

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN052324\  
 Data File : VN082323.D  
 Acq On : 23 May 2024 15:54  
 Operator : JC\MD  
 Sample : P2558-01 10X  
 Misc : 1.12g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 COMP-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\82N051524W.M  
 Title : SW846 8260

Signal : TIC: VN082323.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         | 2.842       | 139           | 151         | 152          | rBV5     | 19713          | 49778         | 3.89%           | 0.566%        |
| 2         | 8.171       | 1045          | 1057        | 1061         | rBV      | 161409         | 387445        | 30.31%          | 4.402%        |
| 3         | 8.224       | 1061          | 1066        | 1077         | rVV      | 310223         | 703473        | 55.03%          | 7.992%        |
| 4         | 8.324       | 1077          | 1083        | 1092         | rVB4     | 10236          | 27334         | 2.14%           | 0.311%        |
| 5         | 8.447       | 1094          | 1104        | 1112         | rBV3     | 36019          | 86576         | 6.77%           | 0.984%        |
| 6         | 8.582       | 1118          | 1127        | 1138         | rBV      | 193668         | 426396        | 33.36%          | 4.844%        |
| 7         | 8.682       | 1138          | 1144        | 1145         | rBV2     | 8591           | 13105         | 1.03%           | 0.149%        |
| 8         | 8.971       | 1184          | 1193        | 1200         | rVB      | 38219          | 72399         | 5.66%           | 0.823%        |
| 9         | 9.106       | 1207          | 1216        | 1229         | rBV      | 427438         | 894472        | 69.97%          | 10.162%       |
| 10        | 9.600       | 1296          | 1300        | 1305         | rVV8     | 7834           | 14071         | 1.10%           | 0.160%        |
| 11        | 10.159      | 1387          | 1395        | 1397         | rBV7     | 6842           | 14854         | 1.16%           | 0.169%        |
| 12        | 10.570      | 1456          | 1465        | 1470         | rBV      | 700282         | 1278307       | 100.00%         | 14.523%       |
| 13        | 10.635      | 1470          | 1476        | 1485         | rVB      | 605879         | 1137571       | 88.99%          | 12.924%       |
| 14        | 11.864      | 1679          | 1685        | 1694         | rBV      | 638381         | 1134836       | 88.78%          | 12.893%       |
| 15        | 12.070      | 1716          | 1720        | 1726         | rBV4     | 24866          | 44911         | 3.51%           | 0.510%        |
| 16        | 12.853      | 1847          | 1853        | 1861         | rVB      | 518514         | 891731        | 69.76%          | 10.131%       |
| 17        | 13.794      | 2007          | 2013        | 2020         | rVB      | 634662         | 1066663       | 83.44%          | 12.119%       |
| 18        | 14.958      | 2208          | 2211        | 2215         | rVB2     | 81810          | 110496        | 8.64%           | 1.255%        |
| 19        | 15.029      | 2217          | 2223        | 2230         | rVB5     | 116884         | 295050        | 23.08%          | 3.352%        |
| 20        | 15.829      | 2356          | 2359        | 2364         | rVB3     | 100395         | 152434        | 11.92%          | 1.732%        |

