

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120722\  
 Data File : VX033302.D  
 Acq On : 07 Dec 2022 23:24  
 Operator : JC/MD  
 Sample : N5906-05  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 33 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 H-3R

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\_X\Method\82X120722W.M  
 Title : SW846 8260

Signal : TIC: VX033302.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         | 2.343       | 199           | 206         | 217          | rBV      | 15253          | 31226         | 4.96%           | 0.730%        |
| 2         | 2.782       | 271           | 278         | 286          | rBV2     | 5185           | 11748         | 1.86%           | 0.275%        |
| 3         | 2.977       | 300           | 310         | 323          | rBV2     | 7851           | 26174         | 4.15%           | 0.612%        |
| 4         | 3.111       | 323           | 332         | 346          | rVB      | 155159         | 355884        | 56.49%          | 8.316%        |
| 5         | 3.764       | 431           | 439         | 447          | rBV3     | 3476           | 9211          | 1.46%           | 0.215%        |
| 6         | 5.385       | 694           | 705         | 721          | rBV      | 56779          | 166727        | 26.47%          | 3.896%        |
| 7         | 5.556       | 721           | 733         | 747          | rVV      | 144929         | 411237        | 65.28%          | 9.609%        |
| 8         | 5.958       | 790           | 799         | 814          | rBV2     | 45020          | 119221        | 18.93%          | 2.786%        |
| 9         | 6.245       | 835           | 846         | 869          | rBV      | 80062          | 255904        | 40.62%          | 5.980%        |
| 10        | 6.763       | 919           | 931         | 944          | rBV      | 219027         | 518263        | 82.27%          | 12.110%       |
| 11        | 7.988       | 1125          | 1132        | 1139         | rBV2     | 4779           | 10085         | 1.60%           | 0.236%        |
| 12        | 8.104       | 1145          | 1151        | 1157         | rBV5     | 7794           | 17195         | 2.73%           | 0.402%        |
| 13        | 8.427       | 1198          | 1204        | 1211         | rBV      | 29922          | 52724         | 8.37%           | 1.232%        |
| 14        | 8.507       | 1211          | 1217        | 1229         | rVV      | 64384          | 111297        | 17.67%          | 2.601%        |
| 15        | 8.653       | 1232          | 1241        | 1250         | rVB      | 174783         | 280563        | 44.54%          | 6.556%        |
| 16        | 8.842       | 1265          | 1272        | 1281         | rBV      | 62673          | 101315        | 16.08%          | 2.367%        |
| 17        | 8.958       | 1283          | 1291        | 1298         | rVV3     | 13170          | 23434         | 3.72%           | 0.548%        |
| 18        | 9.049       | 1300          | 1306        | 1314         | rVB      | 13908          | 21849         | 3.47%           | 0.511%        |
| 19        | 9.165       | 1319          | 1325        | 1334         | rVB2     | 7374           | 11595         | 1.84%           | 0.271%        |
| 20        | 9.445       | 1364          | 1371        | 1376         | rBV5     | 6444           | 12183         | 1.93%           | 0.285%        |
| 21        | 9.573       | 1386          | 1392        | 1401         | rVB4     | 10178          | 17508         | 2.78%           | 0.409%        |
| 22        | 10.055      | 1459          | 1471        | 1477         | rBV      | 448512         | 629951        | 100.00%         | 14.720%       |
| 23        | 10.104      | 1477          | 1479        | 1482         | rVV2     | 6166           | 8063          | 1.28%           | 0.188%        |
| 24        | 10.147      | 1482          | 1486        | 1492         | rVB      | 27435          | 37593         | 5.97%           | 0.878%        |
| 25        | 10.250      | 1497          | 1503        | 1507         | rBV4     | 5824           | 11792         | 1.87%           | 0.276%        |
| 26        | 11.079      | 1634          | 1639        | 1649         | rBV      | 308629         | 402781        | 63.94%          | 9.412%        |
| 27        | 11.274      | 1667          | 1671        | 1675         | rBV2     | 6000           | 8156          | 1.29%           | 0.191%        |
| 28        | 12.024      | 1788          | 1794        | 1803         | rBV      | 440043         | 560533        | 88.98%          | 13.098%       |
| 29        | 12.317      | 1838          | 1842        | 1850         | rVB      | 8089           | 10456         | 1.66%           | 0.244%        |
| 30        | 13.036      | 1954          | 1960        | 1964         | rBV      | 6195           | 7827          | 1.24%           | 0.183%        |
| 31        | 13.195      | 1979          | 1986        | 1990         | rBV2     | 6428           | 8079          | 1.28%           | 0.189%        |
| 32        | 13.622      | 2052          | 2056        | 2058         | rBV2     | 5870           | 8342          | 1.32%           | 0.195%        |
| 33        | 14.597      | 2211          | 2216        | 2220         | rBV      | 8287           | 10911         | 1.73%           | 0.255%        |
| 34        | 14.786      | 2242          | 2247        | 2251         | rBV2     | 6160           | 9840          | 1.56%           | 0.230%        |

