

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX062122\  
 Data File : VX029680.D  
 Acq On : 21 Jun 2022 22:23  
 Operator : JC/MD  
 Sample : N3286-05  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 MW-6S

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\82X061822W.M  
 Title : SW846 8260

Signal : TIC: VX029680.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         | 1.240       | 21            | 25          | 42           | rBV      | 178969         | 356686        | 16.40%          | 2.761%        |
| 2         | 1.368       | 43            | 46          | 51           | rVV      | 61430          | 65795         | 3.02%           | 0.509%        |
| 3         | 1.746       | 104           | 108         | 120          | rVB      | 69491          | 101974        | 4.69%           | 0.789%        |
| 4         | 2.136       | 167           | 172         | 179          | rVB5     | 12967          | 28140         | 1.29%           | 0.218%        |
| 5         | 2.337       | 199           | 205         | 217          | rVB      | 19667          | 42232         | 1.94%           | 0.327%        |
| 6         | 2.782       | 267           | 278         | 288          | rBV      | 64762          | 156815        | 7.21%           | 1.214%        |
| 7         | 2.867       | 288           | 292         | 301          | rVB2     | 19193          | 38698         | 1.78%           | 0.300%        |
| 8         | 3.105       | 320           | 331         | 341          | rVB2     | 47246          | 106620        | 4.90%           | 0.825%        |
| 9         | 4.215       | 500           | 513         | 520          | rBV5     | 7442           | 22282         | 1.02%           | 0.173%        |
| 10        | 4.306       | 520           | 528         | 538          | rVB3     | 9693           | 28232         | 1.30%           | 0.219%        |
| 11        | 5.391       | 694           | 706         | 718          | rBV      | 254398         | 750577        | 34.50%          | 5.811%        |
| 12        | 5.556       | 722           | 733         | 744          | rBV      | 415226         | 1179983       | 54.24%          | 9.135%        |
| 13        | 5.958       | 788           | 799         | 810          | rBV      | 270647         | 723596        | 33.26%          | 5.602%        |
| 14        | 6.251       | 839           | 847         | 857          | rVB      | 41870          | 131953        | 6.07%           | 1.022%        |
| 15        | 6.763       | 918           | 931         | 943          | rBV      | 636142         | 1525358       | 70.12%          | 11.809%       |
| 16        | 7.988       | 1124          | 1132        | 1139         | rVB3     | 16610          | 34253         | 1.57%           | 0.265%        |
| 17        | 8.110       | 1145          | 1152        | 1163         | rBV2     | 22593          | 51467         | 2.37%           | 0.398%        |
| 18        | 8.653       | 1233          | 1241        | 1250         | rBV      | 1389363        | 2175410       | 100.00%         | 16.842%       |
| 19        | 10.055      | 1466          | 1471        | 1478         | rBV      | 1371659        | 1800130       | 82.75%          | 13.936%       |
| 20        | 11.085      | 1634          | 1640        | 1650         | rBV      | 1092159        | 1431469       | 65.80%          | 11.082%       |
| 21        | 12.024      | 1789          | 1794        | 1801         | rBV      | 1581925        | 1894953       | 87.11%          | 14.670%       |
| 22        | 12.244      | 1824          | 1830        | 1837         | rBV      | 155403         | 194117        | 8.92%           | 1.503%        |
| 23        | 12.701      | 1900          | 1905        | 1912         | rVB      | 60188          | 76105         | 3.50%           | 0.589%        |