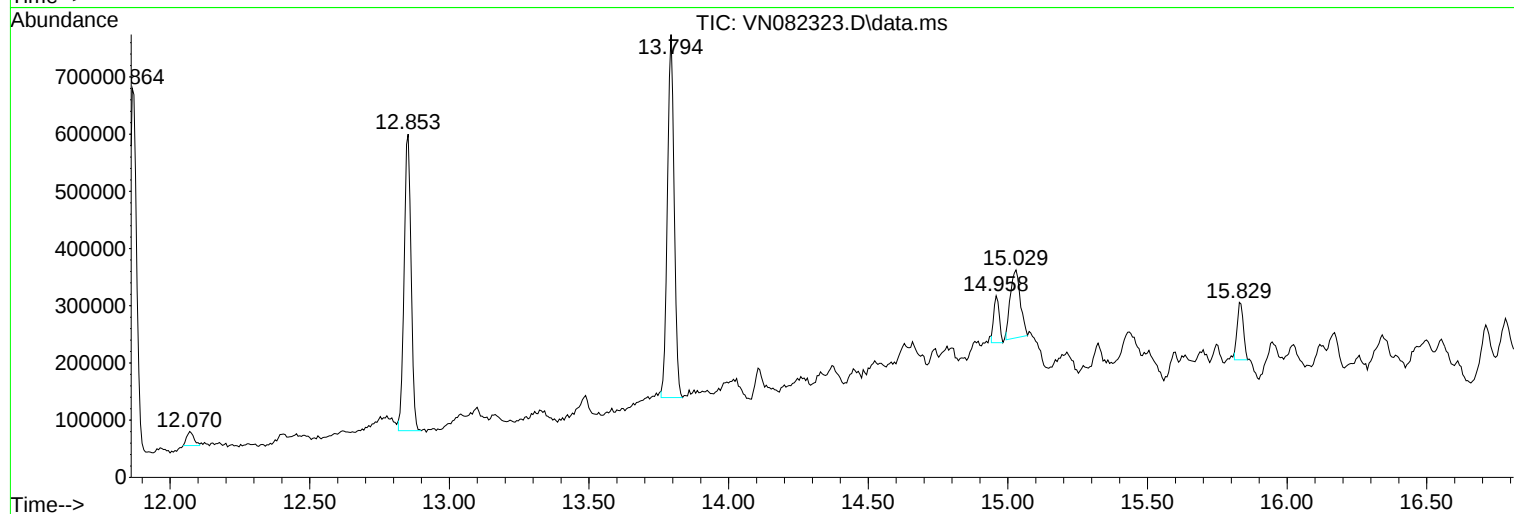
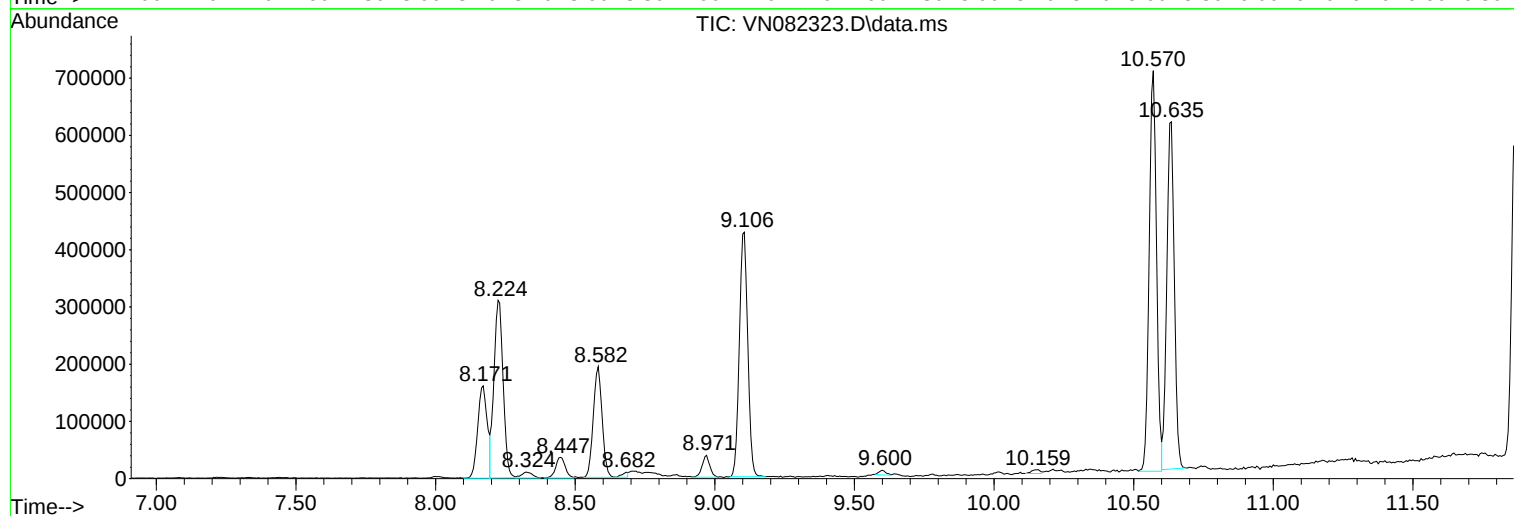
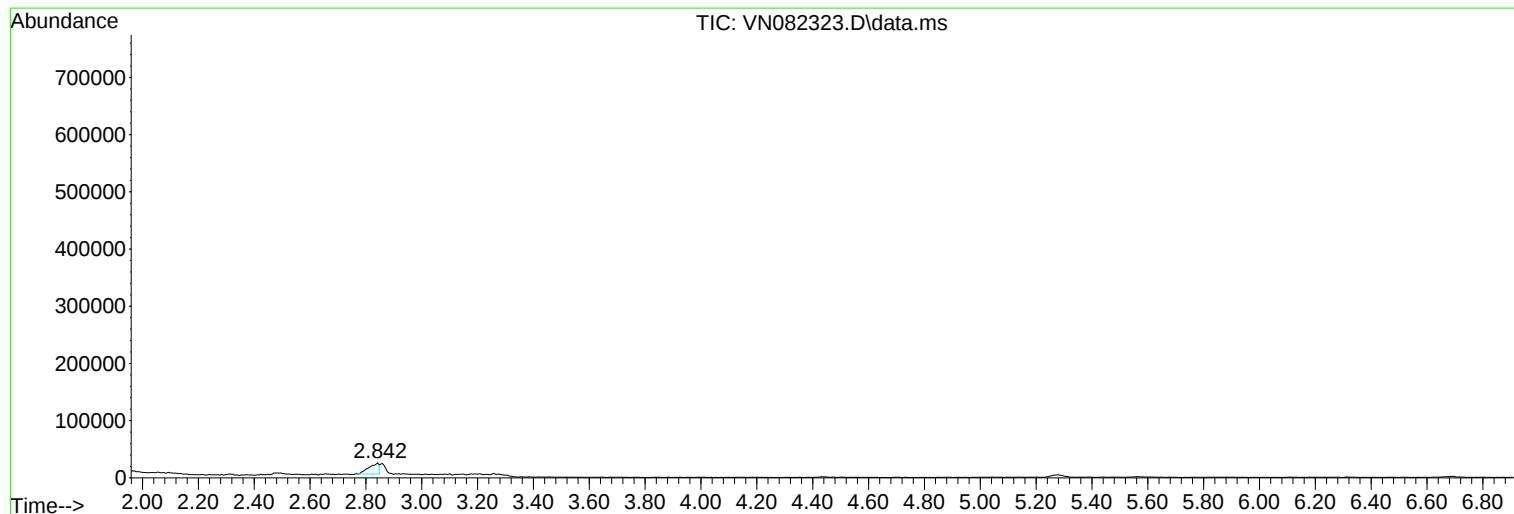
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ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
COMP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051524W.M  
Quant Title : SW846 8260

