

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100720\  
 Data File : VX018823.D  
 Acq On : 07 Oct 2020 20:13  
 Operator : JC/SP  
 Sample : L4286-13  
 Misc : 25.0mL/MSVOA X/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0AW0

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR100220WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

| 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         | 1.386       | 46            | 49          | 60           | rVB      | 59798          | 62672         | 9.61%           | 1.142%        |
| 2         | 1.697       | 96            | 100         | 107          | rBV      | 55416          | 67675         | 10.38%          | 1.233%        |
| 3         | 2.343       | 200           | 206         | 214          | rVB      | 118281         | 181532        | 27.85%          | 3.308%        |
| 4         | 2.459       | 219           | 225         | 230          | rBV      | 6881           | 18143         | 2.78%           | 0.331%        |
| 5         | 2.873       | 289           | 293         | 299          | rVB5     | 6261           | 12006         | 1.84%           | 0.219%        |
| 6         | 3.148       | 331           | 338         | 345          | rBV2     | 9937           | 23183         | 3.56%           | 0.422%        |
| 7         | 3.501       | 387           | 396         | 404          | rBV3     | 25835          | 59970         | 9.20%           | 1.093%        |
| 8         | 4.556       | 557           | 569         | 582          | rBV      | 57882          | 246211        | 37.77%          | 4.486%        |
| 9         | 4.800       | 601           | 609         | 628          | rVB2     | 50609          | 169872        | 26.06%          | 3.095%        |
| 10        | 5.141       | 652           | 665         | 681          | rBV2     | 92922          | 298120        | 45.73%          | 5.432%        |
| 11        | 6.043       | 801           | 813         | 829          | rBV2     | 198896         | 579947        | 88.97%          | 10.567%       |
| 12        | 6.830       | 931           | 942         | 952          | rBV      | 142042         | 351889        | 53.98%          | 6.412%        |
| 13        | 6.982       | 959           | 967         | 968          | rBV5     | 5505           | 11231         | 1.72%           | 0.205%        |
| 14        | 7.372       | 1019          | 1031        | 1042         | rBV      | 123706         | 281894        | 43.24%          | 5.136%        |
| 15        | 8.372       | 1188          | 1195        | 1202         | rBV      | 80973          | 132867        | 20.38%          | 2.421%        |
| 16        | 8.695       | 1241          | 1248        | 1256         | rBV      | 291227         | 449585        | 68.97%          | 8.192%        |
| 17        | 8.762       | 1256          | 1259        | 1270         | rVB      | 20308          | 32686         | 5.01%           | 0.596%        |
| 18        | 8.994       | 1292          | 1297        | 1304         | rBV      | 54106          | 80830         | 12.40%          | 1.473%        |
| 19        | 9.427       | 1362          | 1368        | 1383         | rBV      | 453651         | 651869        | 100.00%         | 11.877%       |
| 20        | 9.561       | 1386          | 1390        | 1397         | rVV2     | 36814          | 53144         | 8.15%           | 0.968%        |
| 21        | 9.616       | 1397          | 1399        | 1408         | rVB2     | 4365           | 6974          | 1.07%           | 0.127%        |
| 22        | 10.098      | 1471          | 1478        | 1487         | rBV      | 300546         | 417943        | 64.11%          | 7.615%        |
| 23        | 10.896      | 1605          | 1609        | 1613         | rVB6     | 5817           | 6838          | 1.05%           | 0.125%        |
| 24        | 11.232      | 1659          | 1664        | 1670         | rBV      | 142275         | 181694        | 27.87%          | 3.311%        |
| 25        | 11.792      | 1751          | 1756        | 1762         | rBV2     | 9844           | 12969         | 1.99%           | 0.236%        |
| 26        | 11.969      | 1781          | 1785        | 1788         | rVB4     | 5727           | 7285          | 1.12%           | 0.133%        |
| 27        | 12.061      | 1795          | 1800        | 1806         | rVB      | 311225         | 383902        | 58.89%          | 6.995%        |
| 28        | 12.256      | 1826          | 1832        | 1843         | rBV      | 62323          | 97543         | 14.96%          | 1.777%        |
| 29        | 12.359      | 1843          | 1849        | 1858         | rVB      | 354801         | 446768        | 68.54%          | 8.140%        |
| 30        | 12.628      | 1888          | 1893        | 1899         | rVB9     | 6089           | 11707         | 1.80%           | 0.213%        |
| 31        | 12.890      | 1933          | 1936        | 1942         | rVB3     | 20190          | 26008         | 3.99%           | 0.474%        |
| 32        | 13.134      | 1968          | 1976        | 1981         | rBV      | 70127          | 88598         | 13.59%          | 1.614%        |
| 33        | 13.634      | 2053          | 2058        | 2064         | rBV9     | 4220           | 7368          | 1.13%           | 0.134%        |
| 34        | 13.835      | 2086          | 2091        | 2095         | rVB3     | 7794           | 9629          | 1.48%           | 0.175%        |

