

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN011123\  
 Data File : VN076212.D  
 Acq On : 11 Jan 2023 16:04  
 Operator : JC\MD  
 Sample : 01081-01  
 Misc : 5.09g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 31963

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\82N121422W.M  
 Title : SW846 8260

Signal : TIC: VN076212.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         | 8.171       | 1030          | 1040        | 1044         | rBV      | 233007         | 572837        | 10.68%          | 2.311%        |
| 2         | 8.224       | 1044          | 1049        | 1063         | rVB      | 488265         | 1090833       | 20.34%          | 4.401%        |
| 3         | 8.582       | 1100          | 1110        | 1123         | rBV2     | 265074         | 754074        | 14.06%          | 3.043%        |
| 4         | 9.100       | 1189          | 1198        | 1213         | rBV      | 649689         | 1311805       | 24.47%          | 5.293%        |
| 5         | 10.565      | 1439          | 1447        | 1453         | rBV      | 947051         | 1754628       | 32.72%          | 7.080%        |
| 6         | 10.629      | 1453          | 1458        | 1470         | rVV      | 340504         | 631765        | 11.78%          | 2.549%        |
| 7         | 11.865      | 1660          | 1668        | 1678         | rBV      | 793465         | 1452331       | 27.09%          | 5.860%        |
| 8         | 11.965      | 1678          | 1685        | 1691         | rBV      | 129507         | 228040        | 4.25%           | 0.920%        |
| 9         | 12.070      | 1696          | 1703        | 1714         | rVB      | 797505         | 1502490       | 28.02%          | 6.062%        |
| 10        | 12.400      | 1746          | 1759        | 1768         | rBV      | 806127         | 1396750       | 26.05%          | 5.636%        |
| 11        | 12.853      | 1829          | 1836        | 1845         | rVB      | 642850         | 1092045       | 20.37%          | 4.406%        |
| 12        | 13.035      | 1860          | 1867        | 1872         | rBV      | 68959          | 122070        | 2.28%           | 0.493%        |
| 13        | 13.100      | 1872          | 1878        | 1886         | rVV      | 248147         | 585584        | 10.92%          | 2.363%        |
| 14        | 13.176      | 1886          | 1891        | 1898         | rVB      | 358468         | 628530        | 11.72%          | 2.536%        |
| 15        | 13.335      | 1910          | 1918        | 1925         | rBV      | 128881         | 249199        | 4.65%           | 1.005%        |
| 16        | 13.482      | 1933          | 1943        | 1950         | rBV      | 695620         | 1188195       | 22.16%          | 4.794%        |
| 17        | 13.794      | 1989          | 1996        | 2015         | rVB2     | 840511         | 1870350       | 34.88%          | 7.547%        |
| 18        | 13.994      | 2025          | 2030        | 2032         | rBV2     | 57697          | 96359         | 1.80%           | 0.389%        |
| 19        | 14.106      | 2045          | 2049        | 2056         | rVB      | 121163         | 186166        | 3.47%           | 0.751%        |
| 20        | 14.182      | 2056          | 2062        | 2067         | rVB2     | 59656          | 101127        | 1.89%           | 0.408%        |
| 21        | 14.253      | 2067          | 2074        | 2075         | rBV2     | 37388          | 59458         | 1.11%           | 0.240%        |
| 22        | 14.270      | 2075          | 2077        | 2083         | rVV2     | 40493          | 63015         | 1.18%           | 0.254%        |
| 23        | 14.329      | 2083          | 2087        | 2092         | rVB      | 51642          | 78309         | 1.46%           | 0.316%        |
| 24        | 14.441      | 2101          | 2106        | 2112         | rBV2     | 36836          | 66176         | 1.23%           | 0.267%        |
| 25        | 14.629      | 2134          | 2138        | 2140         | rBV4     | 50102          | 71071         | 1.33%           | 0.287%        |
| 26        | 14.659      | 2140          | 2143        | 2146         | rVV2     | 55268          | 81358         | 1.52%           | 0.328%        |
| 27        | 14.694      | 2146          | 2149        | 2153         | rVB      | 64255          | 84608         | 1.58%           | 0.341%        |
| 28        | 14.958      | 2185          | 2194        | 2201         | rBV5     | 129893         | 250663        | 4.67%           | 1.011%        |
| 29        | 15.041      | 2202          | 2208        | 2216         | rBV3     | 95304          | 264112        | 4.93%           | 1.066%        |
| 30        | 15.323      | 2251          | 2256        | 2264         | rBV6     | 29053          | 72109         | 1.34%           | 0.291%        |
| 31        | 15.435      | 2270          | 2275        | 2282         | rVB7     | 30559          | 72244         | 1.35%           | 0.291%        |
| 32        | 15.641      | 2298          | 2310        | 2321         | rBV      | 2717125        | 5361790       | 100.00%         | 21.634%       |
| 33        | 15.747      | 2322          | 2328        | 2333         | rVV      | 61677          | 112881        | 2.11%           | 0.455%        |
| 34        | 15.835      | 2339          | 2343        | 2353         | rVB3     | 79251          | 162049        | 3.02%           | 0.654%        |
| 35        | 15.953      | 2354          | 2363        | 2370         | rBV3     | 22743          | 80718         | 1.51%           | 0.326%        |
| 36        | 16.494      | 2447          | 2455        | 2460         | rBV3     | 24469          | 64401         | 1.20%           | 0.260%        |

