

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091724\  
 Data File : VN083965.D  
 Acq On : 18 Sep 2024 06:21  
 Operator : JC\MD  
 Sample : P3964-04  
 Misc : 7.05g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
 ALS Vial : 41 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 SINK-1

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\_N\methods\82N091024W.M  
 Title : SW846 8260

Signal : TIC: VN083965.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         | 5.247       | 546           | 560         | 564          | rBV3     | 82429          | 268320        | 1.05%           | 0.152%        |
| 2         | 5.312       | 565           | 571         | 587          | rVB3     | 141552         | 488317        | 1.92%           | 0.277%        |
| 3         | 5.788       | 639           | 652         | 668          | rVB2     | 95538          | 321978        | 1.26%           | 0.182%        |
| 4         | 7.212       | 883           | 894         | 903          | rBV2     | 208966         | 586987        | 2.30%           | 0.333%        |
| 5         | 7.318       | 903           | 912         | 919          | rBV2     | 116151         | 312683        | 1.23%           | 0.177%        |
| 6         | 8.159       | 1047          | 1055        | 1058         | rBV      | 136236         | 304191        | 1.19%           | 0.172%        |
| 7         | 8.212       | 1058          | 1064        | 1075         | rVV2     | 737757         | 1941224       | 7.62%           | 1.100%        |
| 8         | 8.324       | 1075          | 1083        | 1093         | rVB2     | 385674         | 981165        | 3.85%           | 0.556%        |
| 9         | 8.441       | 1093          | 1103        | 1111         | rBV      | 581639         | 1320090       | 5.18%           | 0.748%        |
| 10        | 8.576       | 1118          | 1126        | 1140         | rBV      | 156780         | 388290        | 1.52%           | 0.220%        |
| 11        | 8.753       | 1140          | 1156        | 1168         | rBV      | 2925019        | 7527101       | 29.54%          | 4.266%        |
| 12        | 8.965       | 1181          | 1192        | 1204         | rVB      | 490164         | 1190595       | 4.67%           | 0.675%        |
| 13        | 9.100       | 1204          | 1215        | 1221         | rBV3     | 649946         | 1519648       | 5.96%           | 0.861%        |
| 14        | 9.335       | 1247          | 1255        | 1260         | rVV2     | 159699         | 396503        | 1.56%           | 0.225%        |
| 15        | 9.588       | 1284          | 1298        | 1303         | rBV3     | 1154122        | 2734304       | 10.73%          | 1.550%        |
| 16        | 9.641       | 1303          | 1307        | 1314         | rVB      | 717894         | 1337607       | 5.25%           | 0.758%        |
| 17        | 9.723       | 1314          | 1321        | 1326         | rBV      | 231223         | 495556        | 1.94%           | 0.281%        |
| 18        | 10.012      | 1362          | 1370        | 1379         | rVB      | 2113035        | 4285112       | 16.81%          | 2.429%        |
| 19        | 10.141      | 1379          | 1392        | 1398         | rBV      | 2962239        | 6236377       | 24.47%          | 3.535%        |
| 20        | 10.200      | 1398          | 1402        | 1406         | rBV      | 512826         | 759221        | 2.98%           | 0.430%        |
| 21        | 10.335      | 1416          | 1425        | 1438         | rBV      | 720122         | 1769055       | 6.94%           | 1.003%        |
| 22        | 10.494      | 1439          | 1452        | 1458         | rVV      | 1874809        | 3522862       | 13.82%          | 1.997%        |
| 23        | 10.565      | 1458          | 1464        | 1470         | rBV2     | 749942         | 1394325       | 5.47%           | 0.790%        |
| 24        | 10.629      | 1470          | 1475        | 1483         | rVV      | 180315         | 475678        | 1.87%           | 0.270%        |
| 25        | 10.741      | 1487          | 1494        | 1501         | rVB3     | 746696         | 1455225       | 5.71%           | 0.825%        |
| 26        | 10.847      | 1508          | 1512        | 1518         | rVB2     | 145140         | 277474        | 1.09%           | 0.157%        |
| 27        | 10.923      | 1518          | 1525        | 1530         | rBV5     | 113368         | 280557        | 1.10%           | 0.159%        |
| 28        | 11.012      | 1530          | 1540        | 1547         | rVV4     | 399770         | 1002329       | 3.93%           | 0.568%        |
| 29        | 11.082      | 1547          | 1552        | 1558         | rVB      | 168673         | 305251        | 1.20%           | 0.173%        |
| 30        | 11.170      | 1558          | 1567        | 1573         | rBV3     | 185806         | 395323        | 1.55%           | 0.224%        |
| 31        | 11.270      | 1574          | 1584        | 1592         | rBV      | 307242         | 712935        | 2.80%           | 0.404%        |
| 32        | 11.641      | 1639          | 1647        | 1659         | rVB2     | 690613         | 1587077       | 6.23%           | 0.900%        |
| 33        | 11.741      | 1659          | 1664        | 1674         | rBV      | 530085         | 885804        | 3.48%           | 0.502%        |
| 34        | 11.864      | 1674          | 1685        | 1690         | rBV2     | 693349         | 1611843       | 6.32%           | 0.914%        |
| 35        | 11.959      | 1690          | 1701        | 1710         | rVV      | 3218942        | 5932609       | 23.28%          | 3.362%        |
| 36        | 12.064      | 1711          | 1719        | 1731         | rVB      | 13028174       | 25484522      | 100.00%         | 14.444%       |

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 Sample : P3964-04  
 Misc : 7.05g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
 ALS Vial : 41 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 SINK-1

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\_N\methods\82N091024W.M  
 Title : SW846 8260

