DATA\VX010320\  
Data File : VX014404.D  
Acq On : 03 Jan 2020 16:37  
Operator : JC/SP  
Sample : K6476-06  
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 15 Sample Multiplier: 1

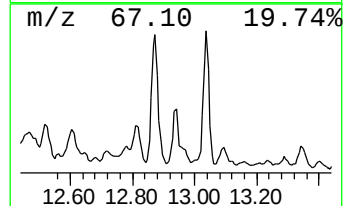
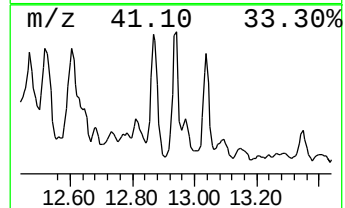
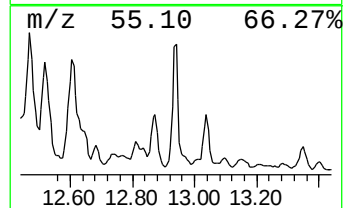
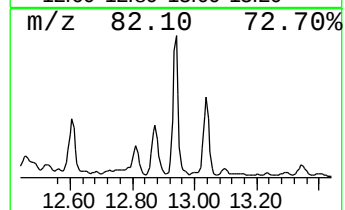
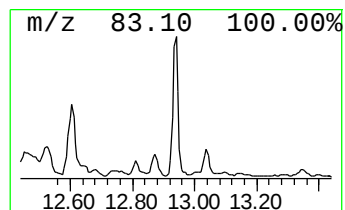
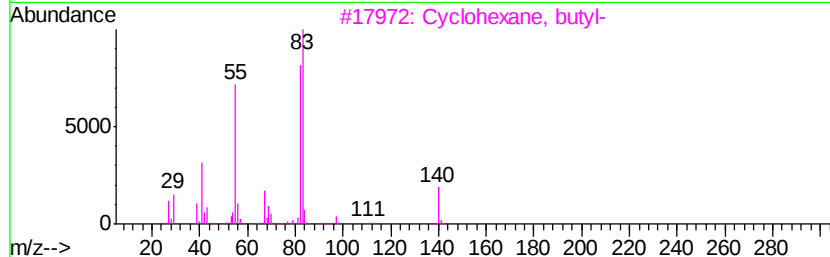
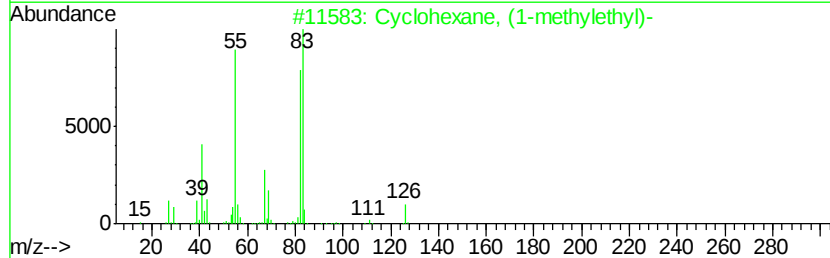
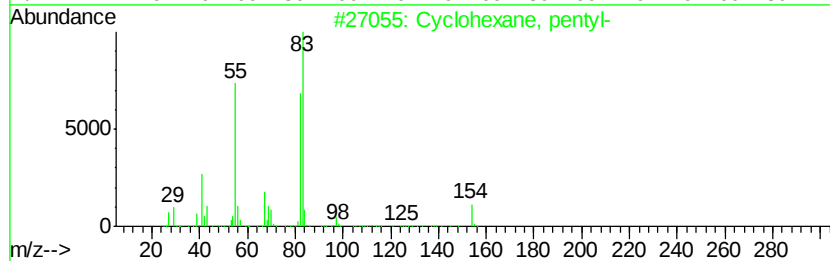
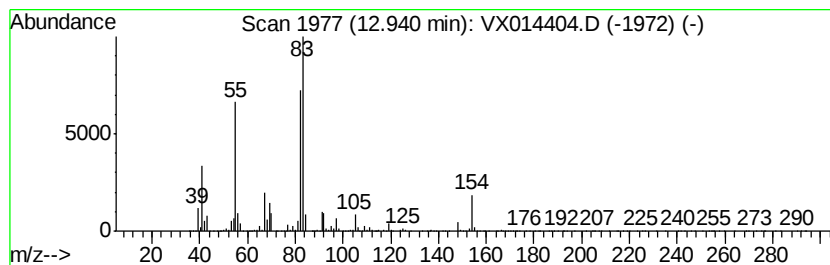
Instrument :  
MSVOA\_X  
ClientSampleId :  
WP022SB455\_191227-14-16ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 10 Cyclohexane, pentyl- Concentration Rank 7

| R.T.    | EstConc    | Area                           | Relative to ISTD       | R.T.           |
|---------|------------|--------------------------------|------------------------|----------------|
| 12.94   | 49.53 ug/l | 3362210                        | 1,4-Dichlorobenzene-d4 | 12.07          |
| Hit# of | 5          | Tentative ID                   | MW MolForm             | CAS# Qual      |
| 1       |            | Cyclohexane, pentyl-           | 154 C11H22             | 004292-92-6 91 |
| 2       |            | Cyclohexane, (1-methylethyl)-  | 126 C9H18              | 000696-29-7 64 |
| 3       |            | Cyclohexane, butyl-            | 140 C10H20             | 001678-93-9 64 |
| 4       |            | Cyclohexane, octyl-            | 196 C14H28             | 001795-15-9 64 |
| 5       |            | Cyclohexane, (2-methylpropyl)- | 140 C10H20             | 001678-98-4 59 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_X\DATA\VX010320\  
Data File : VX014404.D  
Acq On : 03 Jan 2020 16:37  
Operator : JC/SP  
Sample : K6476-06  
Misc : 7.22g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
WP022SB455\_191227-14-16ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X121319W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| Nonane, 3-methyl-    | 10.83 | 68.7    | ug/l  | 4440470  | 3                     | 10.11 | 3229820 | 50.0 |
| Cyclohexanone, 2,... | 10.91 | 67.1    | ug/l  | 4332820  | 3                     | 10.11 | 3229820 | 50.0 |
| 2-Octene, 2,6-dim... | 11.27 | 47.8    | ug/l  | 3244000  | 4                     | 12.07 | 3393940 | 50.0 |
| 3-Hexene, 3-ethyl... | 11.48 | 49.3    | ug/l  | 3346870  | 4                     | 12.07 | 3393940 | 50.0 |
| Cyclohexane, butyl-  | 11.99 | 90.7    | ug/l  | 6155490  | 4                     | 12.07 | 3393940 | 50.0 |
| Oxalic acid, cycl... | 12.47 | 52.1    | ug/l  | 3536310  | 4                     | 12.07 | 3393940 | 50.0 |
| unknown12.52         | 12.52 | 42.5    | ug/l  | 2884260  | 4                     | 12.07 | 3393940 | 50.0 |
| 6-Dodecanol          | 12.60 | 51.9    | ug/l  | 3525600  | 4                     | 12.07 | 3393940 | 50.0 |
| trans-Decalin, 2-... | 12.87 | 70.7    | ug/l  | 4798760  | 4                     | 12.07 | 3393940 | 50.0 |
| Cyclohexane, pentyl- | 12.94 | 49.5    | ug/l  | 3362210  | 4                     | 12.07 | 3393940 | 50.0 |