

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX071524\  
 Data File : VX042323.D  
 Acq On : 15 Jul 2024 13:37  
 Operator : JC/MD  
 Sample : P3206-03  
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 16777

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\82X061824W.M  
 Title : SW846 8260

Signal : TIC: VX042323.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         | 1.258       | 25            | 28          | 37           | rVB      | 22656          | 23972         | 3.30%           | 0.432%        |
| 2         | 1.593       | 68            | 83          | 86           | rBV4     | 7368           | 21384         | 2.95%           | 0.385%        |
| 3         | 2.416       | 211           | 218         | 228          | rVB9     | 2220           | 7482          | 1.03%           | 0.135%        |
| 4         | 5.385       | 693           | 705         | 720          | rBV2     | 72139          | 239725        | 33.03%          | 4.317%        |
| 5         | 5.537       | 720           | 730         | 749          | rVB      | 138821         | 401718        | 55.36%          | 7.234%        |
| 6         | 5.952       | 786           | 798         | 811          | rBV2     | 86771          | 236746        | 32.62%          | 4.263%        |
| 7         | 6.757       | 920           | 930         | 943          | rBV      | 204340         | 499116        | 68.78%          | 8.988%        |
| 8         | 8.646       | 1233          | 1240        | 1250         | rBV      | 458208         | 725670        | 100.00%         | 13.067%       |
| 9         | 10.055      | 1465          | 1471        | 1487         | rBV      | 437117         | 609667        | 84.01%          | 10.979%       |
| 10        | 11.085      | 1634          | 1640        | 1652         | rBV      | 391324         | 540646        | 74.50%          | 9.736%        |
| 11        | 11.384      | 1684          | 1689        | 1692         | rBV      | 5528           | 8392          | 1.16%           | 0.151%        |
| 12        | 11.475      | 1700          | 1704        | 1712         | rVB      | 31336          | 41704         | 5.75%           | 0.751%        |
| 13        | 11.622      | 1722          | 1728        | 1734         | rVB5     | 3893           | 8902          | 1.23%           | 0.160%        |
| 14        | 11.713      | 1740          | 1743        | 1746         | rBV      | 10770          | 12036         | 1.66%           | 0.217%        |
| 15        | 11.756      | 1746          | 1750        | 1759         | rVB2     | 18311          | 32492         | 4.48%           | 0.585%        |
| 16        | 11.890      | 1766          | 1772        | 1777         | rBV7     | 9611           | 17567         | 2.42%           | 0.316%        |
| 17        | 11.945      | 1777          | 1781        | 1784         | rVV3     | 11196          | 15113         | 2.08%           | 0.272%        |
| 18        | 12.024      | 1789          | 1794        | 1800         | rBV      | 495138         | 636742        | 87.75%          | 11.466%       |
| 19        | 12.073      | 1800          | 1802        | 1804         | rVV2     | 12750          | 15033         | 2.07%           | 0.271%        |
| 20        | 12.103      | 1804          | 1807        | 1811         | rVB2     | 18982          | 22602         | 3.11%           | 0.407%        |
| 21        | 12.170      | 1816          | 1818        | 1822         | rVB      | 14795          | 17130         | 2.36%           | 0.308%        |
| 22        | 12.219      | 1822          | 1826        | 1832         | rBV      | 96379          | 147499        | 20.33%          | 2.656%        |
| 23        | 12.310      | 1838          | 1841        | 1848         | rVB7     | 27577          | 51975         | 7.16%           | 0.936%        |
| 24        | 12.377      | 1848          | 1852        | 1855         | rBV4     | 8626           | 16524         | 2.28%           | 0.298%        |
| 25        | 12.426      | 1855          | 1860        | 1864         | rVV      | 160232         | 193359        | 26.65%          | 3.482%        |
| 26        | 12.469      | 1864          | 1867        | 1873         | rVB4     | 21840          | 37019         | 5.10%           | 0.667%        |
| 27        | 12.554      | 1874          | 1881        | 1883         | rBV4     | 20397          | 39692         | 5.47%           | 0.715%        |
| 28        | 12.585      | 1883          | 1886        | 1893         | rVB4     | 17112          | 30592         | 4.22%           | 0.551%        |
| 29        | 12.682      | 1899          | 1902        | 1906         | rBV3     | 17248          | 24094         | 3.32%           | 0.434%        |
| 30        | 12.731      | 1906          | 1910        | 1912         | rVV5     | 7601           | 13738         | 1.89%           | 0.247%        |
| 31        | 12.762      | 1912          | 1915        | 1918         | rVV4     | 9521           | 16009         | 2.21%           | 0.288%        |
| 32        | 12.816      | 1920          | 1924        | 1929         | rVV3     | 23889          | 35660         | 4.91%           | 0.642%        |
| 33        | 12.890      | 1932          | 1936        | 1943         | rVV4     | 32172          | 73024         | 10.06%          | 1.315%        |
| 34        | 12.944      | 1943          | 1945        | 1946         | rVV      | 12794          | 11781         | 1.62%           | 0.212%        |
| 35        | 12.975      | 1946          | 1950        | 1955         | rVB4     | 29341          | 50811         | 7.00%           | 0.915%        |
| 36        | 13.042      | 1957          | 1961        | 1965         | rVB2     | 20187          | 22611         | 3.12%           | 0.407%        |