Sum of corrected areas: 4279667

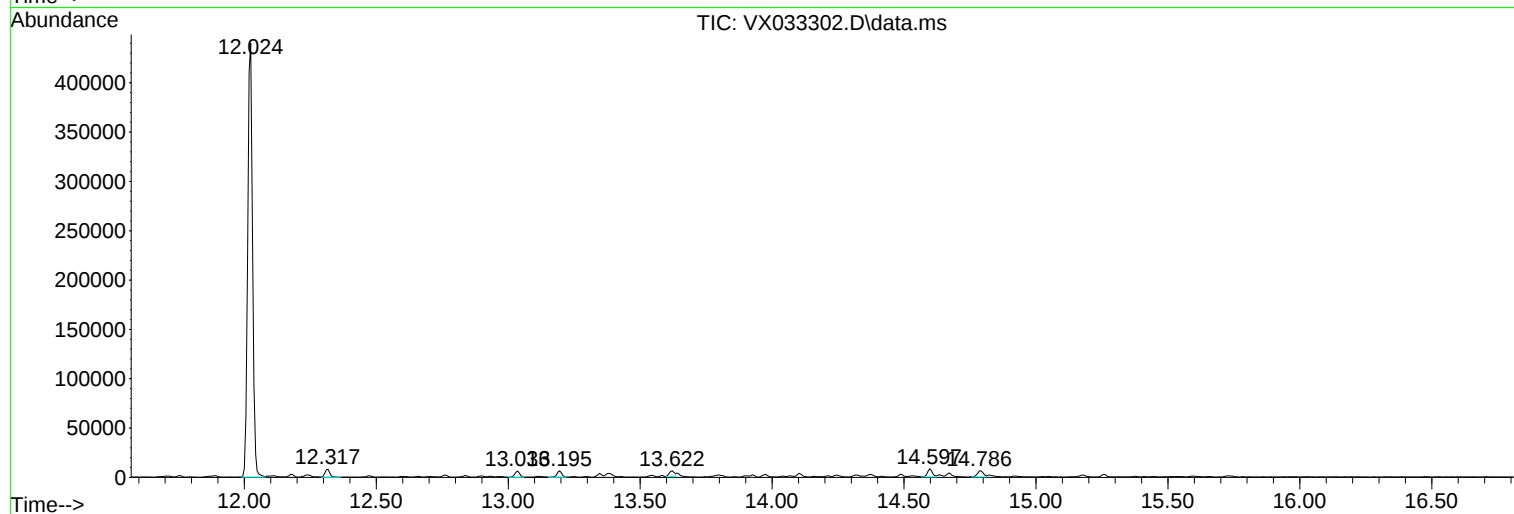
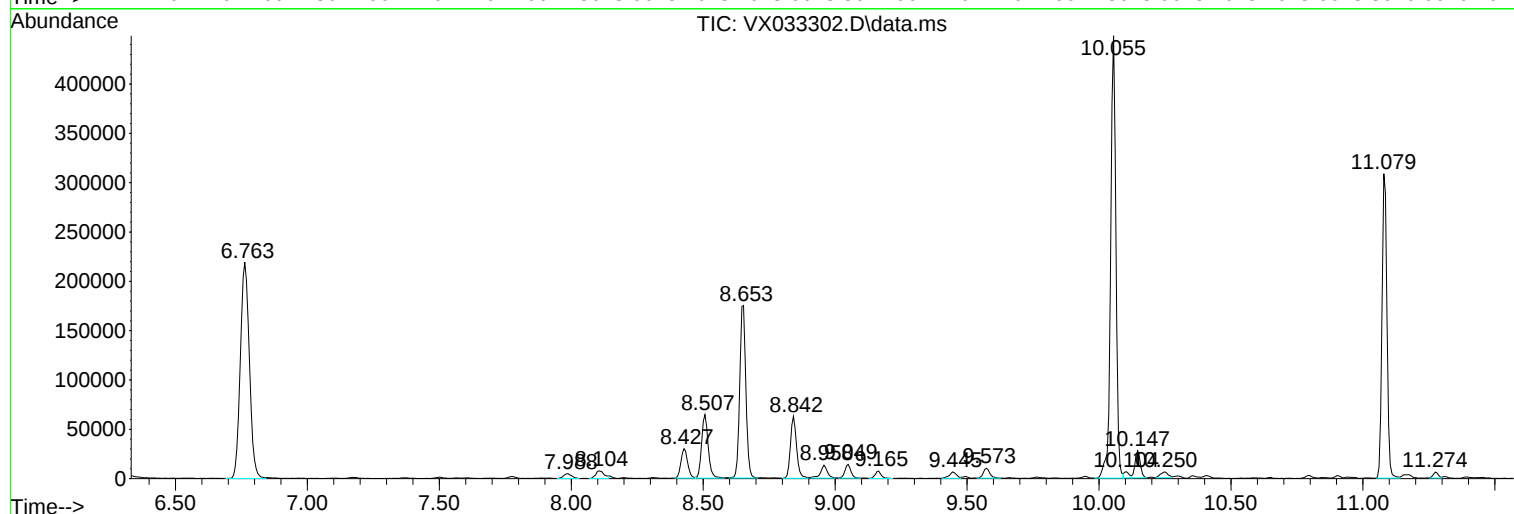
