

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN031622\  
 Data File : VN071322.D  
 Acq On : 16 Mar 2022 16:00  
 Operator : JC\MD  
 Sample : N1886-03 10X  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 30969

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\82N030722W.M

Title : SW846 8260

Signal : TIC: VN071322.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         | 3.681       | 280           | 288         | 305          | rBV2     | 103856         | 294646        | 6.76%           | 1.099%        |
| 2         | 4.287       | 382           | 391         | 401          | rBV      | 80728          | 241322        | 5.53%           | 0.900%        |
| 3         | 4.569       | 427           | 439         | 465          | rVB2     | 45721          | 180326        | 4.13%           | 0.672%        |
| 4         | 4.857       | 476           | 488         | 500          | rBV      | 19599          | 63773         | 1.46%           | 0.238%        |
| 5         | 6.575       | 771           | 780         | 792          | rBV6     | 14758          | 55164         | 1.26%           | 0.206%        |
| 6         | 7.075       | 854           | 865         | 876          | rBV4     | 18192          | 63256         | 1.45%           | 0.236%        |
| 7         | 8.022       | 1015          | 1026        | 1030         | rBV      | 513131         | 1239575       | 28.42%          | 4.622%        |
| 8         | 8.081       | 1030          | 1036        | 1058         | rVB      | 1040466        | 2400445       | 55.04%          | 8.951%        |
| 9         | 8.434       | 1086          | 1096        | 1110         | rBV      | 607734         | 1398855       | 32.07%          | 5.216%        |
| 10        | 8.663       | 1110          | 1135        | 1137         | rBV2     | 47987          | 256473        | 5.88%           | 0.956%        |
| 11        | 8.963       | 1175          | 1186        | 1206         | rBV      | 1519833        | 3132366       | 71.82%          | 11.680%       |
| 12        | 9.157       | 1210          | 1219        | 1235         | rBV      | 455213         | 1247528       | 28.60%          | 4.652%        |
| 13        | 10.328      | 1411          | 1418        | 1428         | rBV      | 271327         | 499722        | 11.46%          | 1.863%        |
| 14        | 10.439      | 1428          | 1437        | 1445         | rBV      | 2357018        | 4361403       | 100.00%         | 16.263%       |
| 15        | 10.939      | 1514          | 1522        | 1537         | rBV      | 277777         | 535329        | 12.27%          | 1.996%        |
| 16        | 11.127      | 1550          | 1554        | 1559         | rVB      | 30536          | 51231         | 1.17%           | 0.191%        |
| 17        | 11.457      | 1604          | 1610        | 1616         | rBV      | 28547          | 46731         | 1.07%           | 0.174%        |
| 18        | 11.739      | 1648          | 1658        | 1670         | rBV      | 2184524        | 3851925       | 88.32%          | 14.363%       |
| 19        | 11.945      | 1684          | 1693        | 1703         | rVB      | 156690         | 273371        | 6.27%           | 1.019%        |
| 20        | 12.727      | 1818          | 1826        | 1835         | rBV      | 1794301        | 3040728       | 69.72%          | 11.339%       |
| 21        | 12.816      | 1836          | 1841        | 1847         | rVV      | 63264          | 108425        | 2.49%           | 0.404%        |
| 22        | 12.927      | 1855          | 1860        | 1867         | rVB3     | 31788          | 54419         | 1.25%           | 0.203%        |
| 23        | 13.668      | 1979          | 1986        | 1995         | rVV      | 1773352        | 3092481       | 70.91%          | 11.532%       |
| 24        | 13.768      | 1995          | 2003        | 2011         | rVB      | 107733         | 229677        | 5.27%           | 0.856%        |
| 25        | 14.416      | 2108          | 2113        | 2124         | rVB2     | 51024          | 98331         | 2.25%           | 0.367%        |