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



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ClientSampleId :  
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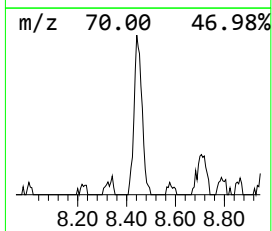
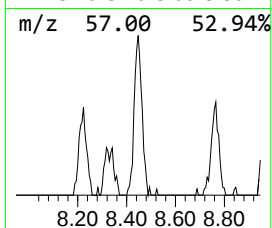
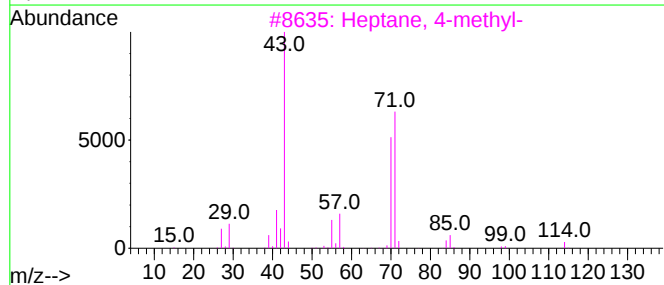
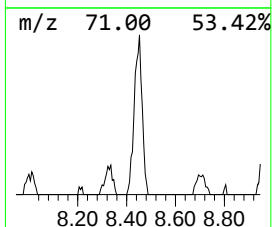
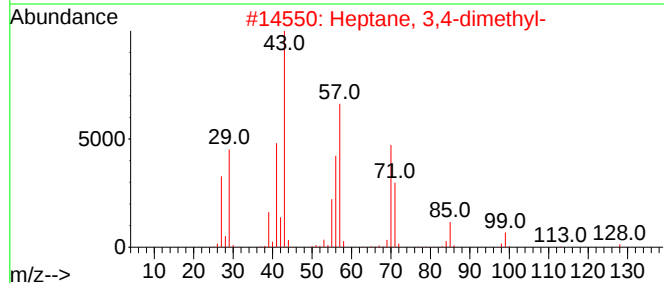
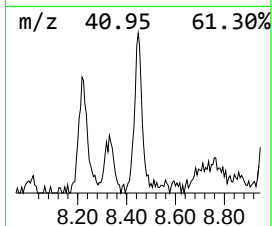
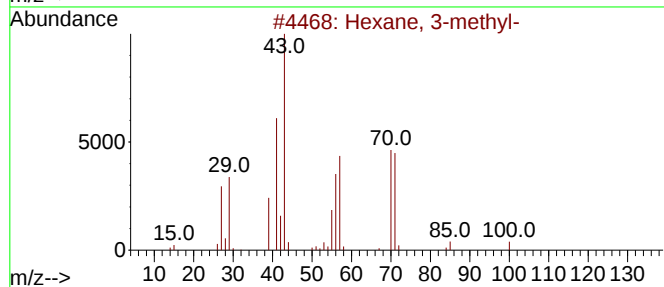
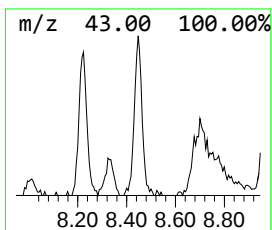
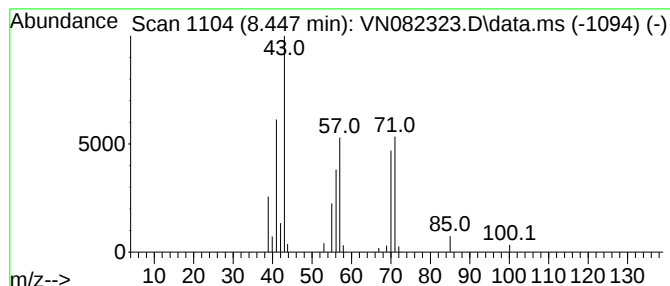
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051524W.M  
Quant Title : SW846 8260

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

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

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 8.447 | 6.15 ug/l | 86576 | Pentafluorobenzene | 8.224 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|-----|---------|-------------|------|
| 1    |    |   | Hexane, 3-methyl-         | 100 | C7H16   | 000589-34-4 | 91   |
| 2    |    |   | Heptane, 3,4-dimethyl-    | 128 | C9H20   | 000922-28-1 | 64   |
| 3    |    |   | Heptane, 4-methyl-        | 114 | C8H18   | 000589-53-7 | 59   |
| 4    |    |   | Heptane                   | 100 | C7H16   | 000142-82-5 | 59   |
| 5    |    |   | Pentane, 2,3,4-trimethyl- | 114 | C8H18   | 000565-75-3 | 59   |



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ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
COMP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051524W.M  
Quant Title : SW846 8260