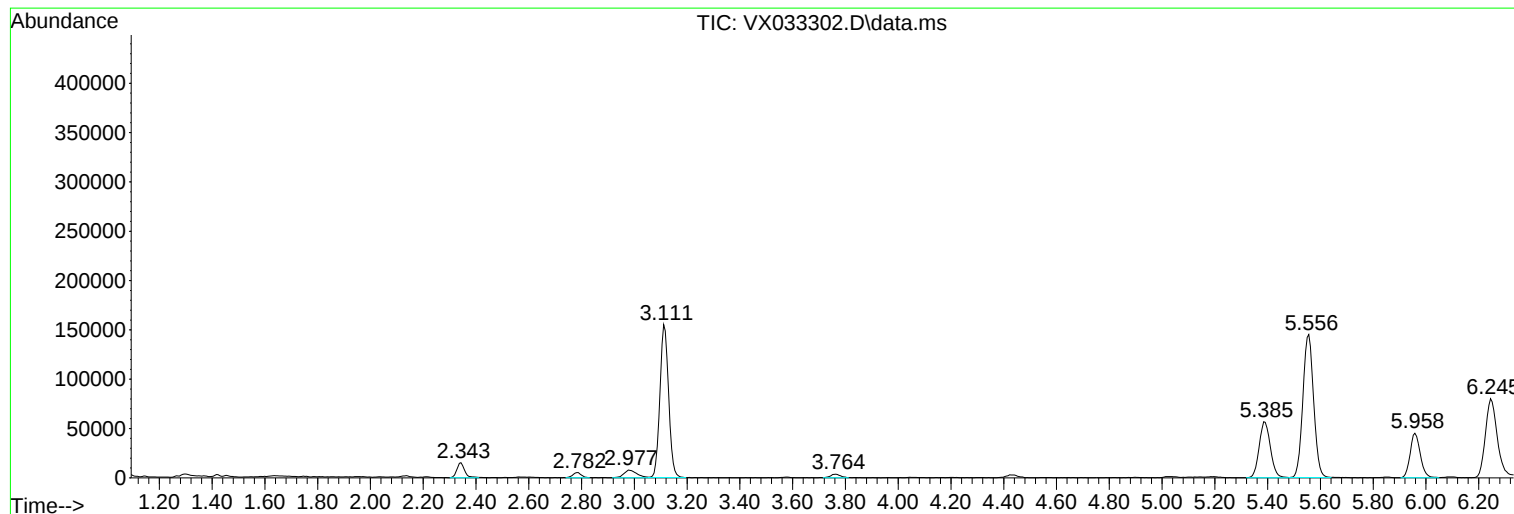
**Instrument :**  
MSVOA\_X  
**ClientSampleId :**  
H-3R

