

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN041824\  
 Data File : VN081797.D  
 Acq On : 18 Apr 2024 19:06  
 Operator : JC\MD  
 Sample : P2121-06  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 4828

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\82N041524W.M  
 Title : SW846 8260

Signal : TIC: VN081797.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         | 4.424       | 410           | 420         | 435          | rBV2     | 40204          | 124345        | 2.13%           | 0.663%        |
| 2         | 7.224       | 887           | 896         | 907          | rBV2     | 31689          | 86510         | 1.48%           | 0.461%        |
| 3         | 8.171       | 1047          | 1057        | 1061         | rBV      | 204876         | 498700        | 8.54%           | 2.660%        |
| 4         | 8.224       | 1061          | 1066        | 1080         | rVB      | 359316         | 807753        | 13.83%          | 4.309%        |
| 5         | 8.582       | 1120          | 1127        | 1138         | rVB2     | 213797         | 494671        | 8.47%           | 2.639%        |
| 6         | 9.100       | 1204          | 1215        | 1227         | rBV      | 522396         | 1064187       | 18.22%          | 5.676%        |
| 7         | 9.265       | 1237          | 1243        | 1250         | rBV3     | 33637          | 75957         | 1.30%           | 0.405%        |
| 8         | 10.571      | 1456          | 1465        | 1473         | rBV      | 796255         | 1490121       | 25.51%          | 7.948%        |
| 9         | 11.865      | 1674          | 1685        | 1696         | rBV      | 733873         | 1323798       | 22.66%          | 7.061%        |
| 10        | 12.423      | 1775          | 1780        | 1784         | rVB2     | 52053          | 78787         | 1.35%           | 0.420%        |
| 11        | 12.847      | 1844          | 1852        | 1863         | rBV      | 591898         | 1090047       | 18.66%          | 5.814%        |
| 12        | 13.259      | 1914          | 1922        | 1930         | rBV      | 3755020        | 5841235       | 100.00%         | 31.157%       |
| 13        | 13.335      | 1930          | 1935        | 1948         | rVB      | 1155303        | 1791440       | 30.67%          | 9.555%        |
| 14        | 13.506      | 1957          | 1964        | 1975         | rBV      | 779262         | 1260579       | 21.58%          | 6.724%        |
| 15        | 13.606      | 1975          | 1981        | 1991         | rVV      | 165629         | 322015        | 5.51%           | 1.718%        |
| 16        | 13.700      | 1993          | 1997        | 2006         | rVB5     | 30397          | 79669         | 1.36%           | 0.425%        |
| 17        | 13.794      | 2006          | 2013        | 2019         | rBV      | 735082         | 1240695       | 21.24%          | 6.618%        |
| 18        | 13.870      | 2019          | 2026        | 2034         | rVB3     | 254465         | 541065        | 9.26%           | 2.886%        |
| 19        | 14.235      | 2082          | 2088        | 2094         | rBV2     | 96627          | 176611        | 3.02%           | 0.942%        |
| 20        | 14.935      | 2202          | 2207        | 2217         | rVB6     | 56516          | 108960        | 1.87%           | 0.581%        |
| 21        | 15.400      | 2280          | 2286        | 2292         | rVB      | 72750          | 124316        | 2.13%           | 0.663%        |
| 22        | 15.517      | 2300          | 2306        | 2311         | rBV4     | 64582          | 126316        | 2.16%           | 0.674%        |