|    |        |      |      |      |      |          |          |        |        |
|----|--------|------|------|------|------|----------|----------|--------|--------|
| 37 | 12.394 | 1766 | 1775 | 1783 | rBV  | 5165402  | 9143913  | 35.88% | 5.183% |
| 38 | 12.476 | 1784 | 1789 | 1795 | rVB  | 199007   | 354981   | 1.39%  | 0.201% |
| 39 | 12.694 | 1820 | 1826 | 1832 | rBV  | 1362598  | 2371428  | 9.31%  | 1.344% |
| 40 | 12.823 | 1840 | 1848 | 1855 | rBV2 | 586510   | 1349377  | 5.29%  | 0.765% |
| 41 | 12.988 | 1871 | 1876 | 1878 | rBV2 | 202821   | 333556   | 1.31%  | 0.189% |
| 42 | 13.035 | 1878 | 1884 | 1889 | rVV  | 2174156  | 3506811  | 13.76% | 1.988% |
| 43 | 13.094 | 1889 | 1894 | 1898 | rVV  | 6842899  | 11640949 | 45.68% | 6.598% |
| 44 | 13.129 | 1898 | 1900 | 1903 | rVV  | 3019175  | 3991666  | 15.66% | 2.262% |
| 45 | 13.170 | 1903 | 1907 | 1915 | rVB  | 3598008  | 6157384  | 24.16% | 3.490% |
| 46 | 13.335 | 1926 | 1935 | 1942 | rBV  | 2438435  | 4220095  | 16.56% | 2.392% |
| 47 | 13.423 | 1942 | 1950 | 1954 | rBV  | 448755   | 834243   | 3.27%  | 0.473% |
| 48 | 13.482 | 1954 | 1960 | 1966 | rBV  | 10833148 | 17005300 | 66.73% | 9.638% |
| 49 | 13.529 | 1966 | 1968 | 1973 | rVB2 | 227391   | 307497   | 1.21%  | 0.174% |
| 50 | 13.641 | 1974 | 1987 | 1990 | rBV3 | 593458   | 1690882  | 6.63%  | 0.958% |
| 51 | 13.817 | 2008 | 2017 | 2030 | rVB3 | 2504558  | 6637181  | 26.04% | 3.762% |
| 52 | 13.953 | 2034 | 2040 | 2041 | rBV2 | 506996   | 777250   | 3.05%  | 0.441% |
| 53 | 13.988 | 2041 | 2046 | 2049 | rBV2 | 1676996  | 3267514  | 12.82% | 1.852% |
| 54 | 14.106 | 2062 | 2066 | 2073 | rVB2 | 354271   | 557469   | 2.19%  | 0.316% |
| 55 | 14.182 | 2074 | 2079 | 2084 | rVB  | 498887   | 812735   | 3.19%  | 0.461% |
| 56 | 14.241 | 2084 | 2089 | 2092 | rBV  | 823774   | 1424506  | 5.59%  | 0.807% |
| 57 | 14.270 | 2092 | 2094 | 2099 | rVV  | 767719   | 998071   | 3.92%  | 0.566% |
| 58 | 14.329 | 2099 | 2104 | 2112 | rVB  | 1468293  | 2279277  | 8.94%  | 1.292% |
| 59 | 14.441 | 2118 | 2123 | 2128 | rVB3 | 440752   | 753406   | 2.96%  | 0.427% |
| 60 | 14.570 | 2140 | 2145 | 2151 | rBV2 | 326794   | 552935   | 2.17%  | 0.313% |
| 61 | 14.653 | 2151 | 2159 | 2162 | rBV  | 910174   | 1596365  | 6.26%  | 0.905% |
| 62 | 14.688 | 2162 | 2165 | 2169 | rVV  | 1097392  | 1618794  | 6.35%  | 0.918% |
| 63 | 14.735 | 2169 | 2173 | 2177 | rVB2 | 382785   | 547875   | 2.15%  | 0.311% |
| 64 | 14.876 | 2192 | 2197 | 2200 | rBV  | 187726   | 260751   | 1.02%  | 0.148% |
| 65 | 14.929 | 2200 | 2206 | 2208 | rBV  | 544130   | 934120   | 3.67%  | 0.529% |
| 66 | 14.958 | 2208 | 2211 | 2216 | rVB2 | 489754   | 766907   | 3.01%  | 0.435% |
| 67 | 15.047 | 2216 | 2226 | 2232 | rBV3 | 837424   | 2674755  | 10.50% | 1.516% |
| 68 | 15.317 | 2261 | 2272 | 2284 | rVV3 | 370756   | 1137832  | 4.46%  | 0.645% |
| 69 | 15.435 | 2285 | 2292 | 2300 | rVV2 | 245745   | 694845   | 2.73%  | 0.394% |
| 70 | 15.594 | 2313 | 2319 | 2321 | rBV3 | 170388   | 332958   | 1.31%  | 0.189% |
| 71 | 15.635 | 2321 | 2326 | 2333 | rVB  | 770955   | 1514539  | 5.94%  | 0.858% |
| 72 | 15.829 | 2349 | 2359 | 2369 | rVB2 | 384158   | 1091448  | 4.28%  | 0.619% |
| 73 | 15.941 | 2370 | 2378 | 2385 | rBV  | 204993   | 519536   | 2.04%  | 0.294% |
| 74 | 16.335 | 2438 | 2445 | 2452 | rVB6 | 128146   | 342286   | 1.34%  | 0.194% |
| 75 | 16.776 | 2513 | 2520 | 2522 | rBV  | 534365   | 945244   | 3.71%  | 0.536% |

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ALS Vial : 41 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

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\_N\methods\82N091024W.M  
Title : SW846 8260

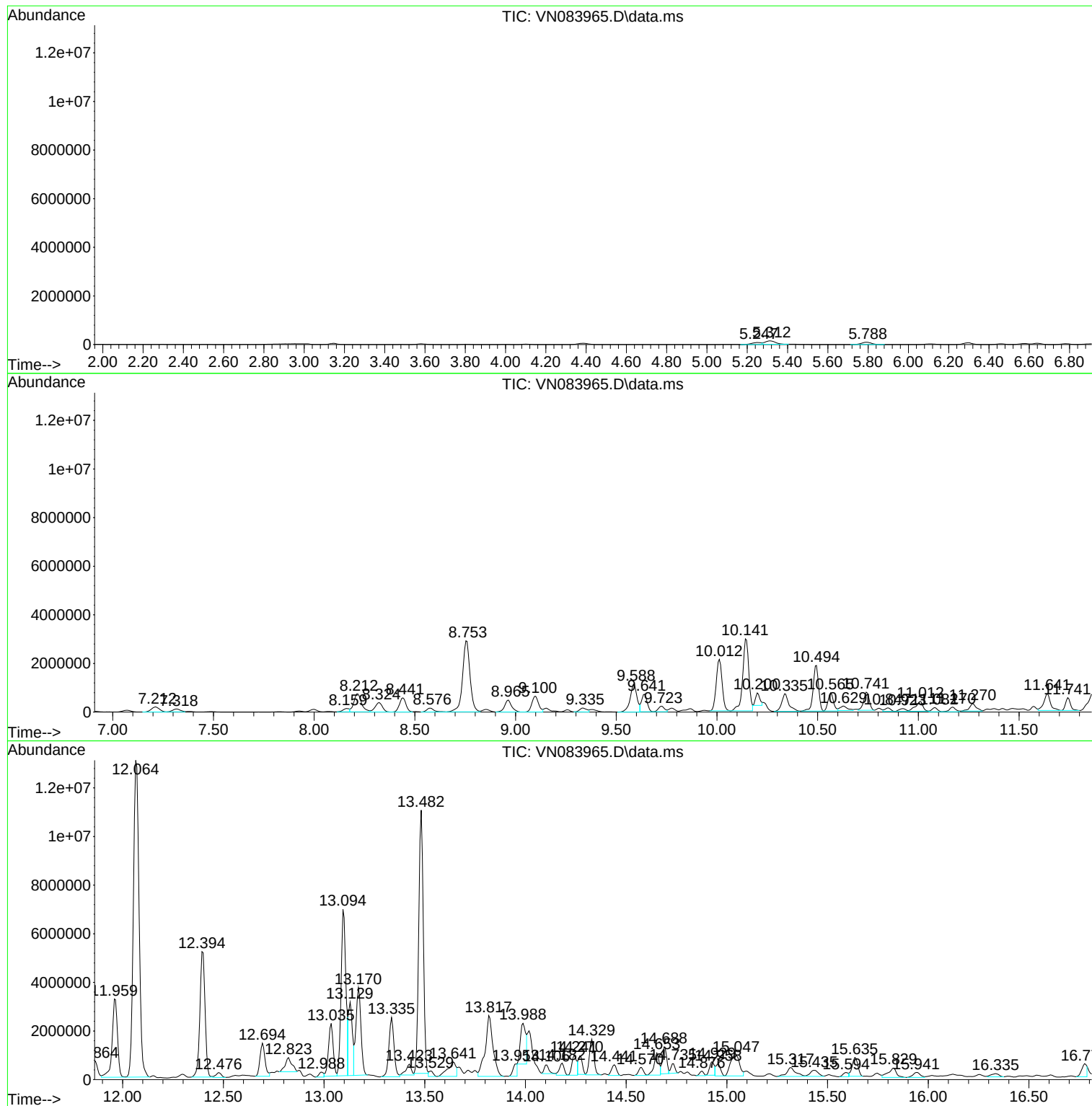
Sum of corrected areas: 176434819

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091724\  
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MSVOA\_N  
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SINK-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.M  
Quant Title : SW846 8260

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



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ALS Vial : 41 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

