

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012121\  
 Data File : VU042153.D  
 Acq On : 21 Jan 2021 16:10  
 Operator : SY/MD  
 Sample : M1170-17  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFT97

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: VU042153.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           | 10           | rBV2     | 14119          | 12559         | 1.19%           | 0.244%        |
| 2         | 1.601       | 71            | 81          | 90           | rVB      | 49954          | 59267         | 5.60%           | 1.152%        |
| 3         | 1.916       | 172           | 179         | 192          | rVB      | 37617          | 48459         | 4.58%           | 0.942%        |
| 4         | 2.568       | 369           | 382         | 394          | rBV      | 86566          | 137945        | 13.03%          | 2.681%        |
| 5         | 3.372       | 613           | 632         | 649          | rVB3     | 8607           | 21066         | 1.99%           | 0.409%        |
| 6         | 4.453       | 954           | 968         | 987          | rBV7     | 4512           | 13466         | 1.27%           | 0.262%        |
| 7         | 4.655       | 1011          | 1031        | 1049         | rBV2     | 49391          | 175796        | 16.60%          | 3.417%        |
| 8         | 5.073       | 1143          | 1161        | 1182         | rBV3     | 76910          | 192014        | 18.13%          | 3.732%        |
| 9         | 5.732       | 1345          | 1366        | 1393         | rBV2     | 149044         | 390942        | 36.91%          | 7.599%        |
| 10        | 6.256       | 1514          | 1529        | 1550         | rVB      | 158927         | 297498        | 28.09%          | 5.783%        |
| 11        | 6.549       | 1594          | 1620        | 1643         | rBV      | 546437         | 1059048       | 100.00%         | 20.586%       |
| 12        | 6.700       | 1654          | 1667        | 1682         | rVB2     | 93139          | 180066        | 17.00%          | 3.500%        |
| 13        | 6.800       | 1685          | 1698        | 1713         | rVB6     | 5810           | 16323         | 1.54%           | 0.317%        |
| 14        | 7.115       | 1783          | 1796        | 1805         | rBV3     | 12084          | 21198         | 2.00%           | 0.412%        |
| 15        | 7.571       | 1926          | 1938        | 1953         | rVB      | 55836          | 98042         | 9.26%           | 1.906%        |
| 16        | 7.803       | 1999          | 2010        | 2024         | rBV4     | 6586           | 12687         | 1.20%           | 0.247%        |
| 17        | 7.906       | 2024          | 2042        | 2056         | rVV      | 183671         | 318279        | 30.05%          | 6.187%        |
| 18        | 8.189       | 2117          | 2130        | 2142         | rBV      | 38094          | 64034         | 6.05%           | 1.245%        |
| 19        | 8.559       | 2236          | 2245        | 2256         | rVB2     | 19916          | 32488         | 3.07%           | 0.632%        |
| 20        | 8.645       | 2258          | 2272        | 2299         | rBV      | 254690         | 507829        | 47.95%          | 9.871%        |
| 21        | 8.800       | 2309          | 2320        | 2337         | rVB4     | 18358          | 44189         | 4.17%           | 0.859%        |
| 22        | 9.423       | 2500          | 2514        | 2535         | rBV      | 221805         | 362133        | 34.19%          | 7.039%        |
| 23        | 9.774       | 2610          | 2623        | 2636         | rBV      | 34806          | 62158         | 5.87%           | 1.208%        |
| 24        | 10.353      | 2793          | 2803        | 2815         | rBV2     | 11579          | 18275         | 1.73%           | 0.355%        |
| 25        | 10.767      | 2918          | 2932        | 2947         | rBV      | 76627          | 122522        | 11.57%          | 2.382%        |
| 26        | 11.697      | 3211          | 3221        | 3231         | rVB2     | 17398          | 26704         | 2.52%           | 0.519%        |
| 27        | 11.819      | 3247          | 3259        | 3278         | rBV      | 238804         | 374583        | 35.37%          | 7.281%        |
| 28        | 12.070      | 3322          | 3337        | 3362         | rBV2     | 31940          | 67459         | 6.37%           | 1.311%        |
| 29        | 12.201      | 3366          | 3378        | 3396         | rVB      | 189817         | 302389        | 28.55%          | 5.878%        |
| 30        | 12.896      | 3583          | 3594        | 3604         | rBV2     | 46724          | 70228         | 6.63%           | 1.365%        |
| 31        | 13.217      | 3684          | 3694        | 3707         | rBV      | 22746          | 34812         | 3.29%           | 0.677%        |