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX071524\  
 Data File : VX042323.D  
 Acq On : 15 Jul 2024 13:37  
 Operator : JC/MD  
 Sample : P3206-03  
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 16777

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\82X061824W.M  
 Title : SW846 8260

|    |        |      |      |      |      |       |       |       |        |
|----|--------|------|------|------|------|-------|-------|-------|--------|
| 37 | 13.170 | 1976 | 1982 | 1986 | rVB4 | 8715  | 16730 | 2.31% | 0.301% |
| 38 | 13.213 | 1986 | 1989 | 1993 | rVV5 | 5213  | 8575  | 1.18% | 0.154% |
| 39 | 13.268 | 1994 | 1998 | 2000 | rVV  | 52305 | 62540 | 8.62% | 1.126% |
| 40 | 13.292 | 2000 | 2002 | 2007 | rVV2 | 28466 | 38117 | 5.25% | 0.686% |
| 41 | 13.383 | 2014 | 2017 | 2020 | rVV2 | 8783  | 11623 | 1.60% | 0.209% |
| 42 | 13.420 | 2020 | 2023 | 2032 | rVB7 | 16634 | 36429 | 5.02% | 0.656% |
| 43 | 13.499 | 2032 | 2036 | 2040 | rBV6 | 4948  | 8546  | 1.18% | 0.154% |
| 44 | 13.585 | 2047 | 2050 | 2054 | rBV5 | 5888  | 9242  | 1.27% | 0.166% |
| 45 | 13.682 | 2061 | 2066 | 2067 | rBV3 | 8986  | 12244 | 1.69% | 0.220% |
| 46 | 13.737 | 2072 | 2075 | 2078 | rVV3 | 11411 | 15328 | 2.11% | 0.276% |
| 47 | 13.774 | 2078 | 2081 | 2087 | rVV2 | 16853 | 28123 | 3.88% | 0.506% |
| 48 | 13.835 | 2087 | 2091 | 2099 | rVB6 | 12603 | 26612 | 3.67% | 0.479% |
| 49 | 13.926 | 2100 | 2106 | 2111 | rBV7 | 7026  | 15407 | 2.12% | 0.277% |
| 50 | 14.036 | 2120 | 2124 | 2128 | rBV  | 25459 | 27962 | 3.85% | 0.504% |
| 51 | 14.231 | 2147 | 2156 | 2164 | rVB8 | 13006 | 36780 | 5.07% | 0.662% |
| 52 | 14.414 | 2182 | 2186 | 2187 | rBV3 | 7930  | 9741  | 1.34% | 0.175% |
| 53 | 14.475 | 2192 | 2196 | 2198 | rVV3 | 10485 | 14339 | 1.98% | 0.258% |
| 54 | 14.499 | 2198 | 2200 | 2206 | rVB5 | 10389 | 14908 | 2.05% | 0.268% |
| 55 | 14.566 | 2206 | 2211 | 2216 | rBV3 | 8329  | 13472 | 1.86% | 0.243% |
| 56 | 14.615 | 2216 | 2219 | 2220 | rBV2 | 14621 | 15337 | 2.11% | 0.276% |
| 57 | 14.639 | 2220 | 2223 | 2226 | rVV  | 17449 | 23327 | 3.21% | 0.420% |
| 58 | 14.670 | 2226 | 2228 | 2234 | rVB5 | 6278  | 7443  | 1.03% | 0.134% |
| 59 | 14.755 | 2238 | 2242 | 2245 | rVV  | 28394 | 33618 | 4.63% | 0.605% |
| 60 | 14.779 | 2245 | 2246 | 2250 | rVV2 | 10406 | 11704 | 1.61% | 0.211% |
| 61 | 14.840 | 2254 | 2256 | 2260 | rVB5 | 6323  | 7864  | 1.08% | 0.142% |
| 62 | 15.103 | 2295 | 2299 | 2302 | rBV5 | 4091  | 7475  | 1.03% | 0.135% |
| 63 | 15.182 | 2308 | 2312 | 2314 | rBV2 | 11307 | 14478 | 2.00% | 0.261% |
| 64 | 15.212 | 2314 | 2317 | 2321 | rVV2 | 10707 | 15669 | 2.16% | 0.282% |
| 65 | 15.279 | 2324 | 2328 | 2331 | rVV5 | 6269  | 8738  | 1.20% | 0.157% |
| 66 | 15.383 | 2340 | 2345 | 2350 | rBV4 | 8976  | 16577 | 2.28% | 0.299% |
| 67 | 15.487 | 2357 | 2362 | 2370 | rBV3 | 22050 | 39408 | 5.43% | 0.710% |
| 68 | 15.615 | 2379 | 2383 | 2388 | rBV5 | 8903  | 13677 | 1.88% | 0.246% |
| 69 | 15.889 | 2424 | 2428 | 2434 | rVB6 | 6571  | 11309 | 1.56% | 0.204% |
| 70 | 16.090 | 2457 | 2461 | 2468 | rBV7 | 4197  | 8100  | 1.12% | 0.146% |
| 71 | 16.371 | 2499 | 2507 | 2513 | rVB8 | 5509  | 13607 | 1.88% | 0.245% |

