

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX072922\  
 Data File : VX030305.D  
 Acq On : 29 Jul 2022 16:09  
 Operator : JC/MD  
 Sample : N3861-08  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 MW-16R

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\82X072522W.M  
 Title : SW846 8260

Signal : TIC: VX030305.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         | 1.227       | 19            | 23          | 27           | rBV2     | 10716          | 15614         | 1.23%           | 0.241%        |
| 2         | 1.368       | 42            | 46          | 50           | rBV      | 32292          | 37923         | 3.00%           | 0.585%        |
| 3         | 1.746       | 103           | 108         | 118          | rVB      | 58245          | 80863         | 6.40%           | 1.248%        |
| 4         | 2.544       | 229           | 239         | 248          | rBV      | 21028          | 41030         | 3.25%           | 0.633%        |
| 5         | 2.782       | 268           | 278         | 284          | rBV      | 27555          | 64567         | 5.11%           | 0.996%        |
| 6         | 2.867       | 287           | 292         | 303          | rVB      | 43980          | 90856         | 7.19%           | 1.402%        |
| 7         | 3.105       | 321           | 331         | 340          | rBV      | 13776          | 31437         | 2.49%           | 0.485%        |
| 8         | 4.306       | 518           | 528         | 539          | rVB2     | 38431          | 110249        | 8.72%           | 1.701%        |
| 9         | 5.391       | 693           | 706         | 715          | rBV      | 141148         | 408444        | 32.31%          | 6.301%        |
| 10        | 5.470       | 715           | 719         | 725          | rVV3     | 19880          | 57972         | 4.59%           | 0.894%        |
| 11        | 5.562       | 725           | 734         | 758          | rVB      | 155761         | 480689        | 38.02%          | 7.416%        |
| 12        | 5.842       | 772           | 780         | 790          | rBV6     | 4446           | 13284         | 1.05%           | 0.205%        |
| 13        | 5.958       | 790           | 799         | 812          | rBV      | 170449         | 449764        | 35.57%          | 6.939%        |
| 14        | 6.257       | 840           | 848         | 857          | rVB4     | 8402           | 24732         | 1.96%           | 0.382%        |
| 15        | 6.367       | 857           | 866         | 877          | rVB5     | 9667           | 28067         | 2.22%           | 0.433%        |
| 16        | 6.769       | 922           | 932         | 944          | rBV      | 257916         | 624973        | 49.43%          | 9.642%        |
| 17        | 7.366       | 1022          | 1030        | 1041         | rVB4     | 19499          | 58565         | 4.63%           | 0.904%        |
| 18        | 7.994       | 1122          | 1133        | 1138         | rVB4     | 6613           | 15386         | 1.22%           | 0.237%        |
| 19        | 8.110       | 1142          | 1152        | 1156         | rBV2     | 18129          | 39476         | 3.12%           | 0.609%        |
| 20        | 8.653       | 1226          | 1241        | 1255         | rBV      | 811637         | 1264322       | 100.00%         | 19.506%       |
| 21        | 9.165       | 1320          | 1325        | 1335         | rVB2     | 12852          | 19016         | 1.50%           | 0.293%        |
| 22        | 10.055      | 1465          | 1471        | 1479         | rBV      | 578862         | 799074        | 63.20%          | 12.328%       |
| 23        | 11.085      | 1634          | 1640        | 1656         | rVB      | 611335         | 774959        | 61.29%          | 11.956%       |
| 24        | 12.024      | 1789          | 1794        | 1803         | rBV      | 802688         | 933989        | 73.87%          | 14.409%       |
| 25        | 12.250      | 1823          | 1831        | 1835         | rBV6     | 8324           | 16562         | 1.31%           | 0.256%        |