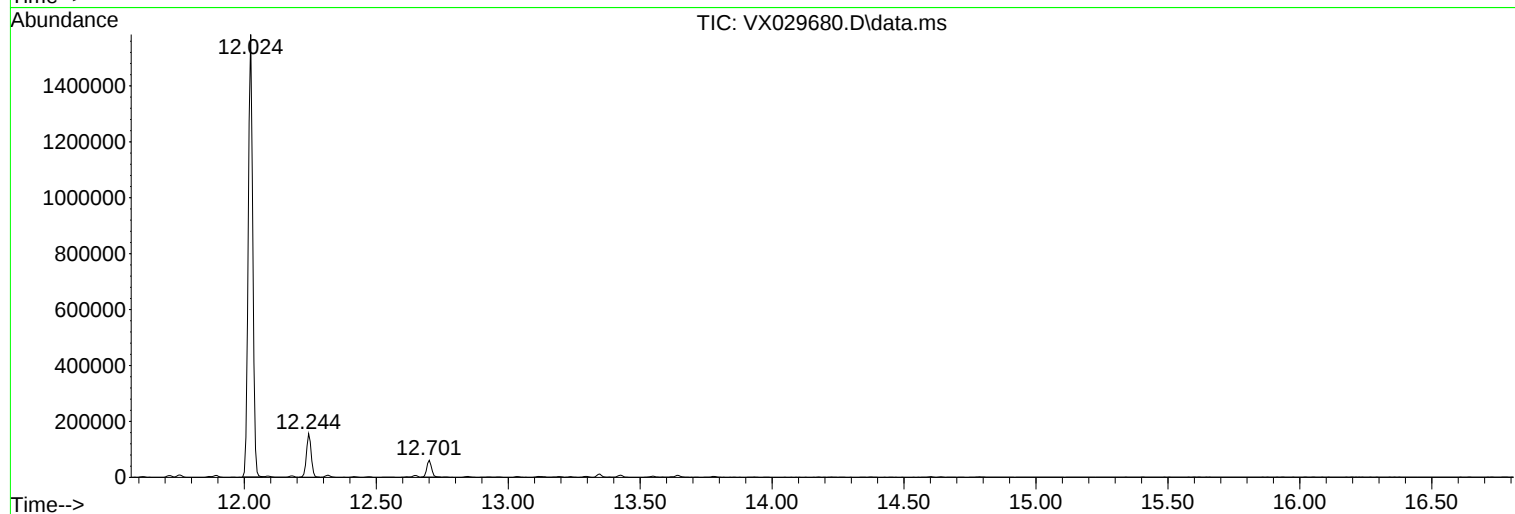
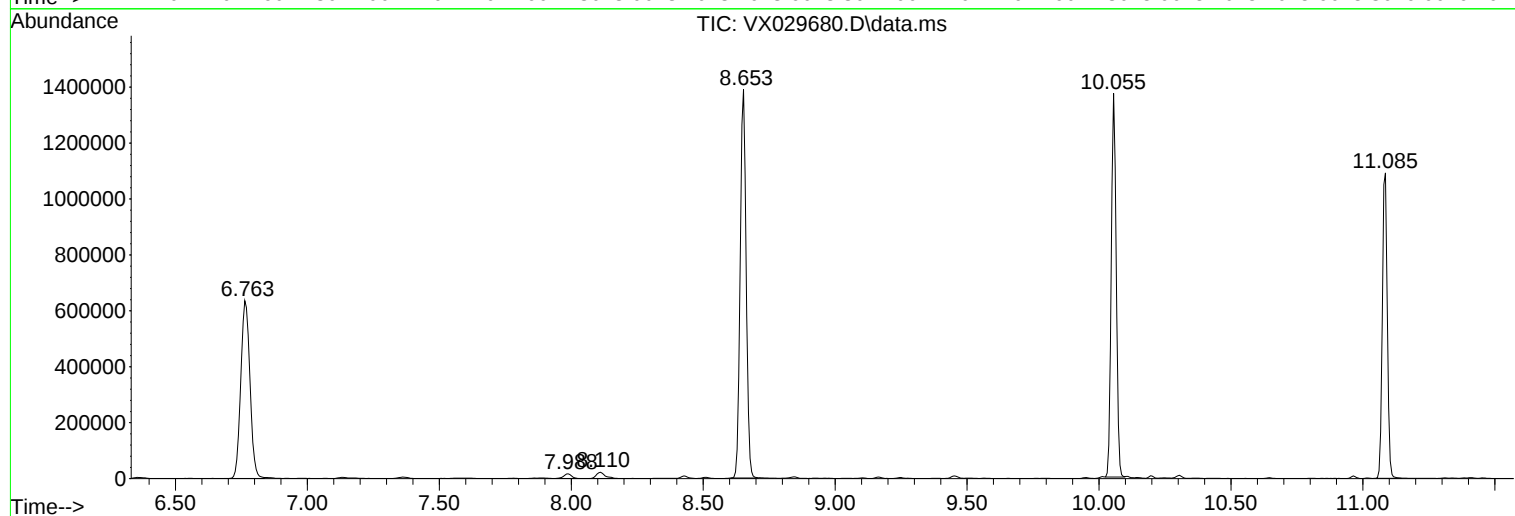
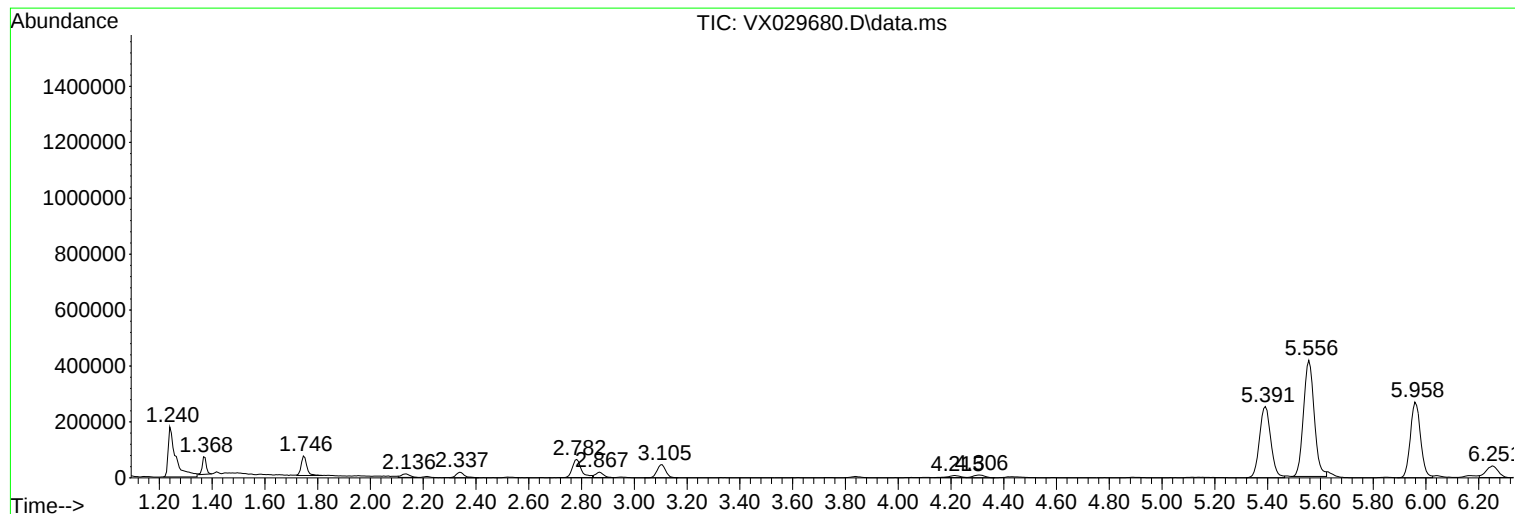
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Instrument :  
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ClientSampleId :  
MW-6S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061822W.M  
Quant Title : SW846 8260