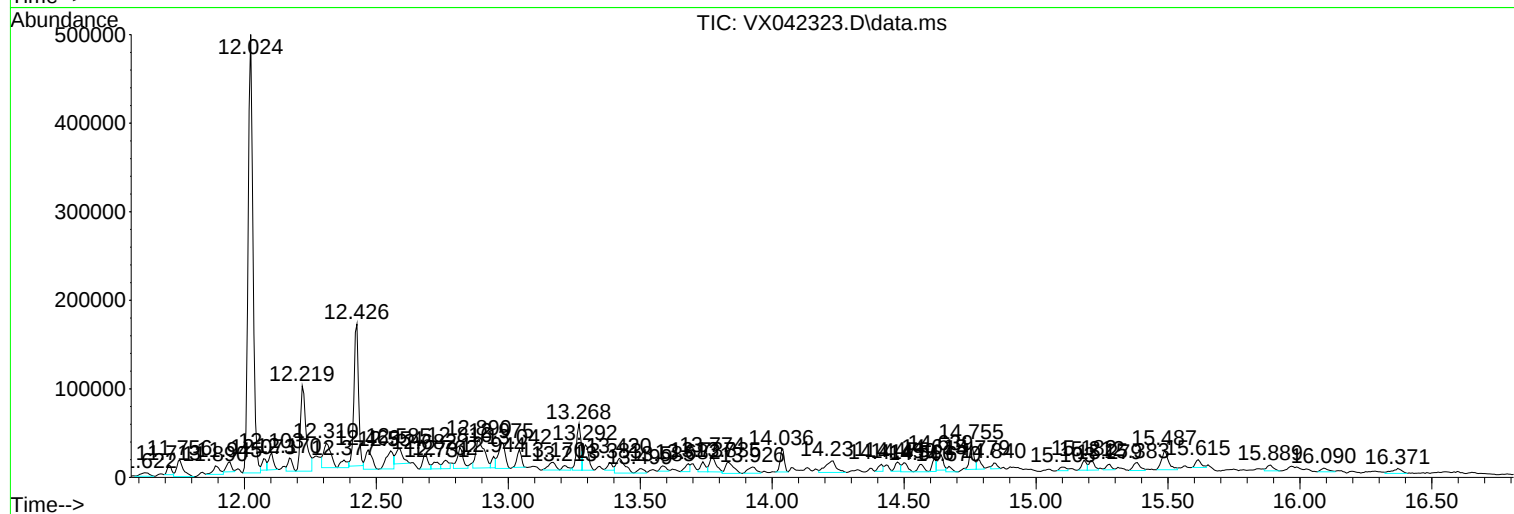
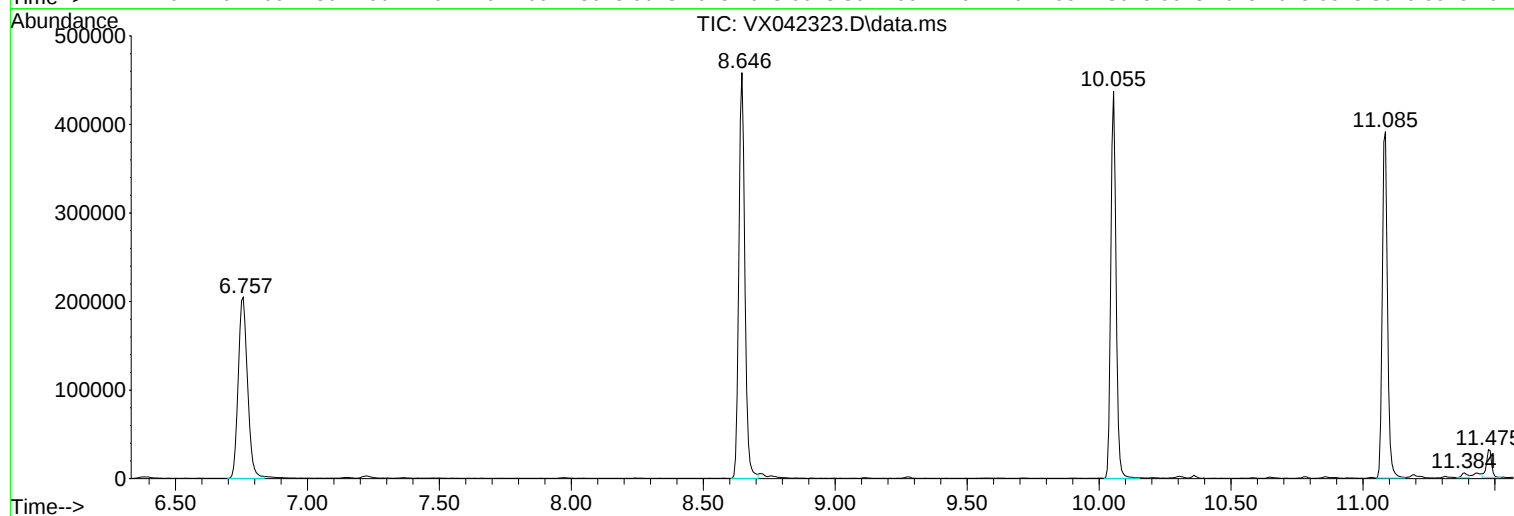
