

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081920\  
Data File : VX018007.D  
Acq On : 20 Aug 2020 01:12  
Operator : JC/SP  
Sample : L3694-07  
Misc : 5.0mL/MSVOA X/WATER  
ALS Vial : 42 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
SLUICEWAY-081320

## Integration Parameters: RTEINT.P

Integrator: RTE  
Smoothing : ON  
Sampling : 1  
Start Thrs: 0.2  
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\82X081920W.M  
Title : SW846 8260

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         | 1.477       | 60            | 64          | 71           | rBV      | 31911          | 41474         | 1.65%           | 0.242%        |
| 2         | 2.093       | 158           | 165         | 172          | rBV      | 164483         | 280233        | 11.12%          | 1.632%        |
| 3         | 2.422       | 213           | 219         | 230          | rVB      | 64215          | 117597        | 4.67%           | 0.685%        |
| 4         | 2.581       | 236           | 245         | 256          | rVB2     | 28787          | 56574         | 2.24%           | 0.329%        |
| 5         | 3.166       | 332           | 341         | 353          | rBV      | 872956         | 2018645       | 80.08%          | 11.755%       |
| 6         | 5.178       | 662           | 671         | 684          | rVB2     | 39582          | 122102        | 4.84%           | 0.711%        |
| 7         | 5.471       | 706           | 719         | 732          | rBV      | 320708         | 921380        | 36.55%          | 5.365%        |
| 8         | 5.629       | 734           | 745         | 760          | rVV      | 540444         | 1515179       | 60.11%          | 8.823%        |
| 9         | 6.032       | 800           | 811         | 823          | rBV2     | 344750         | 903820        | 35.86%          | 5.263%        |
| 10        | 6.830       | 931           | 942         | 954          | rBV      | 780877         | 1853048       | 73.51%          | 10.791%       |
| 11        | 7.879       | 1105          | 1114        | 1123         | rBV3     | 31378          | 67427         | 2.67%           | 0.393%        |
| 12        | 8.458       | 1203          | 1209        | 1215         | rBV2     | 14669          | 29662         | 1.18%           | 0.173%        |
| 13        | 8.696       | 1241          | 1248        | 1256         | rBV      | 1640306        | 2520707       | 100.00%         | 14.679%       |
| 14        | 8.763       | 1256          | 1259        | 1265         | rVB2     | 14287          | 25969         | 1.03%           | 0.151%        |
| 15        | 9.567       | 1384          | 1391        | 1396         | rBV3     | 21168          | 36078         | 1.43%           | 0.210%        |
| 16        | 10.098      | 1470          | 1478        | 1487         | rBV      | 1674798        | 2221566       | 88.13%          | 12.937%       |
| 17        | 10.720      | 1574          | 1580        | 1590         | rVB      | 334131         | 396511        | 15.73%          | 2.309%        |
| 18        | 11.122      | 1638          | 1646        | 1652         | rBV      | 1472466        | 1786619       | 70.88%          | 10.404%       |
| 19        | 12.061      | 1795          | 1800        | 1807         | rBV      | 1880232        | 2207625       | 87.58%          | 12.856%       |
| 20        | 13.628      | 2052          | 2057        | 2063         | rBV9     | 29433          | 50376         | 2.00%           | 0.293%        |