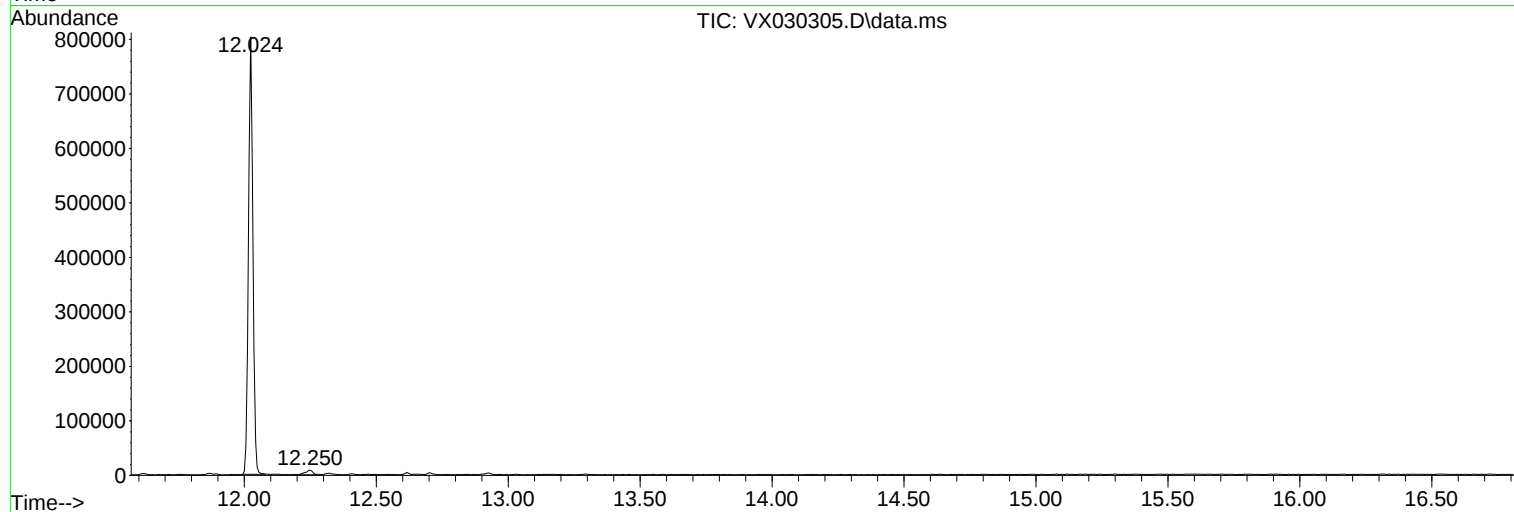
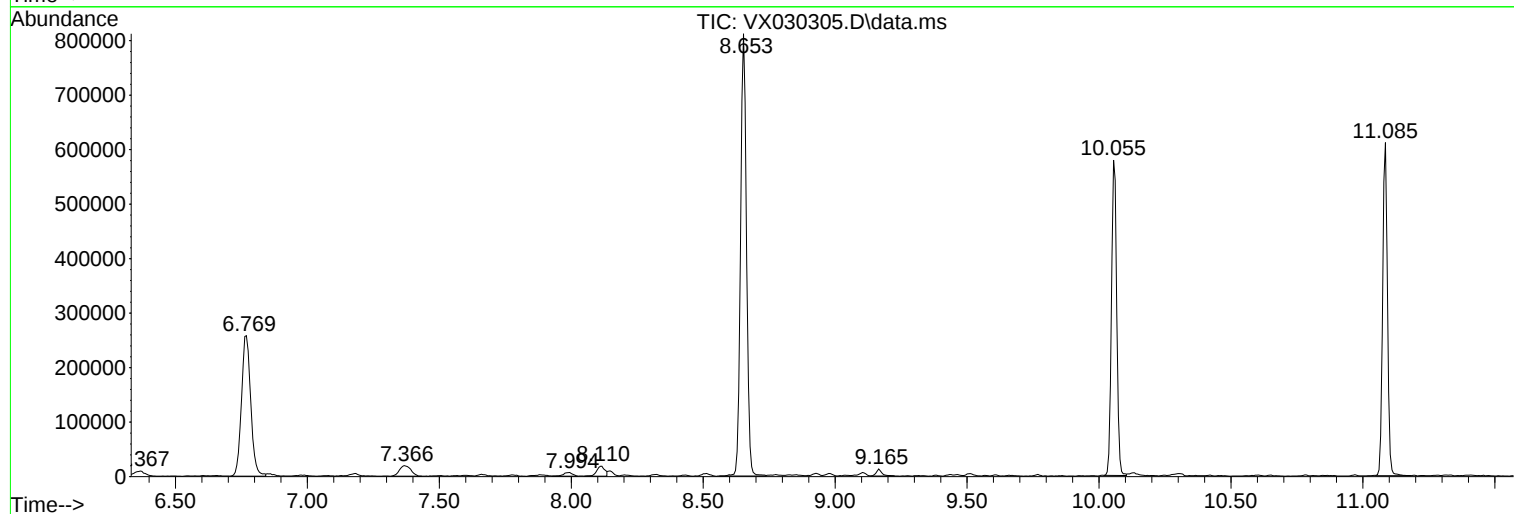
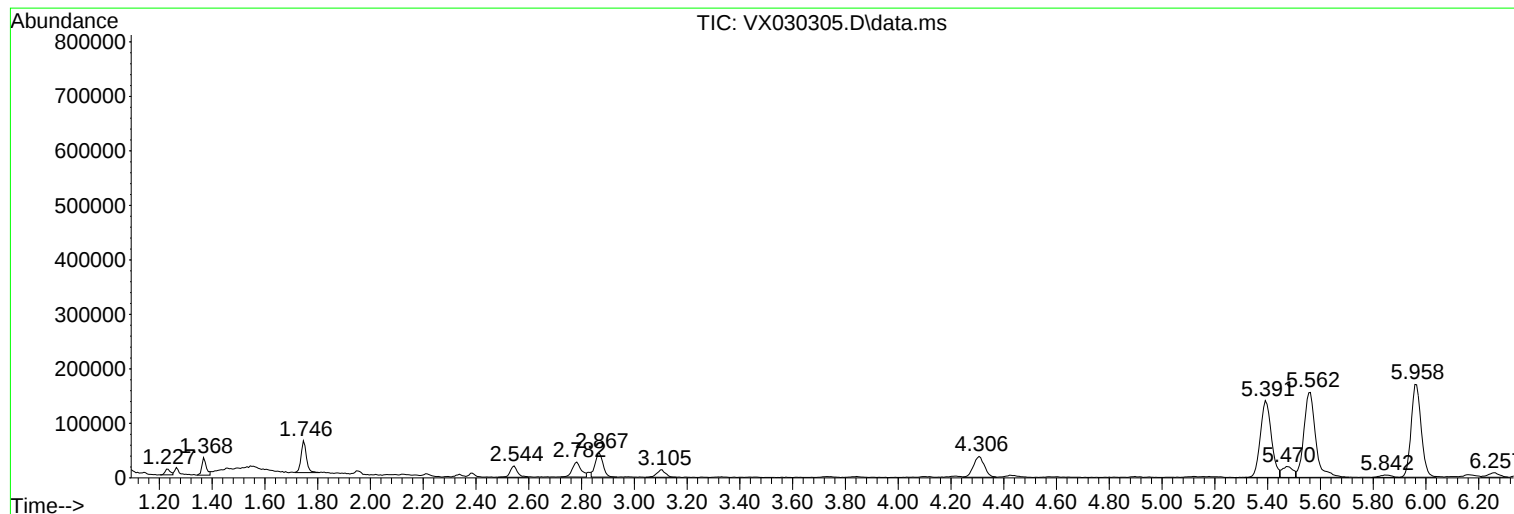
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ALS Vial : 17 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-16R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X072522W.M  
Quant Title : SW846 8260