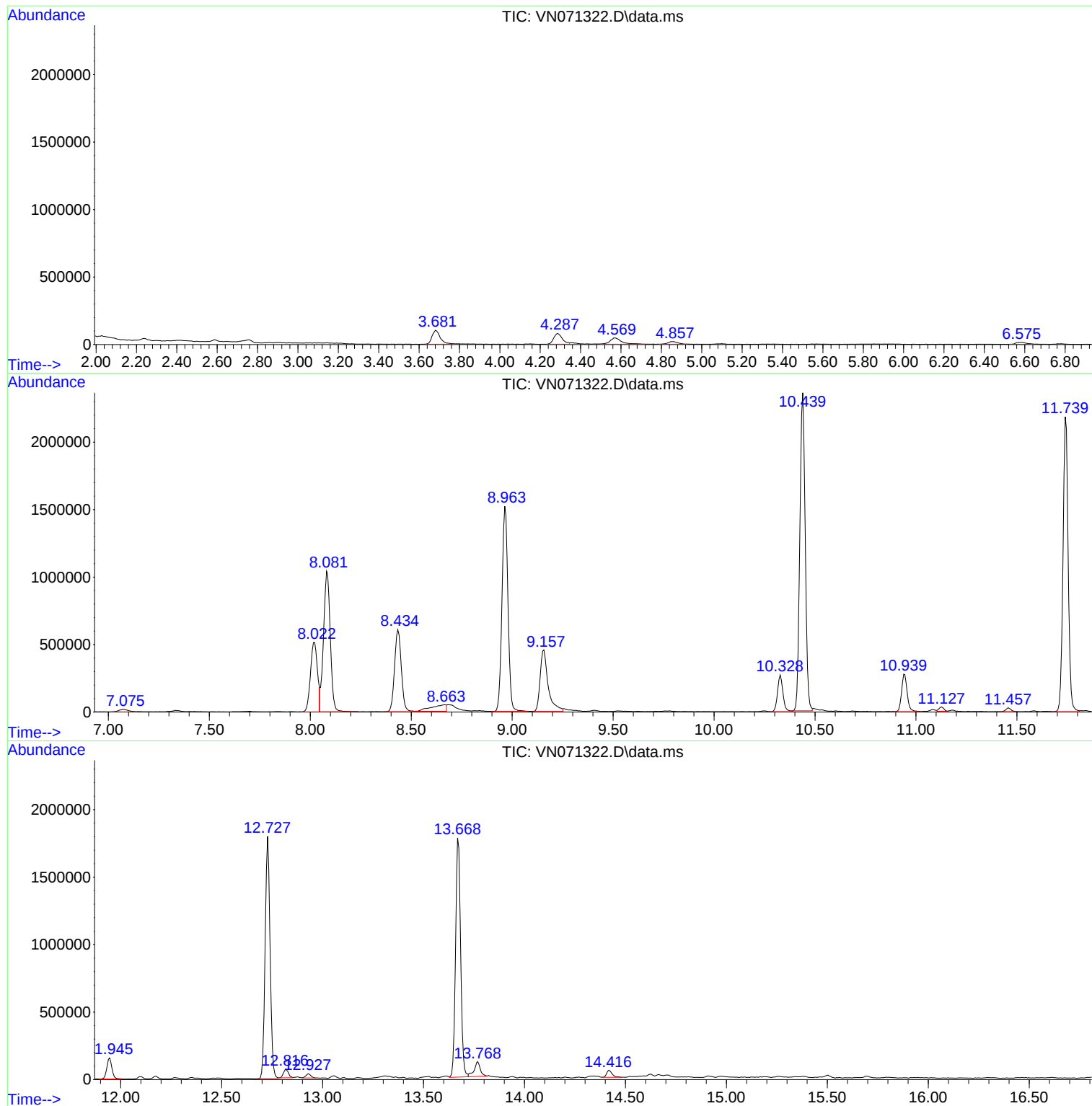
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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
30969

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N030722W.M  
Quant Title : SW846 8260