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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
C0AW0

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\_X\METHOD\SOMXTR100220WMA.M  
Title : TRACE VOA SOM01.0

|    |        |      |      |      |      |       |       |       |        |
|----|--------|------|------|------|------|-------|-------|-------|--------|
| 35 | 13.884 | 2096 | 2099 | 2104 | rVV2 | 13506 | 17818 | 2.73% | 0.325% |
|----|--------|------|------|------|------|-------|-------|-------|--------|

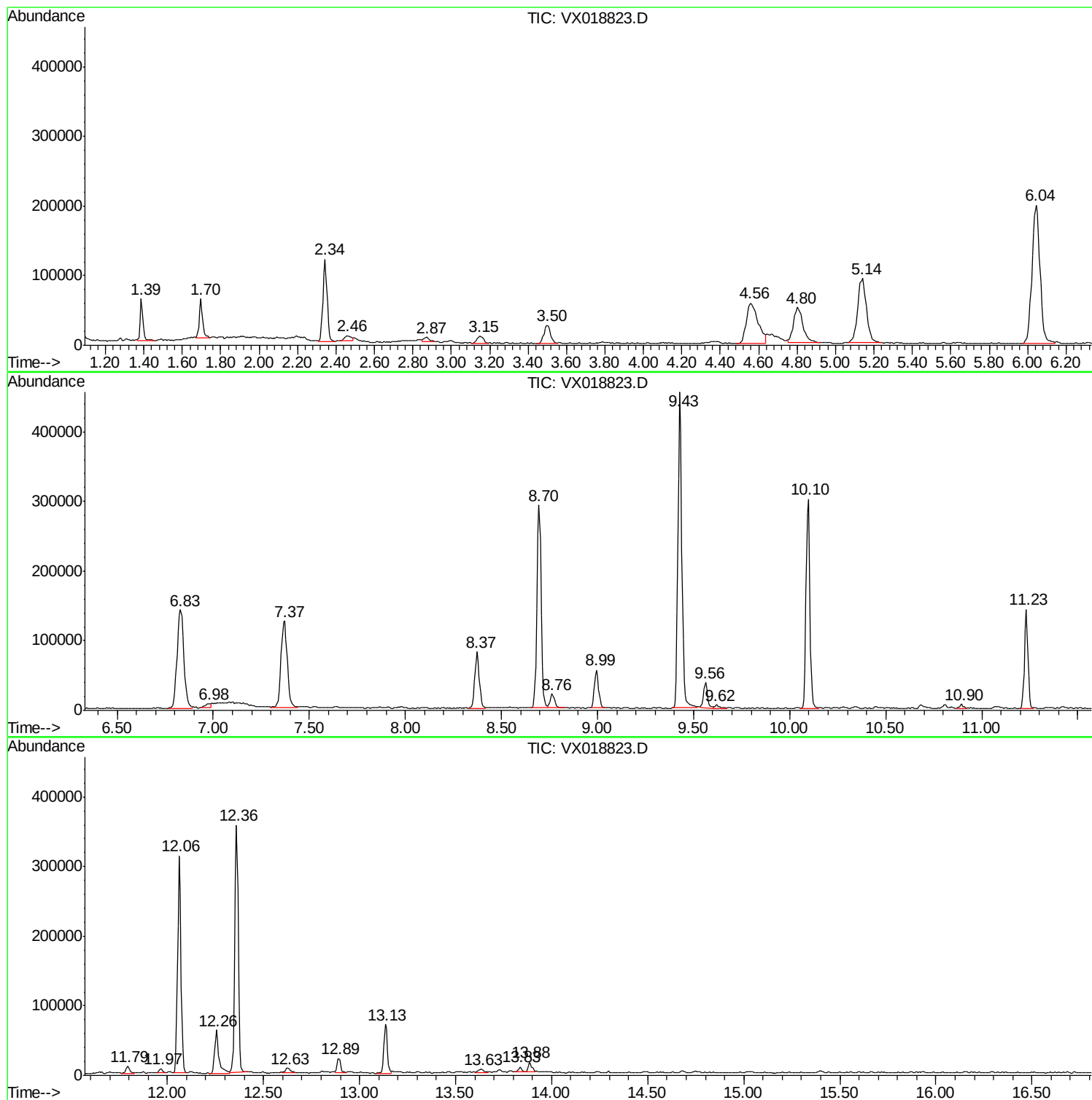
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR100220WMA.M  
Quant Title : TRACE VOA SOM01.0