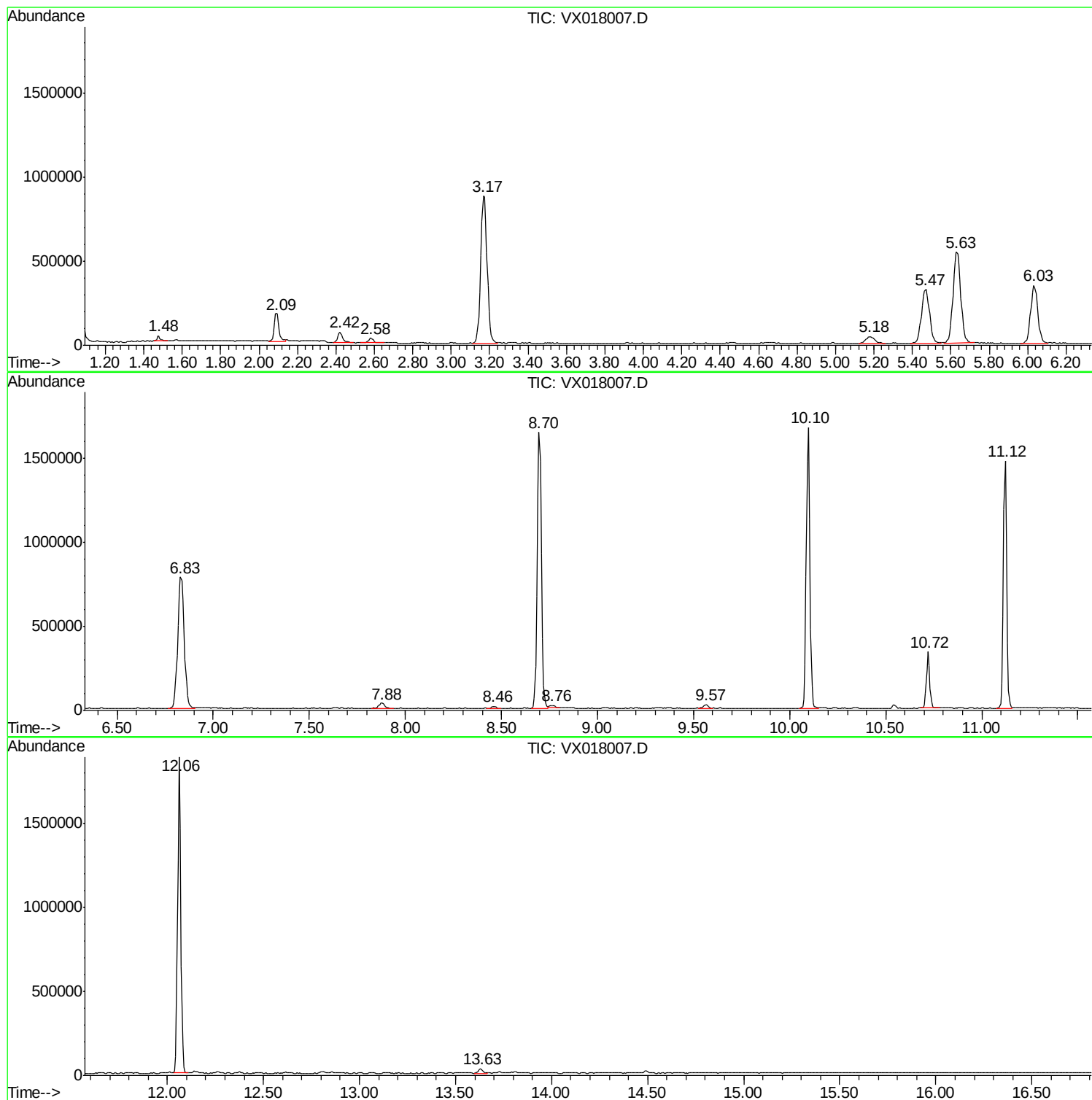
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X081920W.M  
Quant Title : SW846 8260

