

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012121\  
 Data File : VU042151.D  
 Acq On : 21 Jan 2021 15:24  
 Operator : SY/MD  
 Sample : M1170-11DL 4X  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFT92DL

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

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\_U\METHOD\SOMUTR012021WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC: VU042151.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 1.359       | 3             | 6           | 15           | rVB2     | 15392          | 14539         | 2.79%           | 0.328%        |
| 2         | 1.601       | 71            | 81          | 90           | rVB      | 51644          | 59551         | 11.42%          | 1.342%        |
| 3         | 1.694       | 103           | 110         | 118          | rBV2     | 6288           | 10012         | 1.92%           | 0.226%        |
| 4         | 1.916       | 170           | 179         | 191          | rVB      | 38699          | 49779         | 9.55%           | 1.122%        |
| 5         | 2.572       | 371           | 383         | 398          | rBV      | 89970          | 145093        | 27.83%          | 3.271%        |
| 6         | 2.658       | 398           | 410         | 437          | rVV2     | 5650           | 18690         | 3.58%           | 0.421%        |
| 7         | 2.800       | 444           | 454         | 463          | rVB2     | 3121           | 5384          | 1.03%           | 0.121%        |
| 8         | 3.054       | 521           | 533         | 546          | rVB4     | 3663           | 6854          | 1.31%           | 0.155%        |
| 9         | 3.195       | 565           | 577         | 588          | rVB2     | 2105           | 5422          | 1.04%           | 0.122%        |
| 10        | 4.456       | 955           | 969         | 983          | rBV5     | 3846           | 9626          | 1.85%           | 0.217%        |
| 11        | 4.649       | 1011          | 1029        | 1091         | rBV      | 58640          | 237857        | 45.62%          | 5.362%        |
| 12        | 5.073       | 1143          | 1161        | 1183         | rBV      | 77761          | 171679        | 32.93%          | 3.870%        |
| 13        | 5.732       | 1345          | 1366        | 1390         | rBV2     | 155061         | 404541        | 77.60%          | 9.119%        |
| 14        | 6.256       | 1515          | 1529        | 1548         | rBV      | 138664         | 261538        | 50.17%          | 5.896%        |
| 15        | 6.549       | 1594          | 1620        | 1639         | rBV      | 139994         | 271641        | 52.10%          | 6.123%        |
| 16        | 6.700       | 1654          | 1667        | 1686         | rVB      | 98219          | 191049        | 36.65%          | 4.307%        |
| 17        | 6.890       | 1714          | 1726        | 1736         | rBV      | 9757           | 18725         | 3.59%           | 0.422%        |
| 18        | 7.575       | 1926          | 1939        | 1955         | rBV      | 57930          | 102994        | 19.76%          | 2.322%        |
| 19        | 7.906       | 2029          | 2042        | 2056         | rBV      | 192169         | 329271        | 63.16%          | 7.422%        |
| 20        | 7.976       | 2056          | 2064        | 2074         | rVB2     | 5714           | 9564          | 1.83%           | 0.216%        |
| 21        | 8.185       | 2112          | 2129        | 2141         | rBV2     | 38791          | 68908         | 13.22%          | 1.553%        |
| 22        | 8.642       | 2257          | 2271        | 2300         | rBV      | 275993         | 521344        | 100.00%         | 11.752%       |
| 23        | 8.793       | 2307          | 2318        | 2347         | rVB      | 62878          | 107706        | 20.66%          | 2.428%        |
| 24        | 9.423       | 2502          | 2514        | 2534         | rBV      | 190412         | 316445        | 60.70%          | 7.133%        |
| 25        | 9.771       | 2611          | 2622        | 2636         | rVB2     | 12183          | 22018         | 4.22%           | 0.496%        |
| 26        | 10.246      | 2761          | 2770        | 2779         | rBV3     | 3673           | 6949          | 1.33%           | 0.157%        |
| 27        | 10.353      | 2789          | 2803        | 2815         | rBV3     | 23200          | 38134         | 7.31%           | 0.860%        |
| 28        | 10.764      | 2919          | 2931        | 2949         | rBV      | 78376          | 123918        | 23.77%          | 2.793%        |
| 29        | 11.057      | 3012          | 3022        | 3032         | rVB4     | 5234           | 8913          | 1.71%           | 0.201%        |
| 30        | 11.697      | 3208          | 3221        | 3235         | rVB2     | 31125          | 46960         | 9.01%           | 1.059%        |
| 31        | 11.819      | 3248          | 3259        | 3277         | rVB      | 208016         | 324720        | 62.29%          | 7.320%        |
| 32        | 12.070      | 3326          | 3337        | 3360         | rBV      | 32041          | 63791         | 12.24%          | 1.438%        |
| 33        | 12.201      | 3366          | 3378        | 3391         | rVB      | 191510         | 303748        | 58.26%          | 6.847%        |
| 34        | 12.896      | 3581          | 3594        | 3608         | rBV      | 69940          | 105446        | 20.23%          | 2.377%        |
| 35        | 13.217      | 3683          | 3694        | 3707         | rBV      | 35539          | 53318         | 10.23%          | 1.202%        |

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Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFT92DL

Integration Parameters: rteint.p  
Integrator: RTE  
Smoothing : ON Filtering: 5  
Sampling : 1 Min Area: 3 % of largest Peak  
Start Thrs: 0.1 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\_U\METHOD\SOMUTR012021WMA.M  
Title : TRACE VOA SOM01.0