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Sample : 01081-01  
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
31963

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\82N121422W.M  
Title : SW846 8260

|    |        |      |      |      |     |        |         |        |        |
|----|--------|------|------|------|-----|--------|---------|--------|--------|
| 37 | 16.782 | 2496 | 2504 | 2505 | rBV | 693076 | 1023626 | 19.09% | 4.130% |
|----|--------|------|------|------|-----|--------|---------|--------|--------|

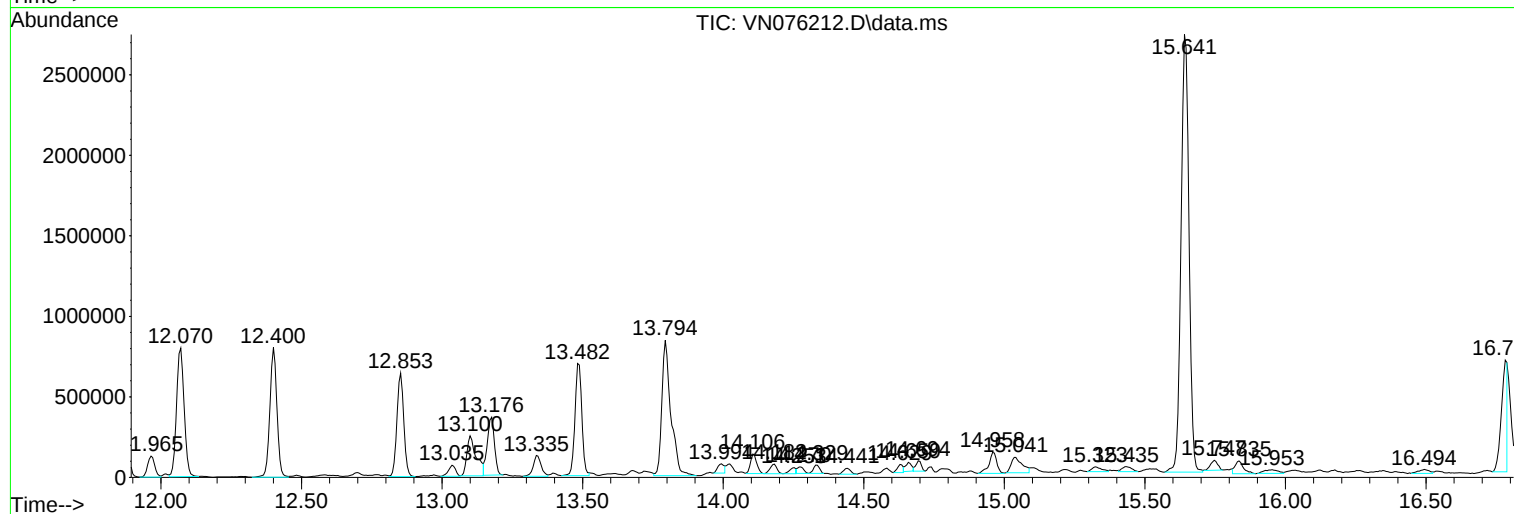
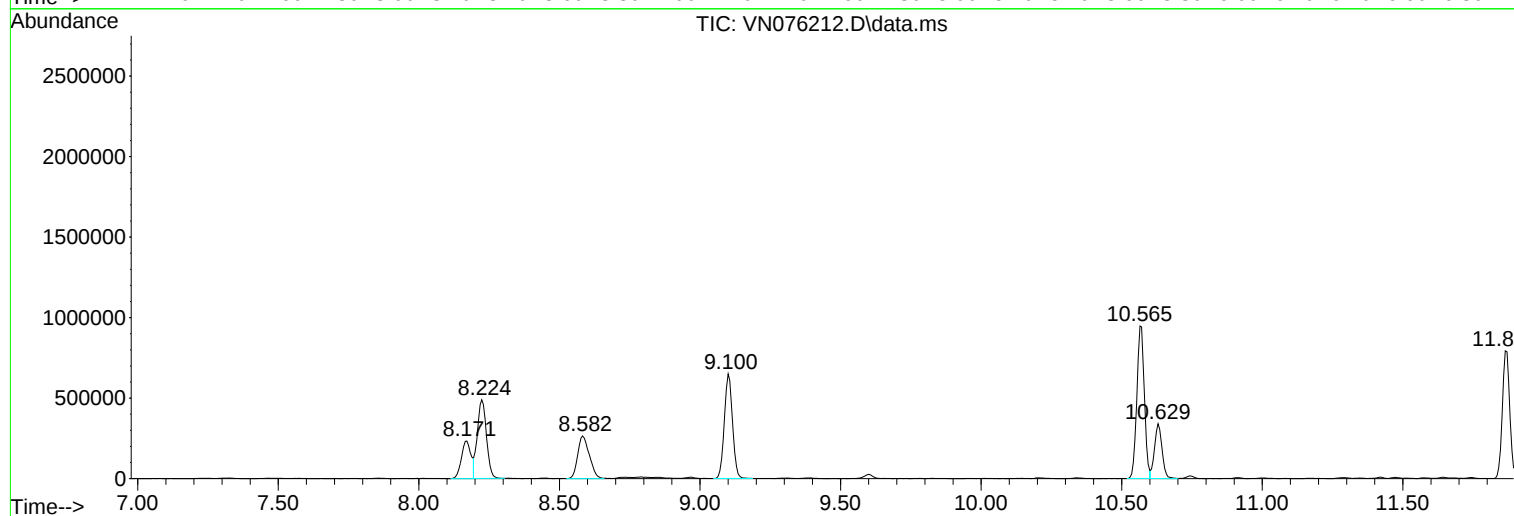
