

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121322\  
 Data File : VX033392.D  
 Acq On : 13 Dec 2022 15:07  
 Operator : JC/MD  
 Sample : N6001-07  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 MW-7

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: VX033392.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         | 1.752       | 103           | 109         | 120          | rVB      | 1056073        | 1400487       | 7.09%           | 3.169%        |
| 2         | 1.959       | 137           | 143         | 155          | rVB      | 239774         | 339955        | 1.72%           | 0.769%        |
| 3         | 2.867       | 288           | 292         | 311          | rVB2     | 196117         | 457026        | 2.31%           | 1.034%        |
| 4         | 3.105       | 320           | 331         | 343          | rBV      | 95326          | 214918        | 1.09%           | 0.486%        |
| 5         | 4.306       | 517           | 528         | 541          | rVB      | 234185         | 665379        | 3.37%           | 1.506%        |
| 6         | 5.556       | 726           | 733         | 758          | rVB      | 142184         | 423253        | 2.14%           | 0.958%        |
| 7         | 6.037       | 803           | 812         | 826          | rVB      | 973000         | 2571620       | 13.01%          | 5.819%        |
| 8         | 6.763       | 920           | 931         | 941          | rBV      | 209747         | 502321        | 2.54%           | 1.137%        |
| 9         | 8.647       | 1234          | 1240        | 1246         | rBV      | 162852         | 257127        | 1.30%           | 0.582%        |
| 10        | 8.720       | 1246          | 1252        | 1262         | rVB      | 1050746        | 1590416       | 8.05%           | 3.599%        |
| 11        | 10.055      | 1460          | 1471        | 1476         | rBV      | 446524         | 632073        | 3.20%           | 1.430%        |
| 12        | 10.195      | 1488          | 1494        | 1505         | rVB      | 7712126        | 10044667      | 50.82%          | 22.730%       |
| 13        | 10.305      | 1505          | 1512        | 1518         | rBV      | 14341042       | 19766182      | 100.00%         | 44.728%       |
| 14        | 10.640      | 1562          | 1567        | 1578         | rVB      | 3140549        | 4001034       | 20.24%          | 9.054%        |
| 15        | 11.079      | 1634          | 1639        | 1648         | rBV      | 308802         | 403292        | 2.04%           | 0.913%        |
| 16        | 12.024      | 1788          | 1794        | 1800         | rBV      | 473277         | 590637        | 2.99%           | 1.337%        |
| 17        | 12.244      | 1824          | 1830        | 1837         | rBV      | 271166         | 331617        | 1.68%           | 0.750%        |