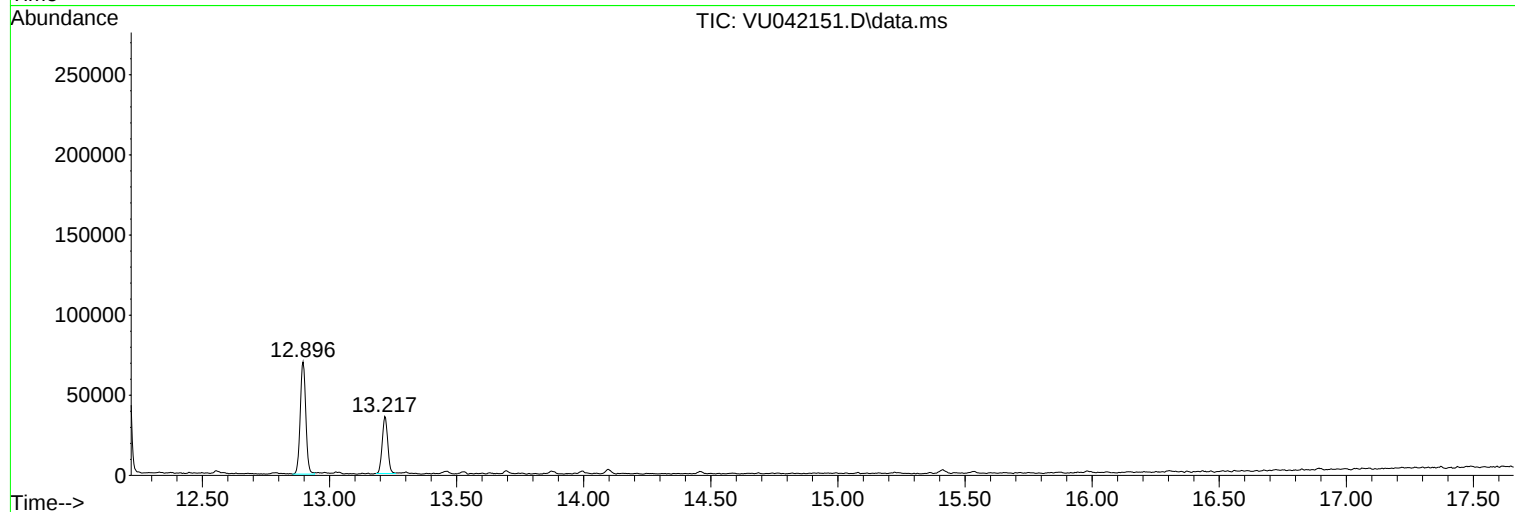
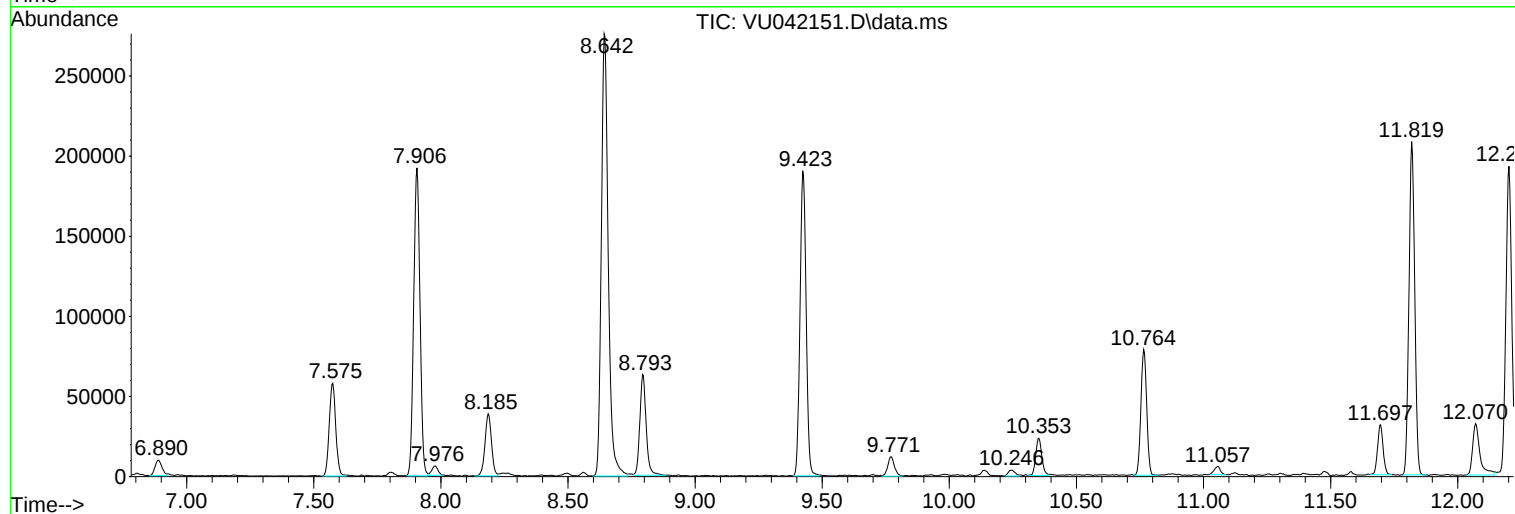
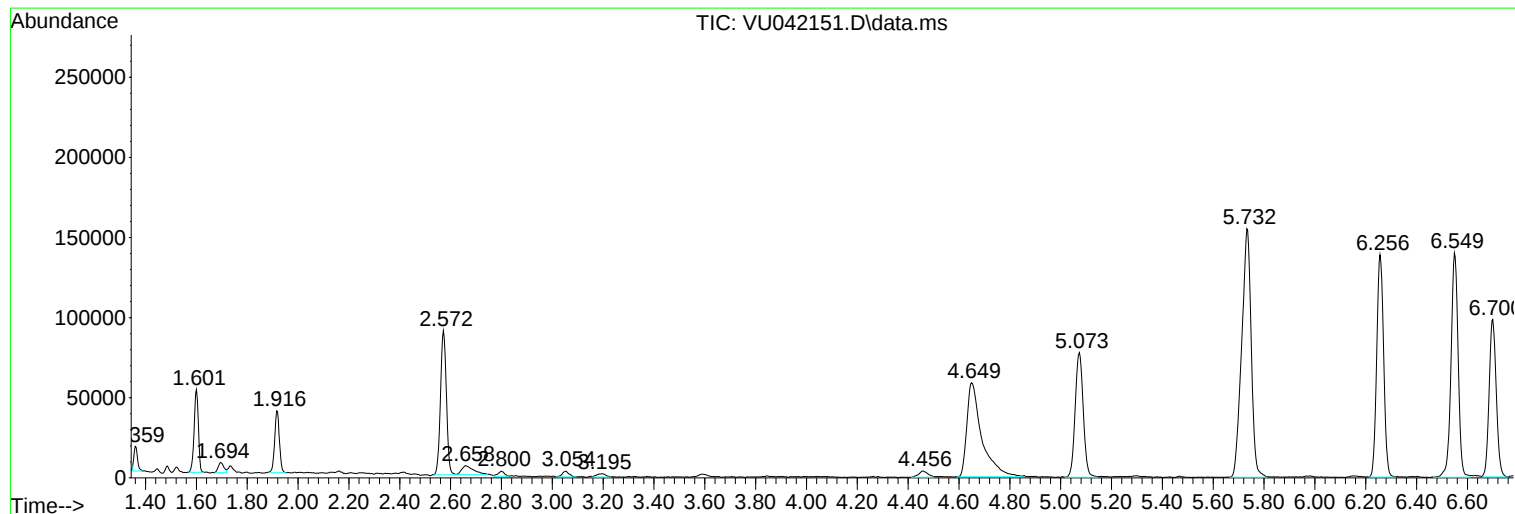
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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Instrument :  
MSVOA\_U  
ClientSampleId :  
BFT92DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