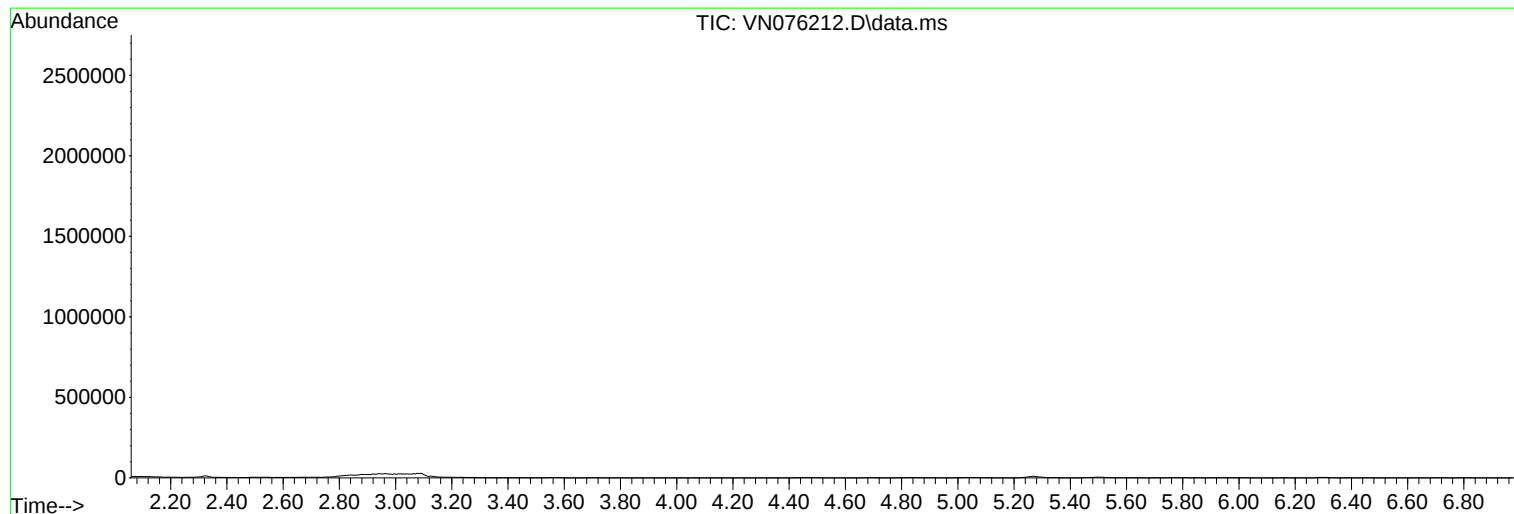
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Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN011123\  
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Instrument :  
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ClientSampleId :  
31963

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121422W.M  
Quant Title : SW846 8260

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



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Operator : JC\MD  
Sample : 01081-01  
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
31963