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



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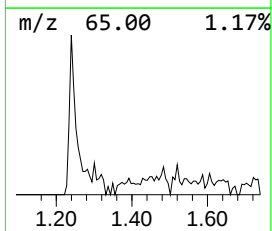
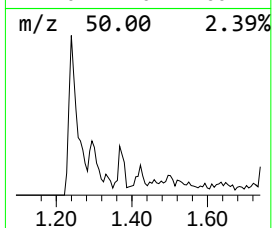
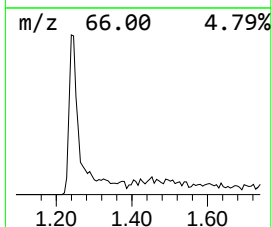
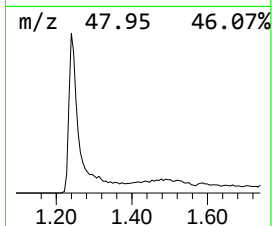
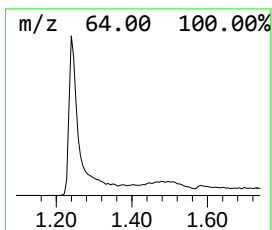
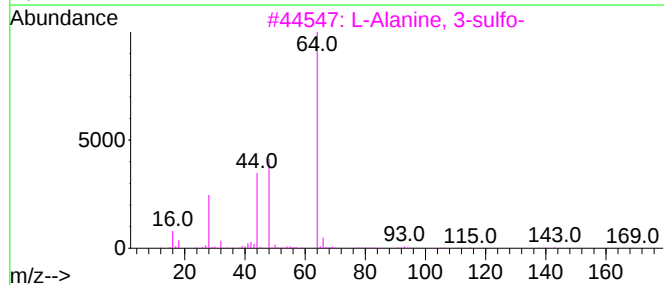
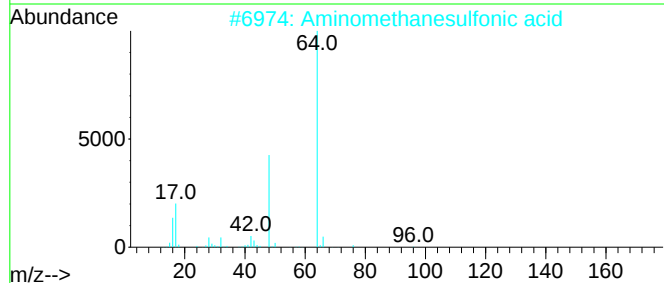
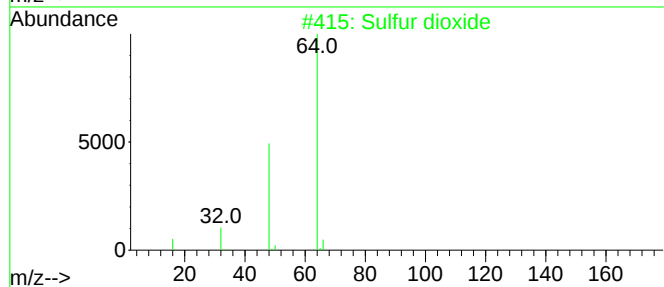
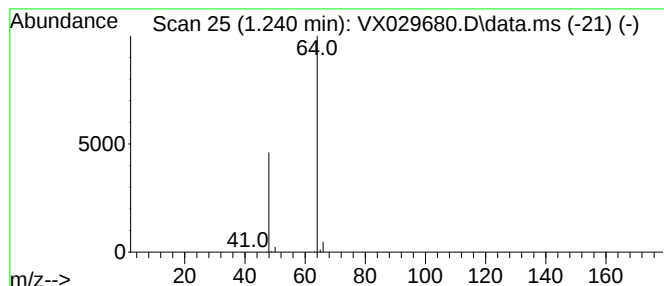
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Sulfur dioxide Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD   | R.T.  |
|-------|------------|--------|--------------------|-------|
| 1.240 | 15.11 ug/l | 356686 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 83   |
| 2    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 74   |
| 3    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 4    |    |   | Ethyl Chloride            | 64  | C2H5Cl   | 000075-00-3 | 3    |
| 5    |    |   | Ethene, 1,1-difluoro-     | 64  | C2H2F2   | 000075-38-7 | 3    |



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MSVOA\_X  
ClientSampleId :  
MW-6S