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



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Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-16R

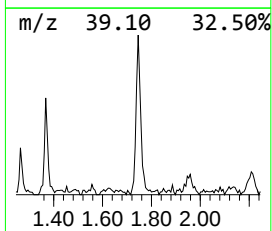
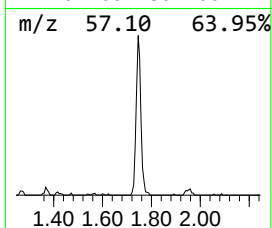
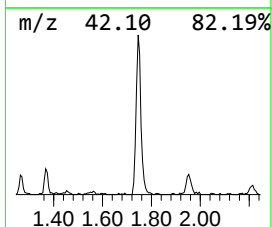
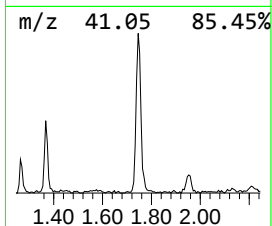
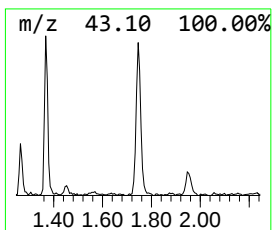
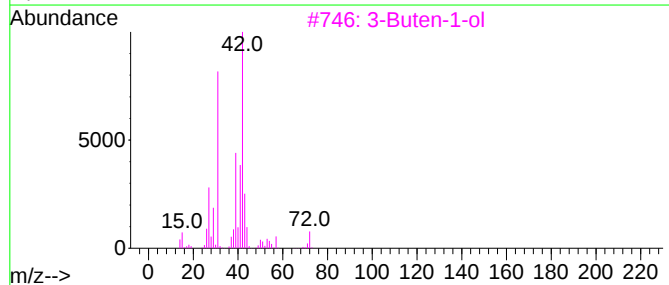
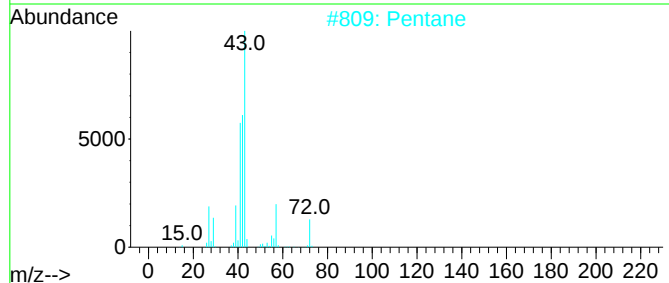
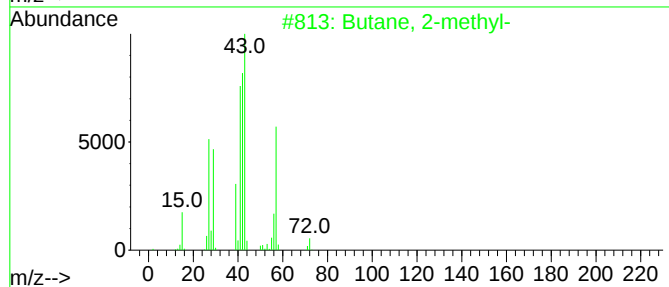
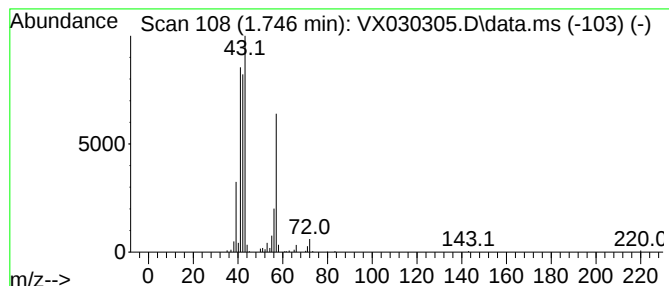
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X072522W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Butane, 2-methyl- Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 1.746 | 8.41 ug/l | 80863 | Pentafluorobenzene | 5.562 |