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120722\  
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ALS Vial : 33 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
H-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X120722W.M  
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX120722\  
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Operator : JC/MD  
Sample : N5906-05  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 33 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
H-3R

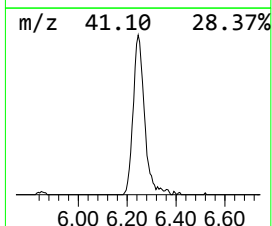
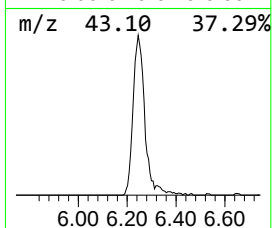
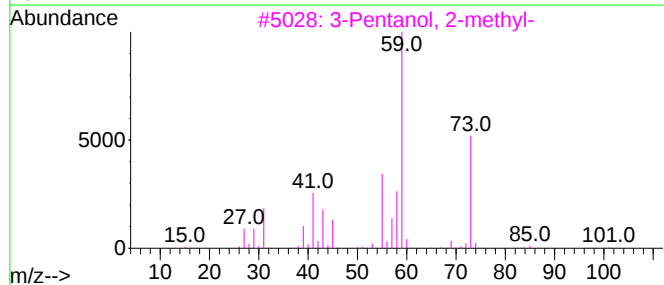
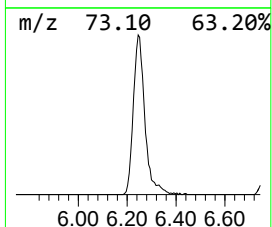
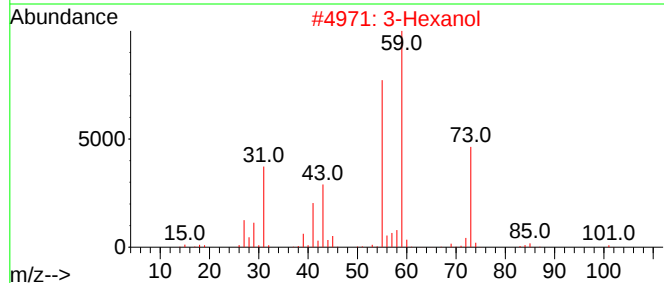
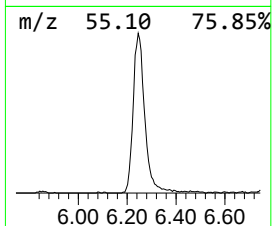
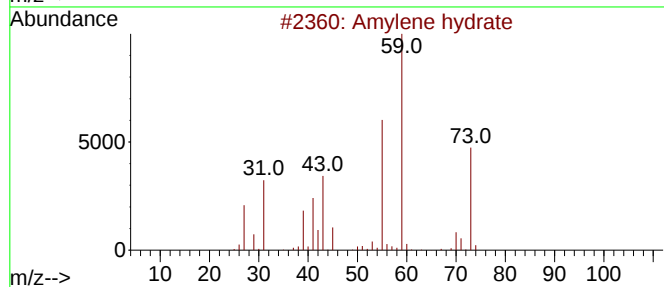
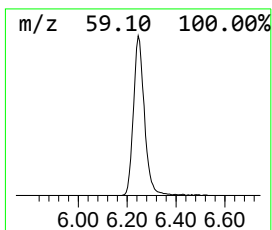
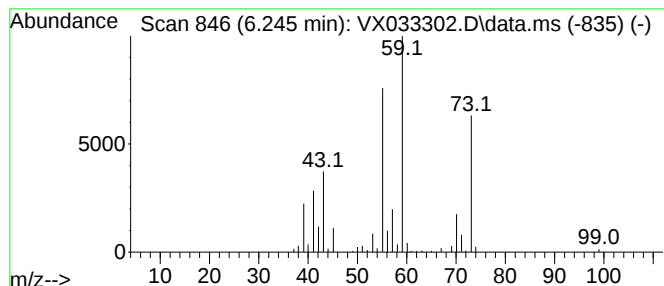
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X120722W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Amylene hydrate Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 6.245 | 24.69 ug/l | 255904 | 1,4-Difluorobenzene | 6.763 |