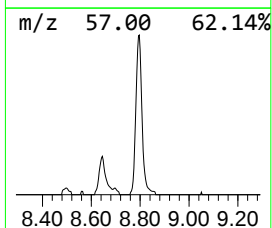
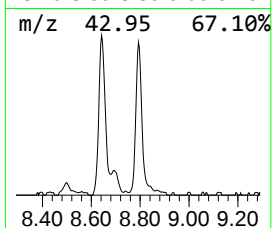
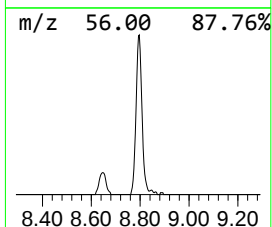
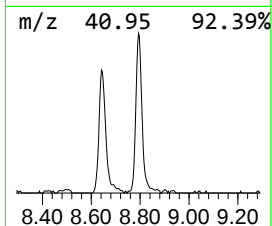
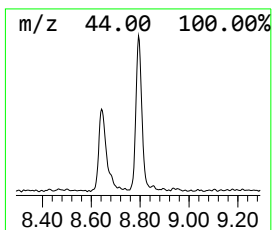
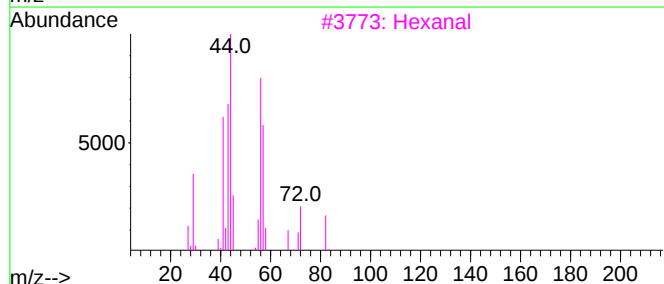
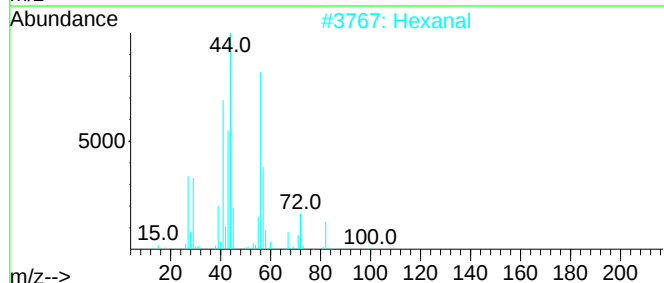
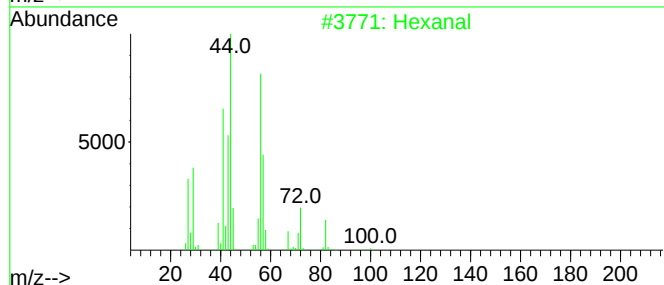
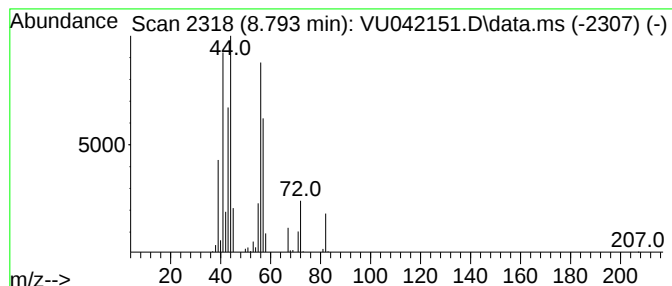
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Hexanal Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.  |
|-------|-----------|--------|------------------|-------|
| 8.793 | 1.70 ug/L | 107706 | Chlorobenzene-d5 | 9.423 |