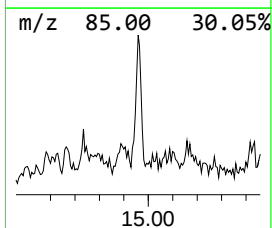
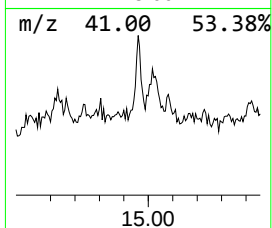
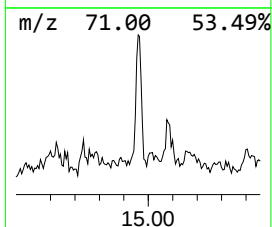
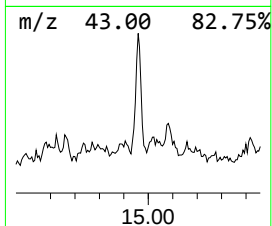
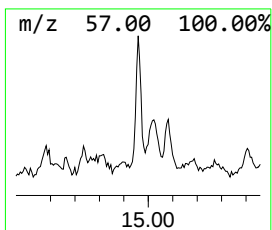
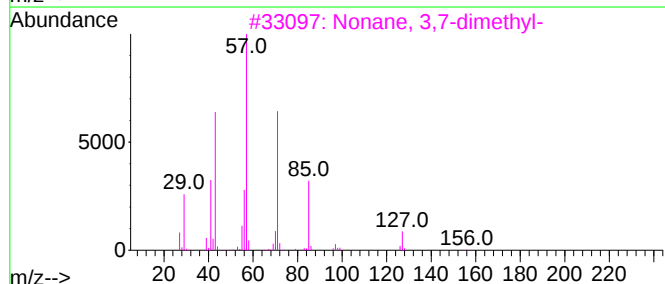
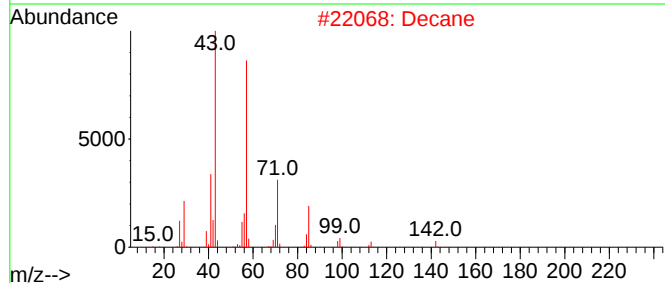
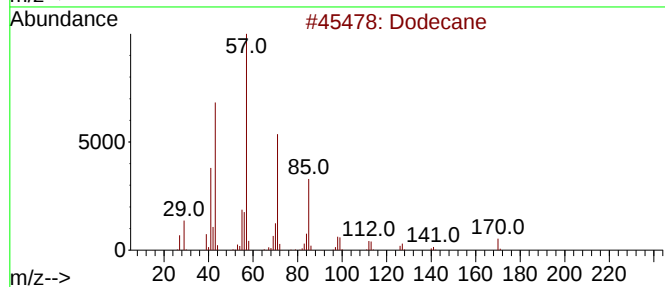
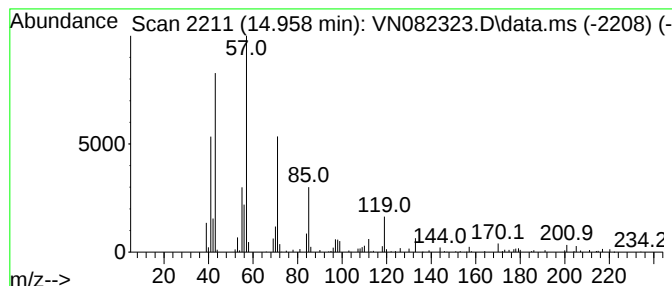
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Dodecane Concentration Rank 4

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 14.958 | 5.18 ug/l | 110496 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Dodecane              | 170 | C12H26  | 000112-40-3 | 81   |
| 2    |    |   | Decane                | 142 | C10H22  | 000124-18-5 | 72   |
| 3    |    |   | Nonane, 3,7-dimethyl- | 156 | C11H24  | 017302-32-8 | 68   |
| 4    |    |   | Undecane              | 156 | C11H24  | 001120-21-4 | 64   |
| 5    |    |   | Decane, 3,8-dimethyl- | 170 | C12H26  | 017312-55-9 | 64   |



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Sample : P2558-01 10X  
Misc : 1.12g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
COMP-1