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



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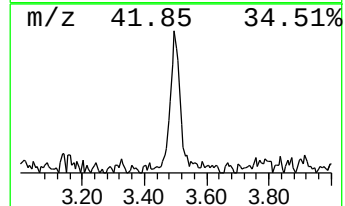
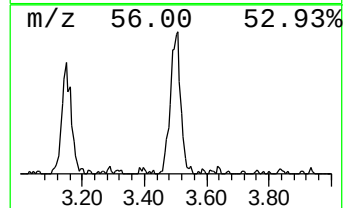
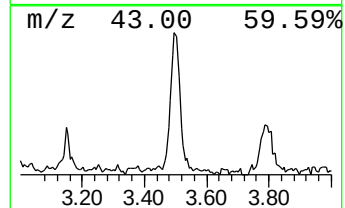
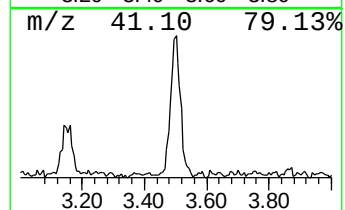
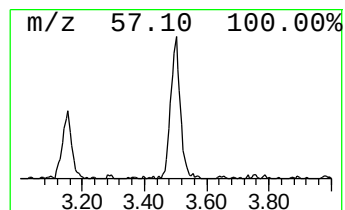
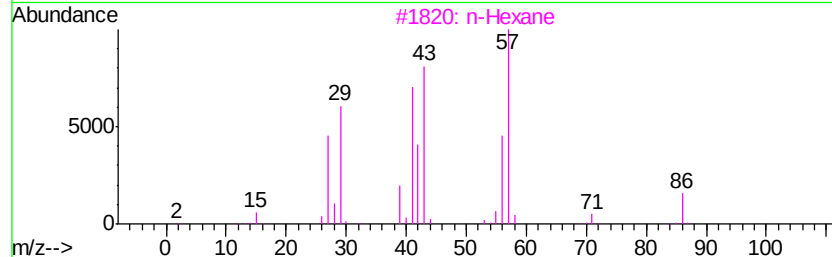
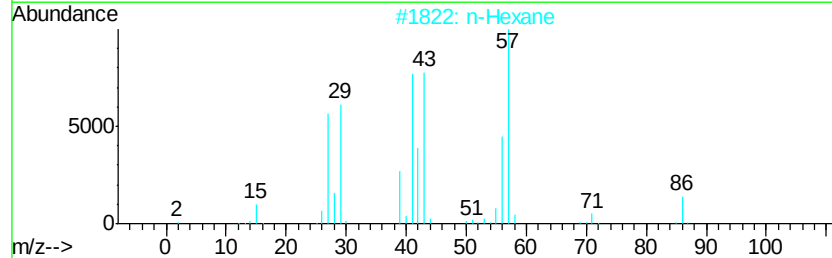
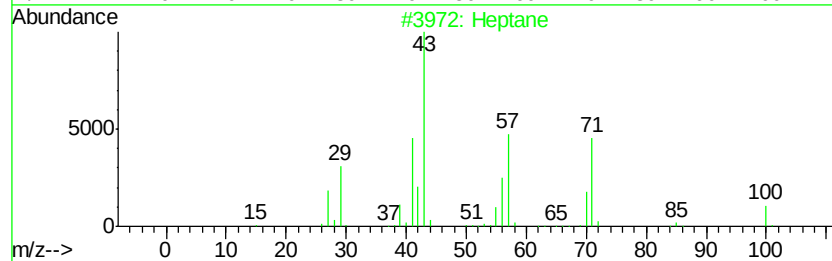
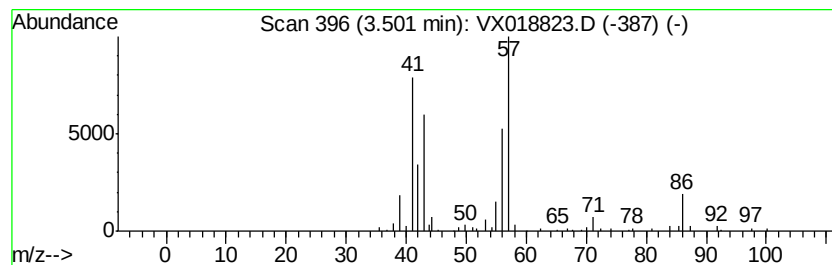
Instrument :  
MSVOA\_X  
ClientSampleId :  
C0AW0