| Hit# | of                     | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|------------------------|---|--------------|-----|---------|-------------|------|
| 1    | Hexanal                |   |              | 100 | C6H12O  | 000066-25-1 | 72   |
| 2    | Hexanal                |   |              | 100 | C6H12O  | 000066-25-1 | 64   |
| 3    | Hexanal                |   |              | 100 | C6H12O  | 000066-25-1 | 64   |
| 4    | Hexanal                |   |              | 100 | C6H12O  | 000066-25-1 | 59   |
| 5    | Cyclobutanol, 2-ethyl- |   |              | 100 | C6H12O  | 035301-43-0 | 42   |



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Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFT92DL

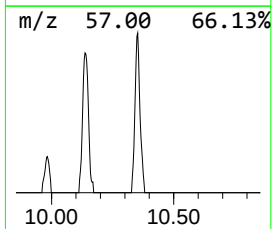
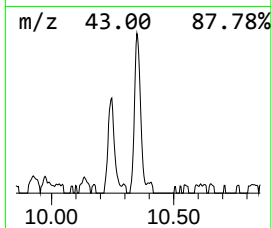
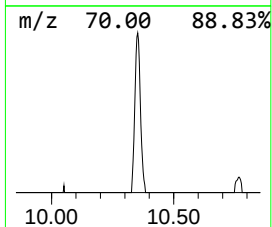
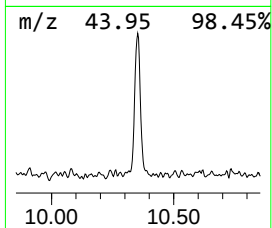
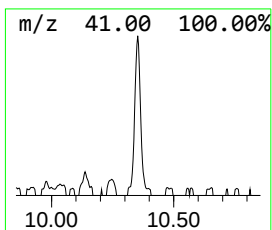
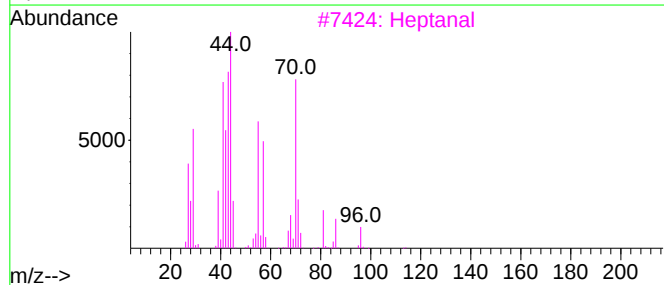
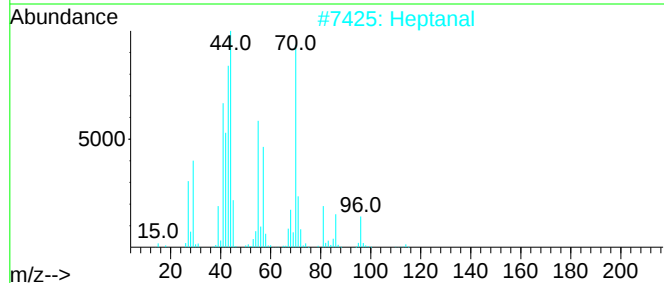
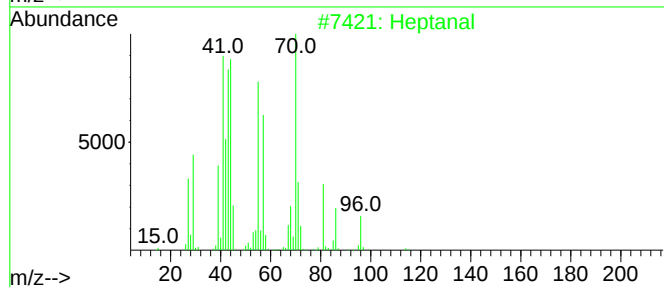
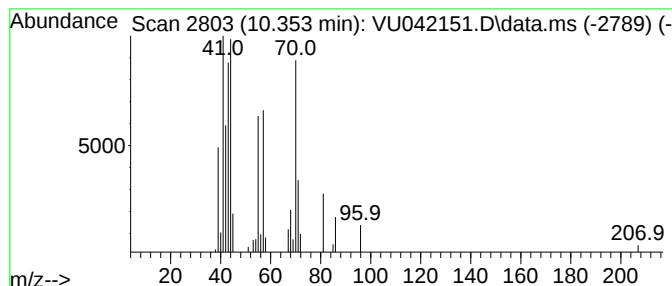
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Heptanal Concentration Rank 7