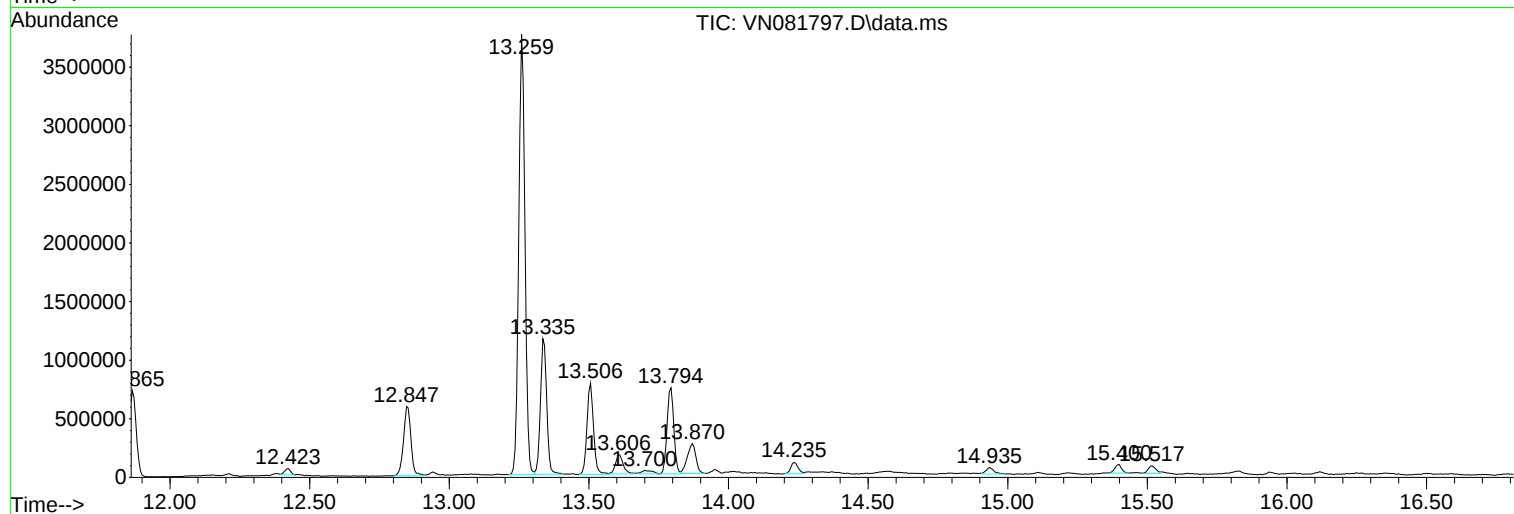
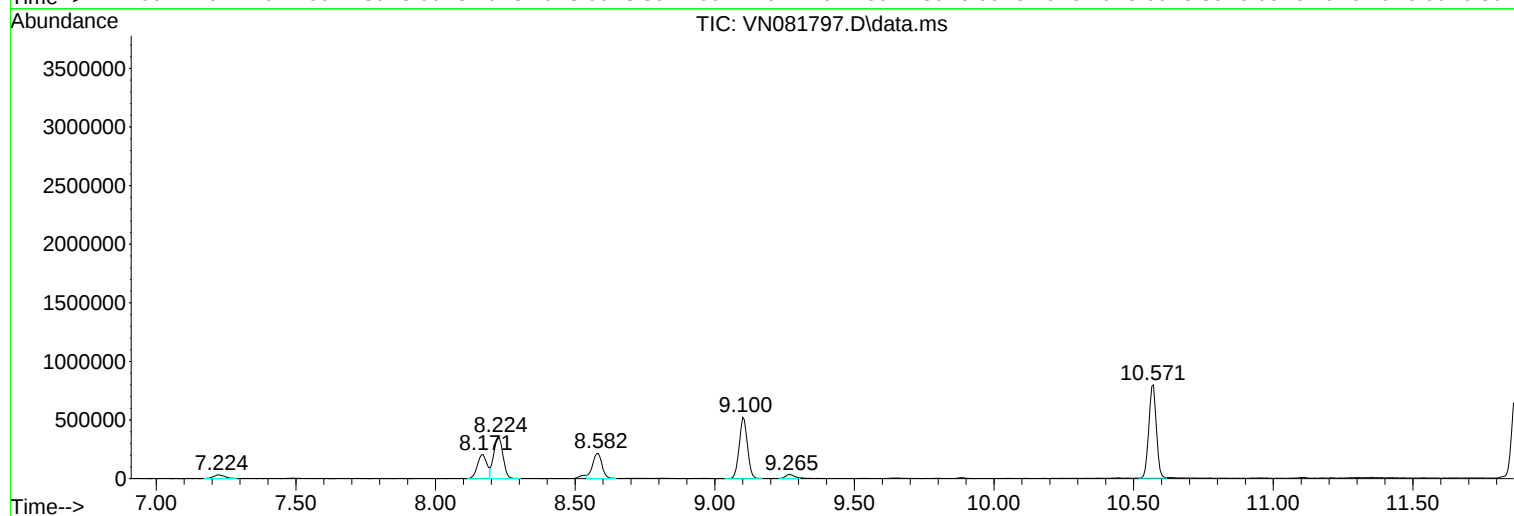
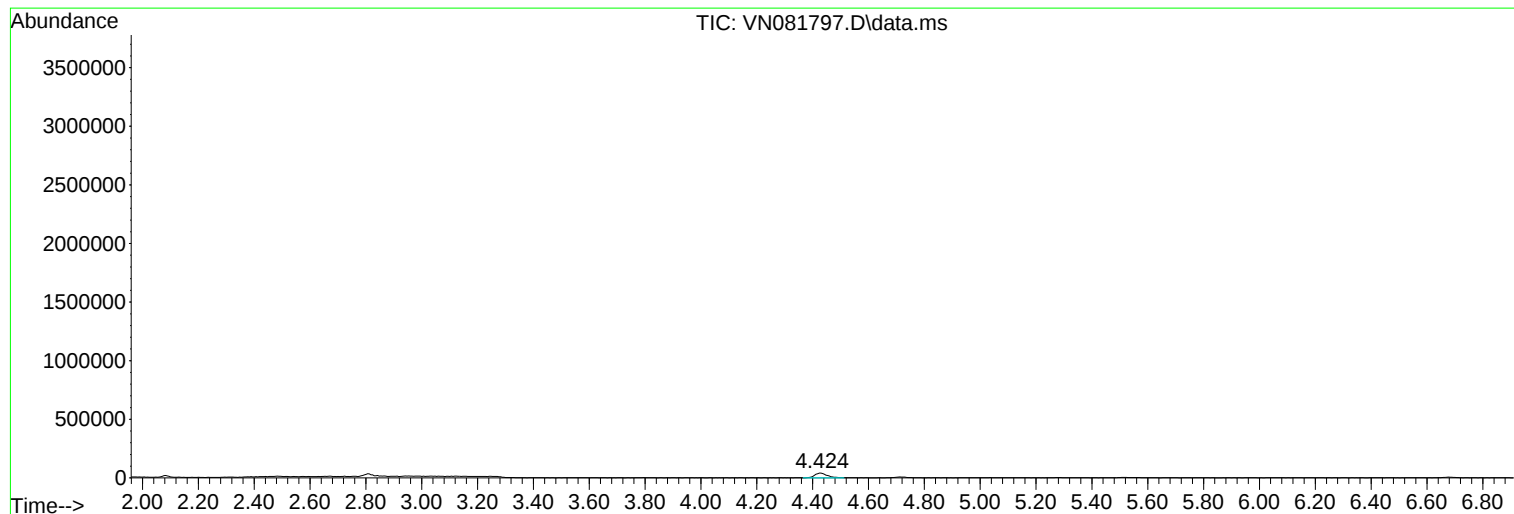
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N041524W.M  
Quant Title : SW846 8260

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



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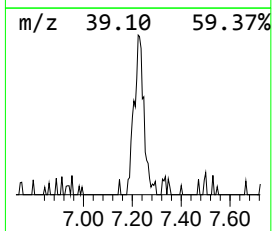
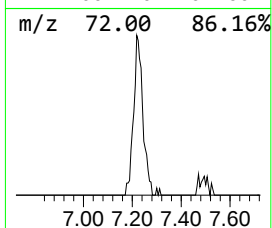
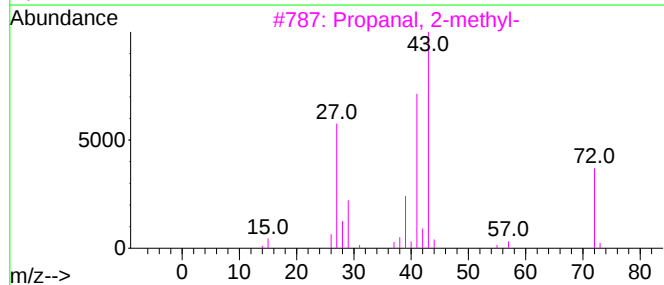
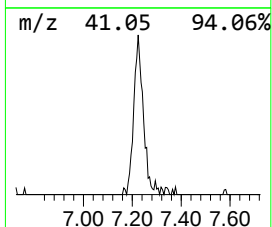
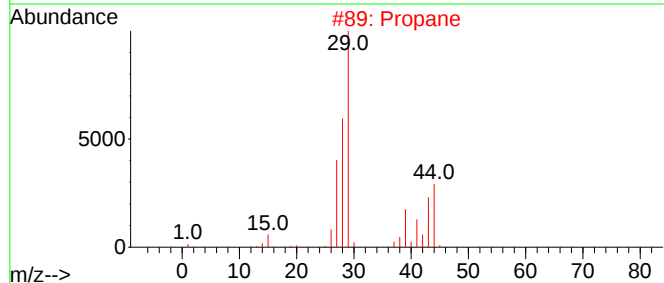
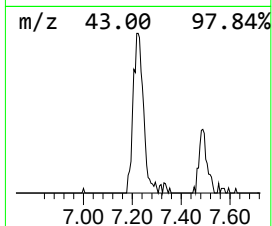
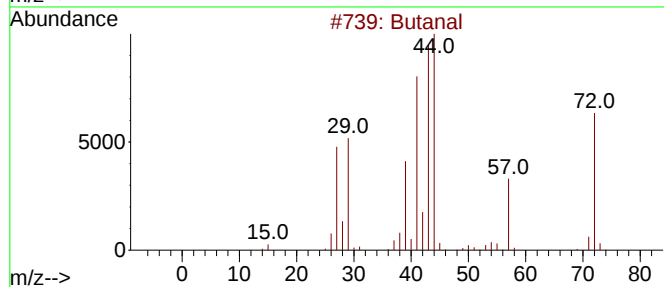
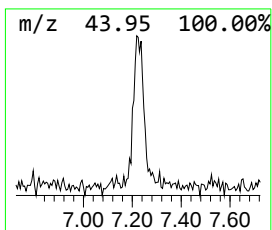
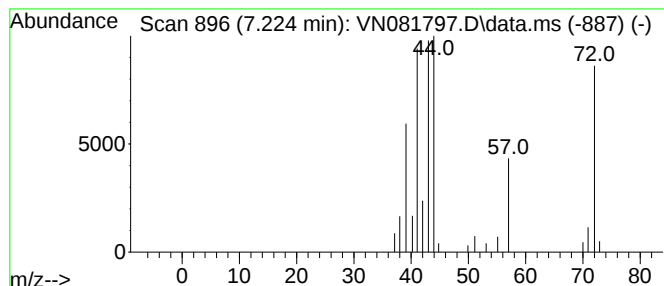
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N041524W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Butanal Concentration Rank 7