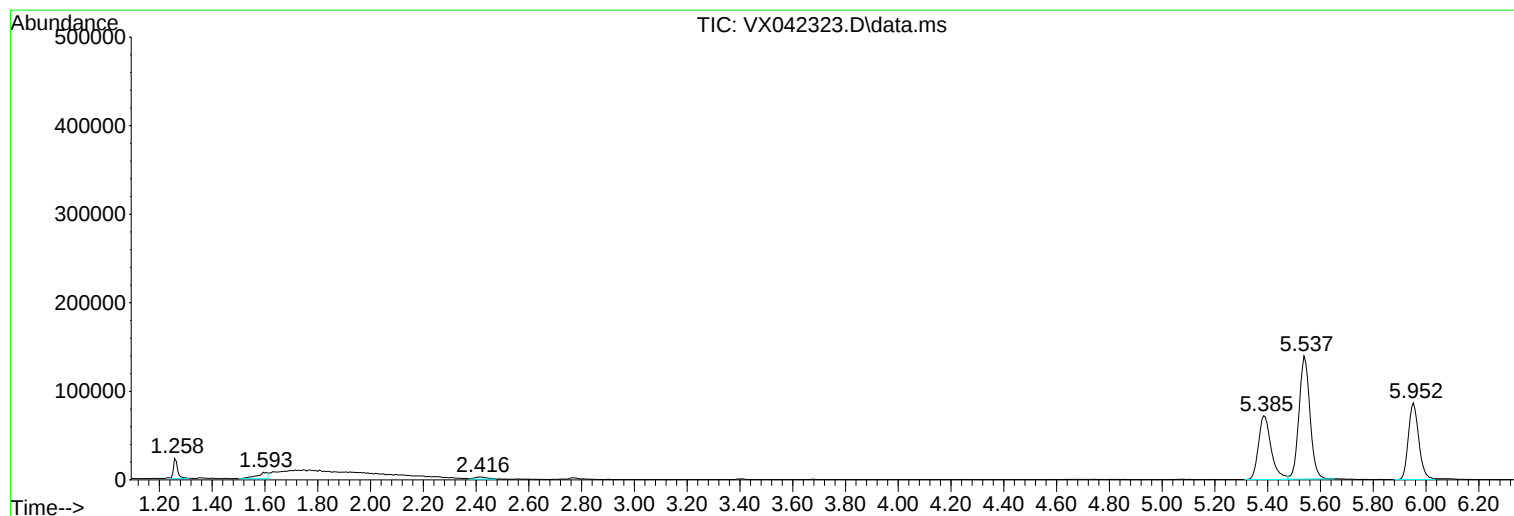
Sum of corrected areas: 5553276