| R.T.   | EstConc   | Area  | Relative to ISTD | R.T.  |
|--------|-----------|-------|------------------|-------|
| 10.353 | 0.60 ug/L | 38134 | Chlorobenzene-d5 | 9.423 |

| Hit# | of       | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----------|---|--------------|-----|---------|-------------|------|
| 1    | Heptanal |   |              | 114 | C7H14O  | 000111-71-7 | 87   |
| 2    | Heptanal |   |              | 114 | C7H14O  | 000111-71-7 | 80   |
| 3    | Heptanal |   |              | 114 | C7H14O  | 000111-71-7 | 72   |
| 4    | Heptanal |   |              | 114 | C7H14O  | 000111-71-7 | 72   |
| 5    | Heptanal |   |              | 114 | C7H14O  | 000111-71-7 | 64   |



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Sample : M1170-11DL 4X  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFT92DL

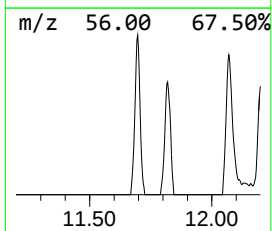
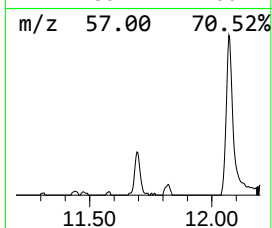
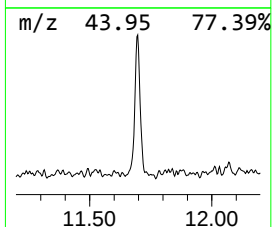
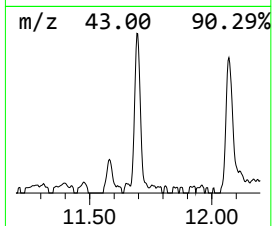
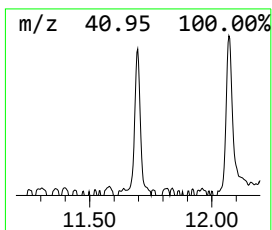
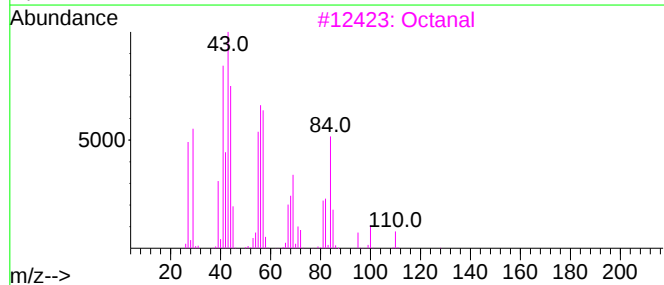
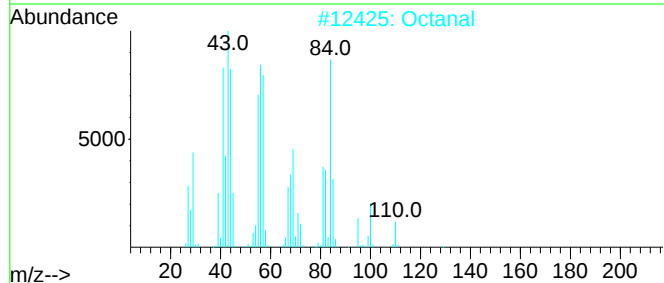
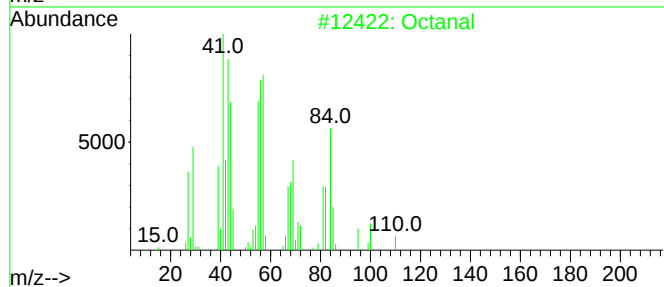
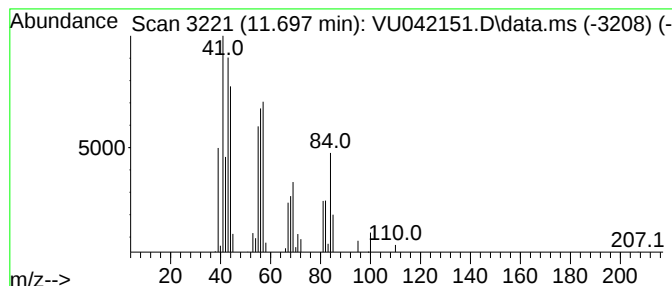
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Octanal Concentration Rank 6

