

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN123021\  
 Data File : VN070409.D  
 Acq On : 30 Dec 2021 19:23  
 Operator : JC/MD  
 Sample : M5212-04  
 Misc : 5.00mL/MSVOA\_N/WATER  
 ALS Vial : 23 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 MW-62

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\82N122721W.M  
 Title : SW846 8260

Signal : TIC: VN070409.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         | 2.236       | 83            | 92          | 101          | rBV2     | 155421         | 288572        | 6.02%           | 1.048%        |
| 2         | 4.296       | 841           | 860         | 878          | rBV3     | 22779          | 65067         | 1.36%           | 0.236%        |
| 3         | 4.594       | 955           | 971         | 993          | rBV2     | 35854          | 108227        | 2.26%           | 0.393%        |
| 4         | 8.024       | 2228          | 2250        | 2261         | rBV2     | 626464         | 1523899       | 31.78%          | 5.533%        |
| 5         | 8.086       | 2261          | 2273        | 2297         | rVB      | 1088505        | 2485334       | 51.84%          | 9.024%        |
| 6         | 8.440       | 2385          | 2405        | 2434         | rBV      | 771663         | 1795662       | 37.45%          | 6.520%        |
| 7         | 8.968       | 2582          | 2602        | 2630         | rBV      | 1713223        | 3606369       | 75.22%          | 13.095%       |
| 8         | 10.443      | 3130          | 3152        | 3176         | rBV      | 2587256        | 4794556       | 100.00%         | 17.409%       |
| 9         | 11.747      | 3620          | 3638        | 3664         | rBV      | 2343340        | 4179223       | 87.17%          | 15.175%       |
| 10        | 12.581      | 3935          | 3949        | 3963         | rVB3     | 76010          | 132476        | 2.76%           | 0.481%        |
| 11        | 12.734      | 3989          | 4006        | 4028         | rBV      | 1750476        | 3119262       | 65.06%          | 11.326%       |
| 12        | 12.921      | 4064          | 4076        | 4092         | rVB2     | 75921          | 131075        | 2.73%           | 0.476%        |
| 13        | 13.675      | 4342          | 4357        | 4385         | rBV      | 1595846        | 2987656       | 62.31%          | 10.848%       |
| 14        | 13.841      | 4408          | 4419        | 4423         | rBV2     | 65975          | 97299         | 2.03%           | 0.353%        |
| 15        | 13.879      | 4423          | 4433        | 4443         | rVB      | 267283         | 408673        | 8.52%           | 1.484%        |
| 16        | 14.002      | 4469          | 4479        | 4493         | rVB5     | 72974          | 122800        | 2.56%           | 0.446%        |
| 17        | 14.150      | 4522          | 4534        | 4547         | rBV3     | 103129         | 181195        | 3.78%           | 0.658%        |
| 18        | 14.214      | 4549          | 4558        | 4572         | rVB3     | 42811          | 77463         | 1.62%           | 0.281%        |
| 19        | 14.329      | 4587          | 4601        | 4616         | rVB      | 236086         | 402148        | 8.39%           | 1.460%        |
| 20        | 14.541      | 4664          | 4680        | 4694         | rVB      | 190073         | 323855        | 6.75%           | 1.176%        |
| 21        | 14.761      | 4750          | 4762        | 4773         | rVB4     | 41349          | 78982         | 1.65%           | 0.287%        |
| 22        | 14.823      | 4775          | 4785        | 4797         | rVB6     | 31441          | 52305         | 1.09%           | 0.190%        |
| 23        | 14.933      | 4811          | 4826        | 4839         | rBV2     | 75853          | 140663        | 2.93%           | 0.511%        |
| 24        | 15.196      | 4911          | 4924        | 4935         | rBV3     | 60535          | 111306        | 2.32%           | 0.404%        |
| 25        | 15.563      | 5049          | 5061        | 5074         | rBV3     | 53080          | 103931        | 2.17%           | 0.377%        |
| 26        | 15.641      | 5079          | 5090        | 5111         | rVB4     | 65681          | 144740        | 3.02%           | 0.526%        |
| 27        | 16.113      | 5252          | 5266        | 5279         | rBV2     | 33443          | 77281         | 1.61%           | 0.281%        |