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX071524\  
Data File : VX042323.D  
Acq On : 15 Jul 2024 13:37  
Operator : JC/MD  
Sample : P3206-03  
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
16777

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061824W.M  
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX071524\  
Data File : VX042323.D  
Acq On : 15 Jul 2024 13:37  
Operator : JC/MD  
Sample : P3206-03  
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
16777

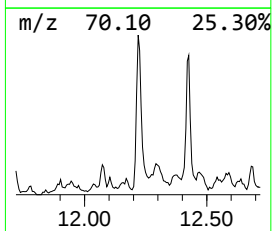
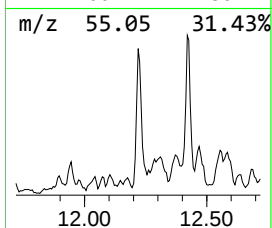
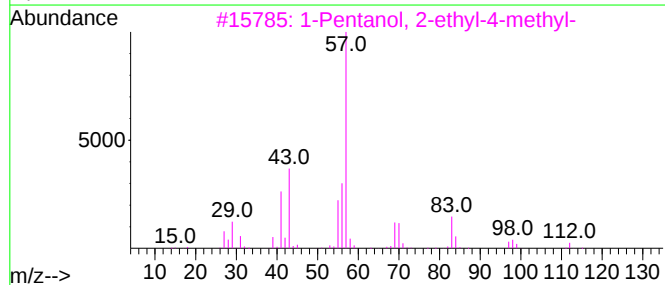
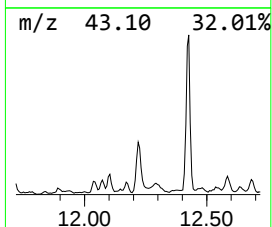
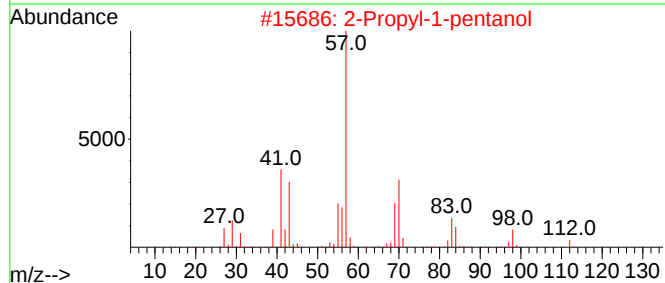
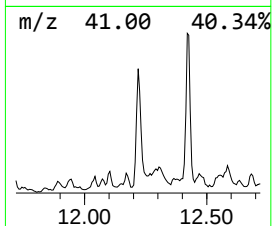
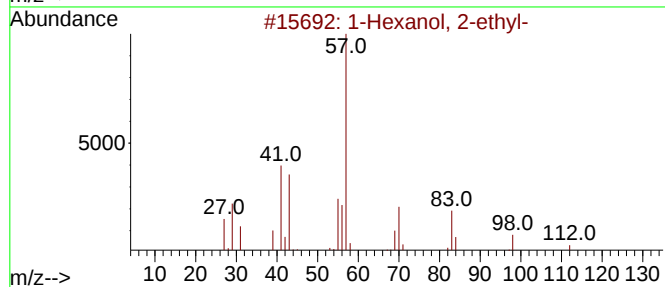
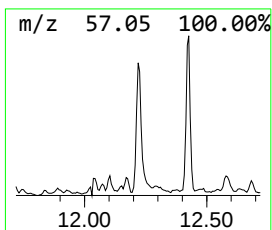
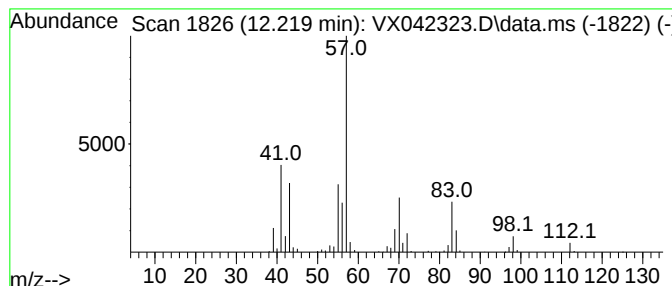
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061824W.M  
Quant Title : SW846 8260