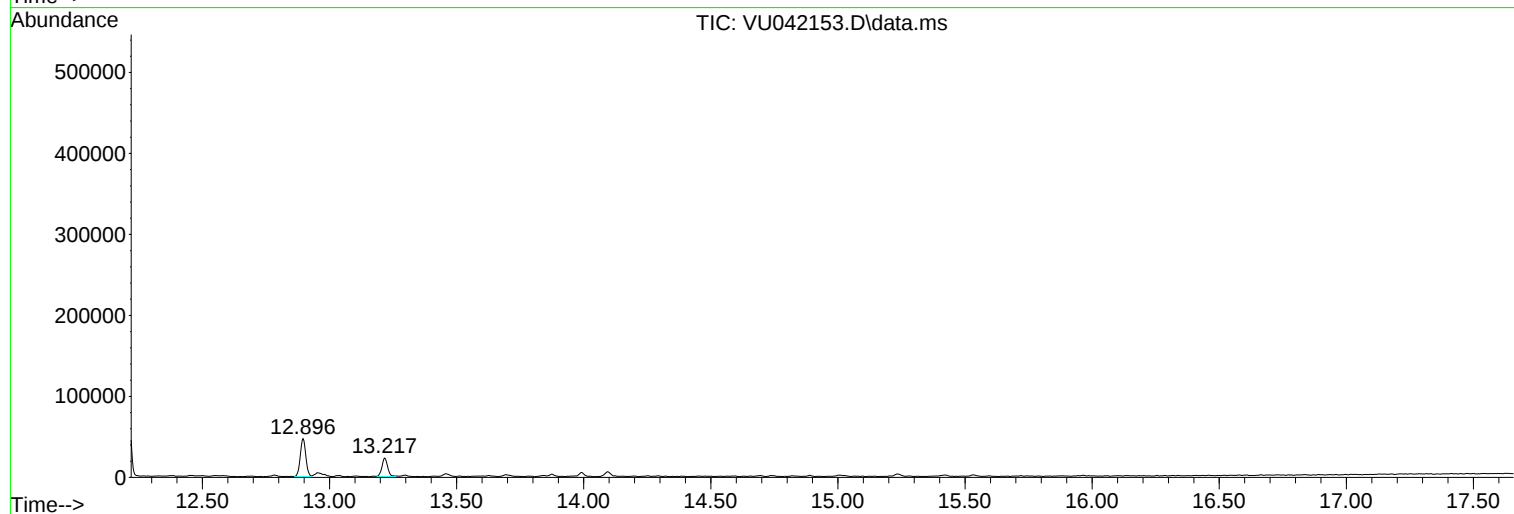
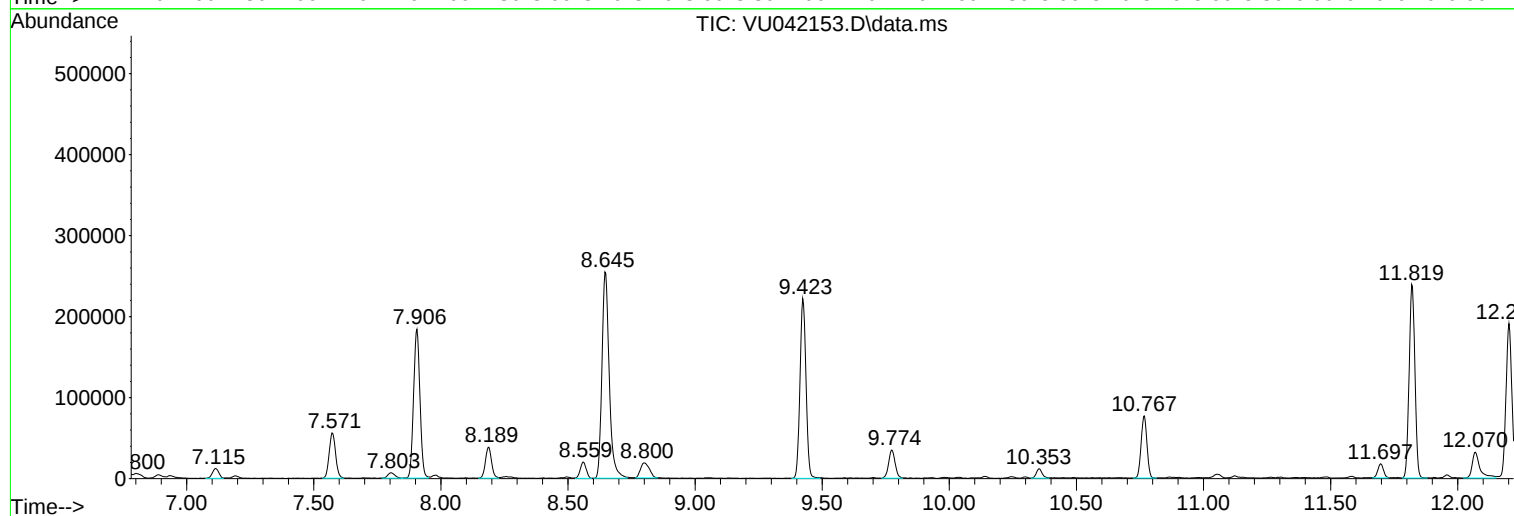
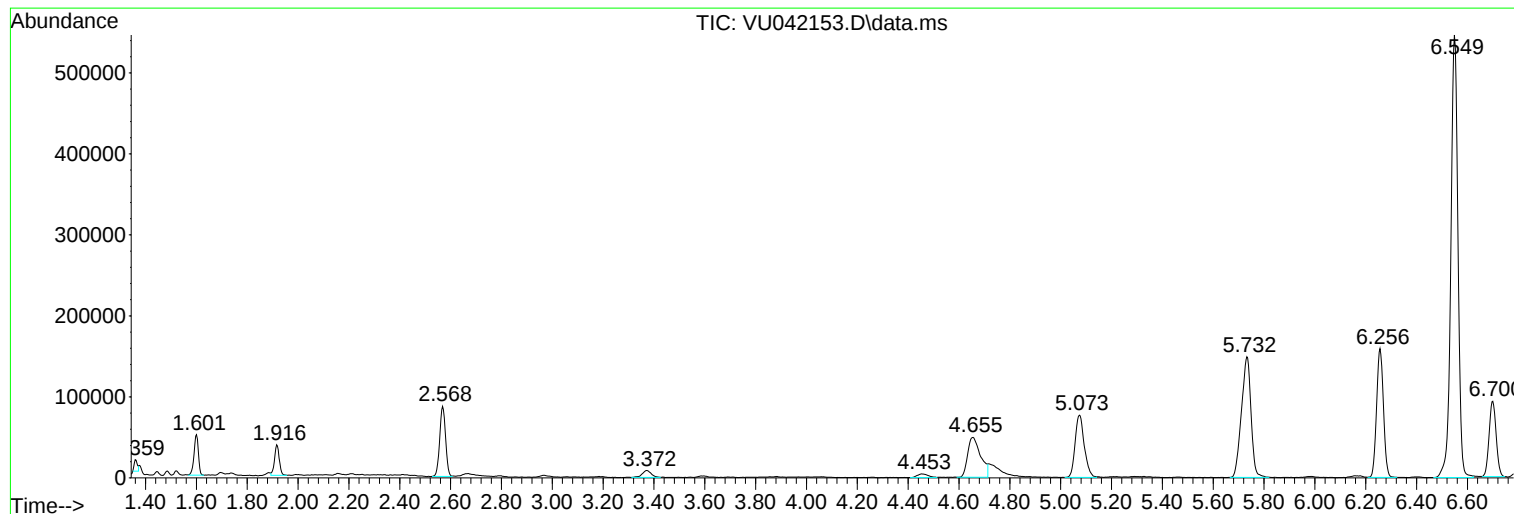
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ALS Vial : 17 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFT97