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 7.224 | 5.35 ug/l | 86510 | Pentafluorobenzene | 8.224 |

| Hit# | of 5 | Tentative ID                      | MW  | MolForm | CAS#        | Qual |
|------|------|-----------------------------------|-----|---------|-------------|------|
| 1    |      | Butanal                           | 72  | C4H8O   | 000123-72-8 | 91   |
| 2    |      | Propane                           | 44  | C3H8    | 000074-98-6 | 47   |
| 3    |      | Propanal, 2-methyl-               | 72  | C4H8O   | 000078-84-2 | 43   |
| 4    |      | 1-Propene, 3-methoxy-             | 72  | C4H8O   | 000627-40-7 | 43   |
| 5    |      | 2-Propen-1-ol, 2-methyl-, acetate | 114 | C6H10O2 | 000820-71-3 | 28   |



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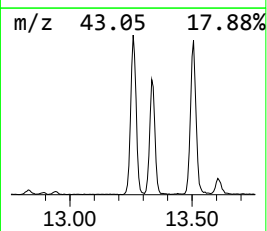
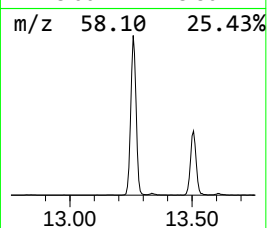
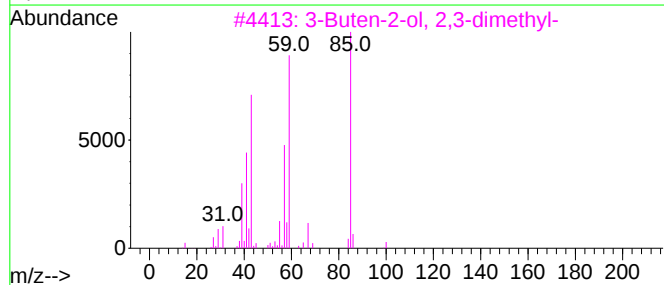
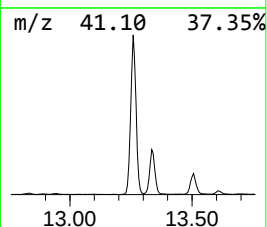
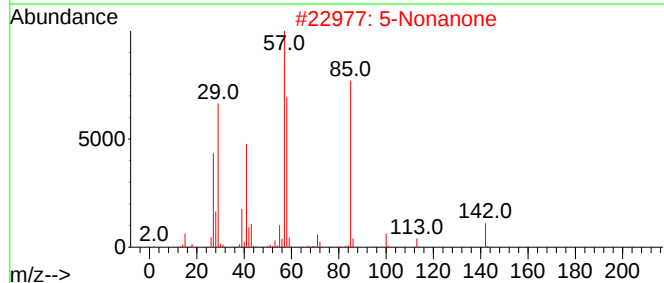
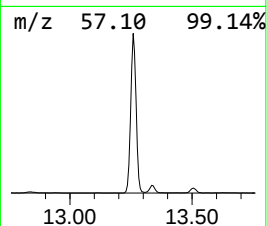
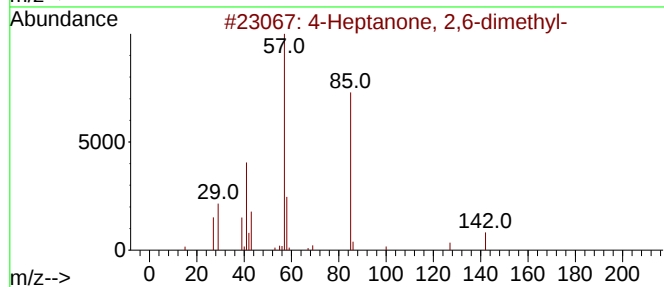
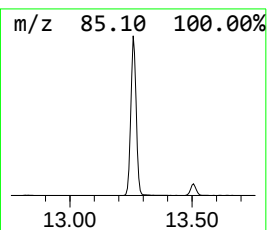
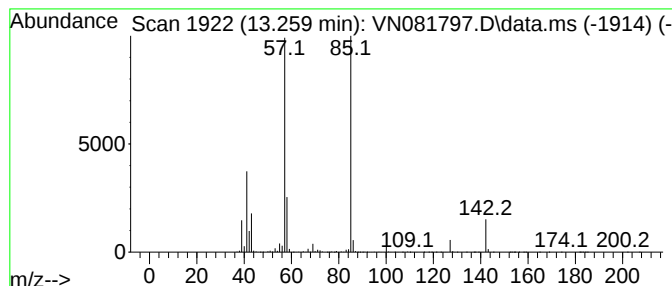
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Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

| R.T.   | EstConc     | Area    | Relative to ISTD       | R.T.   |
|--------|-------------|---------|------------------------|--------|
| 13.259 | 235.40 ug/l | 5841240 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | 4-Heptanone, 2,6-dimethyl-  | 142 | C9H18O  | 000108-83-8 | 94   |
| 2    |    |   | 5-Nonanone                  | 142 | C9H18O  | 000502-56-7 | 64   |
| 3    |    |   | 3-Buten-2-ol, 2,3-dimethyl- | 100 | C6H12O  | 010473-13-9 | 59   |
| 4    |    |   | t-Butyl isobutyl ketone     | 142 | C9H18O  | 014705-50-1 | 50   |
| 5    |    |   | 4-Octanone, 2-methyl-       | 142 | C9H18O  | 007492-38-8 | 50   |