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



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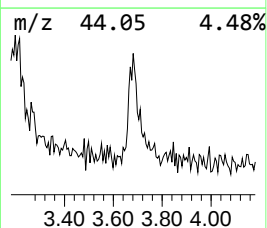
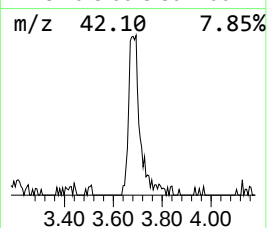
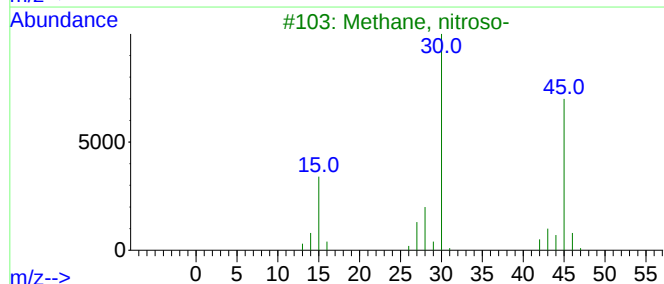
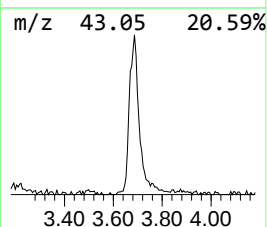
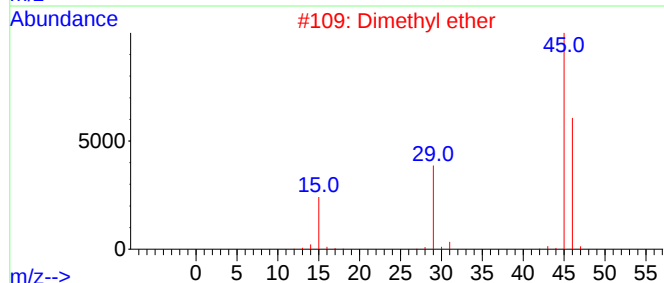
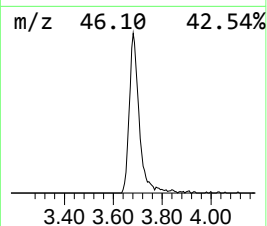
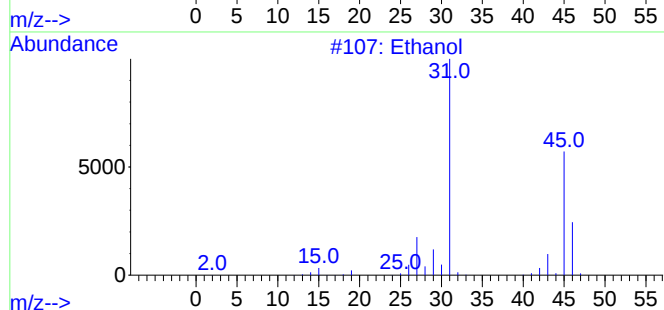
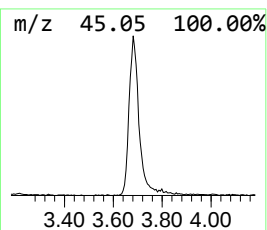
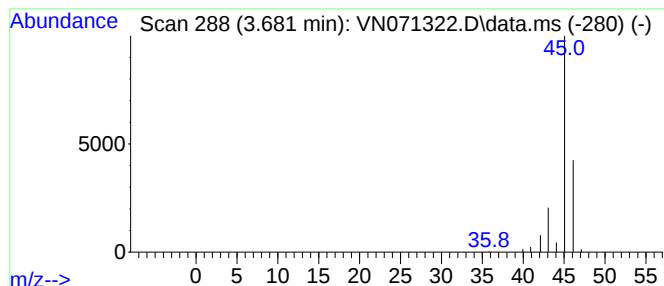
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Ethanol Concentration Rank 3

| R.T.  | EstConc   | Area   | Relative to ISTD   | R.T.  |
|-------|-----------|--------|--------------------|-------|
| 3.681 | 6.14 ug/l | 294646 | Pentafluorobenzene | 8.081 |

| Hit# | of                | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|-------------------|---|--------------|----|---------|-------------|------|
| 1    | Ethanol           |   |              | 46 | C2H6O   | 000064-17-5 | 74   |
| 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    | Oxalic acid       |   |              | 90 | C2H2O4  | 000144-62-7 | 4    |