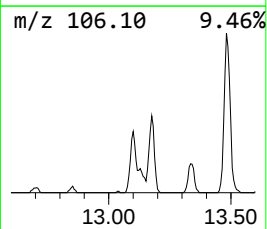
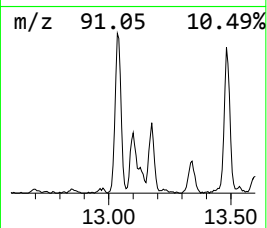
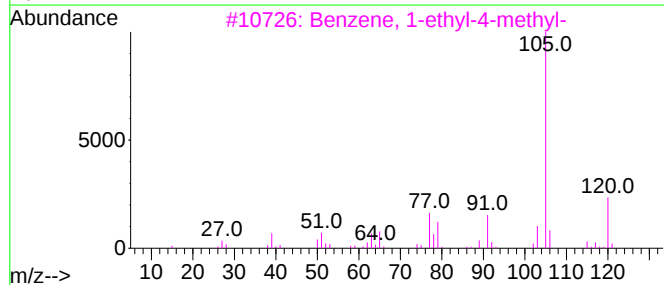
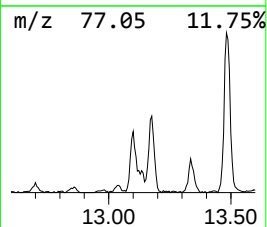
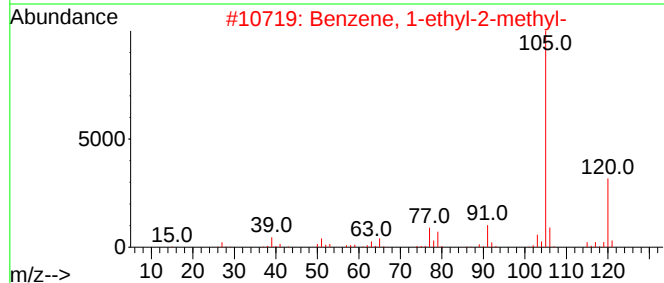
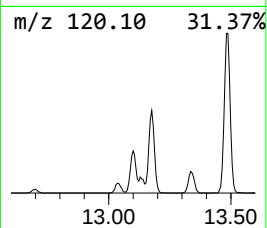
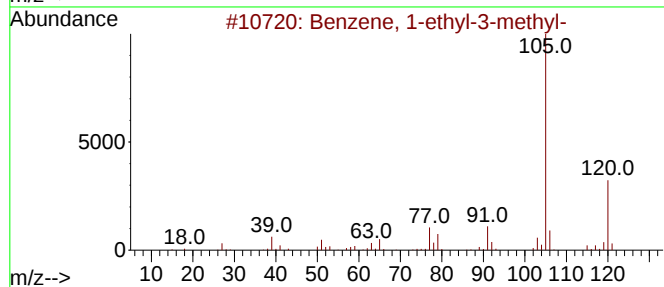
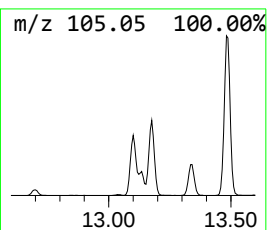
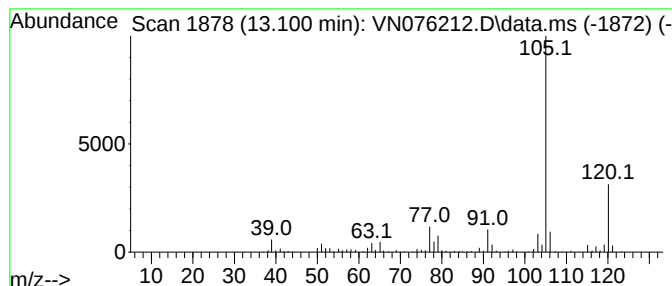
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121422W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 13.100 | 15.65 ug/l | 585584 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID               | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------|-----|---------|-------------|------|
| 1    |    |   | Benzene, 1-ethyl-3-methyl- | 120 | C9H12   | 000620-14-4 | 97   |
| 2    |    |   | Benzene, 1-ethyl-2-methyl- | 120 | C9H12   | 000611-14-3 | 95   |
| 3    |    |   | Benzene, 1-ethyl-4-methyl- | 120 | C9H12   | 000622-96-8 | 94   |
| 4    |    |   | Mesitylene                 | 120 | C9H12   | 000108-67-8 | 91   |
| 5    |    |   | Benzene, 1,2,4-trimethyl-  | 120 | C9H12   | 000095-63-6 | 91   |



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Misc : 5.09g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
31963