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



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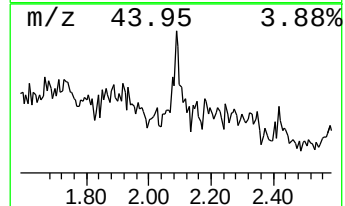
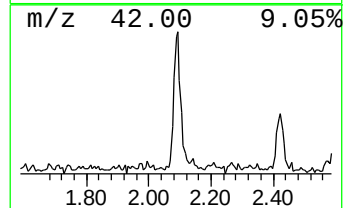
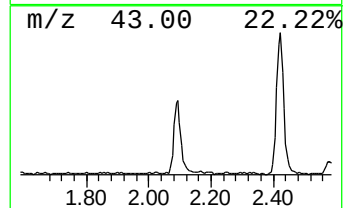
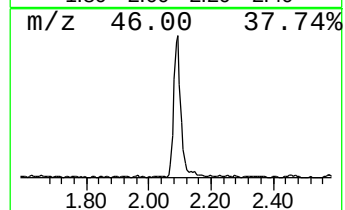
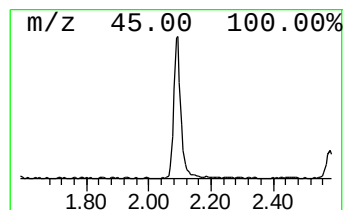
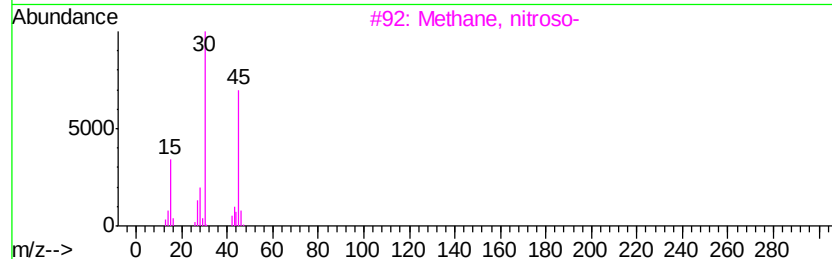
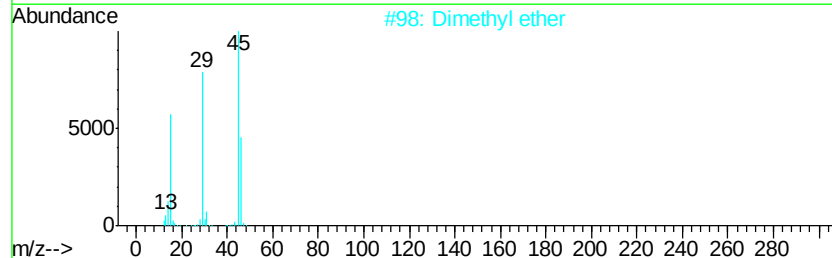
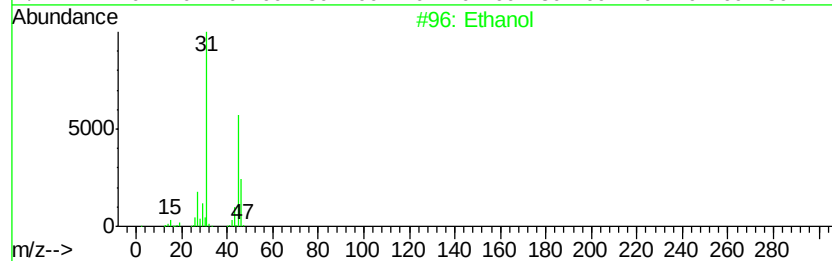
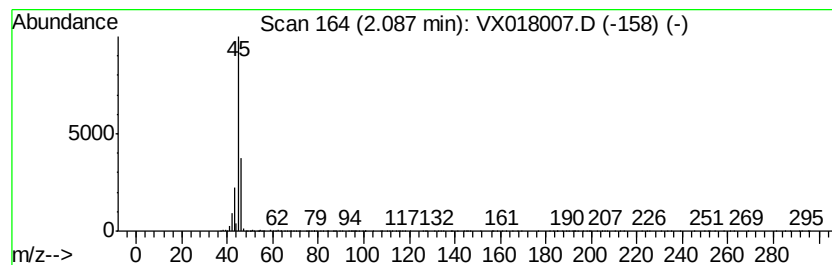
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Quant Title : SW846 8260

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

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Peak Number 1 Ethanol Concentration Rank 1

| R.T.    | EstConc           | Area         | Relative to ISTD   | R.T.    |             |      |
|---------|-------------------|--------------|--------------------|---------|-------------|------|
| 2.09    | 9.25 ug/l         | 280233       | Pentafluorobenzene | 5.64    |             |      |
| Hit# of | 5                 | Tentative ID | MW                 | MolForm | CAS#        | Qual |
| 1       | Ethanol           |              | 46                 | C2H6O   | 000064-17-5 | 64   |
| 2       | Dimethyl ether    |              | 46                 | C2H6O   | 000115-10-6 | 9    |
| 3       | Methane, nitroso- |              | 45                 | CH3NO   | 000865-40-7 | 4    |
| 4       | Formic acid       |              | 46                 | CH2O2   | 000064-18-6 | 4    |
| 5       | 4-Penten-2-ol     |              | 86                 | C5H10O  | 000625-31-0 | 4    |