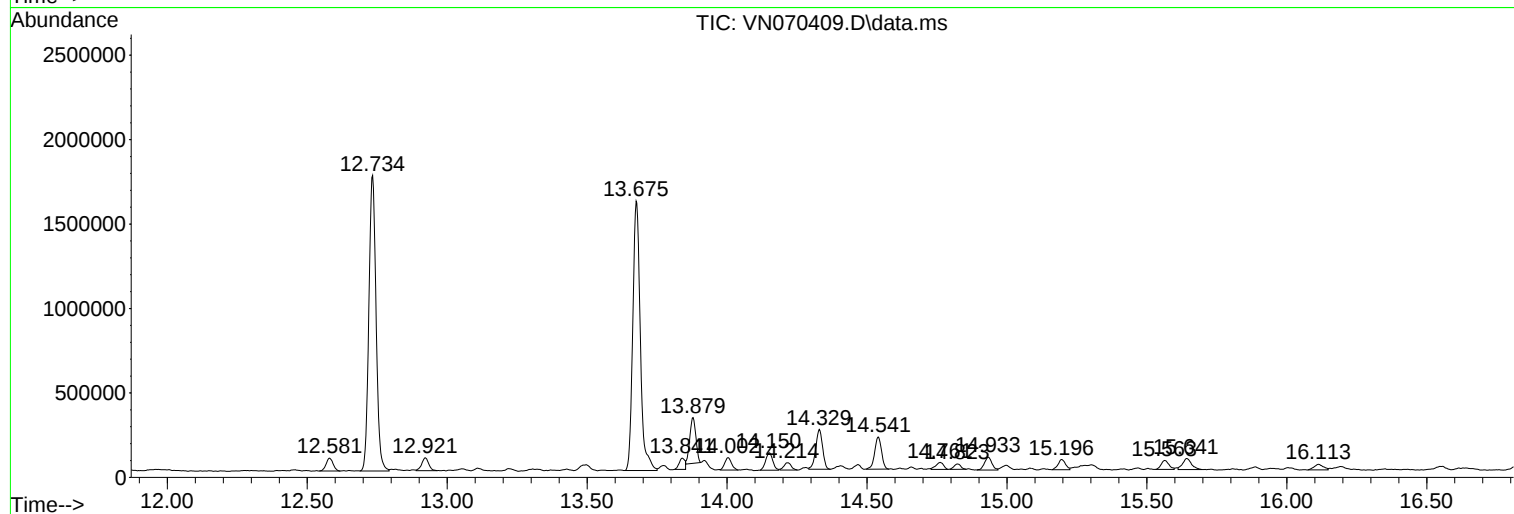
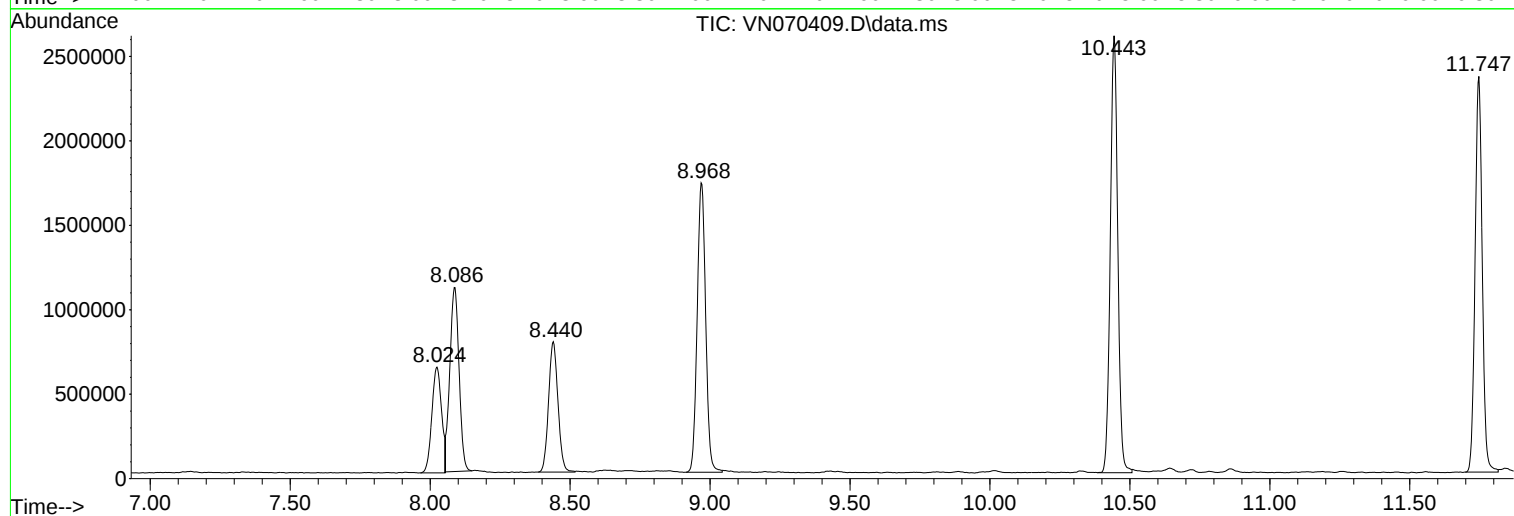
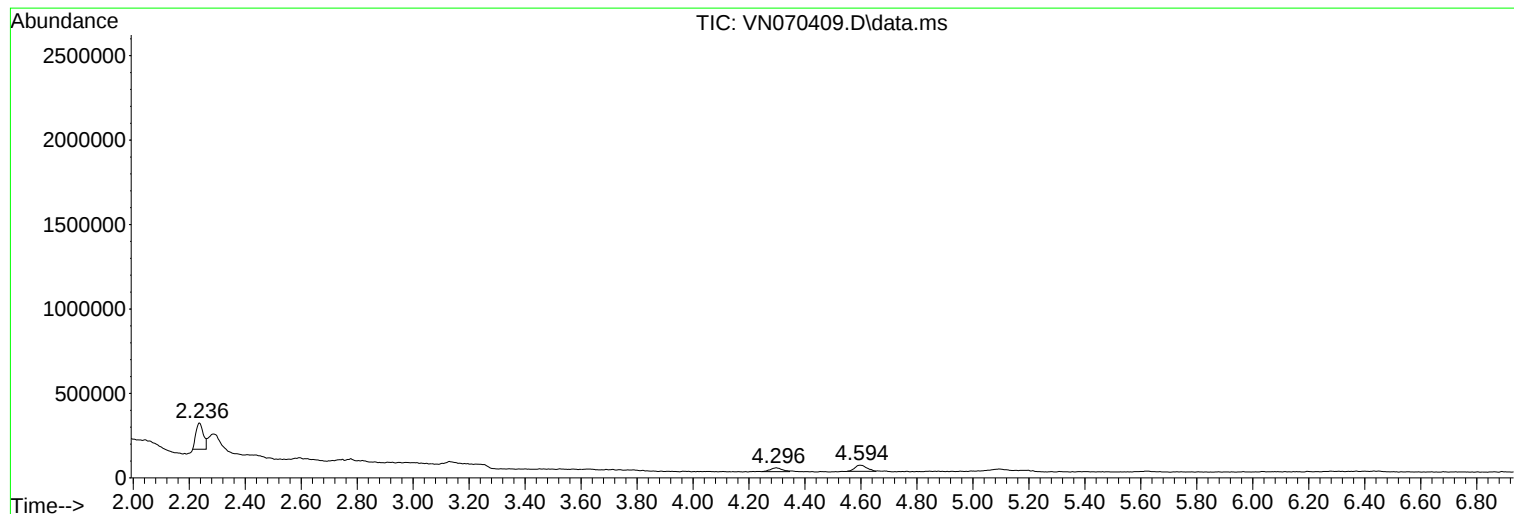
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ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
MW-62