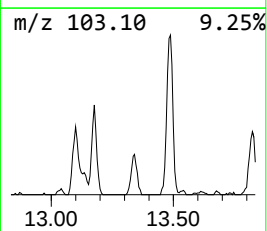
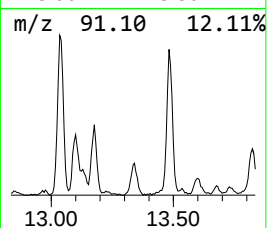
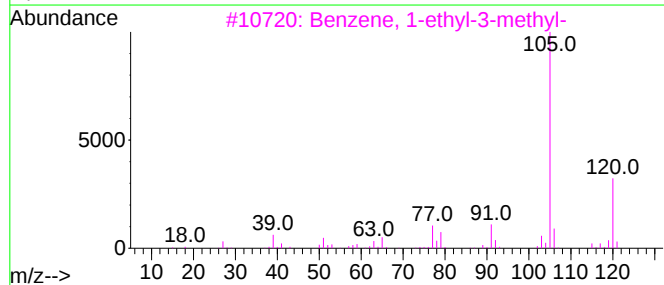
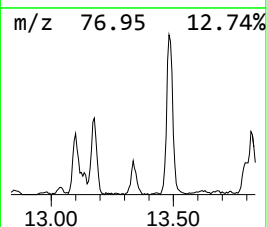
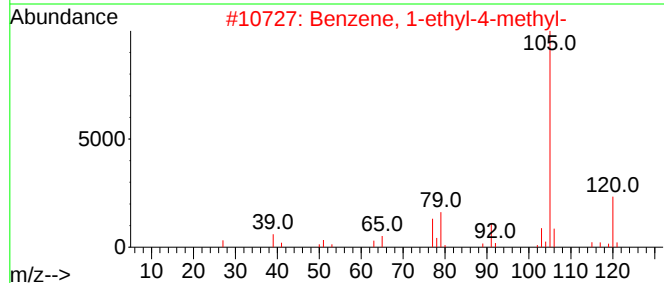
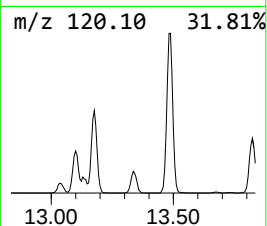
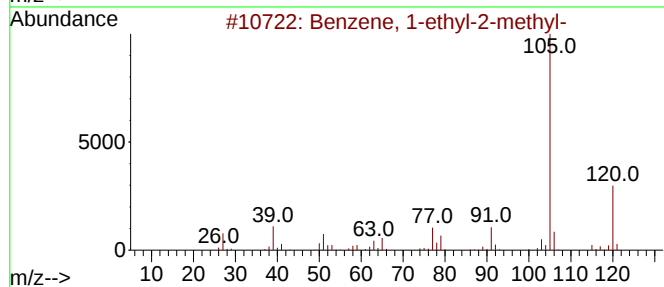
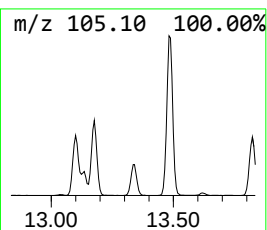
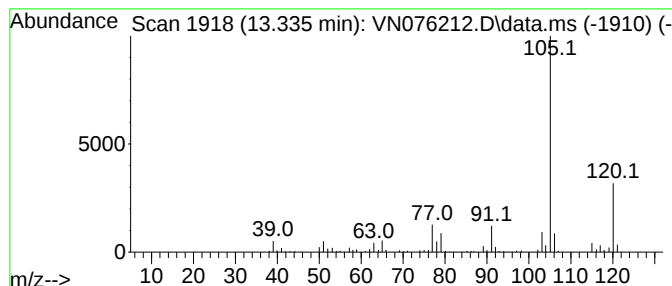
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121422W.M  
Quant Title : SW846 8260

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

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

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 13.335 | 6.66 ug/l | 249199 | 1,4-Dichlorobenzene-d4 | 13.794 |

| 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-4-methyl- | 120 | C9H12   | 000622-96-8 | 94   |
| 3    |    |   | Benzene, 1-ethyl-3-methyl- | 120 | C9H12   | 000620-14-4 | 91   |
| 4    |    |   | Benzene, 1,2,3-trimethyl-  | 120 | C9H12   | 000526-73-8 | 91   |
| 5    |    |   | Mesitylene                 | 120 | C9H12   | 000108-67-8 | 91   |



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ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
31963