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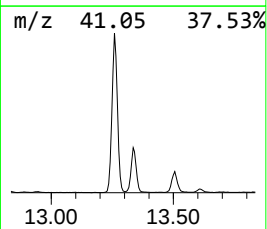
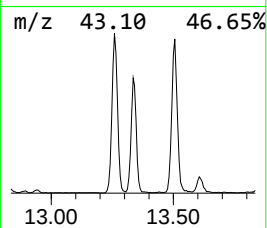
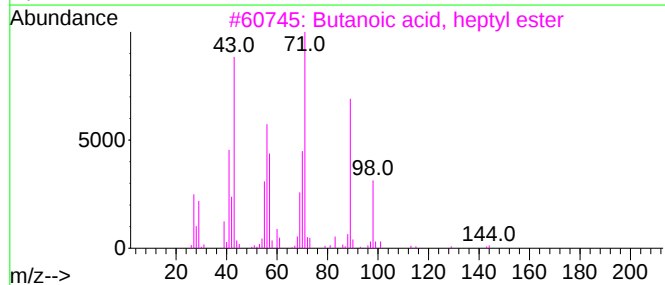
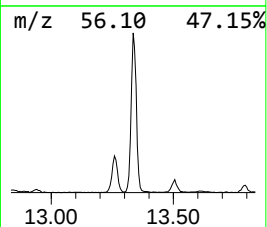
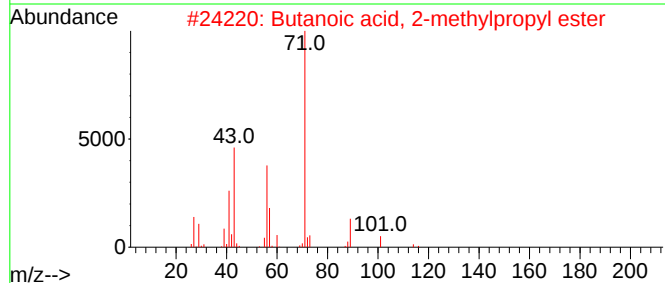
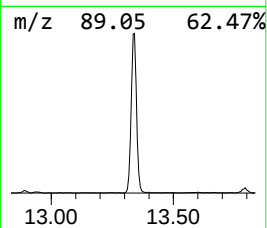
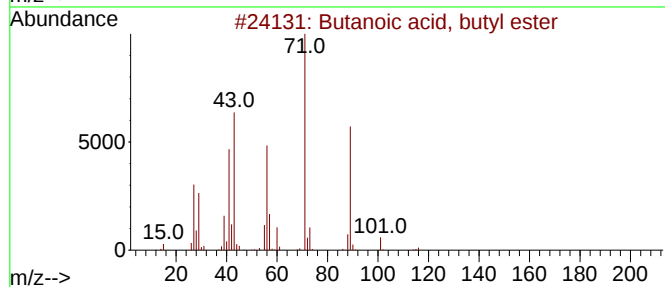
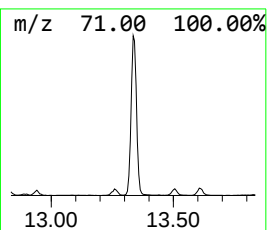
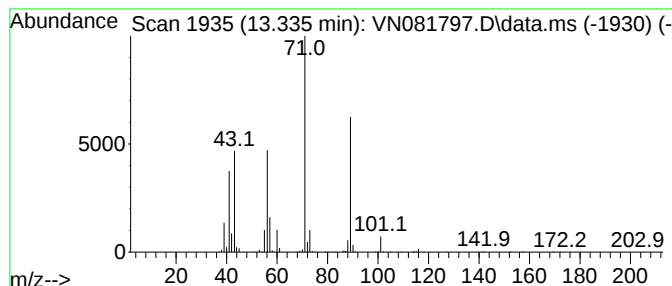
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Butanoic acid, butyl ester Concentration Rank 2

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 13.335 | 72.19 ug/l | 1791440 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Butanoic acid, butyl ester          | 144 | C8H16O2  | 000109-21-7 | 90   |
| 2    |    |   | Butanoic acid, 2-methylpropyl ester | 144 | C8H16O2  | 000539-90-2 | 64   |
| 3    |    |   | Butanoic acid, heptyl ester         | 186 | C11H22O2 | 005870-93-9 | 64   |
| 4    |    |   | Propanoic acid, 2-methyl-, 2-met... | 144 | C8H16O2  | 000097-85-8 | 59   |
| 5    |    |   | Propanoic acid, 2-methyl-, 2-eth... | 216 | C12H24O3 | 074367-31-0 | 50   |



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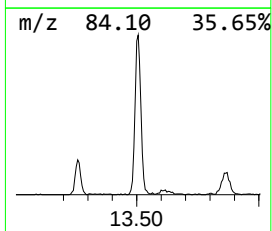
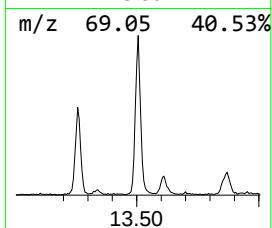
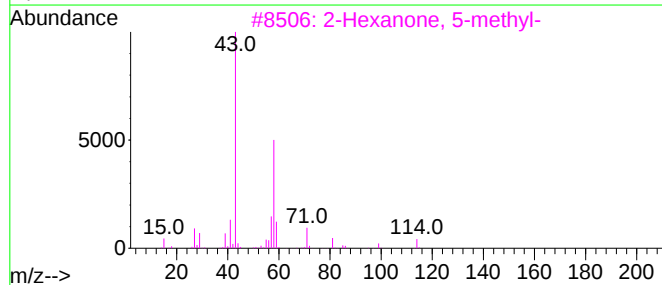
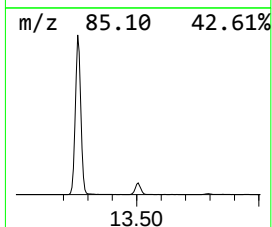
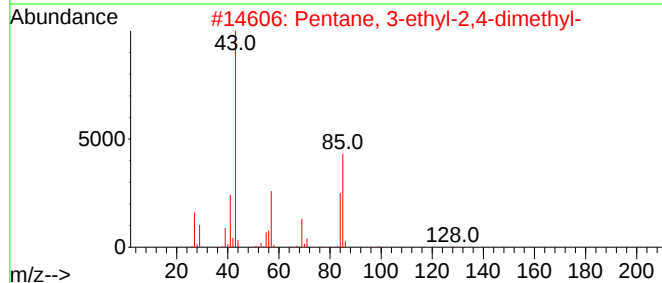
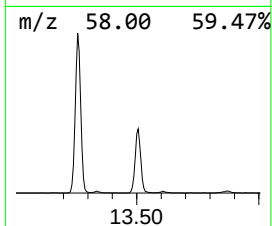
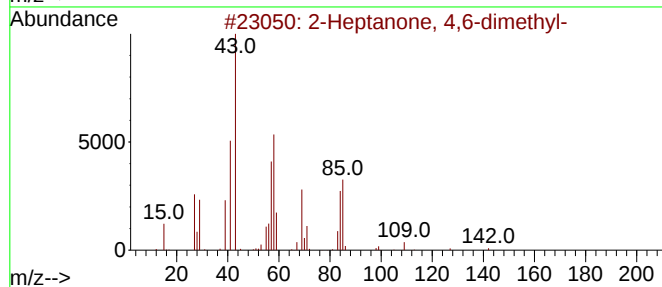
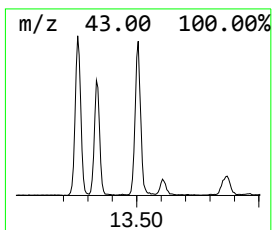
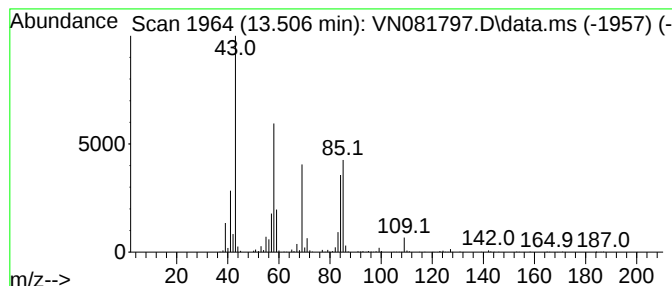
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 2-Heptanone, 4,6-dimethyl- Concentration Rank 3