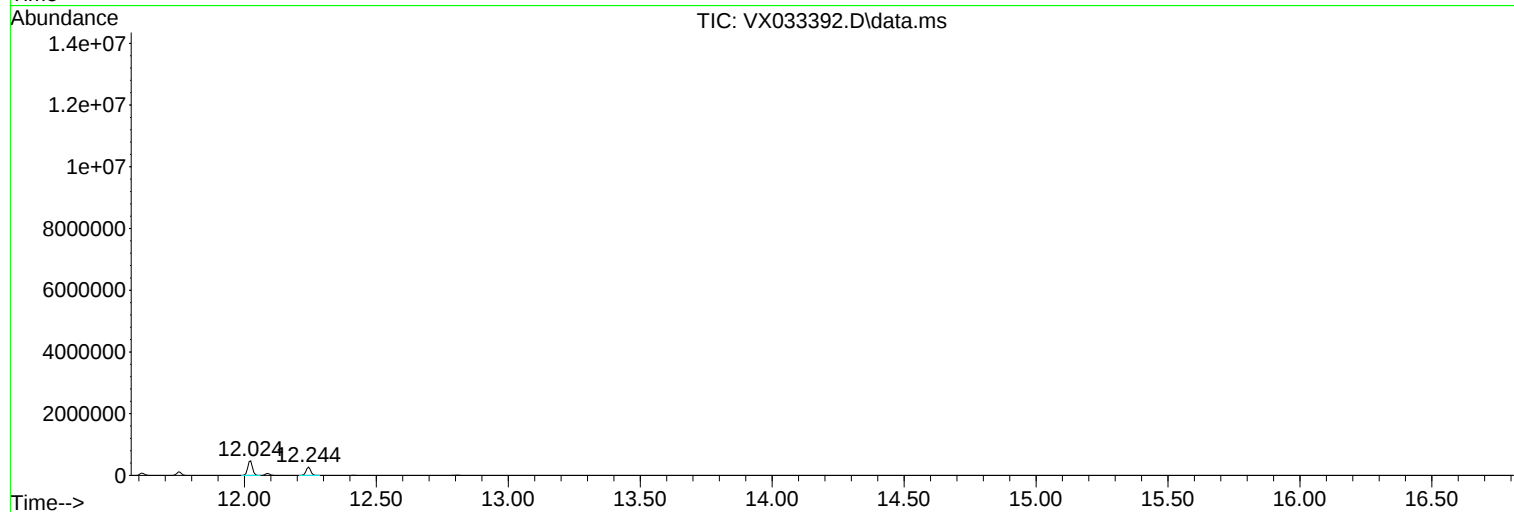
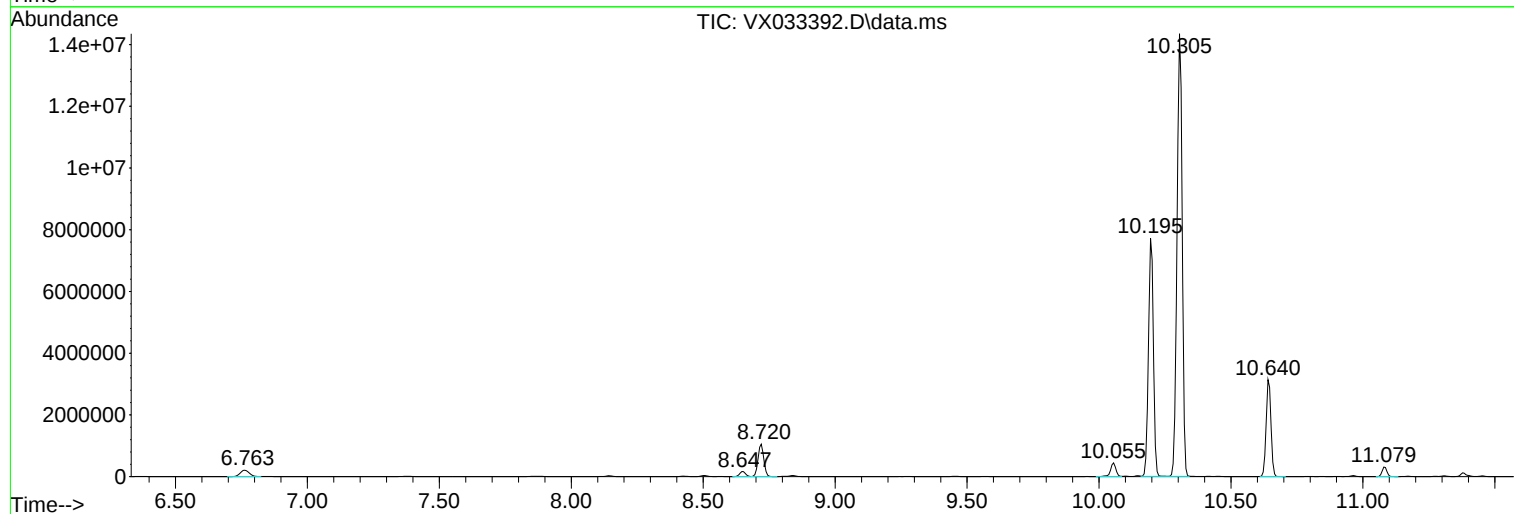
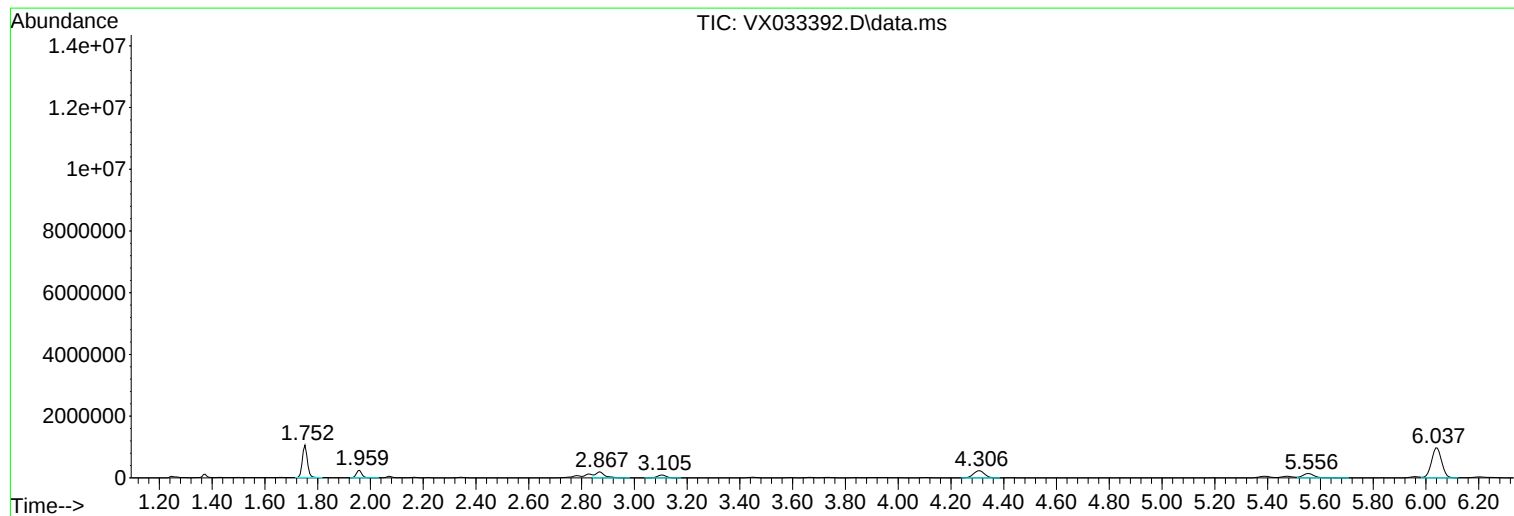
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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-7