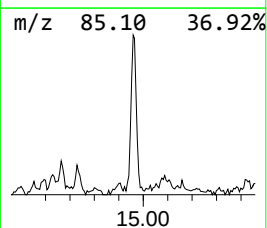
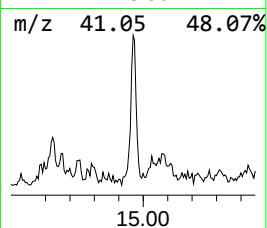
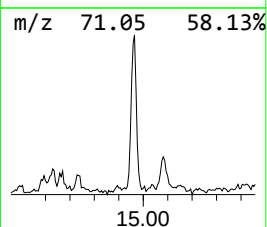
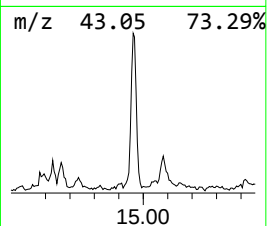
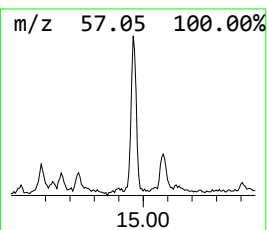
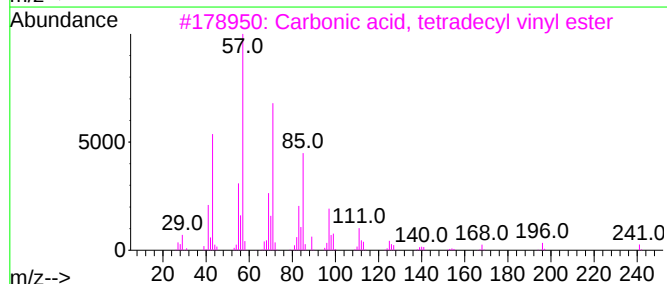
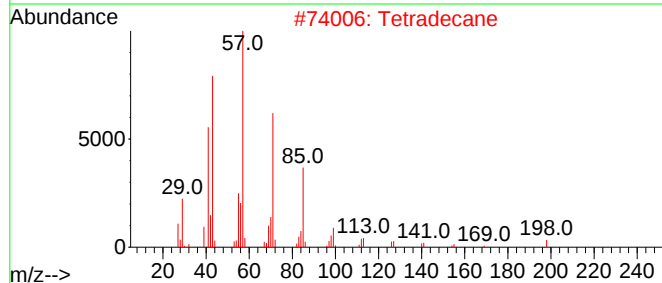
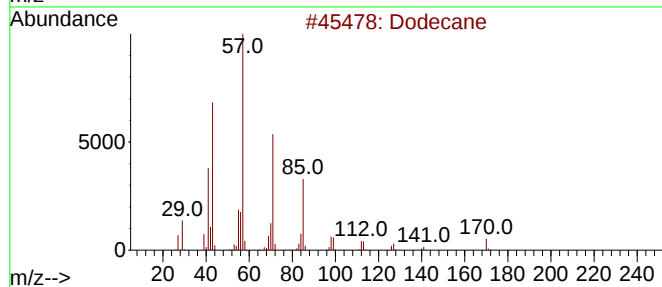
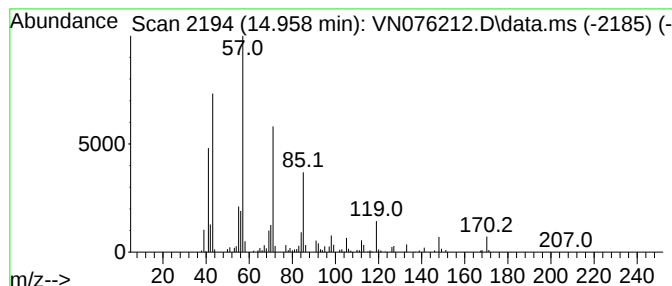
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121422W.M  
Quant Title : SW846 8260

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

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Peak Number 3 Dodecane Concentration Rank 4

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 14.959 | 6.70 ug/l | 250663 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Dodecane                            | 170 | C12H26   | 000112-40-3  | 90   |
| 2    |    |   | Tetradecane                         | 198 | C14H30   | 000629-59-4  | 72   |
| 3    |    |   | Carbonic acid, tetradecyl vinyl ... | 284 | C17H32O3 | 1000382-54-5 | 64   |
| 4    |    |   | Hexadecane                          | 226 | C16H34   | 000544-76-3  | 59   |
| 5    |    |   | Decane, 5-propyl-                   | 184 | C13H28   | 017312-62-8  | 53   |



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ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
31963

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121422W.M  
Quant Title : SW846 8260