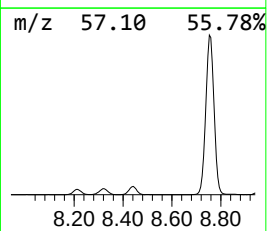
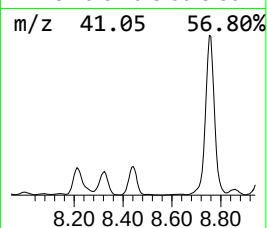
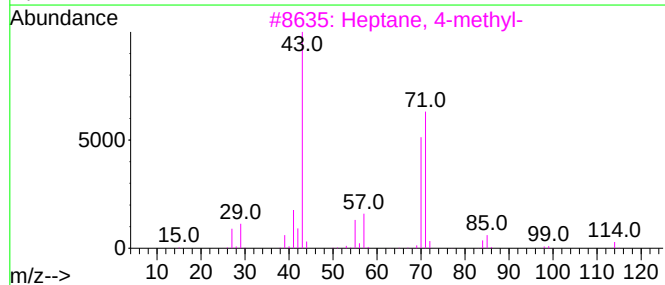
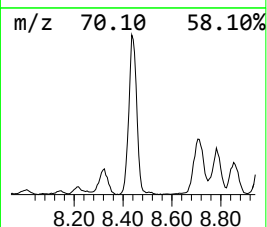
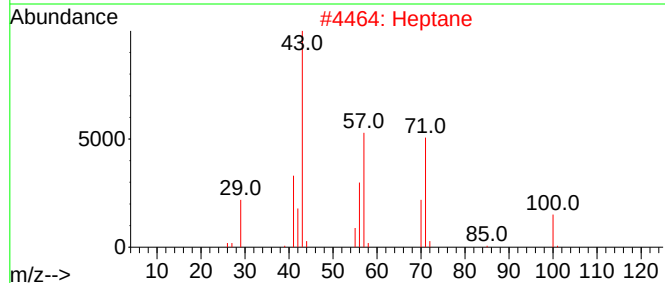
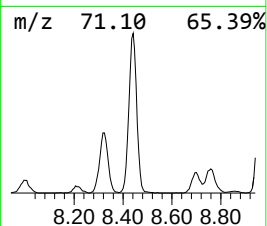
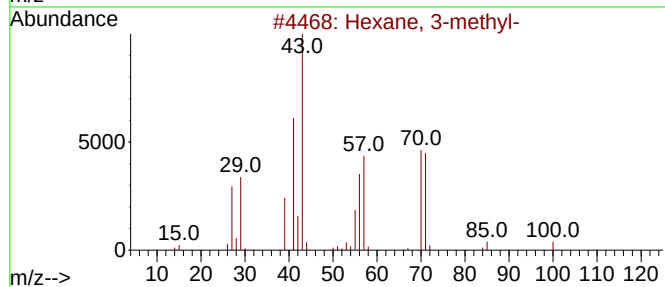
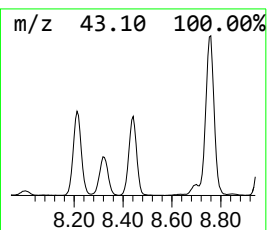
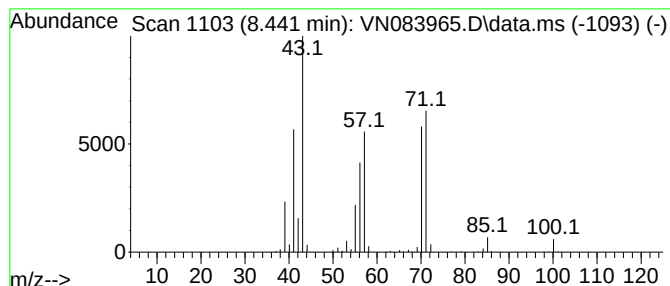
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Hexane, 3-methyl- Concentration Rank 10

| R.T.  | EstConc    | Area    | Relative to ISTD   | R.T.  |
|-------|------------|---------|--------------------|-------|
| 8.441 | 34.00 ug/l | 1320090 | Pentafluorobenzene | 8.218 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|-----|---------|-------------|------|
| 1    |    |   | Hexane, 3-methyl-         | 100 | C7H16   | 000589-34-4 | 91   |
| 2    |    |   | Heptane                   | 100 | C7H16   | 000142-82-5 | 80   |
| 3    |    |   | Heptane, 4-methyl-        | 114 | C8H18   | 000589-53-7 | 59   |
| 4    |    |   | Heptane, 3,3,4-trimethyl- | 142 | C10H22  | 020278-87-9 | 53   |
| 5    |    |   | Pentane, 2,3,4-trimethyl- | 114 | C8H18   | 000565-75-3 | 53   |



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ALS Vial : 41 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

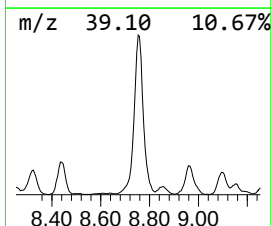
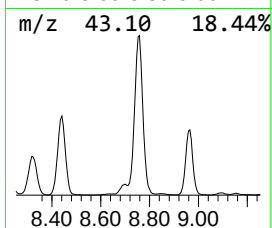
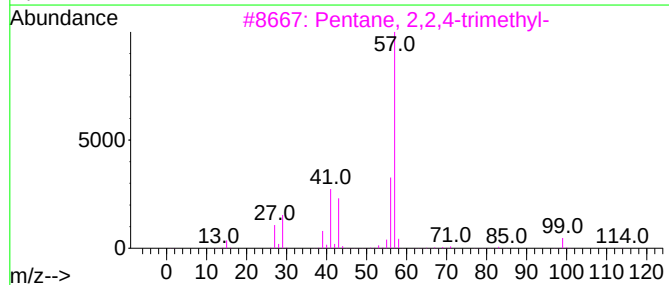
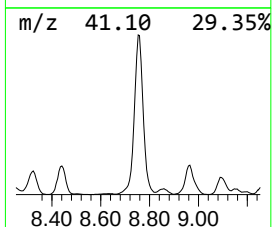
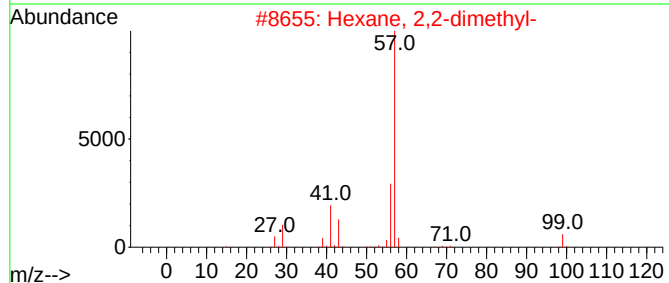
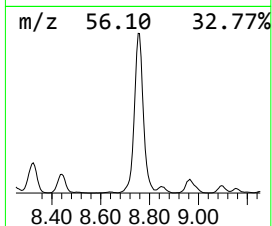
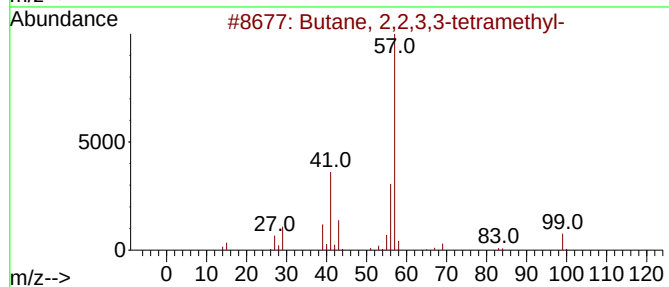
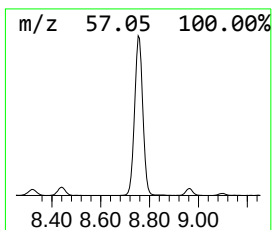
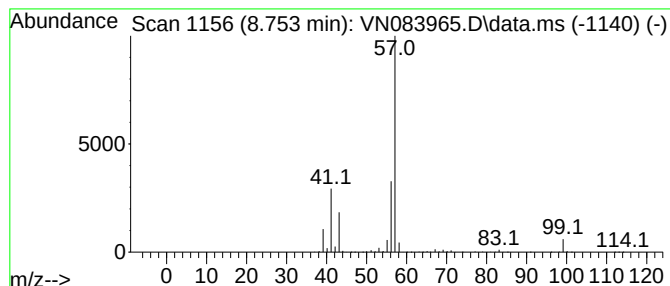
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.M  
Quant Title : SW846 8260

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

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Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

| R.T.  | EstConc     | Area    | Relative to ISTD    | R.T.  |
|-------|-------------|---------|---------------------|-------|
| 8.753 | 247.66 ug/l | 7527100 | 1,4-Difluorobenzene | 9.094 |

| Hit# | of | 5 | Tentative ID                  | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2,2,3,3-tetramethyl-  | 114 | C8H18   | 000594-82-1 | 78   |
| 2    |    |   | Hexane, 2,2-dimethyl-         | 114 | C8H18   | 000590-73-8 | 72   |
| 3    |    |   | Pentane, 2,2,4-trimethyl-     | 114 | C8H18   | 000540-84-1 | 72   |
| 4    |    |   | Hexane, 2,2,4-trimethyl-      | 128 | C9H20   | 016747-26-5 | 64   |
| 5    |    |   | Pentane, 2,2,4,4-tetramethyl- | 128 | C9H20   | 001070-87-7 | 59   |



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Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