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\VX121322\  
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Operator : JC/MD  
Sample : N6001-07  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-7

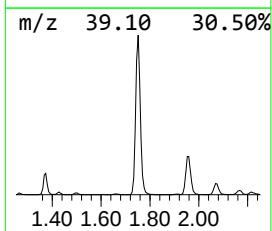
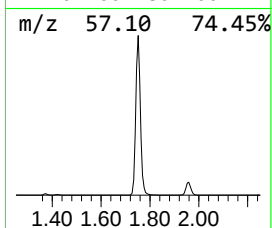
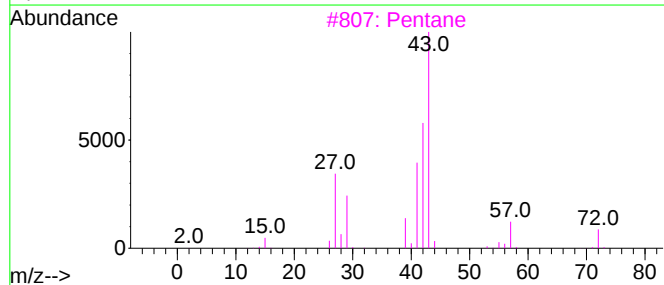
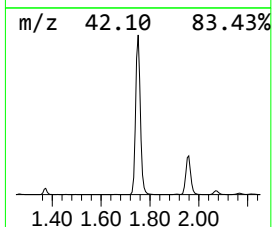
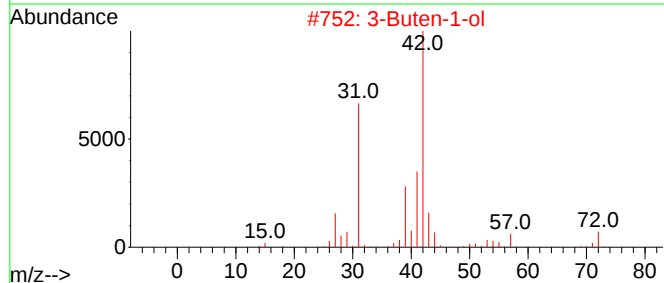
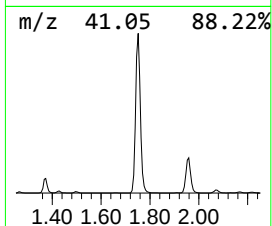
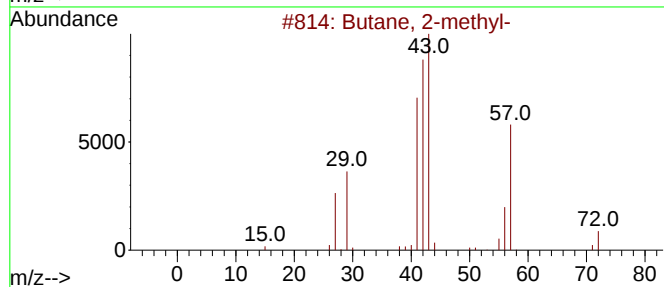
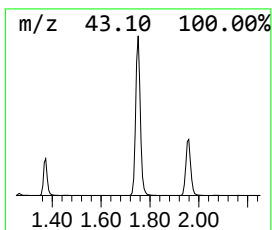
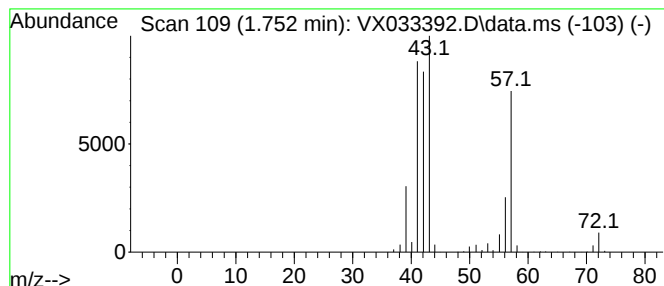
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X120722W.M  
Quant Title : SW846 8260

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

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

| R.T.  | EstConc     | Area    | Relative to ISTD   | R.T.  |
|-------|-------------|---------|--------------------|-------|
| 1.752 | 165.44 ug/l | 1400490 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID               | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methyl-          | 72  | C5H12   | 000078-78-4 | 91   |
| 2    |    |   | 3-Buten-1-ol               | 72  | C4H8O   | 000627-27-0 | 43   |
| 3    |    |   | Pentane                    | 72  | C5H12   | 000109-66-0 | 42   |
| 4    |    |   | Propane, 2-methyl-2-nitro- | 103 | C4H9NO2 | 000594-70-7 | 10   |
| 5    |    |   | 1-Butene                   | 56  | C4H8    | 000106-98-9 | 10   |