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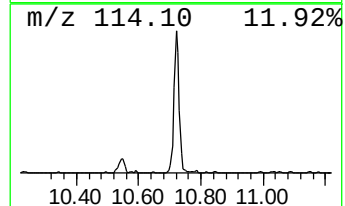
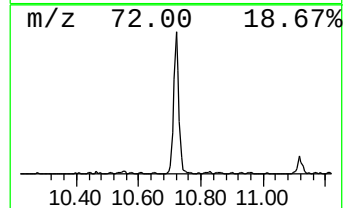
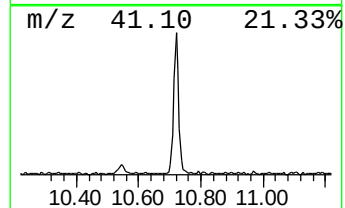
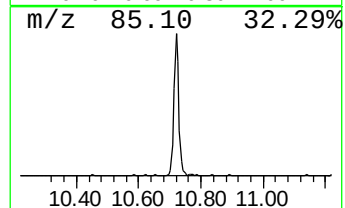
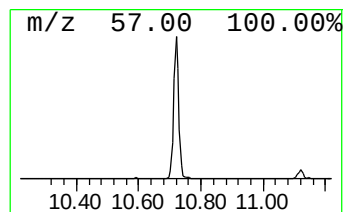
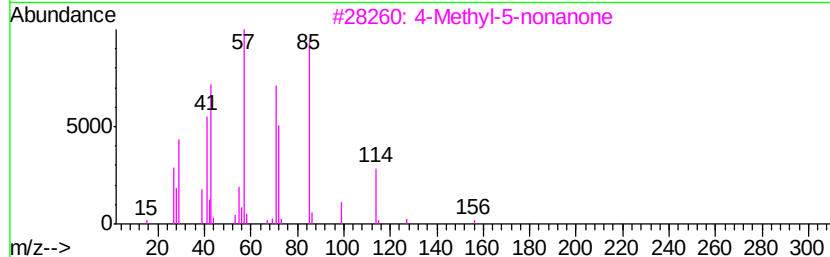
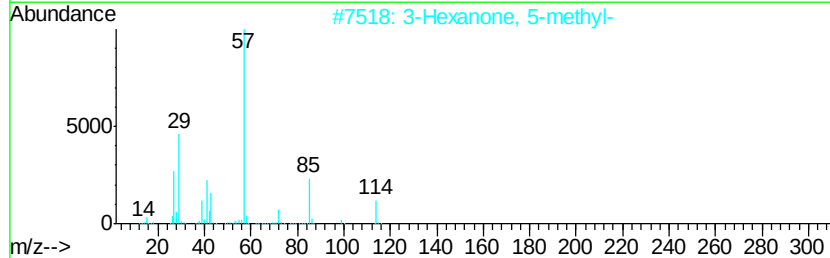
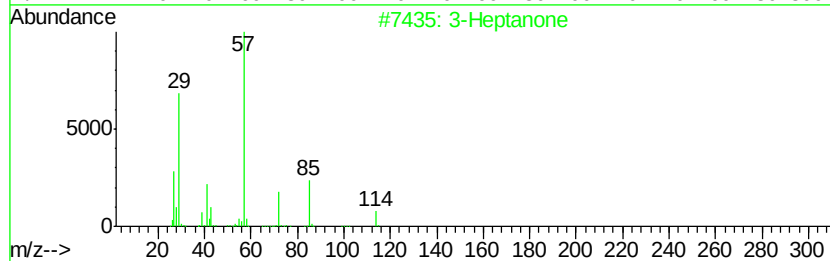
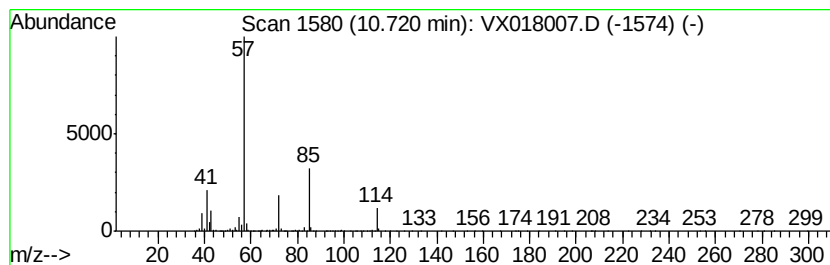
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Peak Number 2 3-Heptanone Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.  |
|-------|-----------|--------|------------------|-------|
| 10.72 | 8.92 ug/l | 396511 | Chlorobenzene-d5 | 10.10 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 3-Heptanone                         | 114 | C7H14O   | 000106-35-4 | 91   |
| 2    |    |   | 3-Hexanone, 5-methyl-               | 114 | C7H14O   | 000623-56-3 | 64   |
| 3    |    |   | 4-Methyl-5-nonanone                 | 156 | C10H20O  | 035900-26-6 | 53   |
| 4    |    |   | 2-Butanone, 1-chloro-3,3-dimethyl-  | 134 | C6H11ClO | 013547-70-1 | 53   |
| 5    |    |   | 2-Butanone, 3,3-dimethyl-1-thioc... | 157 | C7H11NOS | 057518-71-5 | 53   |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                  |       |         |       |          | #                     | RT    | Resp    | Conc |
| Ethanol          | 2.09  | 9.3     | ug/l  | 280233   | 1                     | 5.64  | 1515180 | 50.0 |
| 3-Heptanone      | 10.72 | 8.9     | ug/l  | 396511   | 3                     | 10.10 | 2221570 | 50.0 |