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 13.506 | 50.80 ug/l | 1260580 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 2-Heptanone, 4,6-dimethyl-          | 142 | C9H18O   | 019549-80-5  | 80   |
| 2    |    |   | Pentane, 3-ethyl-2,4-dimethyl-      | 128 | C9H20    | 001068-87-7  | 43   |
| 3    |    |   | 2-Hexanone, 5-methyl-               | 114 | C7H14O   | 000110-12-3  | 38   |
| 4    |    |   | Oxalic acid, diisohexyl ester       | 258 | C14H26O4 | 1010309-32-9 | 38   |
| 5    |    |   | 4-Methylpentan-2-yl propyl carbo... | 188 | C10H20O3 | 1000372-81-8 | 38   |



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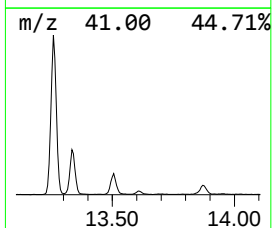
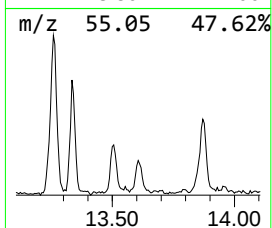
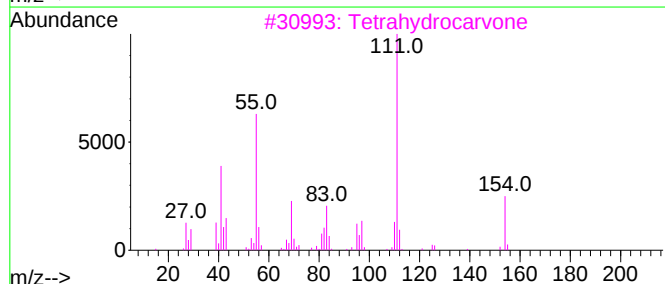
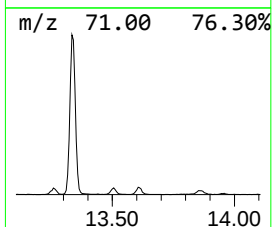
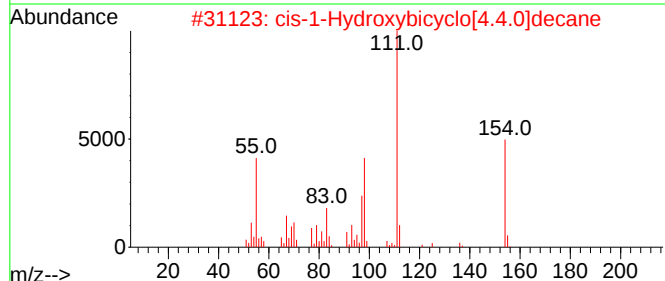
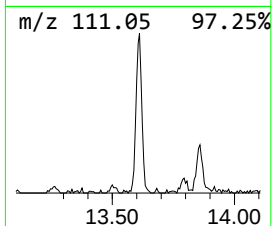
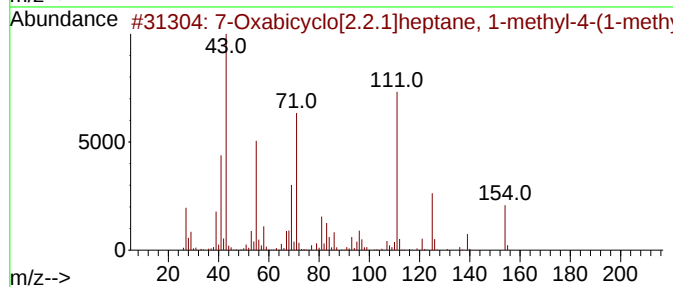
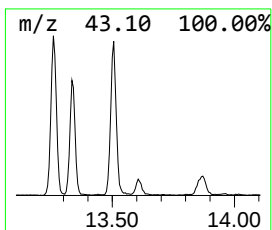
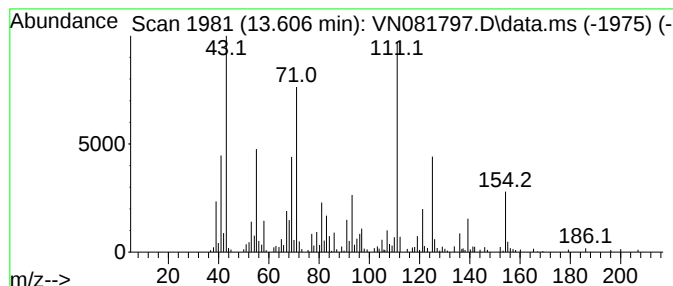
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TIC Integration Parameters: LSCINT.P

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Peak Number 5 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 5

| R.T.      | EstConc                             | Area   | Relative to ISTD       |         |             | R.T.   |
|-----------|-------------------------------------|--------|------------------------|---------|-------------|--------|
| 13.606    | 12.98 ug/l                          | 322015 | 1,4-Dichlorobenzene-d4 |         |             | 13.794 |
| Hit# of 5 | Tentative ID                        |        | MW                     | MolForm | CAS#        | Qual   |
| 1         | 7-Oxabicyclo[2.2.1]heptane, 1-me... |        | 154                    | C10H18O | 000470-67-7 | 87     |
| 2         | cis-1-Hydroxybicyclo[4.4.0]decane   |        | 154                    | C10H18O | 003574-58-1 | 30     |
| 3         | Tetrahydrocarvone                   |        | 154                    | C10H18O | 000499-70-7 | 25     |
| 4         | Octahydronaphthalen-4a-ol           |        | 154                    | C10H18O | 055693-34-0 | 25     |
| 5         | 2(5H)-Furanone, 3,5,5-trimethyl-    |        | 126                    | C7H10O2 | 050598-50-0 | 25     |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN041824\  
Data File : VN081797.D  
Acq On : 18 Apr 2024 19:06  
Operator : JC\MD  
Sample : P2121-06  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
4828