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 11.697 | 0.72 ug/L | 46960 | 1,4-Dichlorobenzene-d4 | 11.819 |

| Hit# | of                            | 5 | Tentative ID | MW  | MolForm   | CAS#        | Qual |
|------|-------------------------------|---|--------------|-----|-----------|-------------|------|
| 1    | Octanal                       |   |              | 128 | C8H16O    | 000124-13-0 | 91   |
| 2    | Octanal                       |   |              | 128 | C8H16O    | 000124-13-0 | 91   |
| 3    | Octanal                       |   |              | 128 | C8H16O    | 000124-13-0 | 90   |
| 4    | Octanal                       |   |              | 128 | C8H16O    | 000124-13-0 | 86   |
| 5    | Bromoacetic acid, hexyl ester |   |              | 222 | C8H15BrO2 | 013048-32-3 | 27   |



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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFT92DL

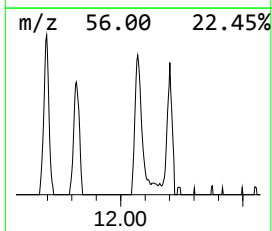
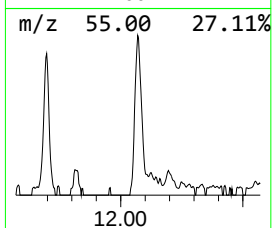
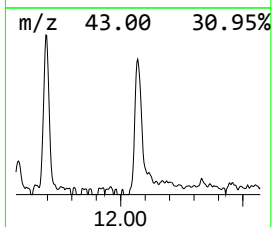
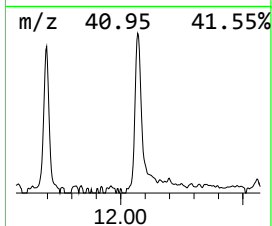
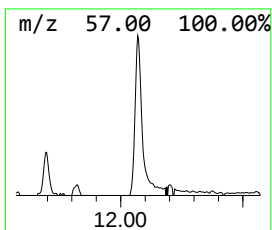
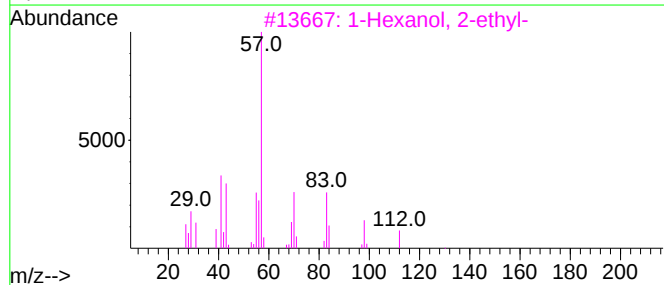
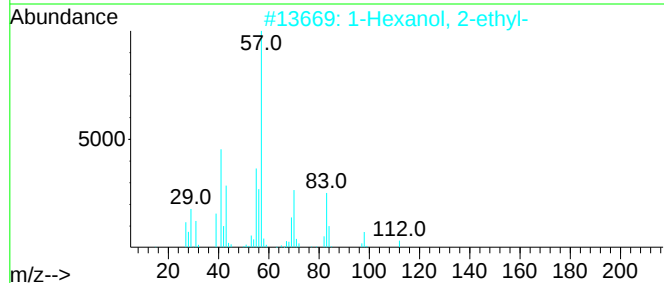
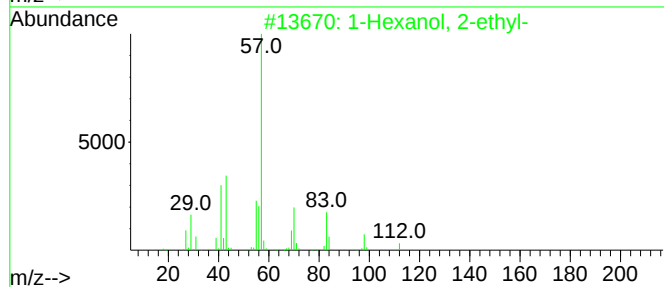
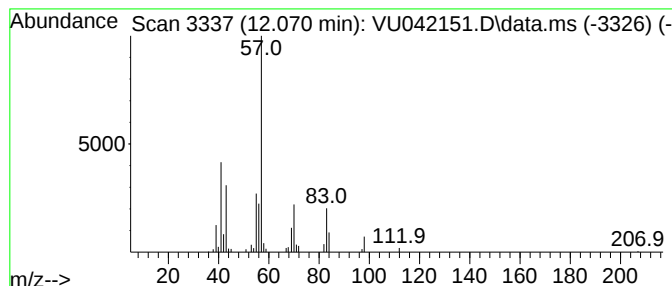
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.070 | 0.98 ug/L | 63791 | 1,4-Dichlorobenzene-d4 | 11.819 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 1-Hexanol, 2-ethyl-                 | 130 | C8H18O   | 000104-76-7  | 83   |
| 2    |    |   | 1-Hexanol, 2-ethyl-                 | 130 | C8H18O   | 000104-76-7  | 78   |
| 3    |    |   | 1-Hexanol, 2-ethyl-                 | 130 | C8H18O   | 000104-76-7  | 59   |
| 4    |    |   | Carbonic acid, isobutyl 2-ethylh... | 230 | C13H26O3 | 1000357-82-9 | 59   |
| 5    |    |   | Heptane, 1,1'-oxybis-               | 214 | C14H30O  | 000629-64-1  | 50   |