| Hit# | of 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|------|---------------------------|-----|---------|-------------|------|
| 1    |      | Amylene hydrate           | 88  | C5H12O  | 000075-85-4 | 78   |
| 2    |      | 3-Hexanol                 | 102 | C6H14O  | 000623-37-0 | 50   |
| 3    |      | 3-Pentanol, 2-methyl-     | 102 | C6H14O  | 000565-67-3 | 42   |
| 4    |      | HEX-5-EN-3-OL             | 100 | C6H12O  | 000688-99-3 | 38   |
| 5    |      | Propanenitrile, 3-ethoxy- | 99  | C5H9NO  | 002141-62-0 | 28   |



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ALS Vial : 33 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
H-3R

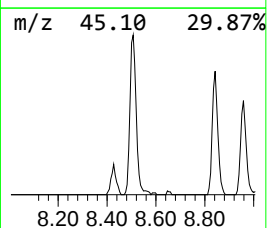
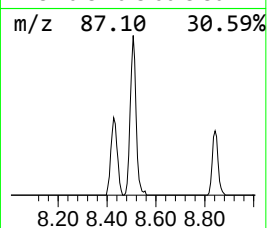
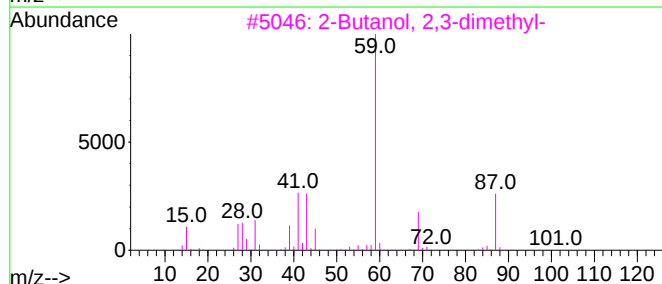
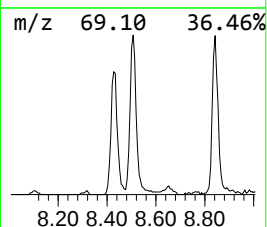
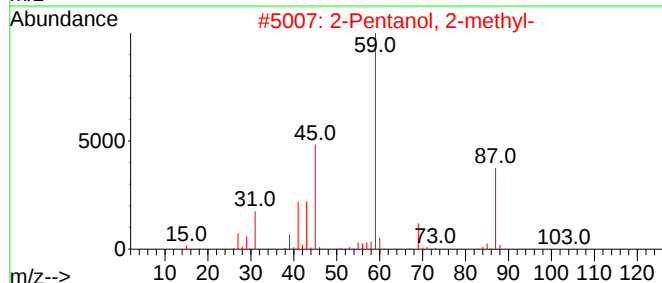
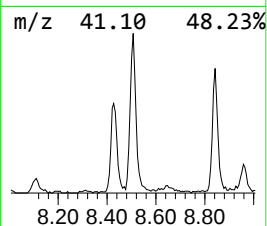
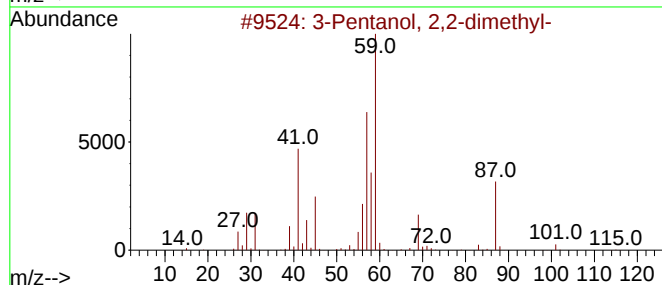
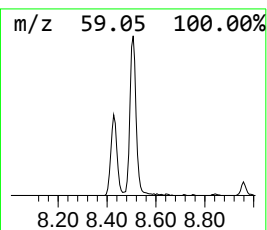
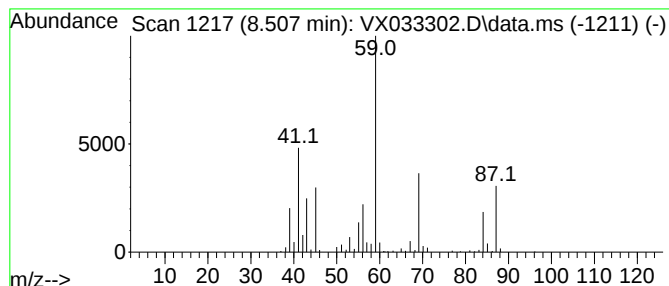
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X120722W.M  
Quant Title : SW846 8260