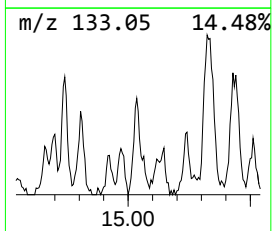
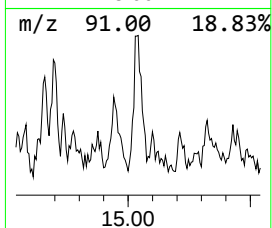
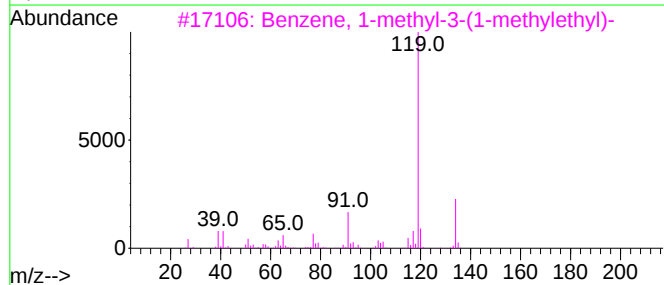
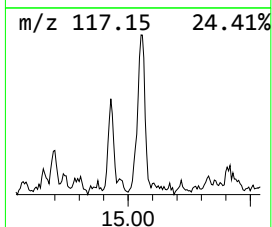
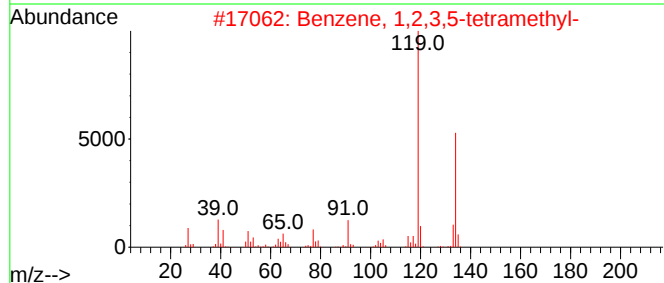
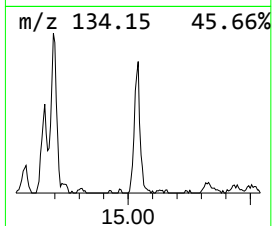
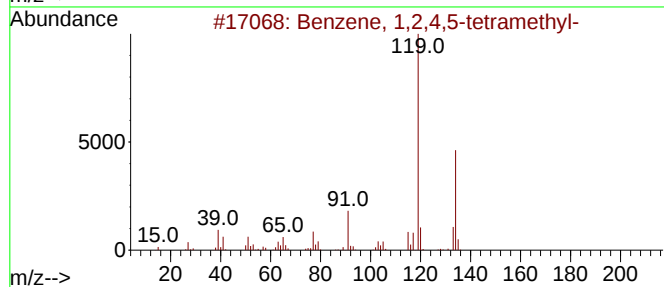
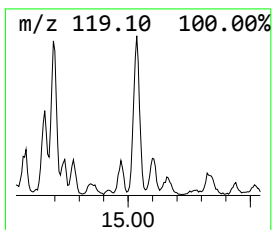
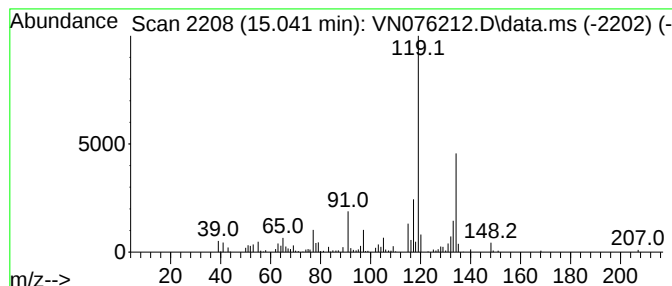
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 3

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 15.041 | 7.06 ug/l | 264112 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Benzene, 1,2,4,5-tetramethyl-       | 134 | C10H14  | 000095-93-2 | 93   |
| 2    |    |   | Benzene, 1,2,3,5-tetramethyl-       | 134 | C10H14  | 000527-53-7 | 76   |
| 3    |    |   | Benzene, 1-methyl-3-(1-methyleth... | 134 | C10H14  | 000535-77-3 | 76   |
| 4    |    |   | 1,3-Cyclopentadiene, 1,2,3,4-tet... | 134 | C10H14  | 076089-59-3 | 76   |
| 5    |    |   | Benzene, 4-ethyl-1,2-dimethyl-      | 134 | C10H14  | 000934-80-5 | 70   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN011123\  
Data File : VN076212.D  
Acq On : 11 Jan 2023 16:04  
Operator : JC\MD  
Sample : 01081-01  
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
31963