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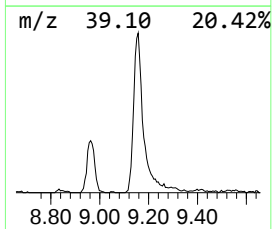
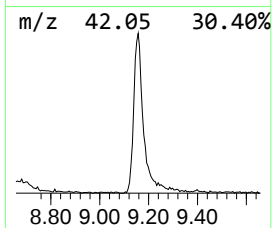
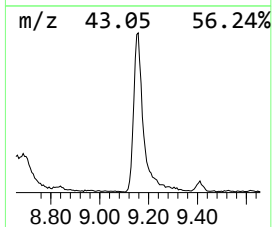
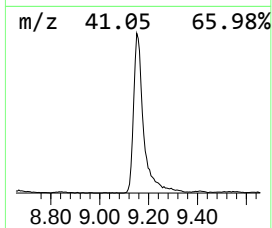
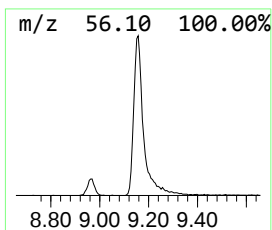
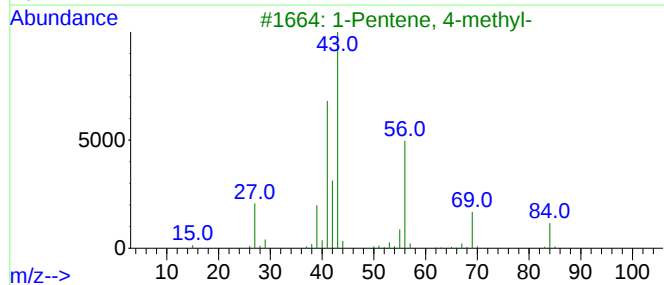
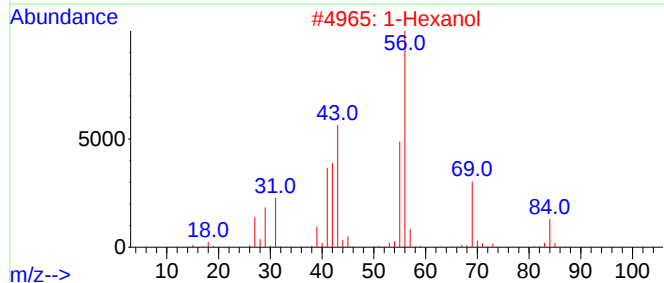
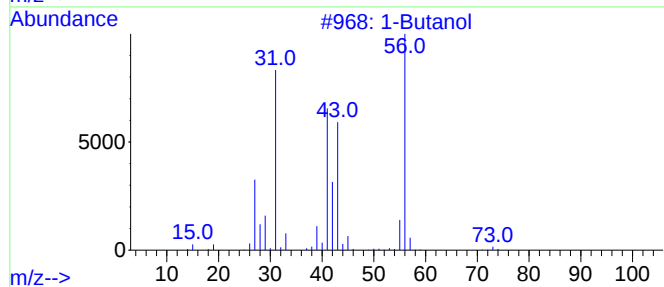
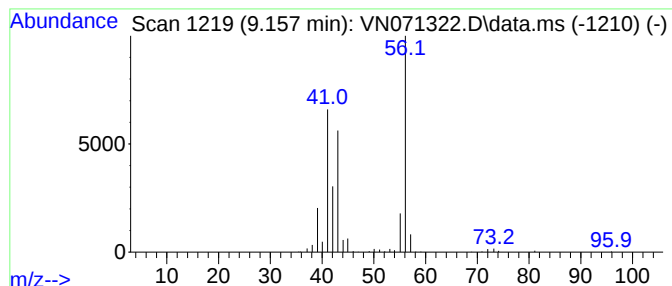
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N030722W.M  
Quant Title : SW846 8260

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

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Peak Number 2 1-Butanol Concentration Rank 1

| R.T.  | EstConc    | Area    | Relative to ISTD    | R.T.  |
|-------|------------|---------|---------------------|-------|
| 9.157 | 19.91 ug/l | 1247530 | 1,4-Difluorobenzene | 8.963 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|-------------------------------------|---|--------------|-----|---------|-------------|------|
| 1    | 1-Butanol                           |   |              | 74  | C4H10O  | 000071-36-3 | 86   |
| 2    | 1-Hexanol                           |   |              | 102 | C6H14O  | 000111-27-3 | 40   |
| 3    | 1-Pentene, 4-methyl-                |   |              | 84  | C6H12   | 000691-37-2 | 40   |
| 4    | 2H-Pyran-2-one, tetrahydro-5,6-d... |   |              | 128 | C7H12O2 | 024405-16-1 | 36   |
| 5    | Hydroperoxide, hexyl                |   |              | 118 | C6H14O2 | 004312-76-9 | 23   |