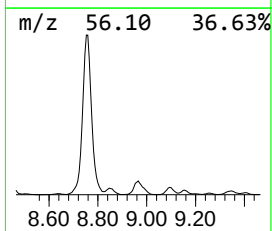
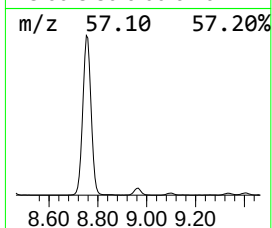
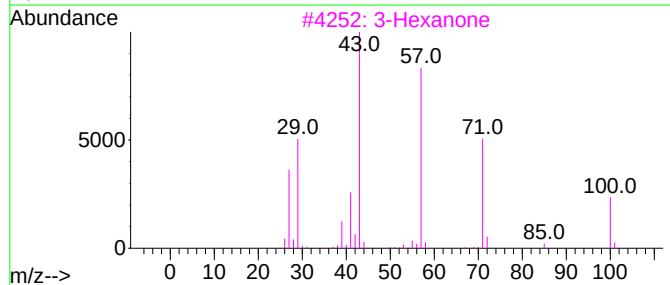
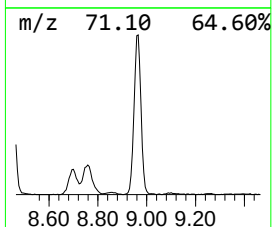
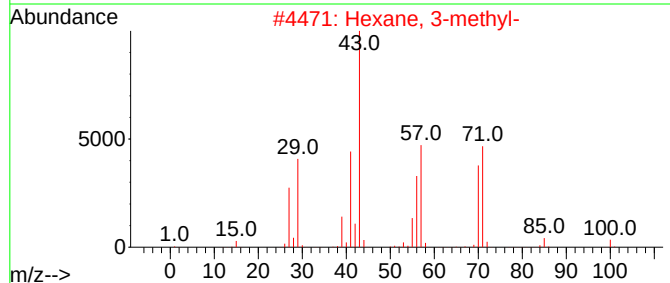
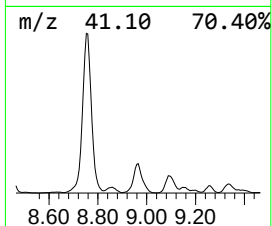
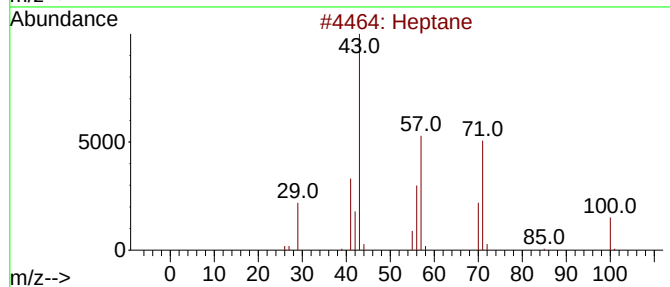
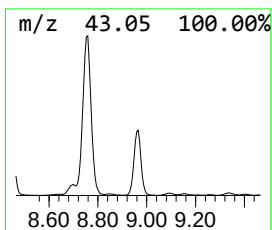
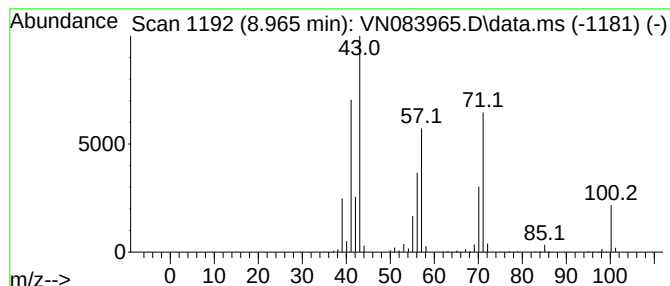
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Quant Title : SW846 8260

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

\*\*\*\*\*  
Peak Number 3 Heptane Concentration Rank 9

| R.T.  | EstConc    | Area    | Relative to ISTD    | R.T.  |
|-------|------------|---------|---------------------|-------|
| 8.965 | 39.17 ug/l | 1190600 | 1,4-Difluorobenzene | 9.094 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Heptane               | 100 | C7H16   | 000142-82-5 | 91   |
| 2    |    |   | Hexane, 3-methyl-     | 100 | C7H16   | 000589-34-4 | 50   |
| 3    |    |   | 3-Hexanone            | 100 | C6H12O  | 000589-38-8 | 38   |
| 4    |    |   | Oxirane, butyl-       | 100 | C6H12O  | 001436-34-6 | 38   |
| 5    |    |   | Butane, 2,2-dimethyl- | 86  | C6H14   | 000075-83-2 | 38   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091724\  
Data File : VN083965.D  
Acq On : 18 Sep 2024 06:21  
Operator : JC\MD  
Sample : P3964-04  
Misc : 7.05g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 41 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

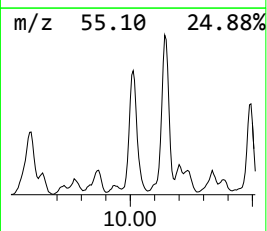
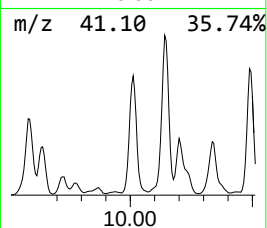
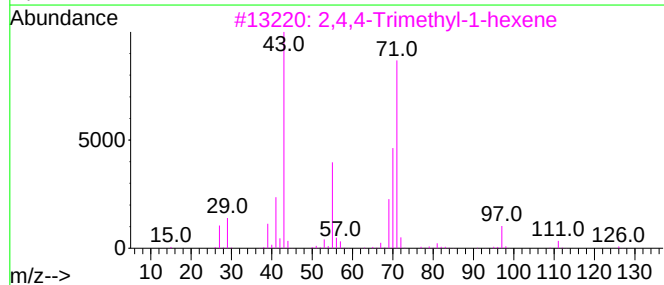
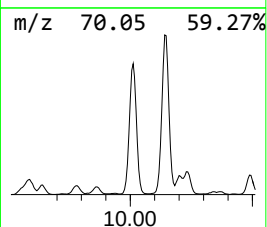
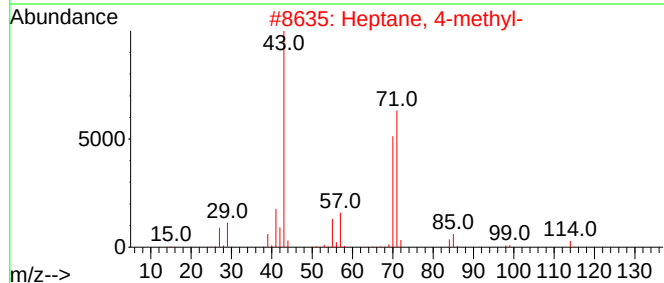
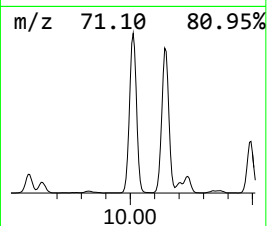
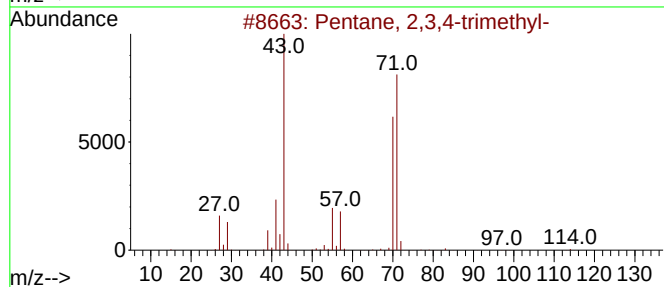
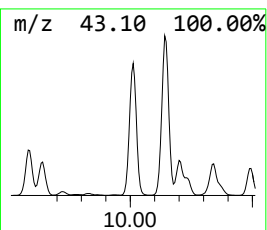
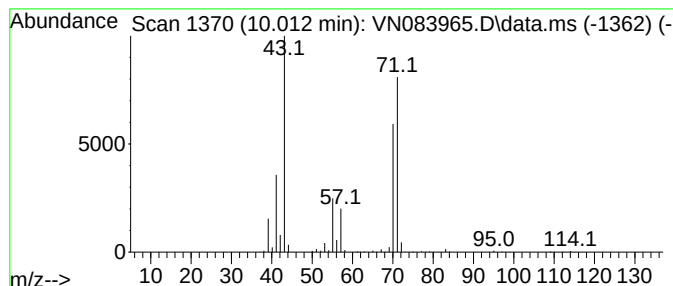
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Quant Title : SW846 8260