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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-7

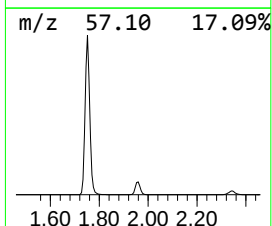
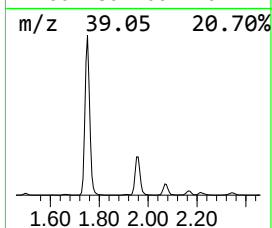
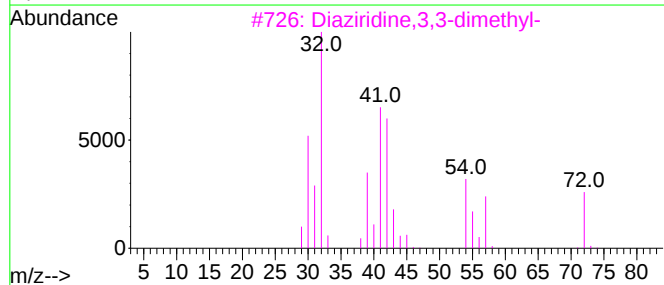
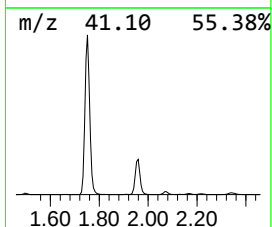
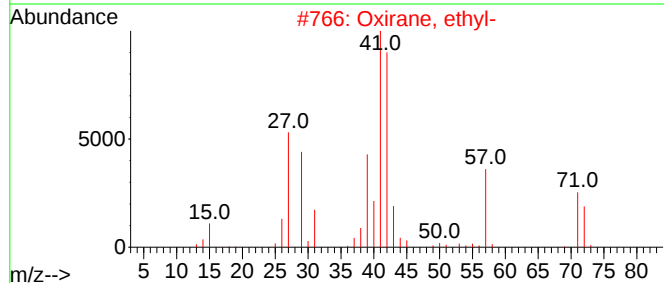
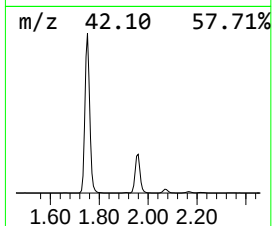
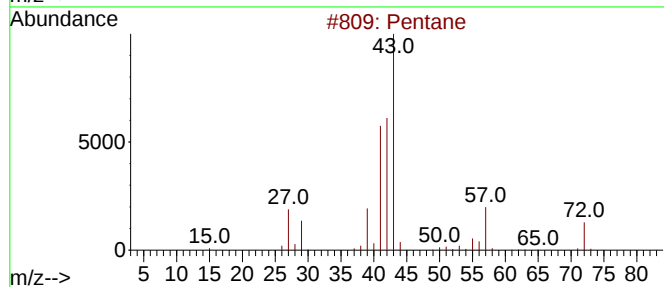
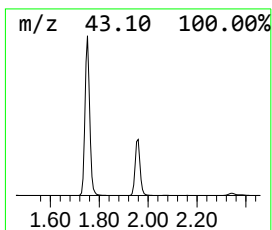
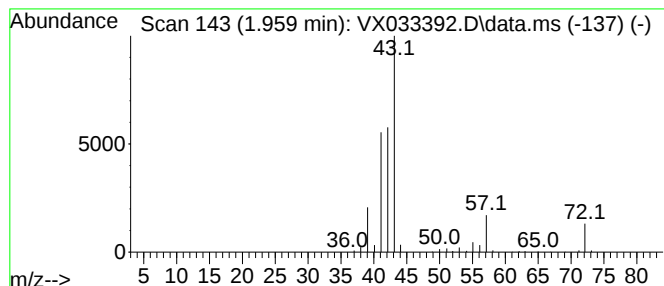
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X120722W.M  
Quant Title : SW846 8260

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

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Peak Number 2 Pentane Concentration Rank 4

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 1.959 | 40.16 ug/l | 339955 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID              | MW | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|----|---------|-------------|------|
| 1    |    |   | Pentane                   | 72 | C5H12   | 000109-66-0 | 91   |
| 2    |    |   | Oxirane, ethyl-           | 72 | C4H8O   | 000106-88-7 | 53   |
| 3    |    |   | Diaziridine,3,3-dimethyl- | 72 | C3H8N2  | 004901-76-2 | 38   |
| 4    |    |   | Butane, 2-methyl-         | 72 | C5H12   | 000078-78-4 | 9    |
| 5    |    |   | Tetrahydrofuran           | 72 | C4H8O   | 000109-99-9 | 9    |



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Sample : N6001-07  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-7