| Hit# | of | 5 | Tentative ID           | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methyl-      | 72  | C5H12   | 000078-78-4 | 90   |
| 2    |    |   | Pentane                | 72  | C5H12   | 000109-66-0 | 33   |
| 3    |    |   | 3-Buten-1-ol           | 72  | C4H8O   | 000627-27-0 | 25   |
| 4    |    |   | 1-Pentene, 4-methyl-   | 84  | C6H12   | 000691-37-2 | 12   |
| 5    |    |   | 2-Pentanone, 3-methyl- | 100 | C6H12O  | 000565-61-7 | 10   |



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Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-16R

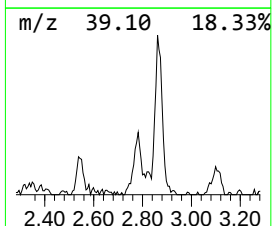
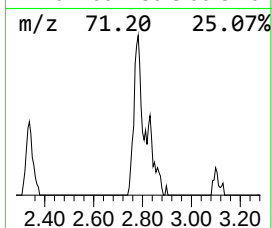
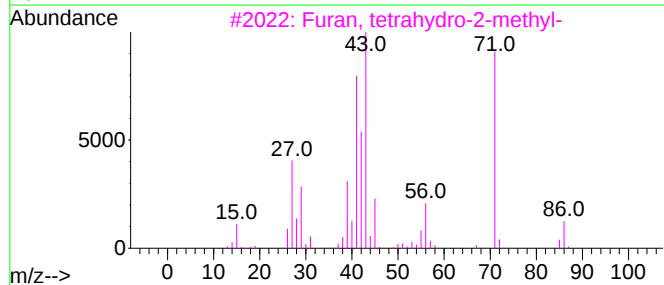
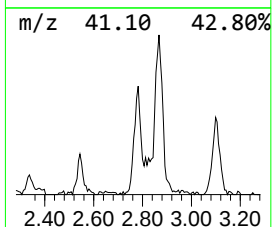
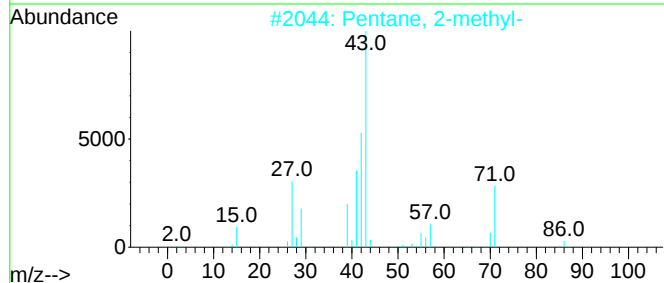
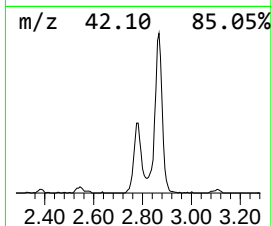
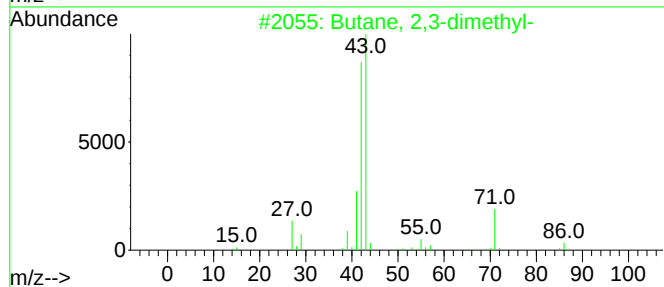
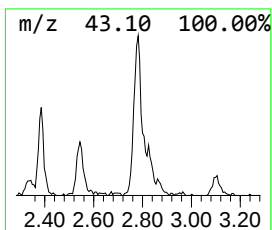
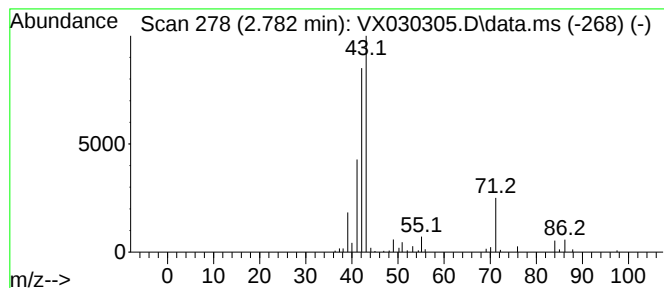
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X072522W.M  
Quant Title : SW846 8260