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR100220WMA.M  
Quant Title : TRACE VOA SOM01.0

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

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Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

| R.T.      | EstConc              | Area  | Relative to ISTD    | R.T.        |      |
|-----------|----------------------|-------|---------------------|-------------|------|
| 3.50      | 0.85 ug/L            | 59970 | 1,4-Difluorobenzene | 6.83        |      |
| Hit# of 5 | Tentative ID         | MW    | MolForm             | CAS#        | Qual |
| 1         | Heptane              | 100   | C7H16               | 000142-82-5 | 56   |
| 2         | n-Hexane             | 86    | C6H14               | 000110-54-3 | 53   |
| 3         | n-Hexane             | 86    | C6H14               | 000110-54-3 | 42   |
| 4         | 1-Pentene, 4-methyl- | 84    | C6H12               | 000691-37-2 | 40   |
| 5         | Cyclobutane          | 56    | C4H8                | 000287-23-0 | 38   |



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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
C0AW0

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR100220WMA.M  
Quant Title : TRACE VOA SOM01.0

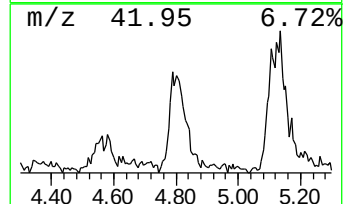
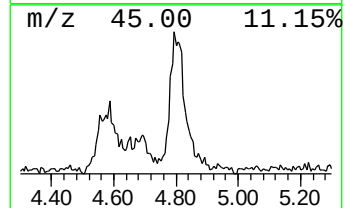
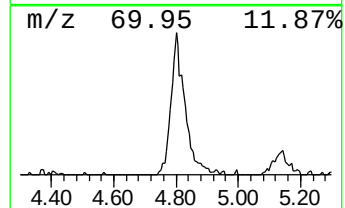
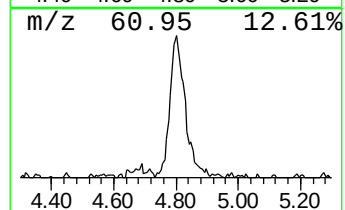
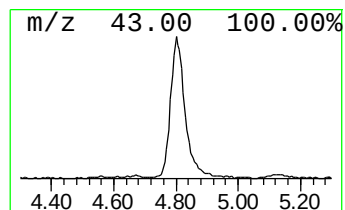
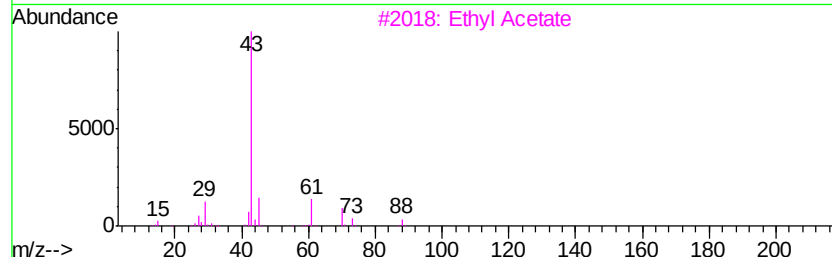
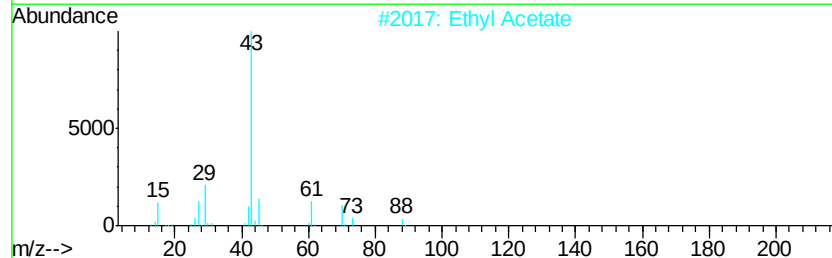
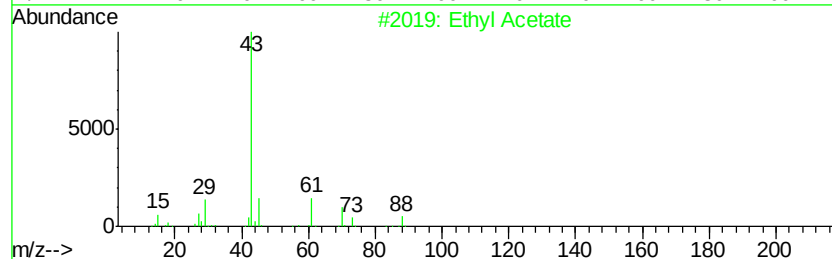
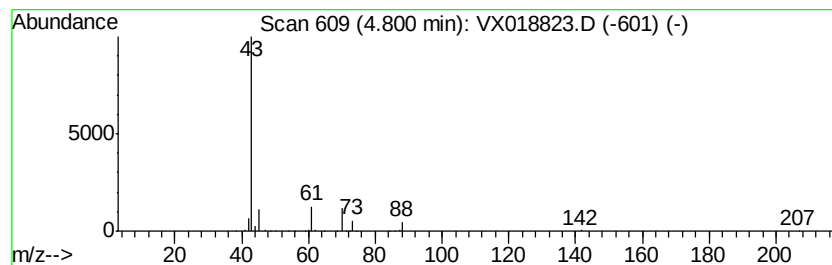
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Ethyl Acetate Concentration Rank 1

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 4.80 | 2.41 ug/L | 169872 | 1,4-Difluorobenzene | 6.83 |

| Hit# | of | Tentative ID    | MW | MolForm | CAS#        | Qual |
|------|----|-----------------|----|---------|-------------|------|
| 1    | 5  | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 86   |
| 2    |    | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 86   |
| 3    |    | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 86   |
| 4    |    | Ethyl Acetate   | 88 | C4H8O2  | 000141-78-6 | 78   |
| 5    |    | CH3C(O)CH2CH2OH | 88 | C4H8O2  | 000590-90-9 | 59   |