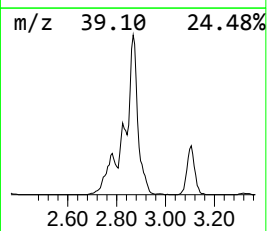
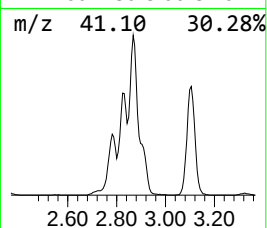
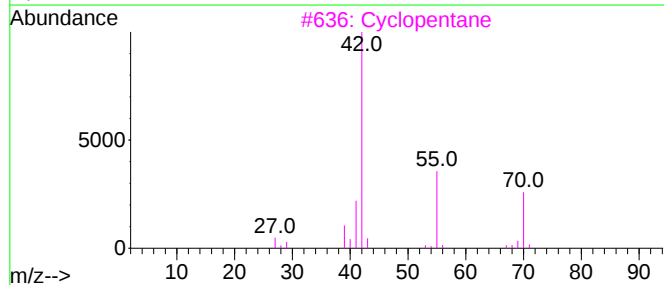
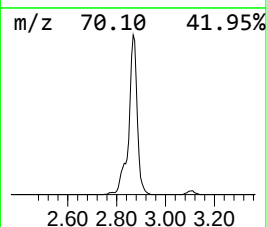
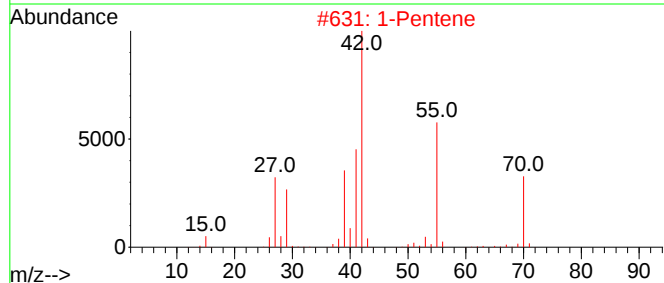
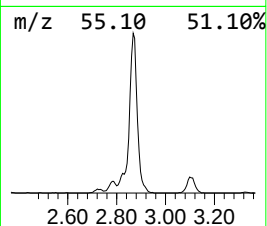
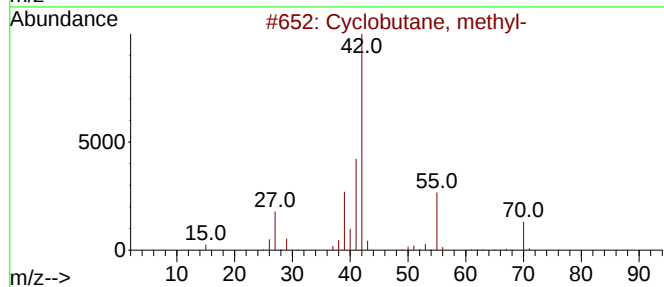
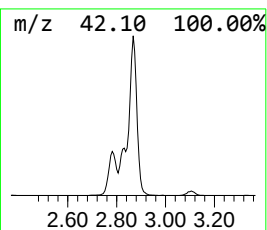
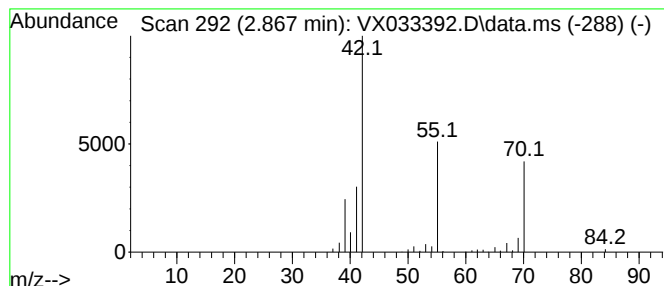
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X120722W.M  
Quant Title : SW846 8260

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

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Peak Number 3 Cyclobutane, methyl- Concentration Rank 3

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 2.867 | 53.99 ug/l | 457026 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID                        | MW | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|----|---------|-------------|------|
| 1    |    |   | Cyclobutane, methyl-                | 70 | C5H10   | 000598-61-8 | 78   |
| 2    |    |   | 1-Pentene                           | 70 | C5H10   | 000109-67-1 | 78   |
| 3    |    |   | Cyclopentane                        | 70 | C5H10   | 000287-92-3 | 78   |
| 4    |    |   | 2-Pentene, (E)-                     | 70 | C5H10   | 000646-04-8 | 47   |
| 5    |    |   | Cyclopropane, 1,2-dimethyl-, trans- | 70 | C5H10   | 002402-06-4 | 38   |



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Sample : N6001-07  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-7