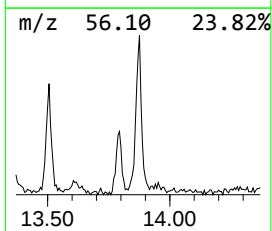
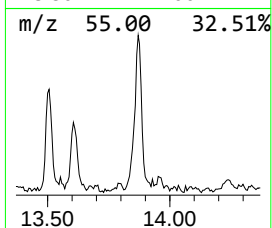
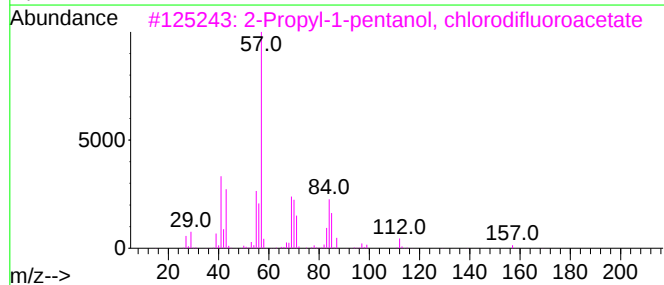
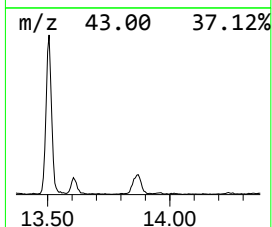
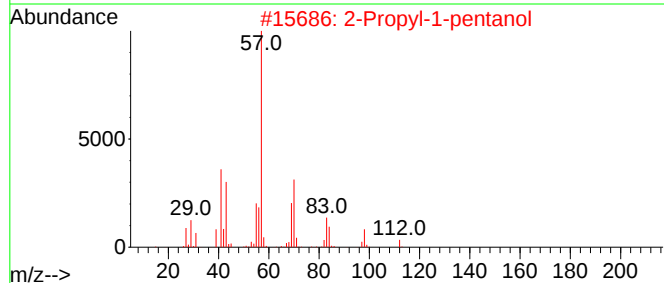
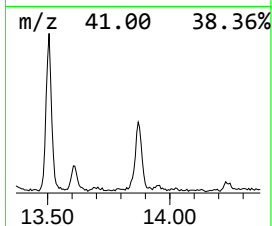
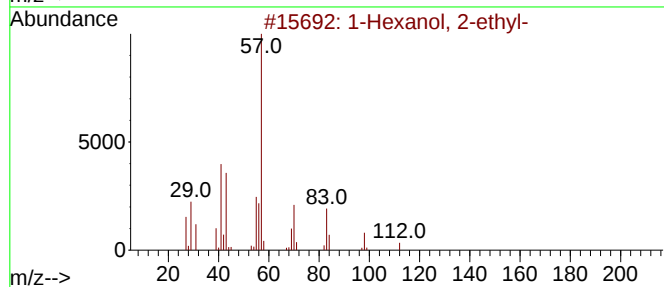
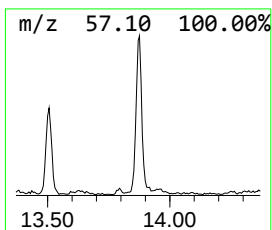
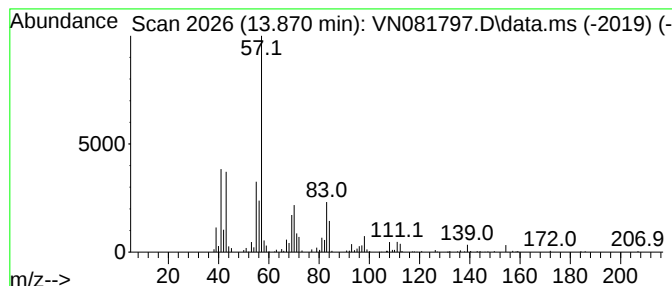
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Quant Title : SW846 8260

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

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Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 13.870 | 21.80 ug/l | 541065 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm      | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|--------------|--------------|------|
| 1    |    |   | 1-Hexanol, 2-ethyl-                 | 130 | C8H18O       | 000104-76-7  | 72   |
| 2    |    |   | 2-Propyl-1-pentanol                 | 130 | C8H18O       | 058175-57-8  | 53   |
| 3    |    |   | 2-Propyl-1-pentanol, chlorodiflu... | 242 | C10H17ClF2O2 | 1000447-27-3 | 50   |
| 4    |    |   | Butyl decyl ether                   | 214 | C14H30O      | 1000406-40-2 | 42   |
| 5    |    |   | 1-Decene, 2,4-dimethyl-             | 168 | C12H24       | 055170-80-4  | 40   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN041824\  
Data File : VN081797.D  
Acq On : 18 Apr 2024 19:06  
Operator : JC\MD  
Sample : P2121-06  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
4828

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N041524W.M  
Quant Title : SW846 8260

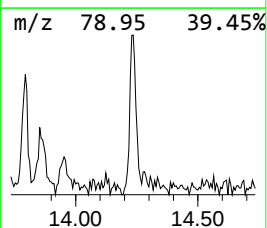
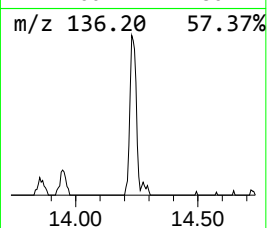
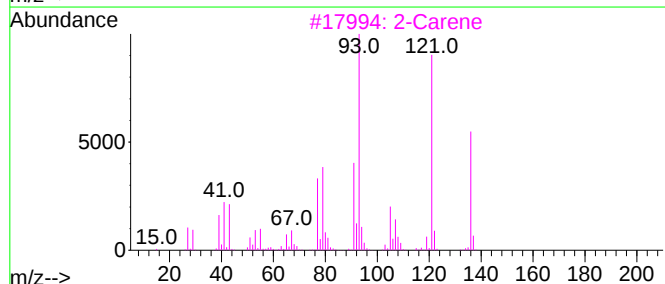
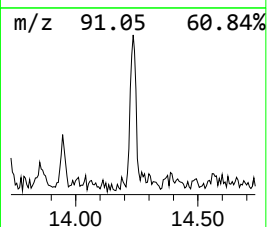
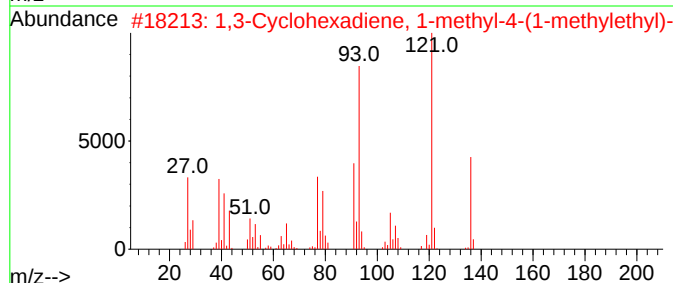
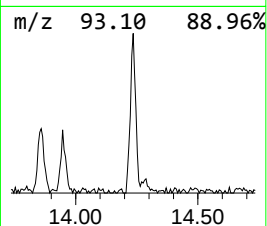
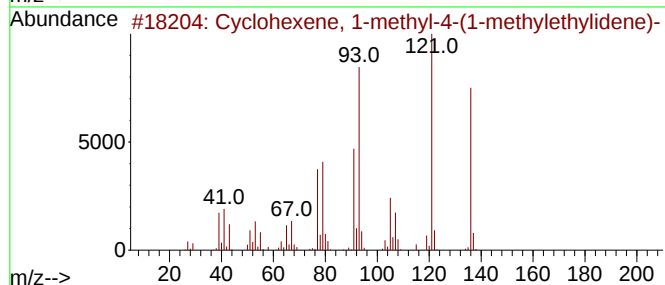
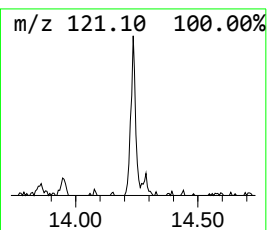
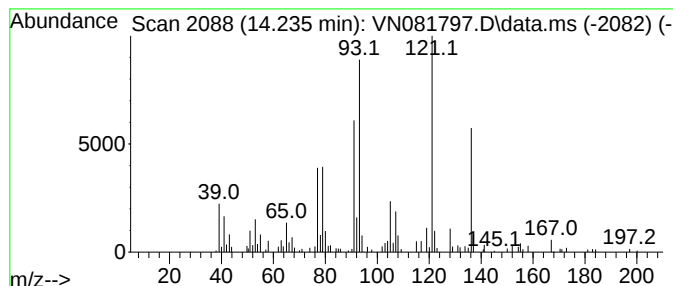
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 6