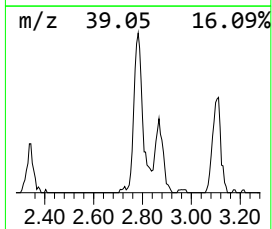
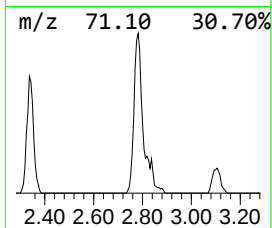
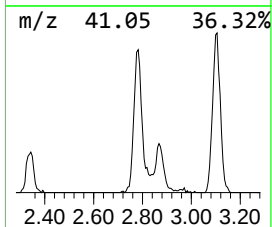
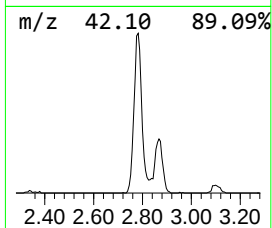
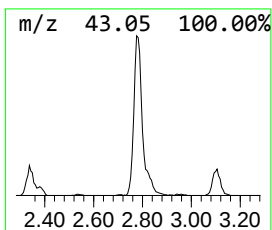
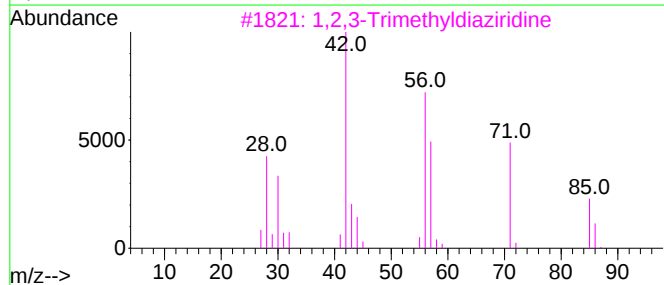
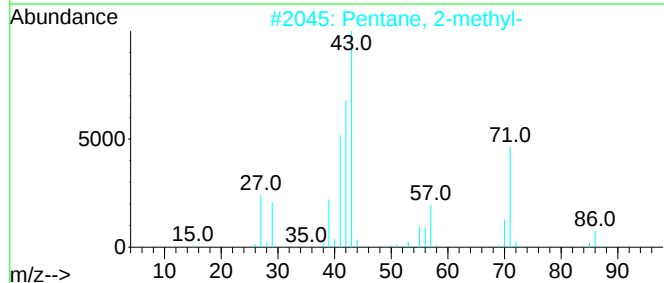
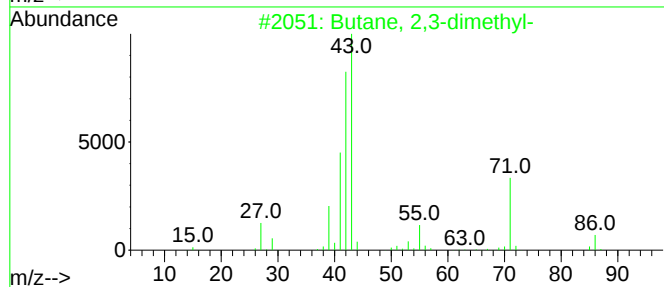
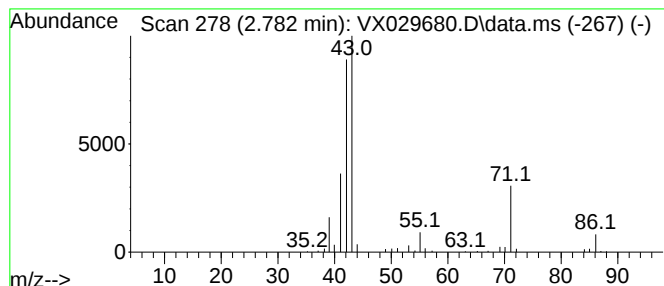
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061822W.M  
Quant Title : SW846 8260

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

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

| R.T.  | EstConc   | Area   | Relative to ISTD   | R.T.  |
|-------|-----------|--------|--------------------|-------|
| 2.782 | 6.64 ug/l | 156815 | Pentafluorobenzene | 5.556 |

| Hit# | of | 5 | Tentative ID               | MW | MolForm | CAS#        | Qual |
|------|----|---|----------------------------|----|---------|-------------|------|
| 1    |    |   | Butane, 2,3-dimethyl-      | 86 | C6H14   | 000079-29-8 | 91   |
| 2    |    |   | Pentane, 2-methyl-         | 86 | C6H14   | 000107-83-5 | 47   |
| 3    |    |   | 1,2,3-Trimethyldiaziridine | 86 | C4H10N2 | 113604-56-1 | 38   |
| 4    |    |   | Tetrahydrofuran            | 72 | C4H8O   | 000109-99-9 | 38   |
| 5    |    |   | Pyrrolidine                | 71 | C4H9N   | 000123-75-1 | 27   |



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Instrument :  
MSVOA\_X  
ClientSampleId :  
MW-6S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X061822W.M  
Quant Title : SW846 8260