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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
C0AW0

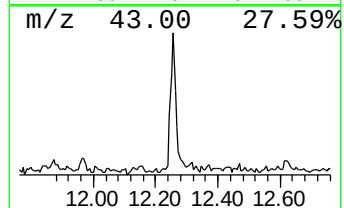
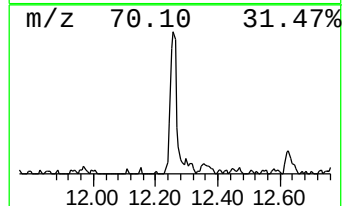
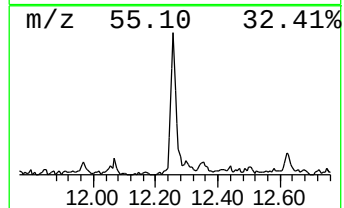
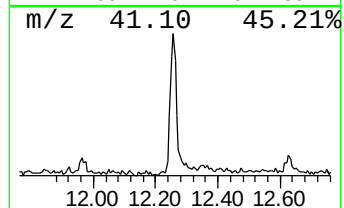
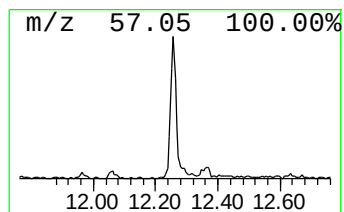
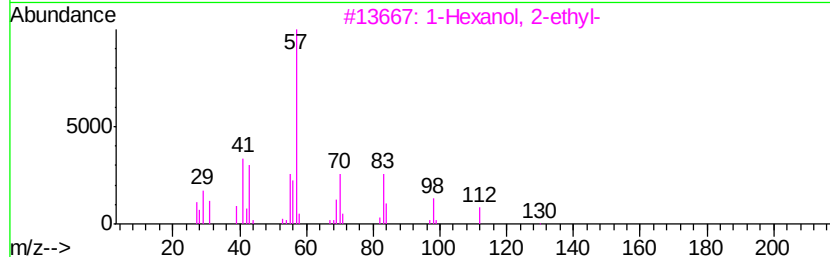
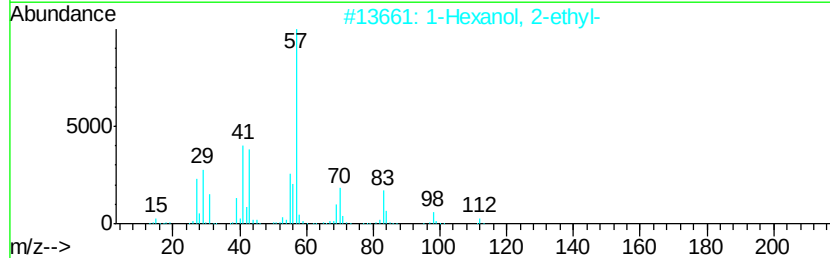
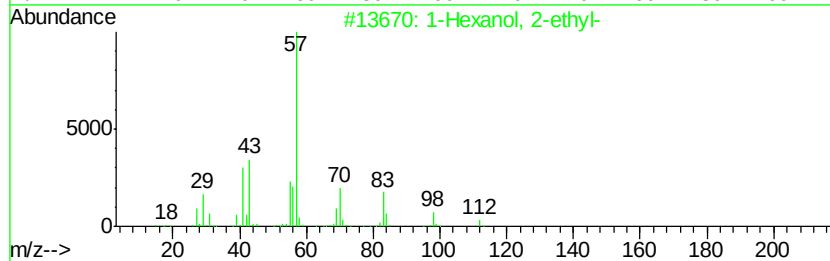
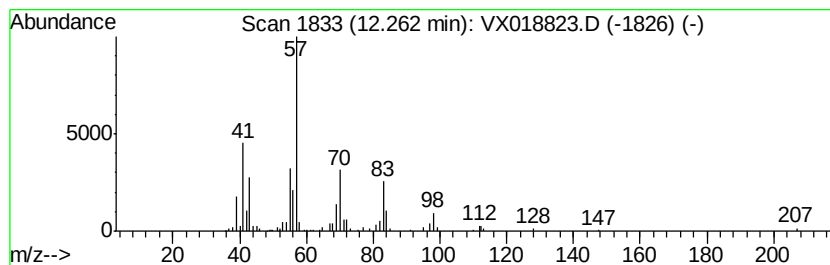
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR100220WMA.M  
Quant Title : TRACE VOA SOM01.0