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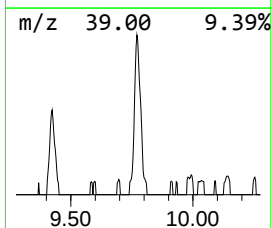
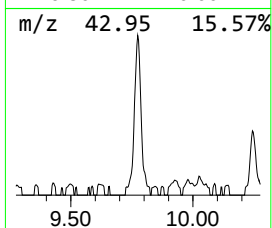
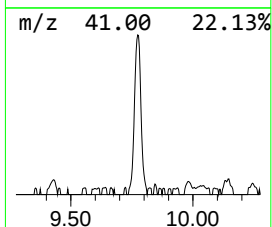
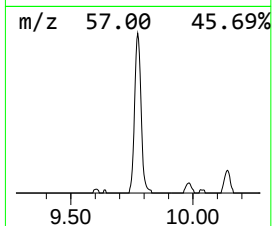
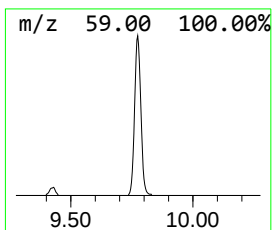
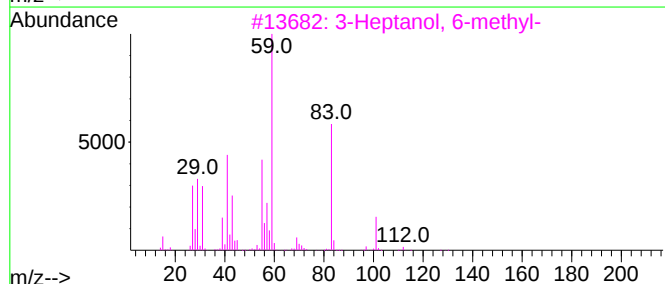
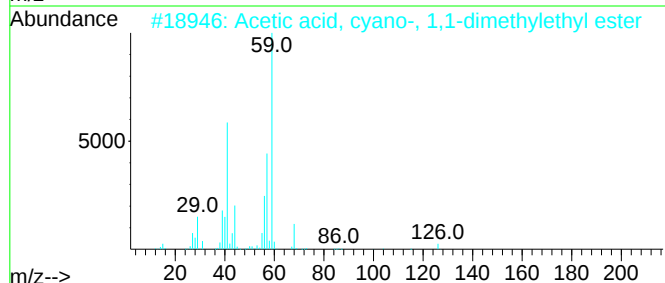
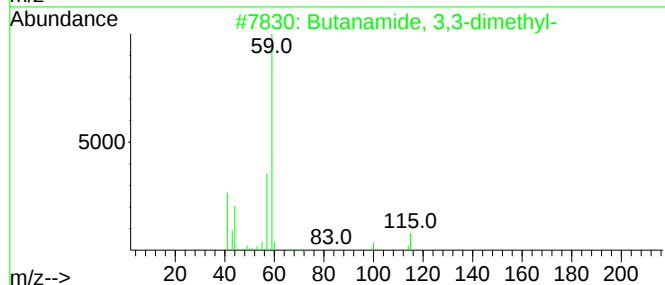
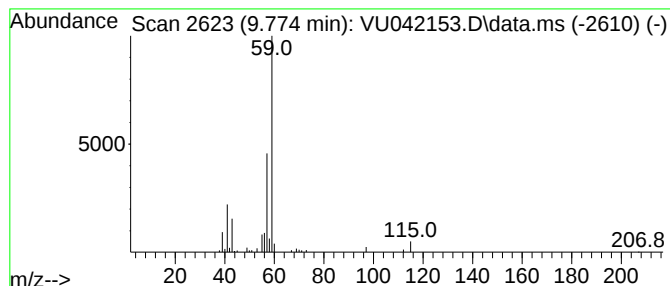
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