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

\*\*\*\*\*  
Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 2

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 12.219 | 11.58 ug/l | 147499 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of                            | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|-------------------------------|---|--------------|-----|---------|-------------|------|
| 1    | 1-Hexanol, 2-ethyl-           |   |              | 130 | C8H18O  | 000104-76-7 | 90   |
| 2    | 2-Propyl-1-pentanol           |   |              | 130 | C8H18O  | 058175-57-8 | 64   |
| 3    | 1-Pentanol, 2-ethyl-4-methyl- |   |              | 130 | C8H18O  | 000106-67-2 | 56   |
| 4    | Heptane, 1,1'-oxybis-         |   |              | 214 | C14H30O | 000629-64-1 | 50   |
| 5    | 1-Decene, 2,4-dimethyl-       |   |              | 168 | C12H24  | 055170-80-4 | 47   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX071524\  
Data File : VX042323.D  
Acq On : 15 Jul 2024 13:37  
Operator : JC/MD  
Sample : P3206-03  
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
16777

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061824W.M  
Quant Title : SW846 8260

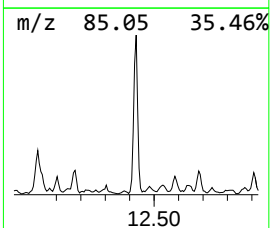
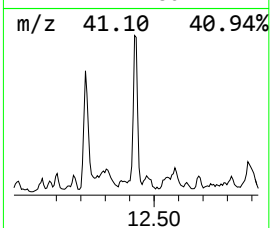
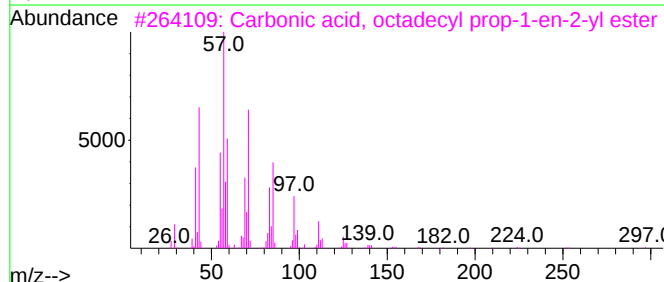