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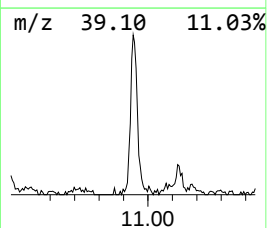
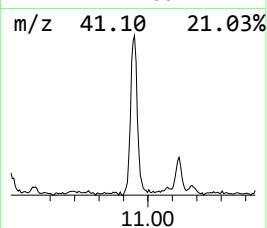
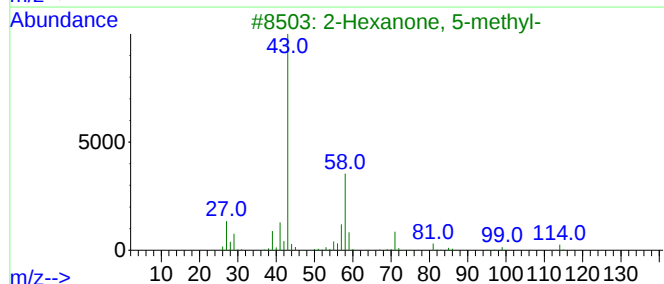
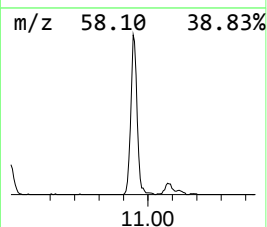
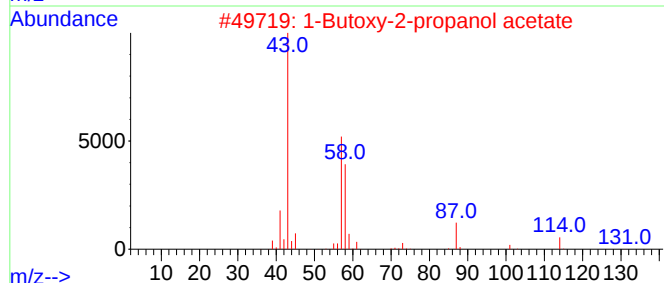
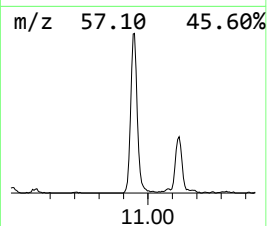
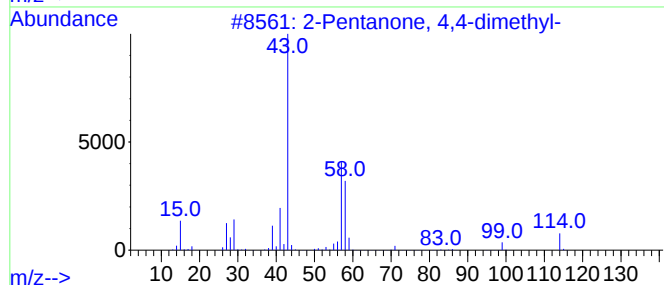
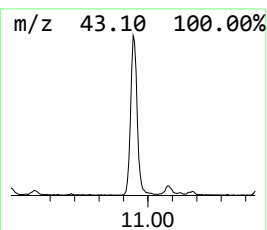
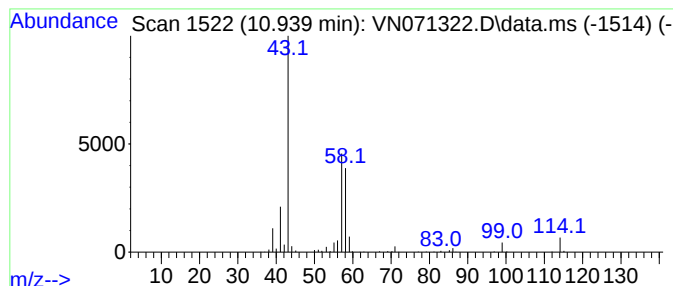
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TIC Integration Parameters: LSCINT.P

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

| R.T.   | EstConc   | Area   | Relative to ISTD | R.T.   |
|--------|-----------|--------|------------------|--------|
| 10.939 | 6.95 ug/l | 535329 | Chlorobenzene-d5 | 11.739 |

| Hit# | of                          | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-----------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4,4-dimethyl-  | 114 | C7H14O       | 000590-50-1 | 91      |      |      |
| 2    | 1-Butoxy-2-propanol acetate | 174 | C9H18O3      | 085409-76-3 | 72      |      |      |
| 3    | 2-Hexanone, 5-methyl-       | 114 | C7H14O       | 000110-12-3 | 64      |      |      |
| 4    | 2-Heptanone                 | 114 | C7H14O       | 000110-43-0 | 59      |      |      |
| 5    | 2-Hexanone, 4-methyl-       | 114 | C7H14O       | 000105-42-0 | 53      |      |      |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Ethanol            | 3.681  | 6.1     | ug/l  | 294646   | 1                     | 8.081  | 2400450 | 50.0 |
| 1-Butanol          | 9.157  | 19.9    | ug/l  | 1247530  | 2                     | 8.963  | 3132370 | 50.0 |
| 2-Pentanone, 4,... | 10.939 | 7.0     | ug/l  | 535329   | 3                     | 11.739 | 3851930 | 50.0 |