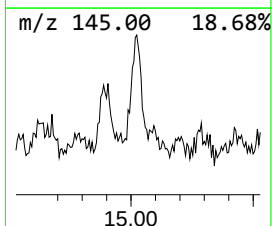
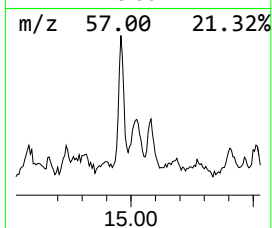
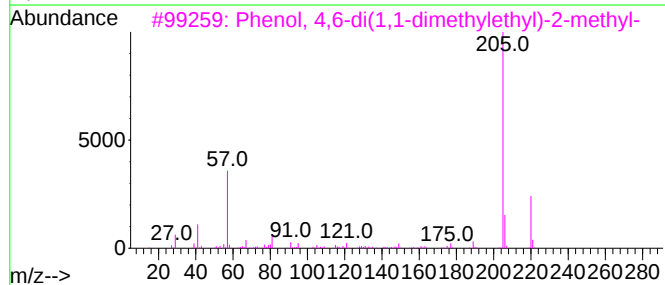
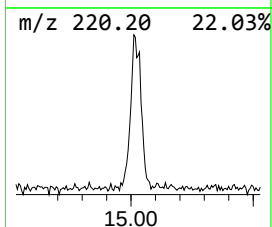
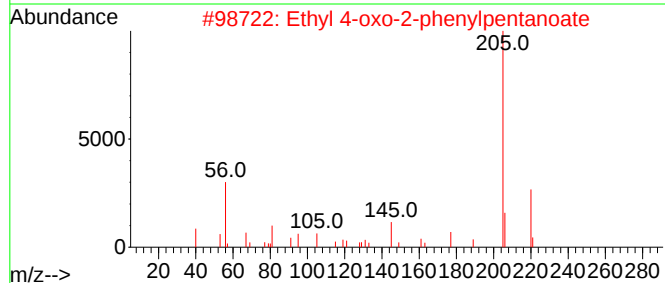
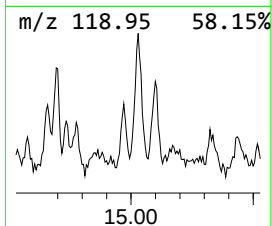
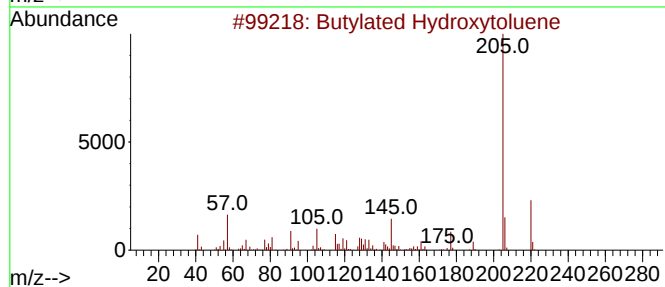
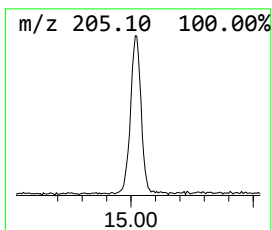
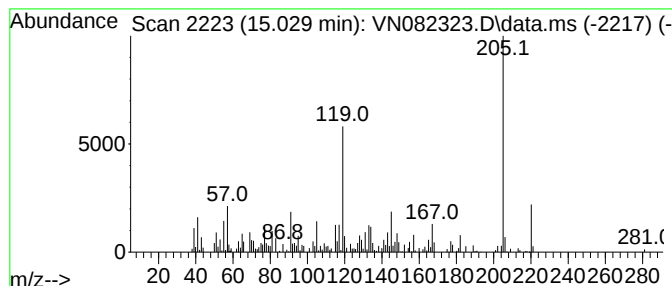
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051524W.M  
Quant Title : SW846 8260

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

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Peak Number 3 Butylated Hydroxytoluene Concentration Rank 1

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 15.029 | 13.83 ug/l | 295050 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Butylated Hydroxytoluene             | 220 | C15H24O    | 000128-37-0  | 53   |
| 2    |    |   | Ethyl 4-oxo-2-phenylpentanoate       | 220 | C13H16O3   | 1000427-11-2 | 46   |
| 3    |    |   | Phenol, 4,6-di(1,1-dimethylethyl)... | 220 | C15H24O    | 000616-55-7  | 38   |
| 4    |    |   | Pyridine, 4-iodo-                    | 205 | C5H4IN     | 015854-87-2  | 30   |
| 5    |    |   | Benzenamine, N,N-diethyl-4-(2-ni...  | 220 | C12H16N2O2 | 064462-51-7  | 30   |



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Instrument :  
MSVOA\_N  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051524W.M  
Quant Title : SW846 8260