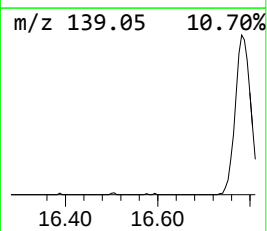
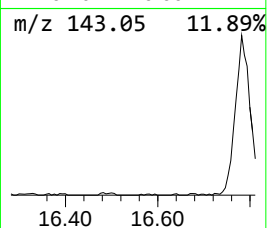
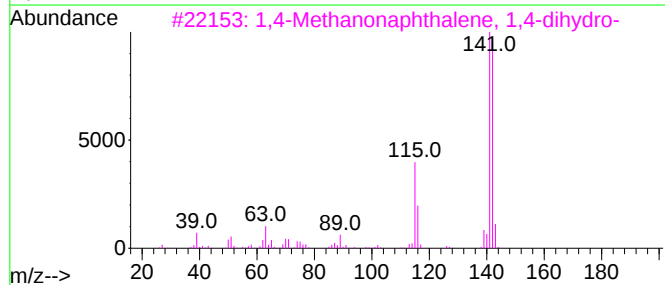
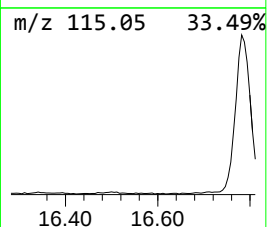
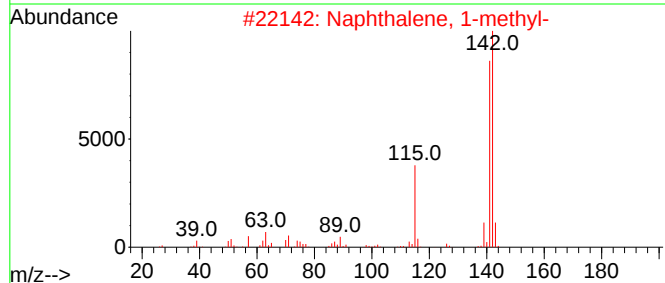
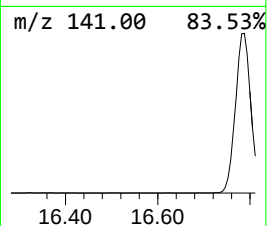
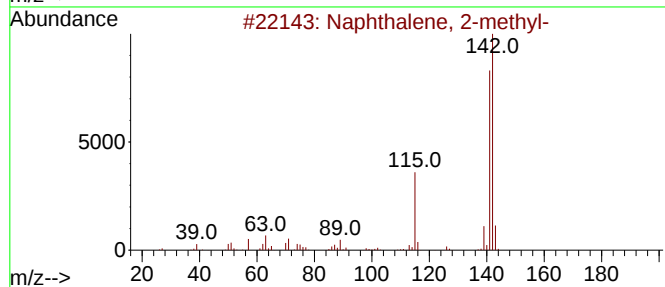
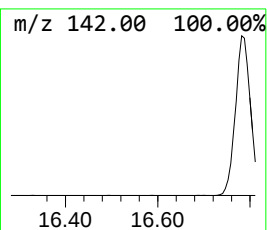
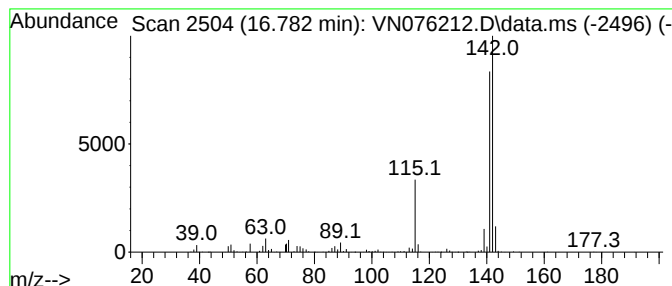
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121422W.M  
Quant Title : SW846 8260

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

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Peak Number 5 Naphthalene, 2-methyl- Concentration Rank 1

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 16.782 | 27.36 ug/l | 1023630 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Naphthalene, 2-methyl-              | 142 | C11H10  | 000091-57-6 | 96   |
| 2    |    |   | Naphthalene, 1-methyl-              | 142 | C11H10  | 000090-12-0 | 96   |
| 3    |    |   | 1,4-Methanonaphthalene, 1,4-dihy... | 142 | C11H10  | 004453-90-1 | 91   |
| 4    |    |   | Benzocycloheptatriene               | 142 | C11H10  | 000264-09-5 | 91   |
| 5    |    |   | 1H-Indene, 1-ethylidene-            | 142 | C11H10  | 002471-83-2 | 64   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN011123\  
Data File : VN076212.D  
Acq On : 11 Jan 2023 16:04  
Operator : JC\MD  
Sample : 01081-01  
Misc : 5.09g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
31963

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N121422W.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 |
| Benzene, 1-ethy... | 13.100 | 15.7    | ug/l  | 585584   | 4                     | 13.794 | 1870350 | 50.0 |
| Benzene, 1-ethy... | 13.335 | 6.7     | ug/l  | 249199   | 4                     | 13.794 | 1870350 | 50.0 |
| Dodecane           | 14.959 | 6.7     | ug/l  | 250663   | 4                     | 13.794 | 1870350 | 50.0 |
| Benzene, 1,2,4,... | 15.041 | 7.1     | ug/l  | 264112   | 4                     | 13.794 | 1870350 | 50.0 |
| Naphthalene, 2-... | 16.782 | 27.4    | ug/l  | 1023630  | 4                     | 13.794 | 1870350 | 50.0 |