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

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Peak Number 4 Pentane, 2,3,4-trimethyl- Concentration Rank 3

| R.T.   | EstConc     | Area    | Relative to ISTD    | R.T.  |
|--------|-------------|---------|---------------------|-------|
| 10.012 | 140.99 ug/l | 4285110 | 1,4-Difluorobenzene | 9.094 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|-----|---------|-------------|------|
| 1    |    |   | Pentane, 2,3,4-trimethyl- | 114 | C8H18   | 000565-75-3 | 91   |
| 2    |    |   | Heptane, 4-methyl-        | 114 | C8H18   | 000589-53-7 | 83   |
| 3    |    |   | 2,4,4-Trimethyl-1-hexene  | 126 | C9H18   | 051174-12-0 | 78   |
| 4    |    |   | Decane, 3,3,4-trimethyl-  | 184 | C13H28  | 049622-18-6 | 78   |
| 5    |    |   | Hexane, 3-methyl-         | 100 | C7H16   | 000589-34-4 | 78   |





Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091724\  
Data File : VN083965.D  
Acq On : 18 Sep 2024 06:21  
Operator : JC\MD  
Sample : P3964-04  
Misc : 7.05g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 41 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

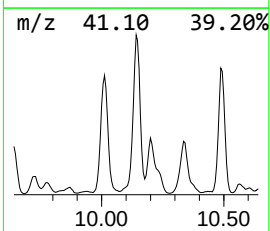
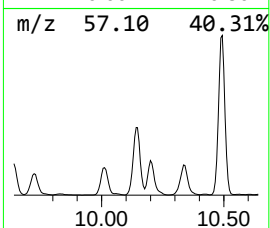
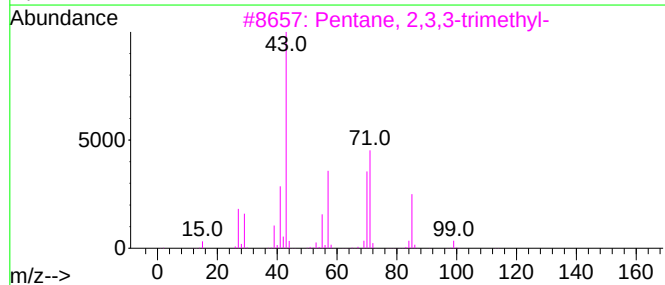
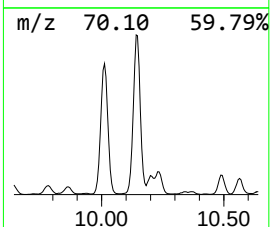
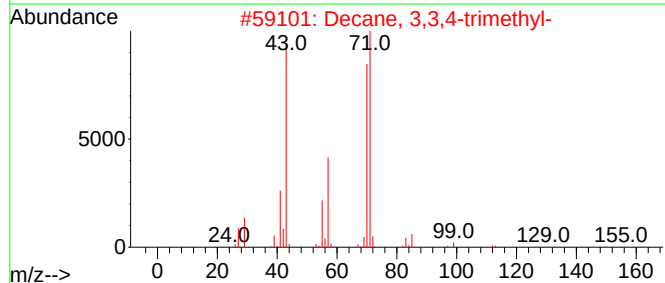
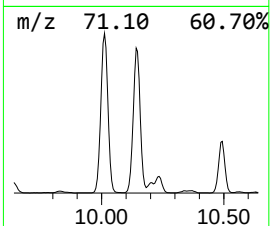
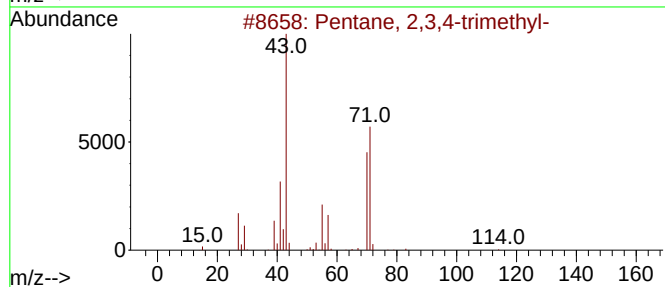
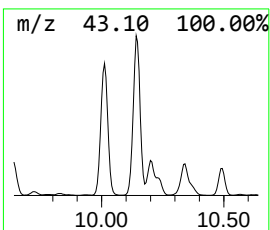
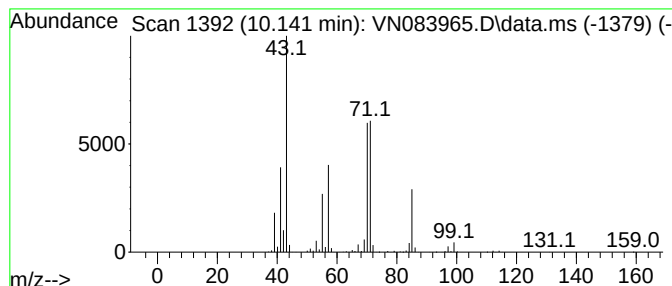
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Quant Title : SW846 8260

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

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Peak Number 5 Decane, 3,3,4-trimethyl- Concentration Rank 2

| R.T.   | EstConc     | Area    | Relative to ISTD    | R.T.  |
|--------|-------------|---------|---------------------|-------|
| 10.141 | 205.19 ug/l | 6236380 | 1,4-Difluorobenzene | 9.094 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|-----|---------|-------------|------|
| 1    |    |   | Pentane, 2,3,4-trimethyl- | 114 | C8H18   | 000565-75-3 | 81   |
| 2    |    |   | Decane, 3,3,4-trimethyl-  | 184 | C13H28  | 049622-18-6 | 64   |
| 3    |    |   | Pentane, 2,3,3-trimethyl- | 114 | C8H18   | 000560-21-4 | 64   |
| 4    |    |   | Heptane, 4-methyl-        | 114 | C8H18   | 000589-53-7 | 64   |
| 5    |    |   | Hexane, 2,3,4-trimethyl-  | 128 | C9H20   | 000921-47-1 | 59   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091724\  
Data File : VN083965.D  
Acq On : 18 Sep 2024 06:21  
Operator : JC\MD  
Sample : P3964-04  
Misc : 7.05g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 41 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.M  
Quant Title : SW846 8260