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MSVOA\_U  
ClientSampleId :  
BFT92DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

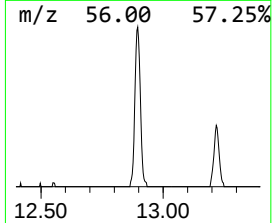
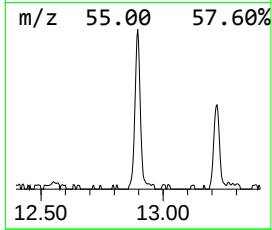
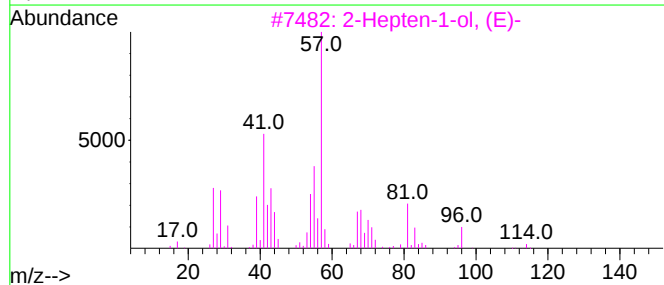
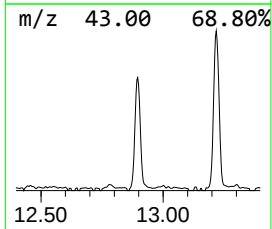
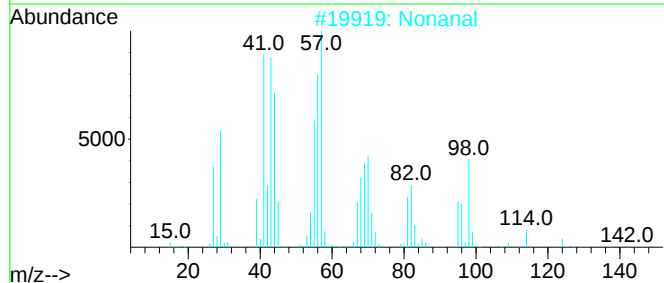
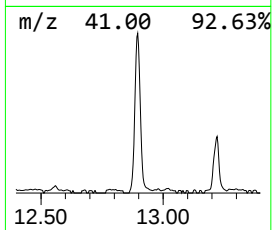
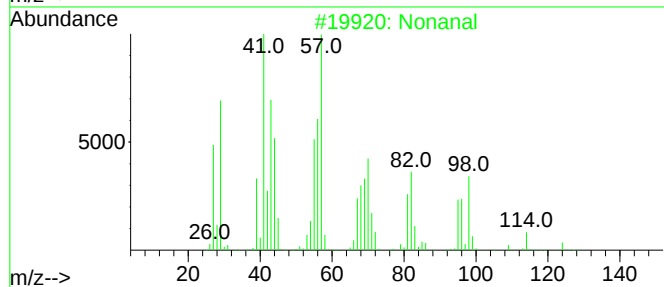
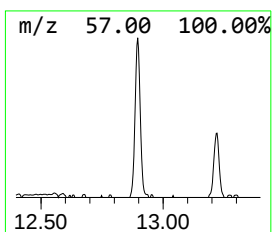
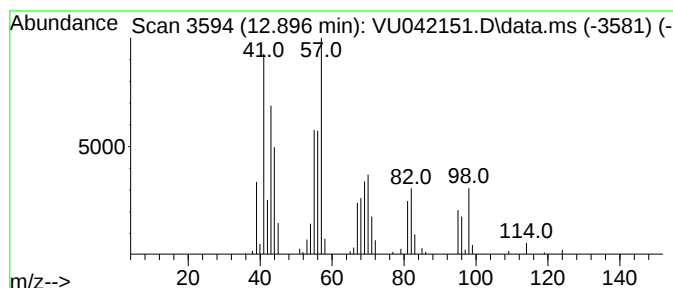
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Nonanal Concentration Rank 3

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 12.896 | 1.62 ug/L | 105446 | 1,4-Dichlorobenzene-d4 | 11.819 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|-----|---------|-------------|------|
| 1    |    |   | Nonanal                   | 142 | C9H18O  | 000124-19-6 | 91   |
| 2    |    |   | Nonanal                   | 142 | C9H18O  | 000124-19-6 | 90   |
| 3    |    |   | 2-Hepten-1-ol, (E)-       | 114 | C7H14O  | 033467-76-4 | 38   |
| 4    |    |   | 6-Hepten-1-ol, 3-methyl-  | 128 | C8H16O  | 004048-32-2 | 27   |
| 5    |    |   | 2-Hexene, 5-methyl-, (E)- | 98  | C7H14   | 007385-82-2 | 27   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012121\  
Data File : VU042151.D  
Acq On : 21 Jan 2021 15:24  
Operator : SY/MD  
Sample : M1170-11DL 4X  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFT92DL