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

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Peak Number 2 3-Pentanol, 2,2-dimethyl- Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.   |
|-------|-----------|--------|------------------|--------|
| 8.507 | 8.83 ug/l | 111297 | Chlorobenzene-d5 | 10.055 |

| Hit# | of 5 | Tentative ID                      | MW  | MolForm | CAS#        | Qual |
|------|------|-----------------------------------|-----|---------|-------------|------|
| 1    |      | 3-Pentanol, 2,2-dimethyl-         | 116 | C7H16O  | 003970-62-5 | 78   |
| 2    |      | 2-Pentanol, 2-methyl-             | 102 | C6H14O  | 000590-36-3 | 72   |
| 3    |      | 2-Butanol, 2,3-dimethyl-          | 102 | C6H14O  | 000594-60-5 | 53   |
| 4    |      | 2-Hydroxy-2-methylhept-6-en-3-one | 142 | C8H14O2 | 000996-61-2 | 38   |
| 5    |      | 3-Hexanol, 4-methyl-              | 116 | C7H16O  | 000615-29-2 | 38   |



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Sample : N5906-05  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 33 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
H-3R

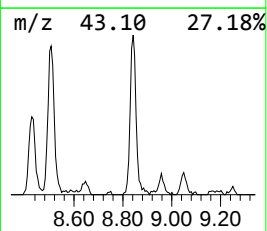
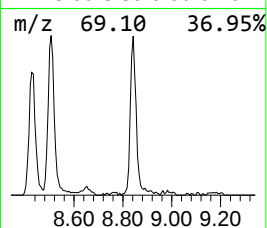
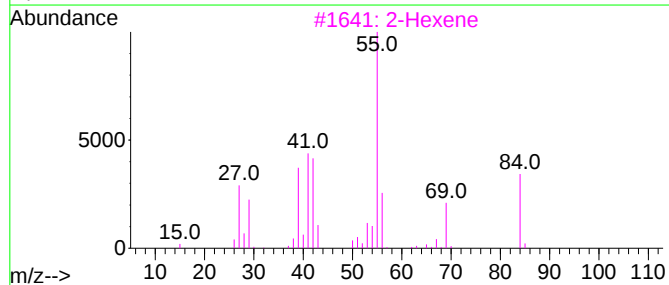
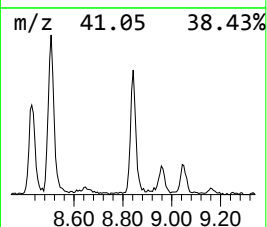
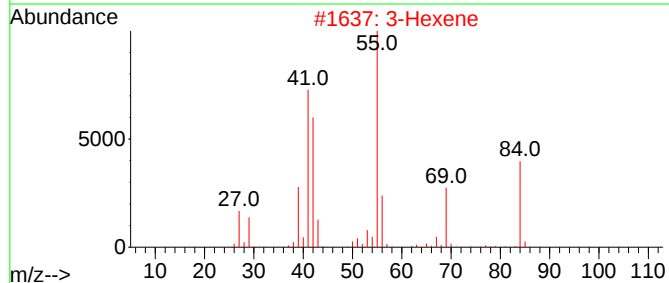
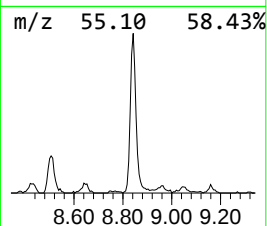
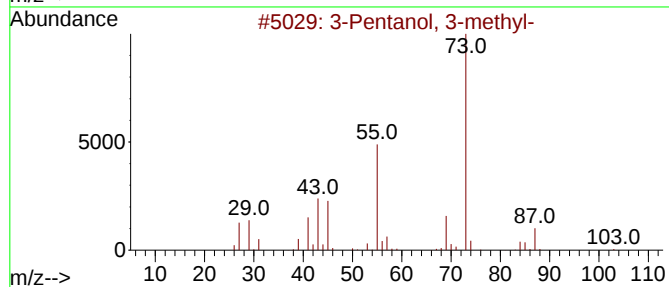
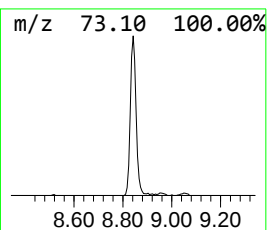
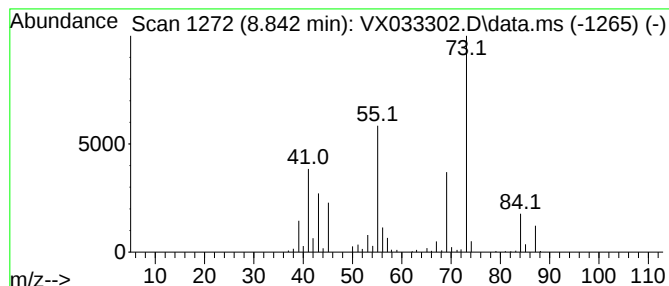
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X120722W.M  