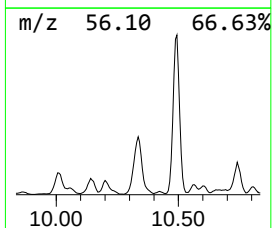
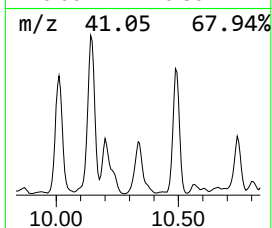
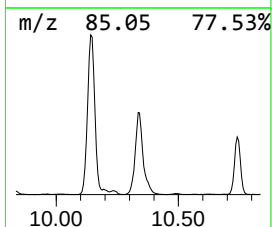
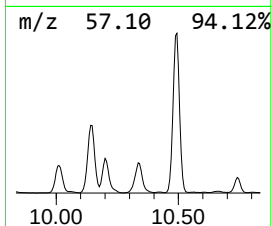
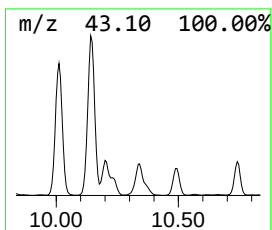
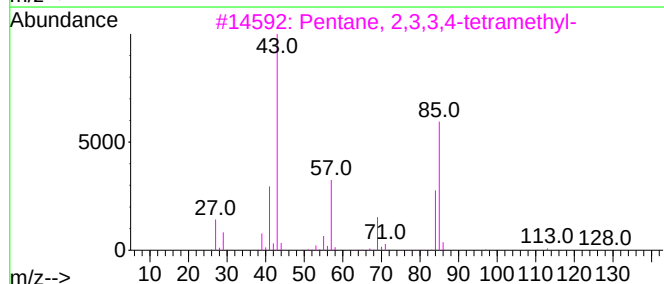
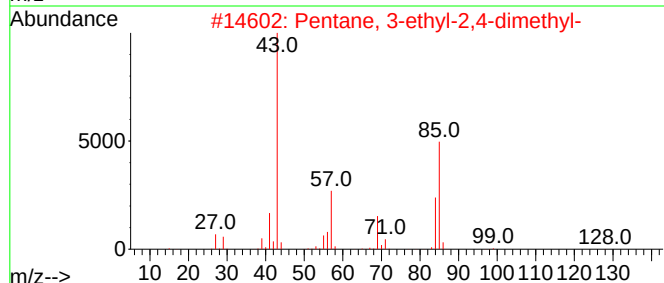
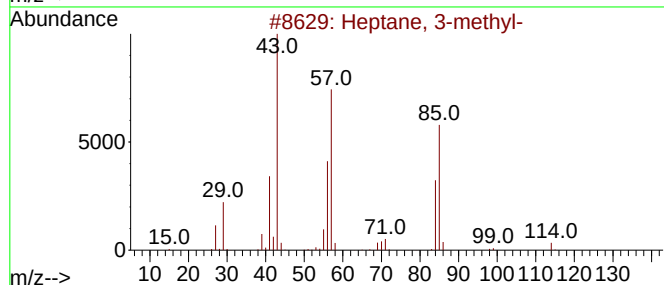
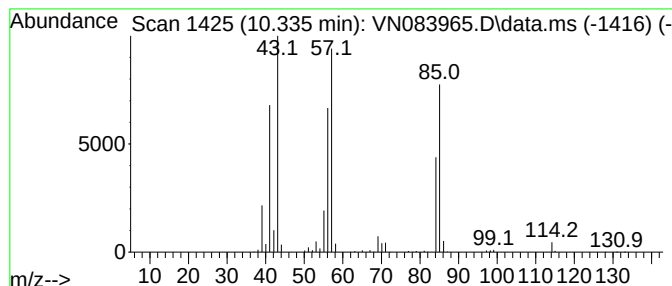
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Pentane, 3-ethyl-2,4-dimethyl- Concentration Rank 6

| R.T.   | EstConc    | Area    | Relative to ISTD    | R.T.  |
|--------|------------|---------|---------------------|-------|
| 10.335 | 58.21 ug/l | 1769060 | 1,4-Difluorobenzene | 9.094 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|-----|---------|-------------|------|
| 1    |    |   | Heptane, 3-methyl-             | 114 | C8H18   | 000589-81-1 | 91   |
| 2    |    |   | Pentane, 3-ethyl-2,4-dimethyl- | 128 | C9H20   | 001068-87-7 | 53   |
| 3    |    |   | Pentane, 2,3,3,4-tetramethyl-  | 128 | C9H20   | 016747-38-9 | 53   |
| 4    |    |   | Heptane, 4-ethyl-              | 128 | C9H20   | 002216-32-2 | 50   |
| 5    |    |   | Pentanoic acid, butyl ester    | 158 | C9H18O2 | 000591-68-4 | 50   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091724\  
Data File : VN083965.D  
Acq On : 18 Sep 2024 06:21  
Operator : JC\MD  
Sample : P3964-04  
Misc : 7.05g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 41 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

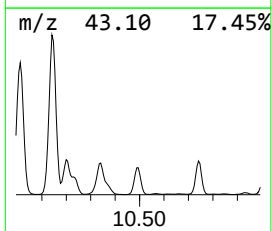
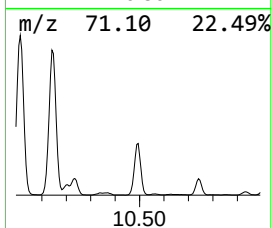
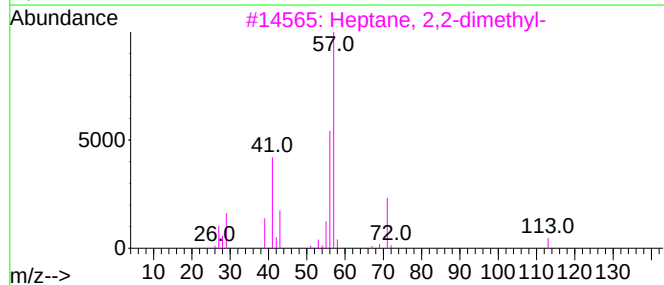
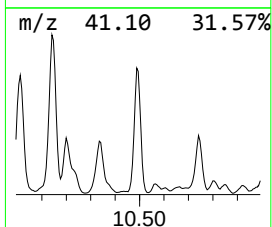
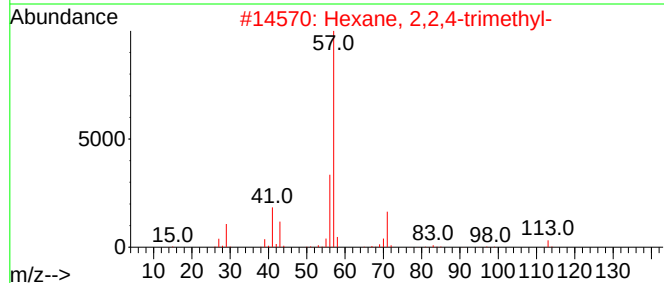
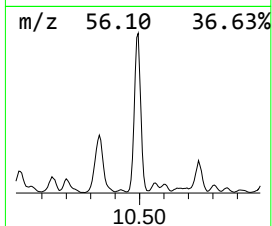
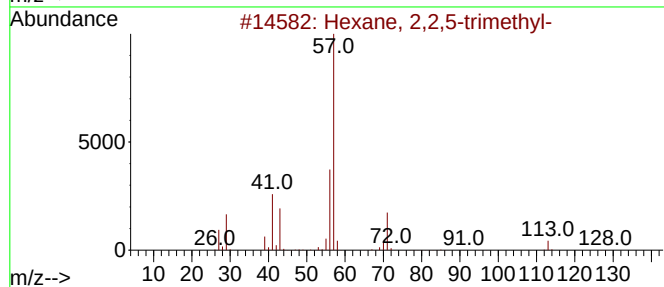
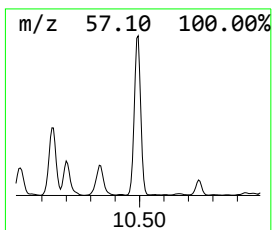
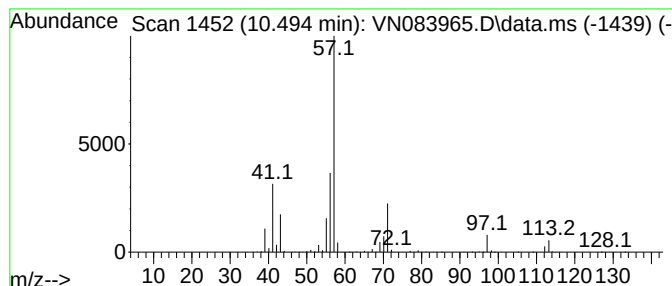
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Quant Title : SW846 8260

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

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Peak Number 7 Hexane, 2,2,5-trimethyl- Concentration Rank 4

| R.T.   | EstConc     | Area    | Relative to ISTD | R.T.   |
|--------|-------------|---------|------------------|--------|
| 10.494 | 109.28 ug/l | 3522860 | Chlorobenzene-d5 | 11.865 |

| Hit# | of | 5 | Tentative ID             | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------|-----|---------|-------------|------|
| 1    |    |   | Hexane, 2,2,5-trimethyl- | 128 | C9H20   | 003522-94-9 | 72   |
| 2    |    |   | Hexane, 2,2,4-trimethyl- | 128 | C9H20   | 016747-26-5 | 72   |
| 3    |    |   | Heptane, 2,2-dimethyl-   | 128 | C9H20   | 001071-26-7 | 64   |
| 4    |    |   | Undecane, 2,6-dimethyl-  | 184 | C13H28  | 017301-23-4 | 64   |
| 5    |    |   | Octane, 2,6-dimethyl-    | 142 | C10H22  | 002051-30-1 | 56   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091724\  
Data File : VN083965.D  
Acq On : 18 Sep 2024 06:21  
Operator : JC\MD  
Sample : P3964-04  
Misc : 7.05g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 41 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