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

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

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 2.782 | 6.72 ug/l | 64567 | Pentafluorobenzene | 5.562 |

| Hit# | of 5 | Tentative ID                    | MW  | MolForm | CAS#        | Qual |
|------|------|---------------------------------|-----|---------|-------------|------|
| 1    |      | Butane, 2,3-dimethyl-           | 86  | C6H14   | 000079-29-8 | 80   |
| 2    |      | Pentane, 2-methyl-              | 86  | C6H14   | 000107-83-5 | 17   |
| 3    |      | Furan, tetrahydro-2-methyl-     | 86  | C5H10O  | 000096-47-9 | 10   |
| 4    |      | 4-Penten-2-one                  | 84  | C5H8O   | 013891-87-7 | 9    |
| 5    |      | 2-Furanmethanamine, tetrahydro- | 101 | C5H11NO | 004795-29-3 | 9    |



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Sample : N3861-08  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-16R

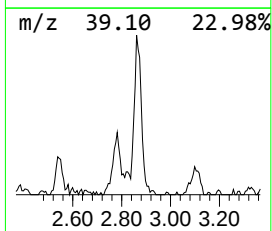
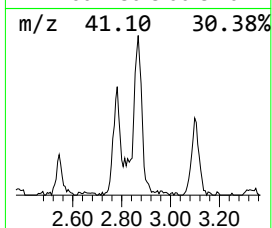
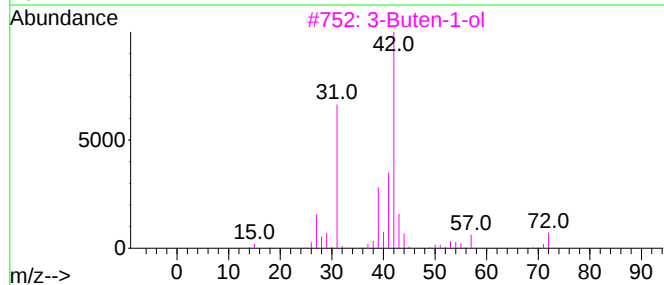
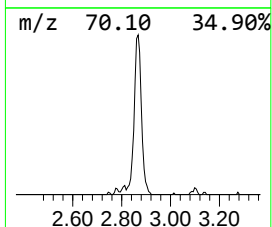
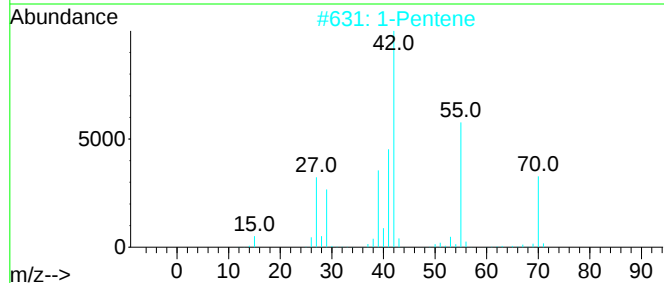
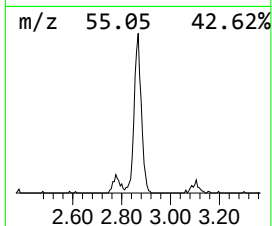
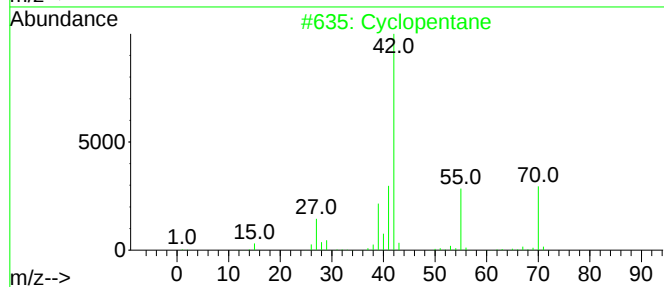
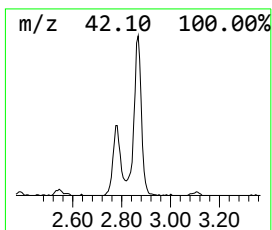
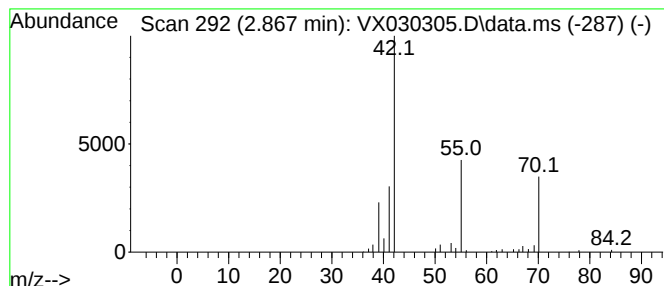
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X072522W.M  
Quant Title : SW846 8260