Quant Title : SW846 8260

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

\*\*\*\*\*  
Peak Number 3 3-Pentanol, 3-methyl- Concentration Rank 3

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.   |
|-------|-----------|--------|------------------|--------|
| 8.842 | 8.04 ug/l | 101315 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID             | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------|-----|---------|-------------|------|
| 1    |    |   | 3-Pentanol, 3-methyl-    | 102 | C6H14O  | 000077-74-7 | 78   |
| 2    |    |   | 3-Hexene                 | 84  | C6H12   | 000592-47-2 | 27   |
| 3    |    |   | 2-Hexene                 | 84  | C6H12   | 000592-43-8 | 27   |
| 4    |    |   | 3-Hexene, (Z)-           | 84  | C6H12   | 007642-09-3 | 27   |
| 5    |    |   | Methane, isothiocyanato- | 73  | C2H3NS  | 000556-61-6 | 25   |



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ALS Vial : 33 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
H-3R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X120722W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |       |         |       |          | #                     | RT     | Resp   | Conc |
| Amylene hydrate    | 6.245 | 24.7    | ug/l  | 255904   | 2                     | 6.763  | 518263 | 50.0 |
| 3-Pentanol, 2,2... | 8.507 | 8.8     | ug/l  | 111297   | 3                     | 10.055 | 629951 | 50.0 |
| 3-Pentanol, 3-m... | 8.842 | 8.0     | ug/l  | 101315   | 3                     | 10.055 | 629951 | 50.0 |