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

\*\*\*\*\*  
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD       | R.T.  |
|-------|-----------|-------|------------------------|-------|
| 12.26 | 1.27 ug/L | 97543 | 1,4-Dichlorobenzene-d4 | 12.06 |

| Hit# | of | Tentative ID              | MW  | MolForm | CAS#         | Qual |
|------|----|---------------------------|-----|---------|--------------|------|
| 1    | 5  | 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  | 64   |
| 4    |    | 1-Hexanol, 2-ethyl-       | 130 | C8H18O  | 000104-76-7  | 64   |
| 5    |    | 1-Isobutoxy-2-ethylhexane | 186 | C12H26O | 1000139-90-3 | 64   |



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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR100220WMA.M  
Quant Title : TRACE VOA SOM01.0

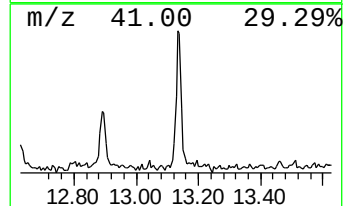
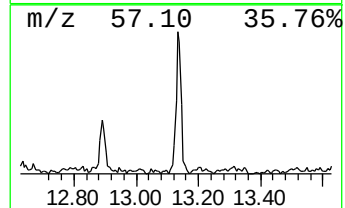
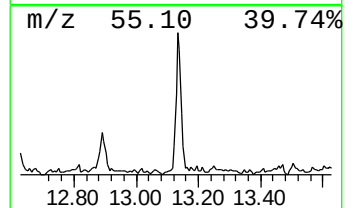
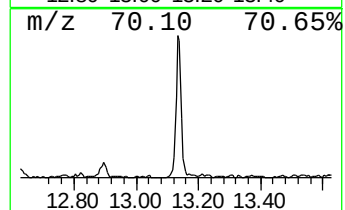
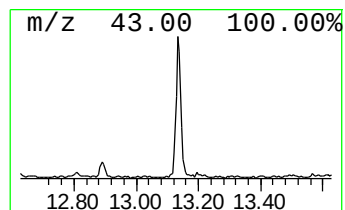
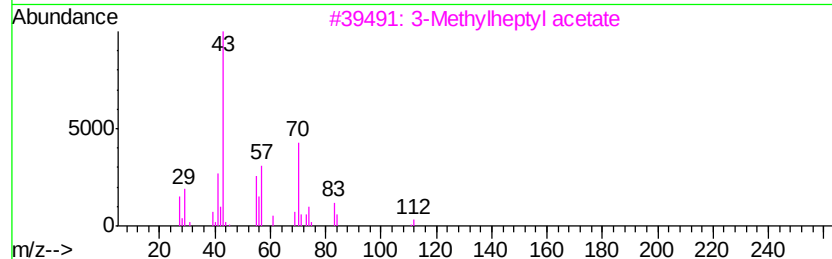
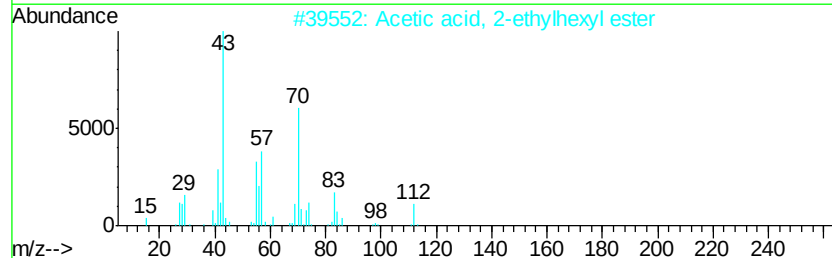
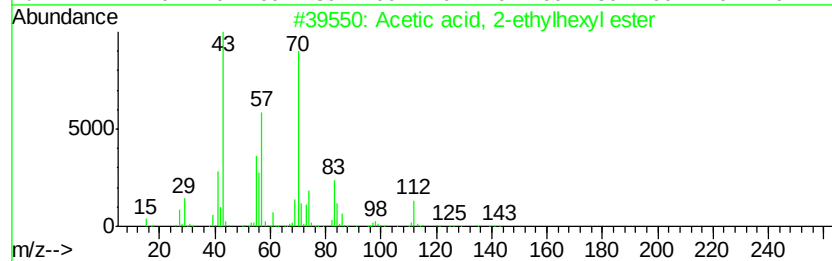
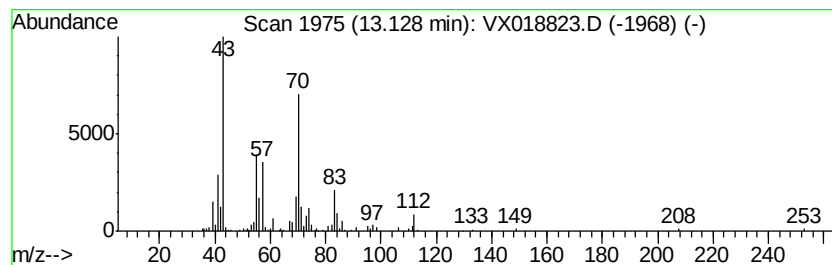
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Acetic acid, 2-ethylhexyl e... Concentration Rank 4