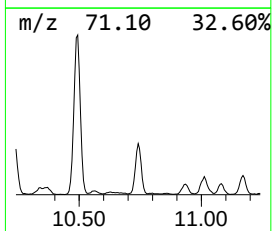
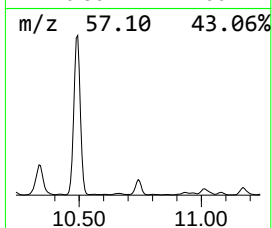
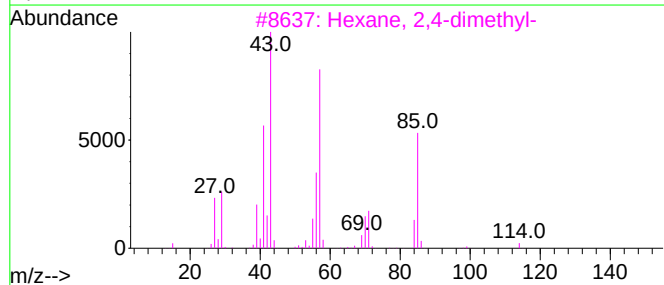
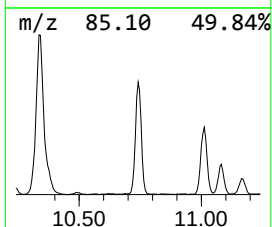
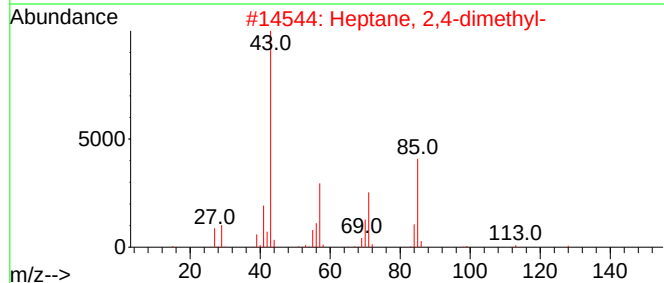
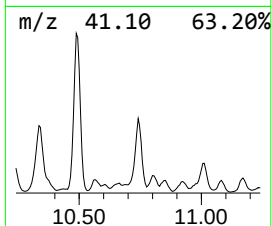
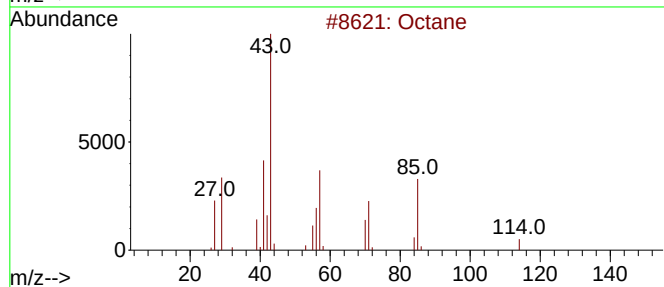
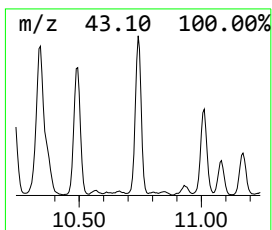
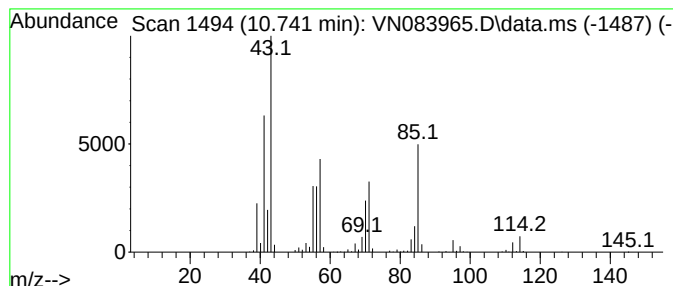
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Quant Title : SW846 8260

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

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Peak Number 8 Octane Concentration Rank 8

| R.T.   | EstConc    | Area    | Relative to ISTD | R.T.   |
|--------|------------|---------|------------------|--------|
| 10.741 | 45.14 ug/l | 1455230 | Chlorobenzene-d5 | 11.865 |

| Hit# | of | 5 | Tentative ID            | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------|-----|---------|-------------|------|
| 1    |    |   | Octane                  | 114 | C8H18   | 000111-65-9 | 90   |
| 2    |    |   | Heptane, 2,4-dimethyl-  | 128 | C9H20   | 002213-23-2 | 58   |
| 3    |    |   | Hexane, 2,4-dimethyl-   | 114 | C8H18   | 000589-43-5 | 53   |
| 4    |    |   | Undecane, 2,4-dimethyl- | 184 | C13H28  | 017312-80-0 | 47   |
| 5    |    |   | Heptane, 4,4-dimethyl-  | 128 | C9H20   | 001068-19-5 | 38   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091724\  
Data File : VN083965.D  
Acq On : 18 Sep 2024 06:21  
Operator : JC\MD  
Sample : P3964-04  
Misc : 7.05g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 41 Sample Multiplier: 1

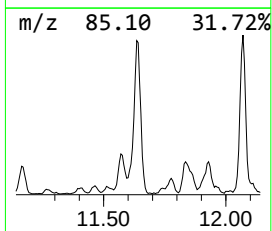
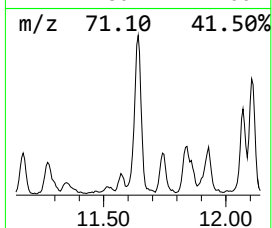
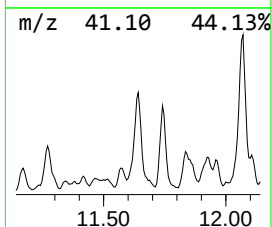
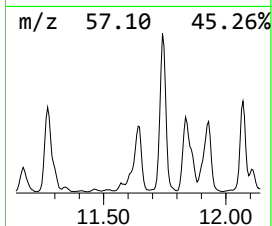
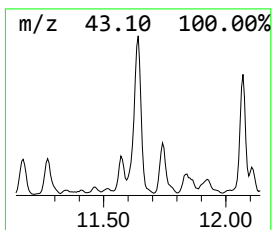
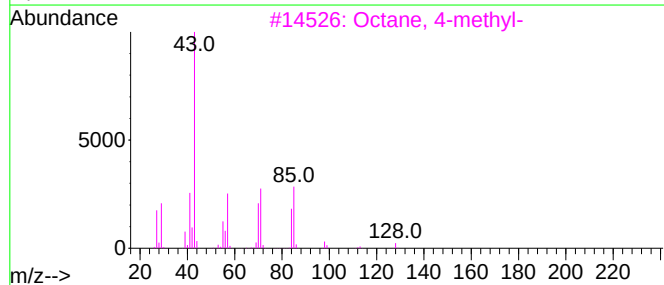
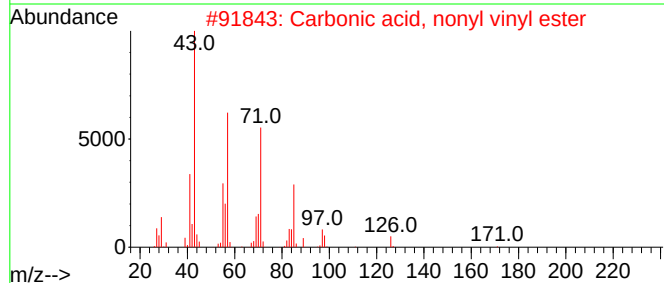
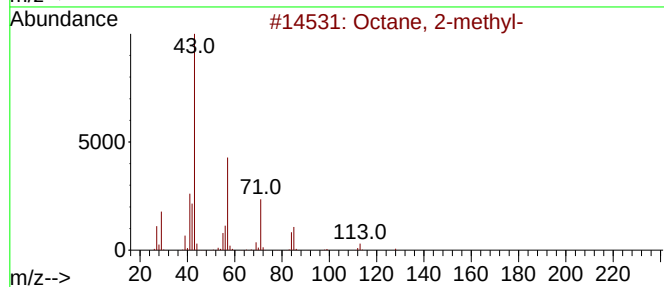
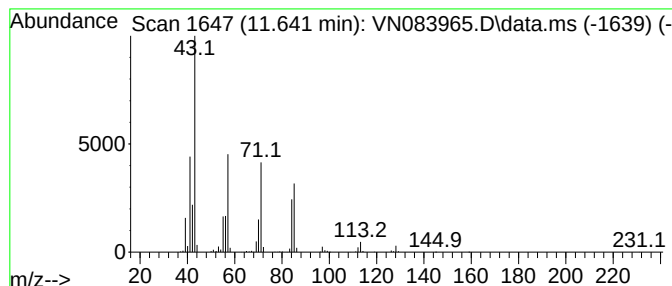
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MSVOA\_N  
ClientSampleId :  
SINK-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.M  
Quant Title : SW846 8260