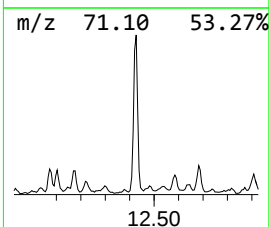
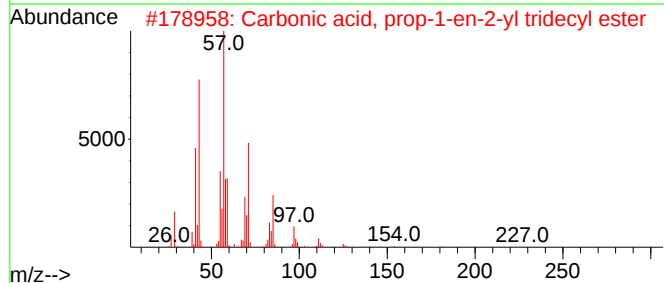
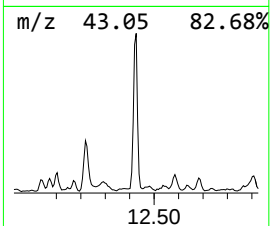
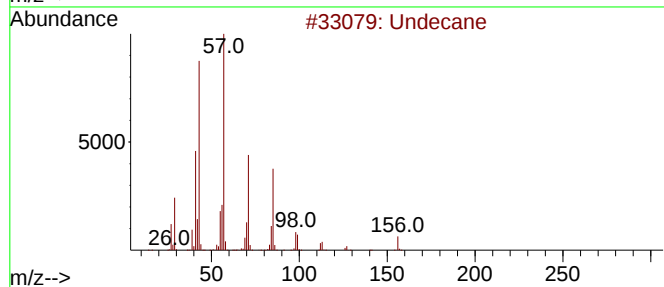
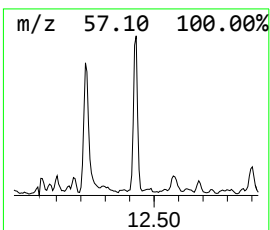
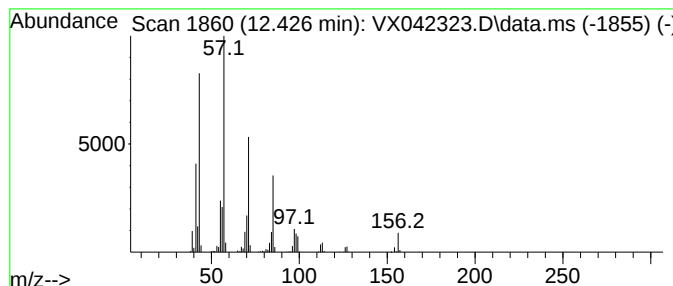
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 2 Undecane Concentration Rank 1

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 12.426 | 15.18 ug/l | 193359 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm  | CAS#         | Qual |
|------|-------------------------------------|---|--------------|-----|----------|--------------|------|
| 1    | Undecane                            |   |              | 156 | C11H24   | 001120-21-4  | 94   |
| 2    | Carbonic acid, prop-1-en-2-yl tr... |   |              | 284 | C17H32O3 | 1000382-90-8 | 86   |
| 3    | Carbonic acid, octadecyl prop-1-... |   |              | 354 | C22H42O3 | 1000383-11-5 | 86   |
| 4    | Tetradecane                         |   |              | 198 | C14H30   | 000629-59-4  | 86   |
| 5    | Nonadecane                          |   |              | 268 | C19H40   | 000629-92-5  | 72   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX071524\  
Data File : VX042323.D  
Acq On : 15 Jul 2024 13:37  
Operator : JC/MD  
Sample : P3206-03  
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
16777