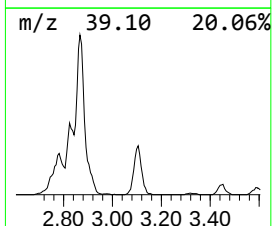
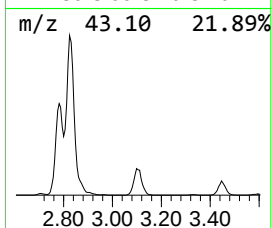
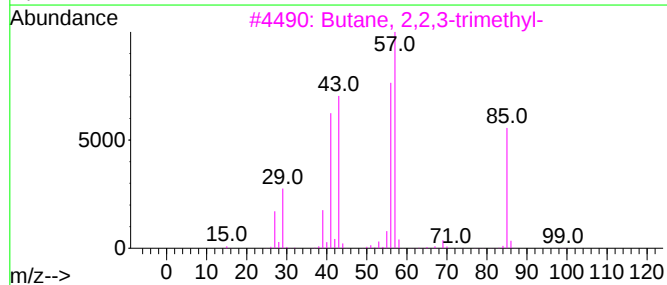
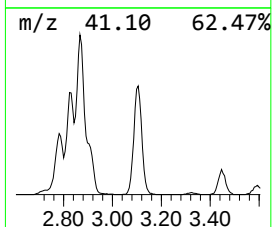
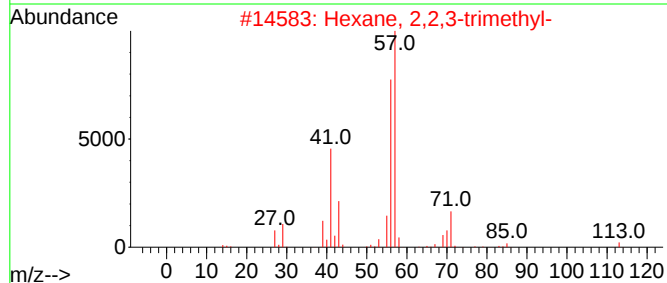
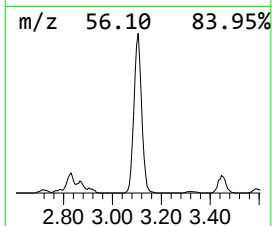
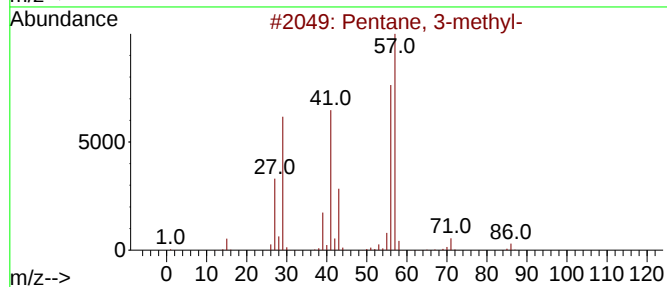
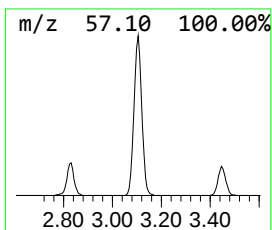
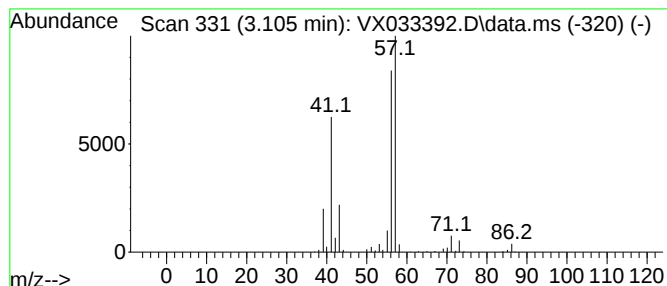
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X120722W.M  
Quant Title : SW846 8260

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

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Peak Number 4 Pentane, 3-methyl- Concentration Rank 6

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 3.105 | 25.39 ug/l | 214918 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------|-----|----------|-------------|------|
| 1    |    |   | Pentane, 3-methyl-             | 86  | C6H14    | 000096-14-0 | 90   |
| 2    |    |   | Hexane, 2,2,3-trimethyl-       | 128 | C9H20    | 016747-25-4 | 78   |
| 3    |    |   | Butane, 2,2,3-trimethyl-       | 100 | C7H16    | 000464-06-2 | 64   |
| 4    |    |   | Pentane, 3-ethyl-2,2-dimethyl- | 128 | C9H20    | 016747-32-3 | 43   |
| 5    |    |   | Sulphuric acid dibutyl ester   | 210 | C8H18O4S | 000625-22-9 | 40   |



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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-7