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

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Peak Number 9 Octane, 2-methyl- Concentration Rank 7

| R.T.      | EstConc                          | Area    | Relative to ISTD |          | R.T.         |      |
|-----------|----------------------------------|---------|------------------|----------|--------------|------|
| 11.641    | 49.23 ug/l                       | 1587080 | Chlorobenzene-d5 |          | 11.865       |      |
| Hit# of 5 | Tentative ID                     |         | MW               | MolForm  | CAS#         | Qual |
| 1         | Octane, 2-methyl-                |         | 128              | C9H20    | 003221-61-2  | 64   |
| 2         | Carbonic acid, nonyl vinyl ester |         | 214              | C12H22O3 | 1000383-25-6 | 64   |
| 3         | Octane, 4-methyl-                |         | 128              | C9H20    | 002216-34-4  | 64   |
| 4         | Hexane, 2,3,4-trimethyl-         |         | 128              | C9H20    | 000921-47-1  | 59   |
| 5         | Heptane, 2,6-dimethyl-           |         | 128              | C9H20    | 001072-05-5  | 59   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091724\  
Data File : VN083965.D  
Acq On : 18 Sep 2024 06:21  
Operator : JC\MD  
Sample : P3964-04  
Misc : 7.05g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 41 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

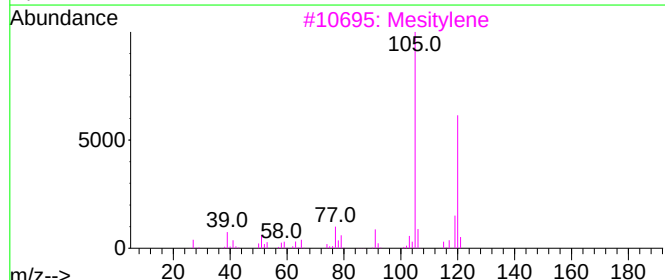
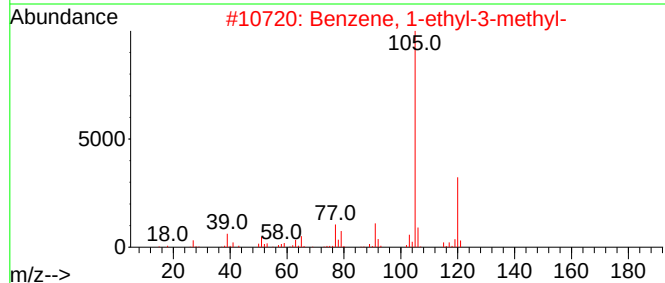
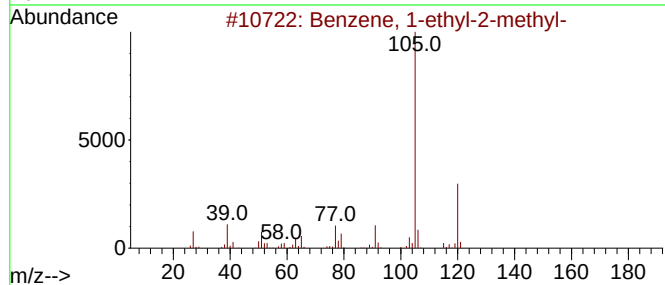
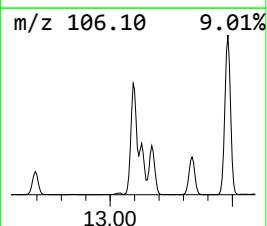
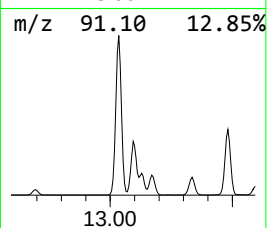
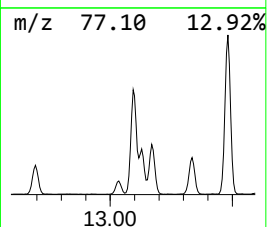
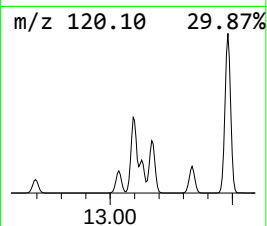
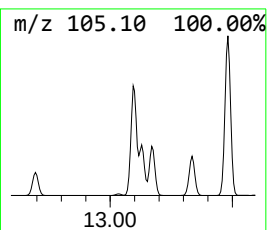
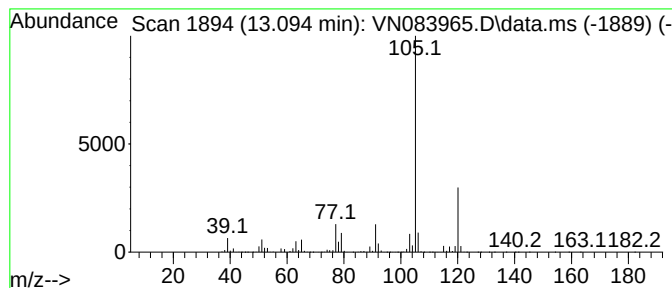
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.M  
Quant Title : SW846 8260

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

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Peak Number 10 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

| R.T.   | EstConc    | Area     | Relative to ISTD       | R.T.   |
|--------|------------|----------|------------------------|--------|
| 13.094 | 87.69 ug/l | 11640900 | 1,4-Dichlorobenzene-d4 | 13.788 |

| Hit# | of | 5 | Tentative ID               | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------|-----|---------|-------------|------|
| 1    |    |   | Benzene, 1-ethyl-2-methyl- | 120 | C9H12   | 000611-14-3 | 95   |
| 2    |    |   | Benzene, 1-ethyl-3-methyl- | 120 | C9H12   | 000620-14-4 | 94   |
| 3    |    |   | Mesitylene                 | 120 | C9H12   | 000108-67-8 | 91   |
| 4    |    |   | Benzene, 1,2,3-trimethyl-  | 120 | C9H12   | 000526-73-8 | 91   |
| 5    |    |   | Benzene, 1,2,4-trimethyl-  | 120 | C9H12   | 000095-63-6 | 91   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091724\  
Data File : VN083965.D  
Acq On : 18 Sep 2024 06:21  
Operator : JC\MD  
Sample : P3964-04  
Misc : 7.05g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 41 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
SINK-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.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 |
| Hexane, 3-methyl-  | 8.441  | 34.0    | ug/l  | 1320090  | 1                     | 8.218  | 1941220 | 50.0 |
| Butane, 2,2,3,3... | 8.753  | 247.7   | ug/l  | 7527100  | 2                     | 9.094  | 1519650 | 50.0 |
| Heptane            | 8.965  | 39.2    | ug/l  | 1190600  | 2                     | 9.094  | 1519650 | 50.0 |
| Pentane, 2,3,4-... | 10.012 | 141.0   | ug/l  | 4285110  | 2                     | 9.094  | 1519650 | 50.0 |
| Decane, 3,3,4-t... | 10.141 | 205.2   | ug/l  | 6236380  | 2                     | 9.094  | 1519650 | 50.0 |
| Pentane, 3-ethy... | 10.335 | 58.2    | ug/l  | 1769060  | 2                     | 9.094  | 1519650 | 50.0 |
| Hexane, 2,2,5-t... | 10.494 | 109.3   | ug/l  | 3522860  | 3                     | 11.865 | 1611840 | 50.0 |
| Octane             | 10.741 | 45.1    | ug/l  | 1455230  | 3                     | 11.865 | 1611840 | 50.0 |
| Octane, 2-methyl-  | 11.641 | 49.2    | ug/l  | 1587080  | 3                     | 11.865 | 1611840 | 50.0 |
| Benzene, 1-ethy... | 13.094 | 87.7    | ug/l  | 11640900 | 4                     | 13.788 | 6637180 | 50.0 |