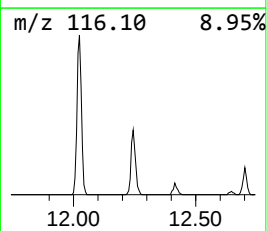
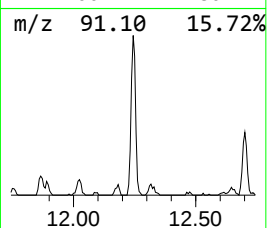
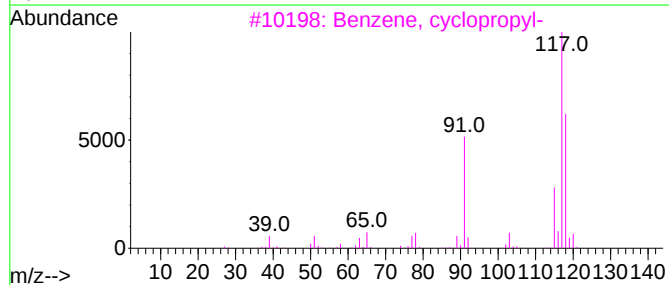
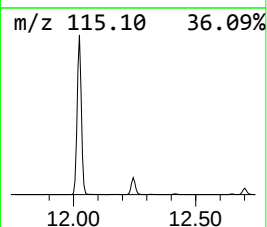
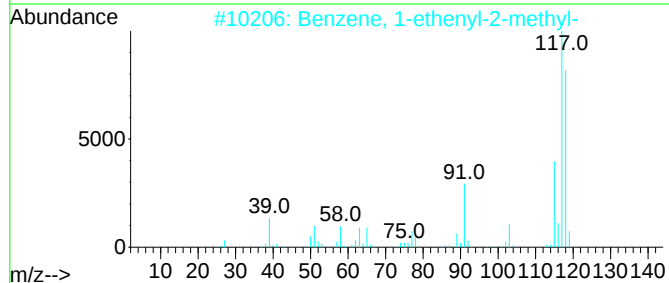
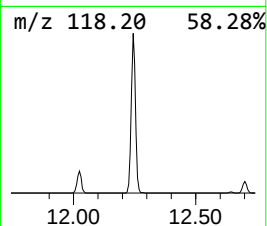
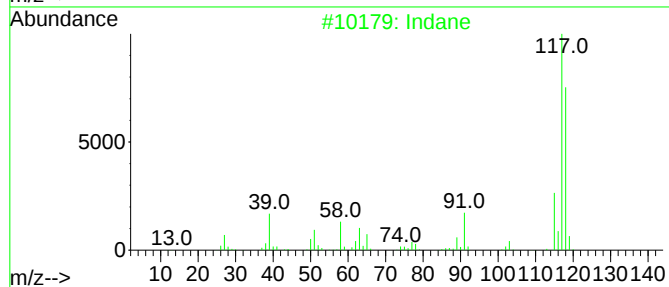
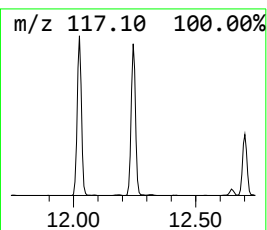
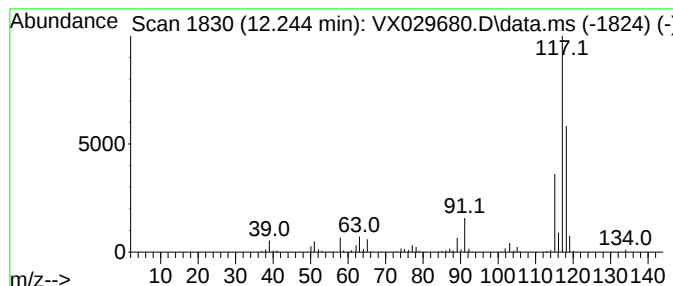
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Indane Concentration Rank 3

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 12.244 | 5.12 ug/l | 194117 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Indane                              | 118 | C9H10   | 000496-11-7  | 91   |
| 2    |    |   | Benzene, 1-ethenyl-2-methyl-        | 118 | C9H10   | 000611-15-4  | 87   |
| 3    |    |   | Benzene, cyclopropyl-               | 118 | C9H10   | 000873-49-4  | 87   |
| 4    |    |   | Benzene, 1-propenyl-                | 118 | C9H10   | 000637-50-3  | 87   |
| 5    |    |   | Tetracyclo[3.3.1.0(2,8).0(4,6)]-... | 118 | C9H10   | 1000191-13-7 | 83   |



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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 |
| Sulfur dioxide     | 1.240  | 15.1    | ug/l  | 356686   | 1                     | 5.556  | 1179980 | 50.0 |
| Butane, 2,3-dim... | 2.782  | 6.6     | ug/l  | 156815   | 1                     | 5.556  | 1179980 | 50.0 |
| Indane             | 12.244 | 5.1     | ug/l  | 194117   | 4                     | 12.024 | 1894950 | 50.0 |