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

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Peak Number 2 Butanamide, 3,3-dimethyl- Concentration Rank 4

| R.T.  | EstConc   | Area  | Relative to ISTD | R.T.  |
|-------|-----------|-------|------------------|-------|
| 9.774 | 0.86 ug/L | 62158 | Chlorobenzene-d5 | 9.423 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Butanamide, 3,3-dimethyl-           | 115 | C6H13NO   | 000926-04-5  | 64   |
| 2    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2  | 001116-98-9  | 50   |
| 3    |    |   | 3-Heptanol, 6-methyl-               | 130 | C8H18O    | 018720-66-6  | 43   |
| 4    |    |   | 2,3-Dimethyl-4-penten-2-ol          | 114 | C7H14O    | 019781-52-3  | 38   |
| 5    |    |   | 4-O-Acetyl-2,5-di-O-methyl-3,6-d... | 215 | C10H17NO4 | 1000101-80-3 | 38   |



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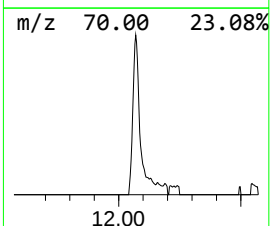
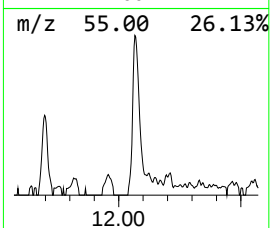
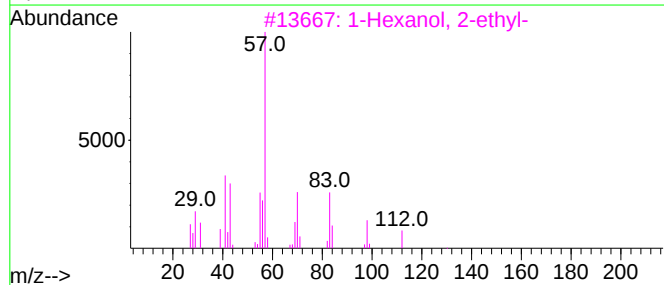
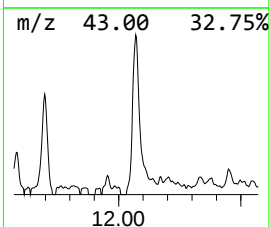
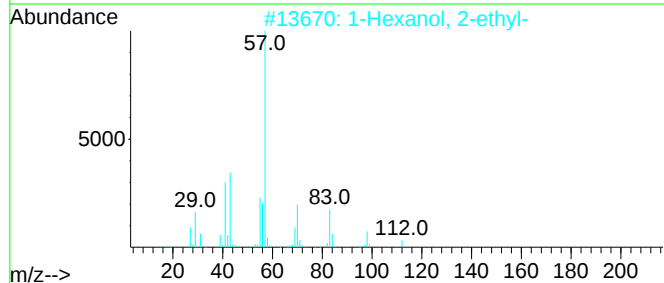
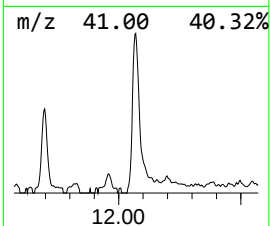
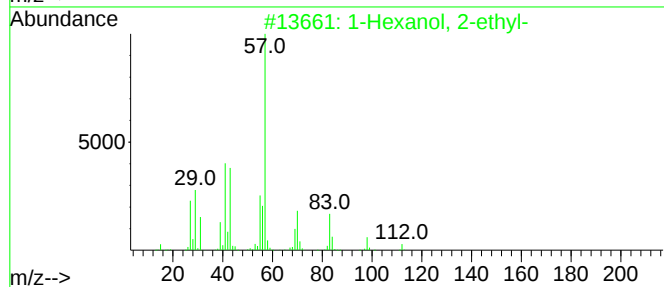
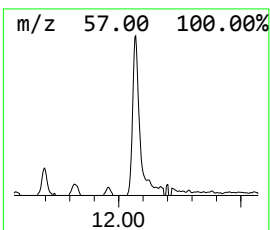
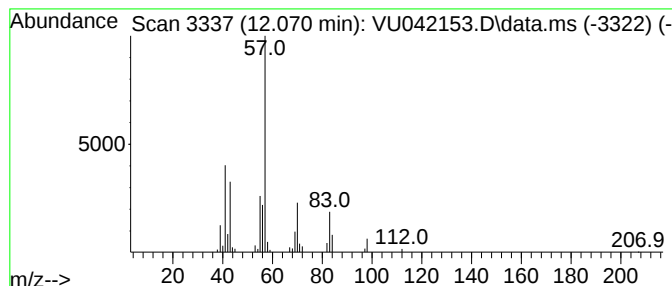
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