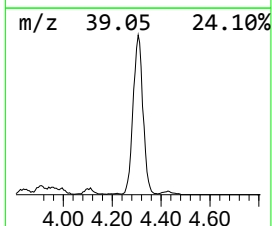
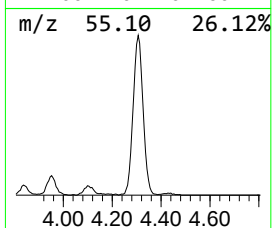
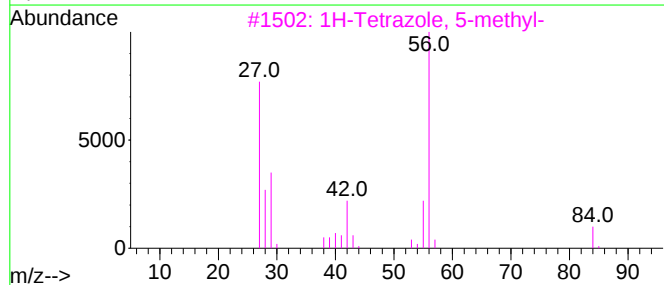
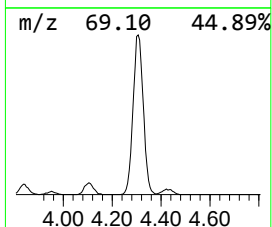
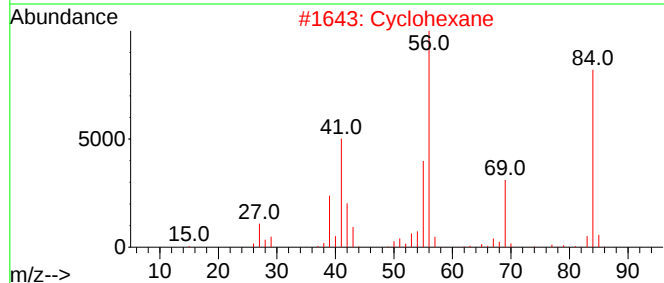
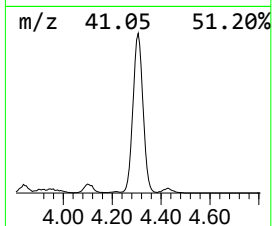
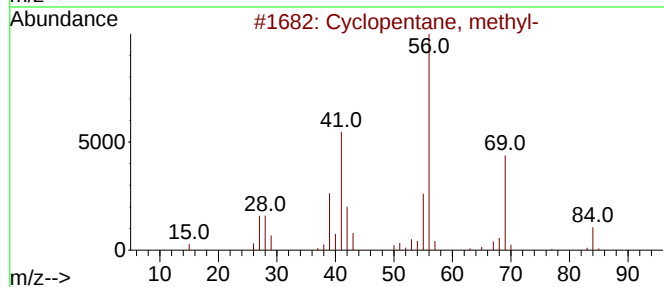
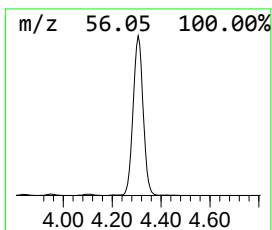
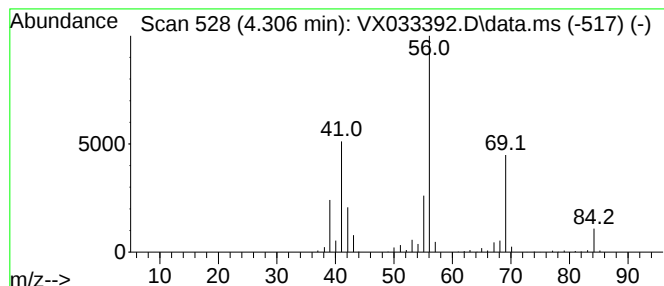
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X120722W.M  
Quant Title : SW846 8260

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

\*\*\*\*\*  
Peak Number 5 Cyclopentane, methyl- Concentration Rank 2

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 4.306 | 78.60 ug/l | 665379 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID            | MW | MolForm | CAS#        | Qual |
|------|----|---|-------------------------|----|---------|-------------|------|
| 1    |    |   | Cyclopentane, methyl-   | 84 | C6H12   | 000096-37-7 | 94   |
| 2    |    |   | Cyclohexane             | 84 | C6H12   | 000110-82-7 | 86   |
| 3    |    |   | 1H-Tetrazole, 5-methyl- | 84 | C2H4N4  | 004076-36-2 | 80   |
| 4    |    |   | Cyclobutane, ethyl-     | 84 | C6H12   | 004806-61-5 | 72   |
| 5    |    |   | 1-Pentene, 2-methyl-    | 84 | C6H12   | 000763-29-1 | 47   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121322\  
Data File : VX033392.D  
Acq On : 13 Dec 2022 15:07  
Operator : JC/MD  
Sample : N6001-07  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-7