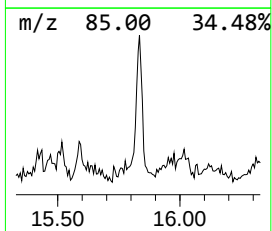
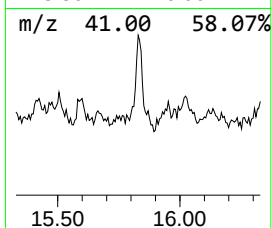
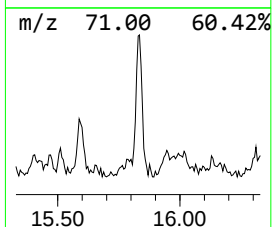
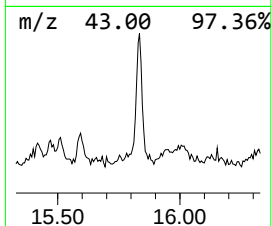
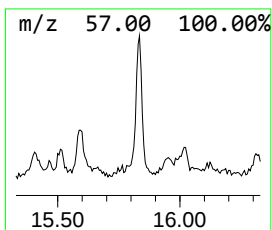
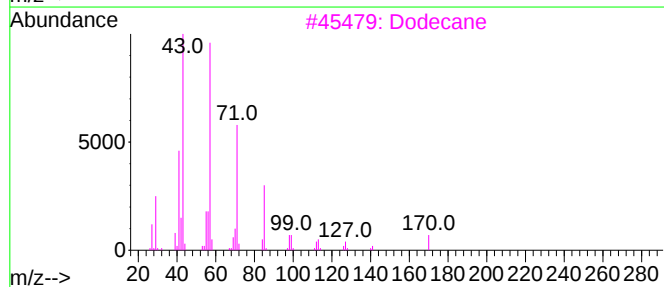
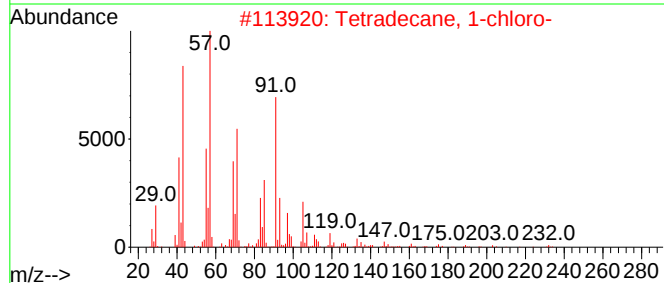
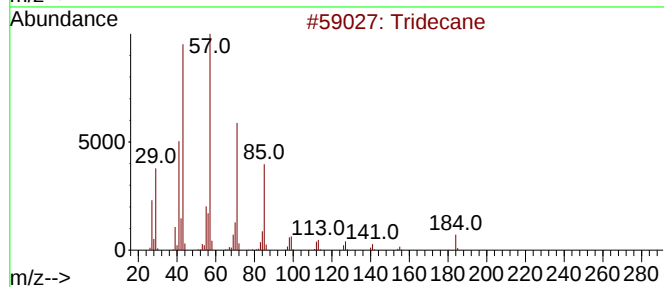
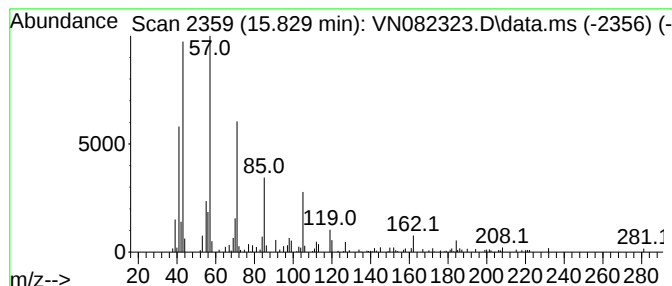
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Tridecane Concentration Rank 2

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 15.829 | 7.15 ug/l | 152434 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID           | MW  | MolForm  | CAS#        | Qual |
|------|----|---|------------------------|-----|----------|-------------|------|
| 1    |    |   | Tridecane              | 184 | C13H28   | 000629-50-5 | 93   |
| 2    |    |   | Tetradecane, 1-chloro- | 232 | C14H29Cl | 002425-54-9 | 90   |
| 3    |    |   | Dodecane               | 170 | C12H26   | 000112-40-3 | 78   |
| 4    |    |   | Undecane               | 156 | C11H24   | 001120-21-4 | 49   |
| 5    |    |   | Undecane, 5-methyl-    | 170 | C12H26   | 001632-70-8 | 49   |



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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 |
| Hexane, 3-methyl-  | 8.447  | 6.2     | ug/l  | 86576    | 1                     | 8.224  | 703473  | 50.0 |
| Dodecane           | 14.958 | 5.2     | ug/l  | 110496   | 4                     | 13.794 | 1066660 | 50.0 |
| Butylated Hydro... | 15.029 | 13.8    | ug/l  | 295050   | 4                     | 13.794 | 1066660 | 50.0 |
| Tridecane          | 15.829 | 7.2     | ug/l  | 152434   | 4                     | 13.794 | 1066660 | 50.0 |