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

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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.070 | 0.90 ug/L | 67459 | 1,4-Dichlorobenzene-d4 | 11.822 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | 1-Hexanol, 2-ethyl-   | 130 | C8H18O  | 000104-76-7 | 78   |
| 2    |    |   | 1-Hexanol, 2-ethyl-   | 130 | C8H18O  | 000104-76-7 | 78   |
| 3    |    |   | 1-Hexanol, 2-ethyl-   | 130 | C8H18O  | 000104-76-7 | 74   |
| 4    |    |   | 2-Propyl-1-pentanol   | 130 | C8H18O  | 058175-57-8 | 59   |
| 5    |    |   | Heptane, 1,1'-oxybis- | 214 | C14H30O | 000629-64-1 | 59   |



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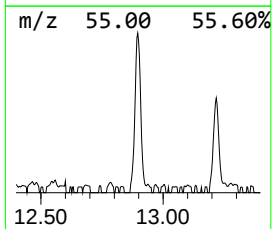
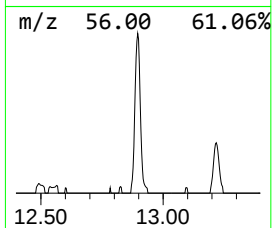
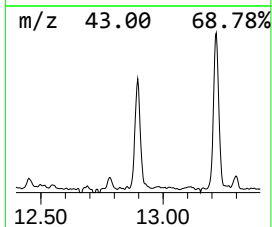
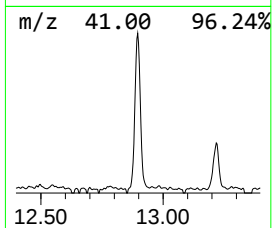
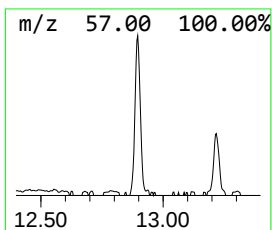
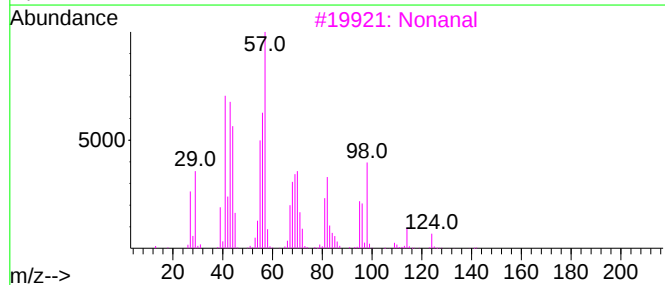
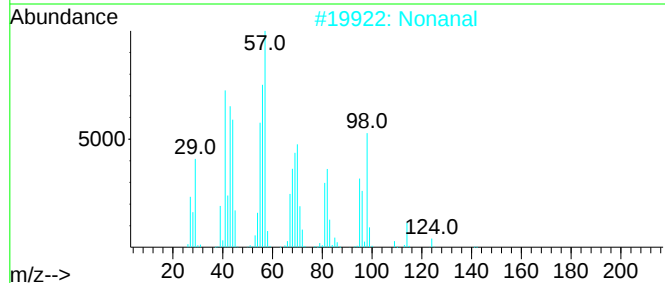
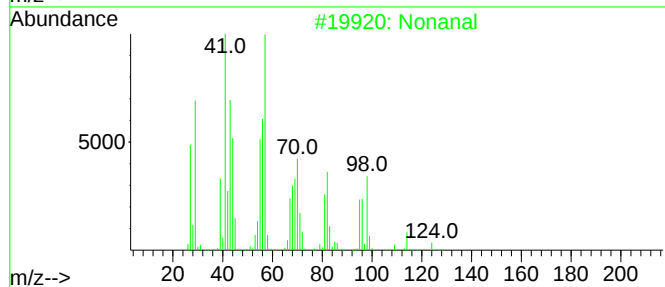
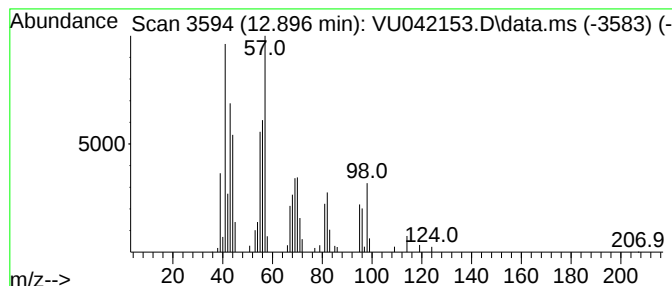
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Quant Title : TRACE VOA SOM01.0

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

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Peak Number 4 Nonanal Concentration Rank 2

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.896 | 0.94 ug/L | 70228 | 1,4-Dichlorobenzene-d4 | 11.822 |

| Hit# | of                              | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------------------------------|---|--------------|-----|---------|-------------|------|
| 1    | Nonanal                         |   |              | 142 | C9H18O  | 000124-19-6 | 87   |
| 2    | Nonanal                         |   |              | 142 | C9H18O  | 000124-19-6 | 86   |
| 3    | Nonanal                         |   |              | 142 | C9H18O  | 000124-19-6 | 86   |
| 4    | Nonanal                         |   |              | 142 | C9H18O  | 000124-19-6 | 80   |
| 5    | Cyclohexanol, 2-methyl-, trans- |   |              | 114 | C7H14O  | 007443-52-9 | 38   |



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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butanamide, 3,3... | 9.774  | 0.9     | ug/L  | 62158    | 2                     | 9.423  | 362133 | 5.0  |
| 1-Hexanol, 2-et... | 12.070 | 0.9     | ug/L  | 67459    | 3                     | 11.822 | 374583 | 5.0  |
| Nonanal            | 12.896 | 0.9     | ug/L  | 70228    | 3                     | 11.822 | 374583 | 5.0  |