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 14.235 | 7.12 ug/l | 176611 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexene, 1-methyl-4-(1-methy... | 136 | C10H16  | 000586-62-9 | 97   |
| 2    |    |   | 1,3-Cyclohexadiene, 1-methyl-4-(... | 136 | C10H16  | 000099-86-5 | 95   |
| 3    |    |   | 2-Carene                            | 136 | C10H16  | 000554-61-0 | 94   |
| 4    |    |   | Bicyclo[4.1.0]hept-2-ene, 3,7,7-... | 136 | C10H16  | 004497-92-1 | 91   |
| 5    |    |   | Cyclohexene, 4-methyl-3-(1-methy... | 136 | C10H16  | 099805-90-0 | 90   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN041824\  
Data File : VN081797.D  
Acq On : 18 Apr 2024 19:06  
Operator : JC\MD  
Sample : P2121-06  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
4828

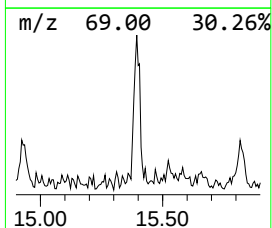
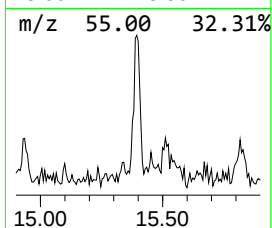
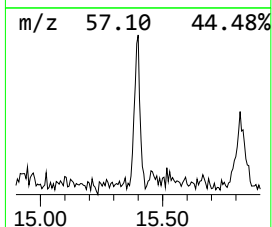
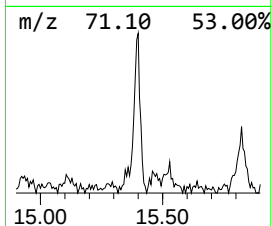
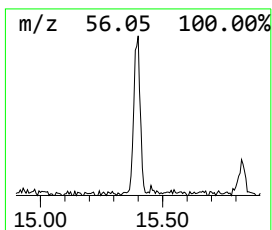
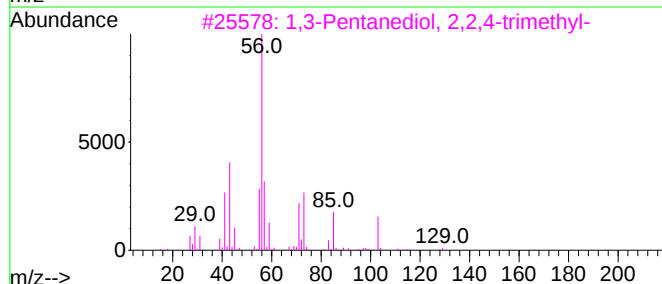
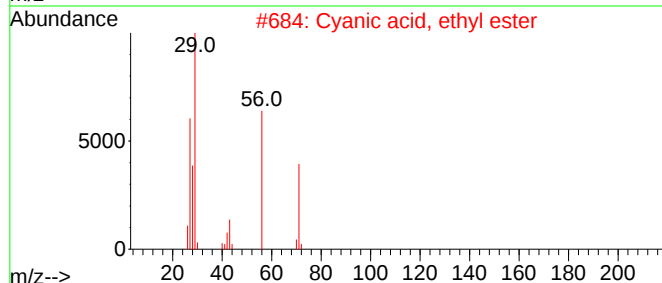
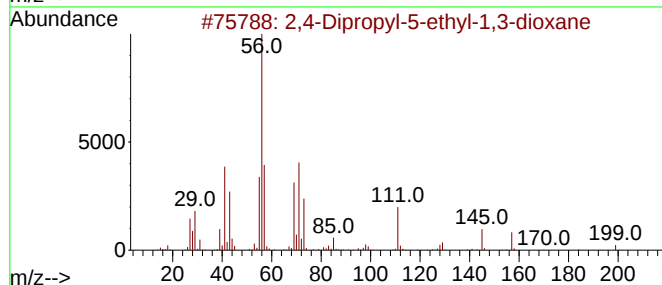
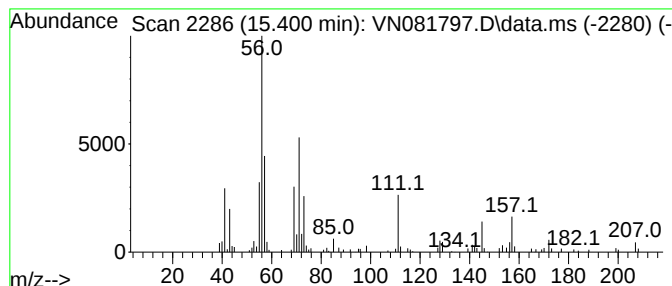
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Quant Title : SW846 8260

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

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Peak Number 8 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 9