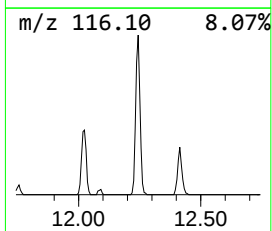
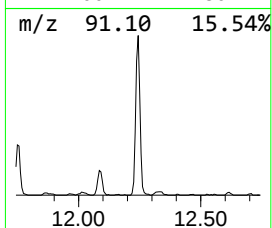
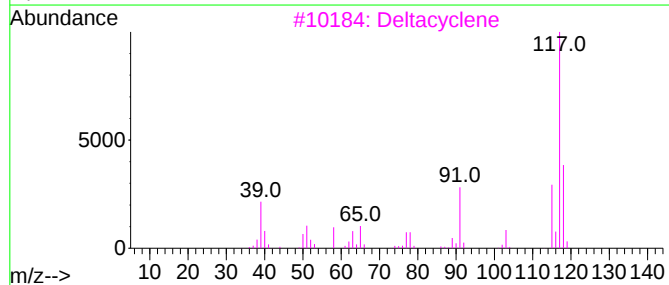
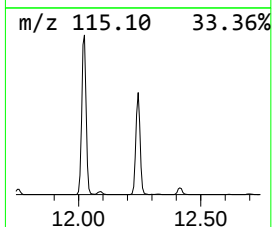
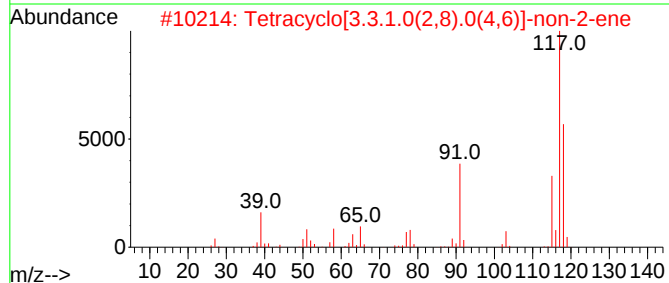
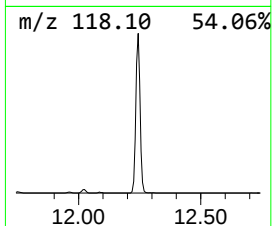
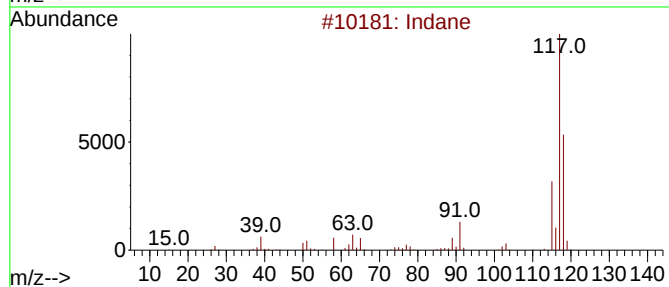
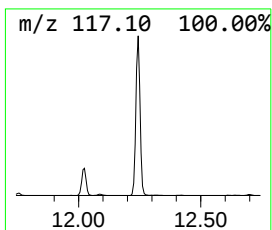
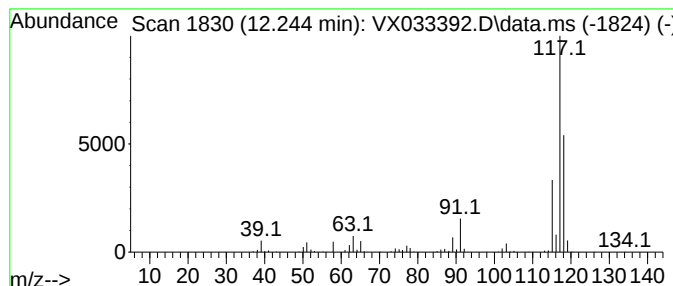
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Quant Title : SW846 8260

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

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Peak Number 6 Indane Concentration Rank 5

| R.T.      | EstConc                             | Area   | Relative to ISTD       | R.T.         |      |
|-----------|-------------------------------------|--------|------------------------|--------------|------|
| 12.244    | 28.07 ug/l                          | 331617 | 1,4-Dichlorobenzene-d4 | 12.024       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm                | CAS#         | Qual |
| 1         | Indane                              | 118    | C9H10                  | 000496-11-7  | 93   |
| 2         | Tetracyclo[3.3.1.0(2,8).0(4,6)]-... | 118    | C9H10                  | 1000191-13-7 | 80   |
| 3         | Deltacyclene                        | 118    | C9H10                  | 007785-10-6  | 72   |
| 4         | Benzene, 2-propenyl-                | 118    | C9H10                  | 000300-57-2  | 64   |
| 5         | Benzene, 1-ethenyl-2-methyl-        | 118    | C9H10                  | 000611-15-4  | 50   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121322\  
Data File : VX033392.D  
Acq On : 13 Dec 2022 15:07  
Operator : JC/MD  
Sample : N6001-07  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-7

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 |
| Butane, 2-methyl-  | 1.752  | 165.4   | ug/l  | 1400490  | 1                     | 5.556  | 423253 | 50.0 |
| Pentane            | 1.959  | 40.2    | ug/l  | 339955   | 1                     | 5.556  | 423253 | 50.0 |
| Cyclobutane, me... | 2.867  | 54.0    | ug/l  | 457026   | 1                     | 5.556  | 423253 | 50.0 |
| Pentane, 3-methyl- | 3.105  | 25.4    | ug/l  | 214918   | 1                     | 5.556  | 423253 | 50.0 |
| Cyclopentane, m... | 4.306  | 78.6    | ug/l  | 665379   | 1                     | 5.556  | 423253 | 50.0 |
| Indane             | 12.244 | 28.1    | ug/l  | 331617   | 4                     | 12.024 | 590637 | 50.0 |