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

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Peak Number 3 Cyclopentane Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 2.867 | 9.45 ug/l | 90856 | Pentafluorobenzene | 5.562 |

| Hit# | of | 5 | Tentative ID         | MW | MolForm | CAS#        | Qual |
|------|----|---|----------------------|----|---------|-------------|------|
| 1    |    |   | Cyclopentane         | 70 | C5H10   | 000287-92-3 | 86   |
| 2    |    |   | 1-Pentene            | 70 | C5H10   | 000109-67-1 | 72   |
| 3    |    |   | 3-Buten-1-ol         | 72 | C4H8O   | 000627-27-0 | 42   |
| 4    |    |   | Cyclopropane, ethyl- | 70 | C5H10   | 001191-96-4 | 9    |
| 5    |    |   | Cyclobutanone        | 70 | C4H6O   | 001191-95-3 | 9    |



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MSVOA\_X  
ClientSampleId :  
MW-16R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X072522W.M  
Quant Title : SW846 8260

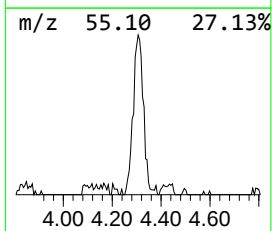
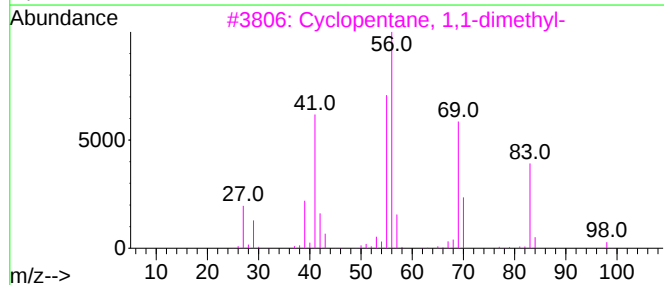
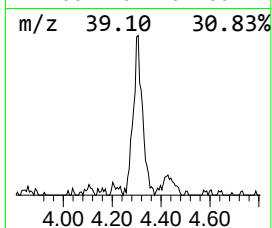
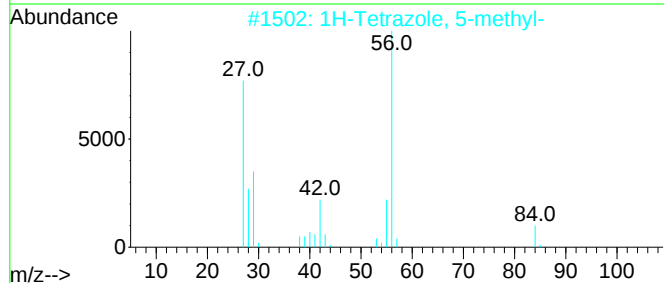
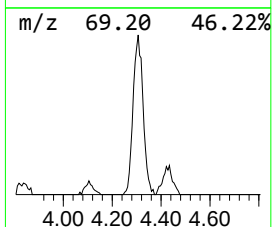
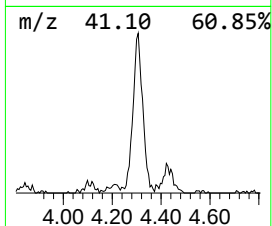
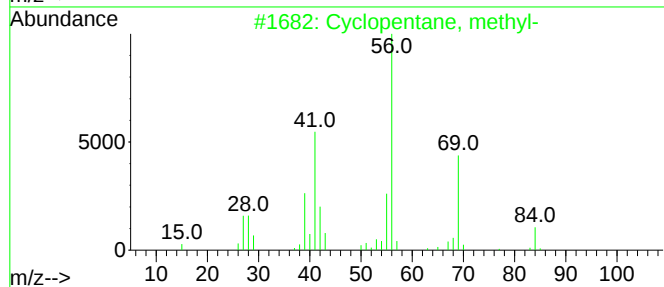
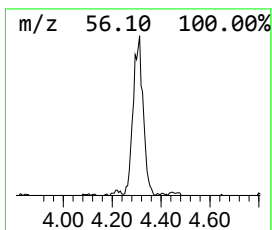
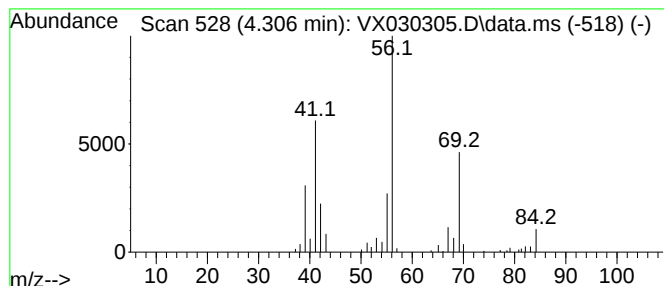