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 15.400 | 5.01 ug/l | 124316 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of 5 | Tentative ID                      | MW  | MolForm  | CAS#        | Qual |
|------|------|-----------------------------------|-----|----------|-------------|------|
| 1    |      | 2,4-Dipropyl-5-ethyl-1,3-dioxane  | 200 | C12H24O2 | 006413-83-8 | 86   |
| 2    |      | Cyanoic acid, ethyl ester         | 71  | C3H5NO   | 000627-48-5 | 49   |
| 3    |      | 1,3-Pentanediol, 2,2,4-trimethyl- | 146 | C8H18O2  | 000144-19-4 | 28   |
| 4    |      | Cyclooctanamine                   | 127 | C8H17N   | 005452-37-9 | 27   |
| 5    |      | 2-Methyl-1-nonene                 | 140 | C10H20   | 002980-71-4 | 16   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN041824\  
Data File : VN081797.D  
Acq On : 18 Apr 2024 19:06  
Operator : JC\MD  
Sample : P2121-06  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
4828

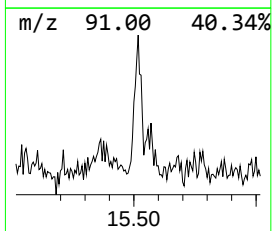
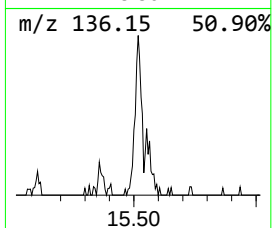
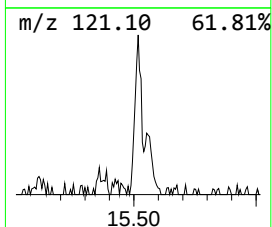
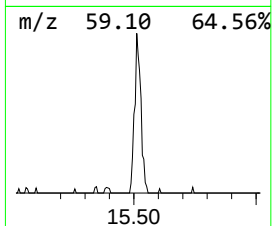
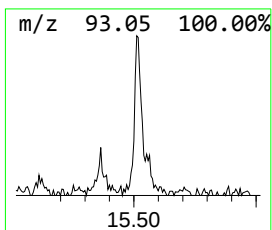
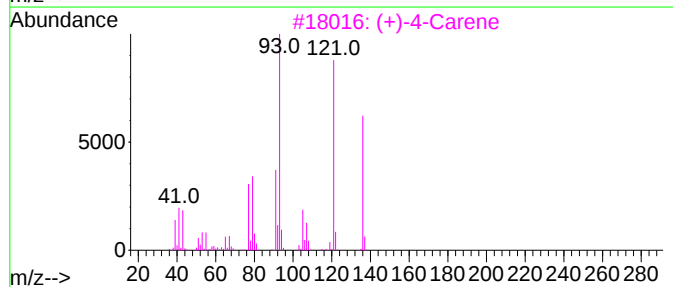
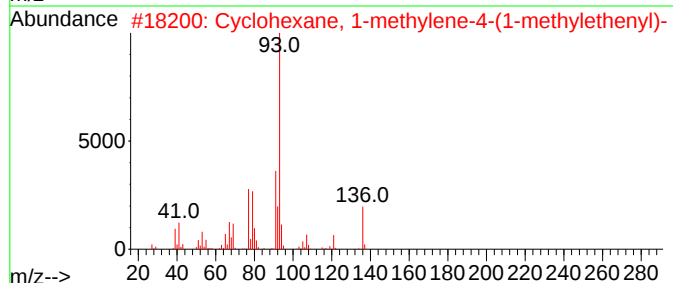
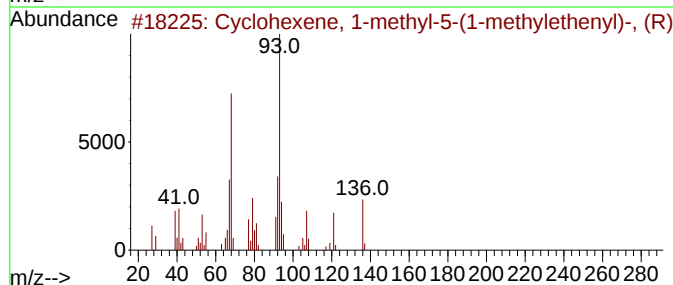
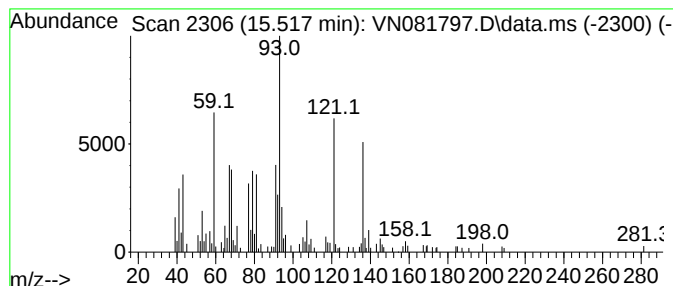
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N041524W.M  
Quant Title : SW846 8260

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

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Peak Number 9 Cyclohexene, 1-methyl-5-(1-... Concentration Rank 8

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 15.517 | 5.09 ug/l | 126316 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexene, 1-methyl-5-(1-methy... | 136 | C10H16  | 001461-27-4 | 58   |
| 2    |    |   | Cyclohexane, 1-methylene-4-(1-me... | 136 | C10H16  | 000499-97-8 | 49   |
| 3    |    |   | (+)-4-Carene                        | 136 | C10H16  | 029050-33-7 | 46   |
| 4    |    |   | 1,3-Cyclohexadiene, 1-methyl-4-(... | 136 | C10H16  | 000099-86-5 | 46   |
| 5    |    |   | Cyclopropane, 1,1-dimethyl-2-(3-... | 136 | C10H16  | 068998-21-0 | 46   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN041824\  
Data File : VN081797.D  
Acq On : 18 Apr 2024 19:06  
Operator : JC\MD  
Sample : P2121-06  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
4828

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N041524W.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 |
| Butanal            | 7.224  | 5.3     | ug/l  | 86510    | 1                     | 8.224  | 807753  | 50.0 |
| 4-Heptanone, 2,... | 13.259 | 235.4   | ug/l  | 5841240  | 4                     | 13.794 | 1240700 | 50.0 |
| Butanoic acid, ... | 13.335 | 72.2    | ug/l  | 1791440  | 4                     | 13.794 | 1240700 | 50.0 |
| 2-Heptanone, 4,... | 13.506 | 50.8    | ug/l  | 1260580  | 4                     | 13.794 | 1240700 | 50.0 |
| 7-Oxabicyclo[2.... | 13.606 | 13.0    | ug/l  | 322015   | 4                     | 13.794 | 1240700 | 50.0 |
| 1-Hexanol, 2-et... | 13.870 | 21.8    | ug/l  | 541065   | 4                     | 13.794 | 1240700 | 50.0 |
| Cyclohexene, 1-... | 14.235 | 7.1     | ug/l  | 176611   | 4                     | 13.794 | 1240700 | 50.0 |
| 2,4-Dipropyl-5-... | 15.400 | 5.0     | ug/l  | 124316   | 4                     | 13.794 | 1240700 | 50.0 |
| Cyclohexene, 1-... | 15.517 | 5.1     | ug/l  | 126316   | 4                     | 13.794 | 1240700 | 50.0 |