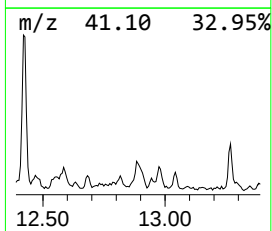
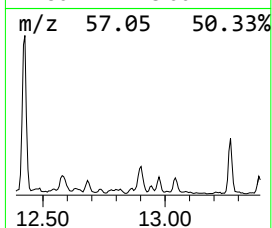
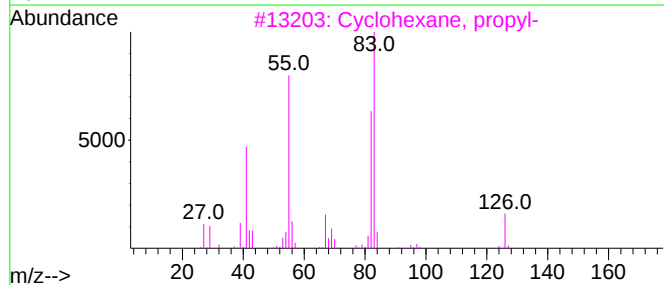
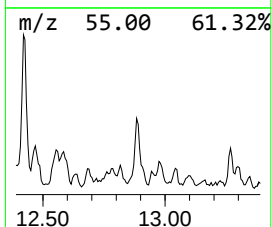
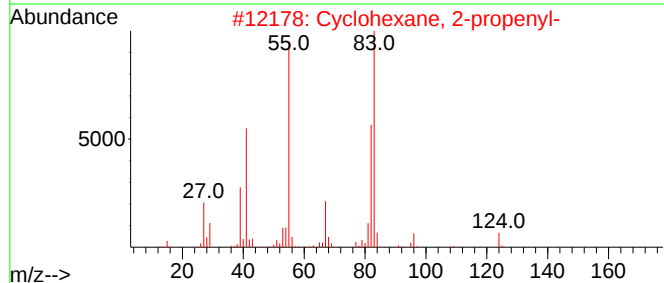
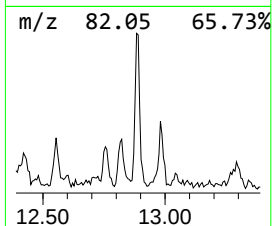
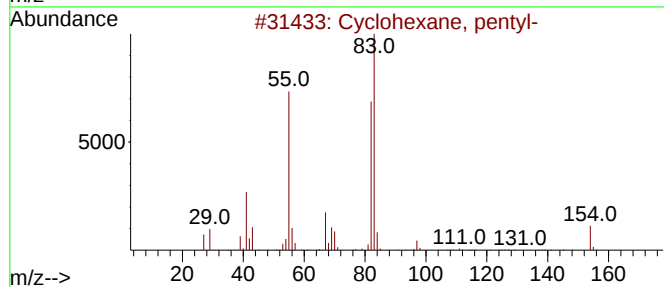
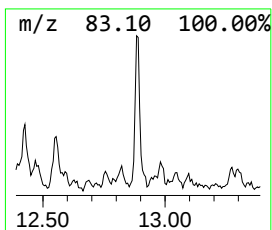
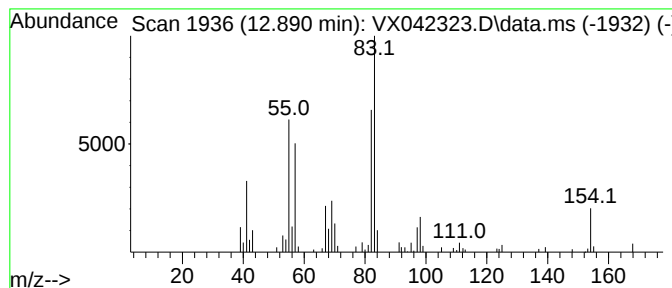
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061824W.M  
Quant Title : SW846 8260

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

\*\*\*\*\*  
Peak Number 3 Cyclohexane, pentyl- Concentration Rank 3

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.890 | 5.73 ug/l | 73024 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexane, pentyl-                | 154 | C11H22  | 004292-92-6 | 87   |
| 2    |    |   | Cyclohexane, 2-propenyl-            | 124 | C9H16   | 002114-42-3 | 59   |
| 3    |    |   | Cyclohexane, propyl-                | 126 | C9H18   | 001678-92-8 | 59   |
| 4    |    |   | Cyclohexane, (1-methylethyl)-       | 126 | C9H18   | 000696-29-7 | 59   |
| 5    |    |   | Cyclohexane, 1,1'-(1,4-butanediyl)- | 222 | C16H30  | 006165-44-2 | 59   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX071524\  
Data File : VX042323.D  
Acq On : 15 Jul 2024 13:37  
Operator : JC/MD  
Sample : P3206-03  
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA\_X/MEOH  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
16777

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061824W.M  
Quant Title : SW846 8260

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 1-Hexanol, 2-et... | 12.219 | 11.6    | ug/l  | 147499   | 4                     | 12.024 | 636742 | 50.0 |
| Undecane           | 12.426 | 15.2    | ug/l  | 193359   | 4                     | 12.024 | 636742 | 50.0 |
| Cyclohexane, pe... | 12.890 | 5.7     | ug/l  | 73024    | 4                     | 12.024 | 636742 | 50.0 |