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Cyclopentane, methyl- Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 4.306 | 11.47 ug/l | 110249 | Pentafluorobenzene | 5.562 |

| Hit# | of | 5 | Tentative ID                | MW | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|----|---------|-------------|------|
| 1    |    |   | Cyclopentane, methyl-       | 84 | C6H12   | 000096-37-7 | 91   |
| 2    |    |   | 1H-Tetrazole, 5-methyl-     | 84 | C2H4N4  | 004076-36-2 | 64   |
| 3    |    |   | Cyclopentane, 1,1-dimethyl- | 98 | C7H14   | 001638-26-2 | 50   |
| 4    |    |   | Cyclobutane                 | 56 | C4H8    | 000287-23-0 | 47   |
| 5    |    |   | Cyclobutane, ethyl-         | 84 | C6H12   | 004806-61-5 | 45   |



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Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-16R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X072522W.M  
Quant Title : SW846 8260

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

| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| Butane, 2-methyl-  | 1.746 | 8.4     | ug/l  | 80863    | 1                     | 5.562 | 480689 | 50.0 |
| Butane, 2,3-dim... | 2.782 | 6.7     | ug/l  | 64567    | 1                     | 5.562 | 480689 | 50.0 |
| Cyclopentane       | 2.867 | 9.4     | ug/l  | 90856    | 1                     | 5.562 | 480689 | 50.0 |
| Cyclopentane, m... | 4.306 | 11.5    | ug/l  | 110249   | 1                     | 5.562 | 480689 | 50.0 |