| R.T.  | EstConc   | Area  | Relative to ISTD       | R.T.  |
|-------|-----------|-------|------------------------|-------|
| 13.13 | 1.15 ug/L | 88598 | 1,4-Dichlorobenzene-d4 | 12.06 |

| Hit# of | 5 | Tentative ID                    | MW  | MolForm  | CAS#        | Qual |
|---------|---|---------------------------------|-----|----------|-------------|------|
| 1       |   | Acetic acid, 2-ethylhexyl ester | 172 | C10H20O2 | 000103-09-3 | 90   |
| 2       |   | Acetic acid, 2-ethylhexyl ester | 172 | C10H20O2 | 000103-09-3 | 80   |
| 3       |   | 3-Methylheptyl acetate          | 172 | C10H20O2 | 072218-58-7 | 59   |
| 4       |   | 2-Ethylhexyl methacrylate       | 198 | C12H22O2 | 000688-84-6 | 53   |
| 5       |   | 3-Undecene, 9-methyl-, (Z)-     | 168 | C12H24   | 074630-50-5 | 50   |



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ALS Vial : 15 Sample Multiplier: 1

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MSVOA\_X  
ClientSampleId :  
C0AW0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\SOMXTR100220WMA.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 |
| (DEL) Alkane: Str... | 3.50  | 0.8     | ug/L  | 59970    | 1                     | 6.83  | 351889 | 5.0  |
| Ethyl Acetate        | 4.80  | 2.4     | ug/L  | 169872   | 1                     | 6.83  | 351889 | 5.0  |
| 1-Hexanol, 2-ethyl-  | 12.26 | 1.3     | ug/L  | 97543    | 3                     | 12.06 | 383902 | 5.0  |
| Acetic acid, 2-et... | 13.13 | 1.1     | ug/L  | 88598    | 3                     | 12.06 | 383902 | 5.0  |