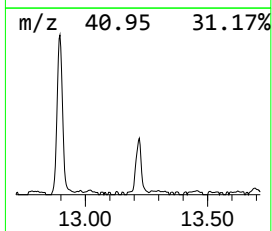
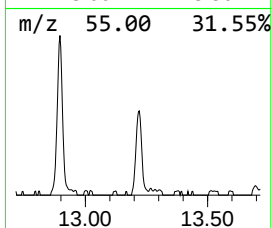
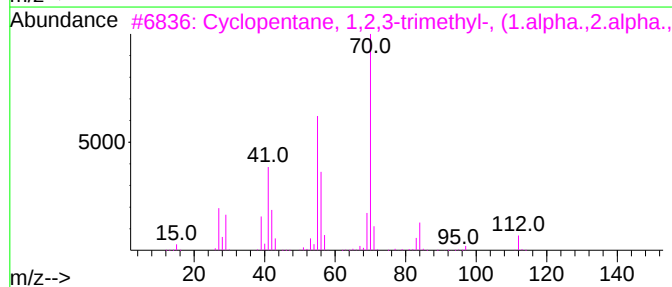
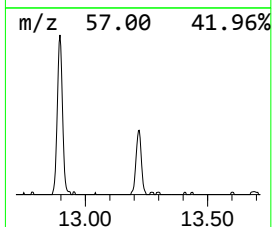
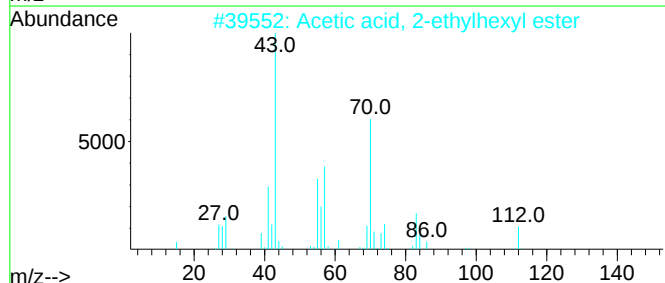
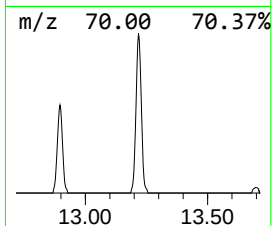
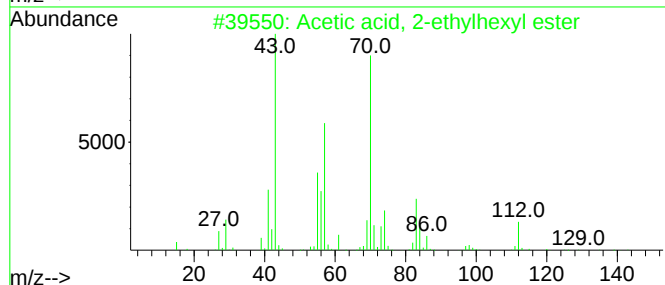
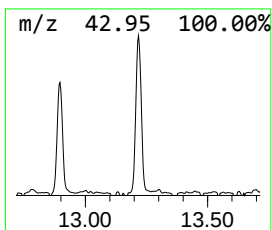
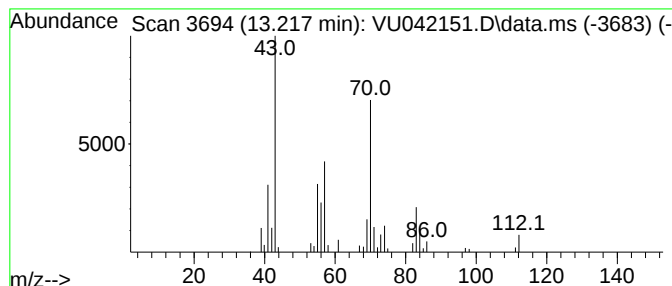
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Acetic acid, 2-ethylhexyl e... Concentration Rank 5

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 13.217 | 0.82 ug/L | 53318 | 1,4-Dichlorobenzene-d4 | 11.819 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Acetic acid, 2-ethylhexyl ester     | 172 | C10H20O2 | 000103-09-3 | 91   |
| 2    |    |   | Acetic acid, 2-ethylhexyl ester     | 172 | C10H20O2 | 000103-09-3 | 90   |
| 3    |    |   | Cyclopentane, 1,2,3-trimethyl-, ... | 112 | C8H16    | 002613-69-6 | 64   |
| 4    |    |   | Cyclopentane, 1,2,3-trimethyl-, ... | 112 | C8H16    | 002613-69-6 | 59   |
| 5    |    |   | Octane, 2-chloro-                   | 148 | C8H17Cl  | 000628-61-5 | 50   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012121\  
Data File : VU042151.D  
Acq On : 21 Jan 2021 15:24  
Operator : SY/MD  
Sample : M1170-11DL 4X  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFT92DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Hexanal            | 8.793  | 1.7     | ug/L  | 107706   | 2                     | 9.423  | 316445 | 5.0  |
| Heptanal           | 10.353 | 0.6     | ug/L  | 38134    | 2                     | 9.423  | 316445 | 5.0  |
| Octanal            | 11.697 | 0.7     | ug/L  | 46960    | 3                     | 11.819 | 324720 | 5.0  |
| 1-Hexanol, 2-et... | 12.070 | 1.0     | ug/L  | 63791    | 3                     | 11.819 | 324720 | 5.0  |
| Nonanal            | 12.896 | 1.6     | ug/L  | 105446   | 3                     | 11.819 | 324720 | 5.0  |
| Acetic acid, 2-... | 13.217 | 0.8     | ug/L  | 53318    | 3                     | 11.819 | 324720 | 5.0  |