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N122721W.M  
Quant Title : SW846 8260

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



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MW-62

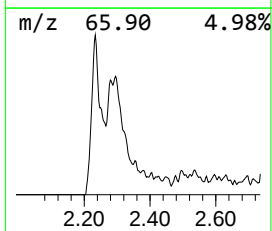
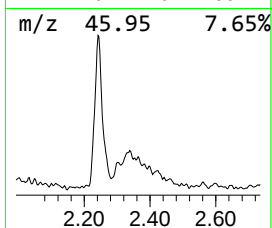
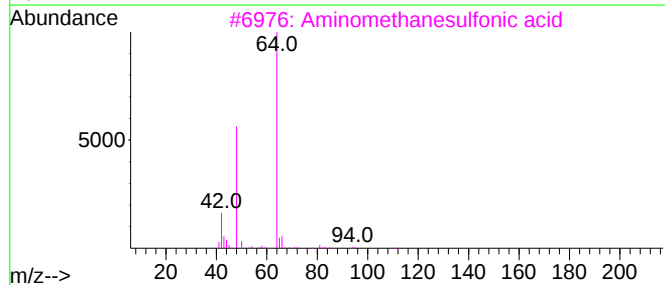
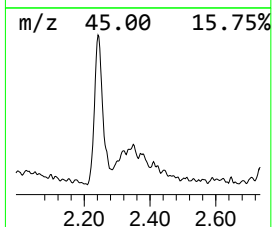
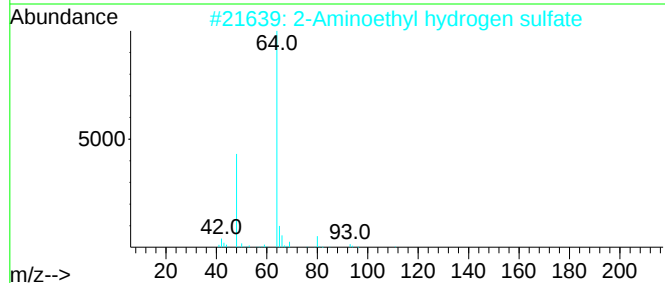
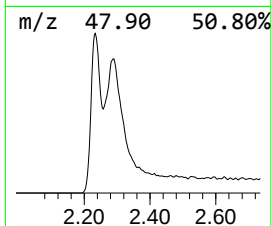
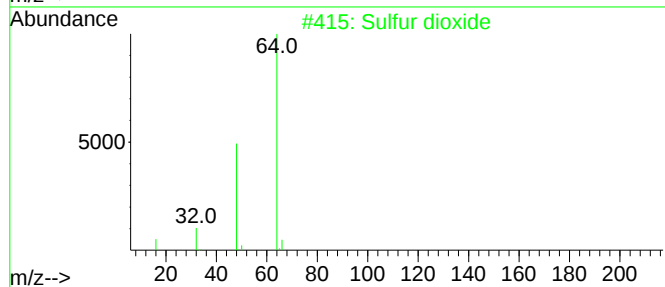
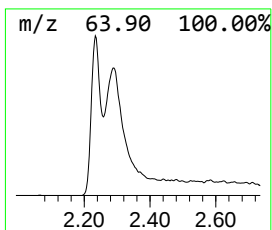
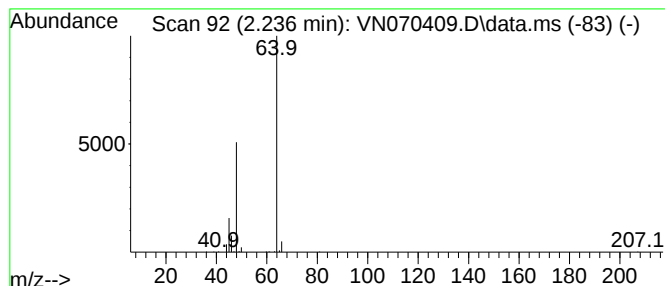
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N122721W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Sulfur dioxide Concentration Rank 3

| R.T.  | EstConc   | Area   | Relative to ISTD   | R.T.  |
|-------|-----------|--------|--------------------|-------|
| 2.236 | 5.81 ug/l | 288572 | Pentafluorobenzene | 8.088 |

| Hit# | of | 5 | Tentative ID                  | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide                | 64  | O2S      | 007446-09-5 | 78   |
| 2    |    |   | 2-Aminoethyl hydrogen sulfate | 141 | C2H7N04S | 000926-39-6 | 64   |
| 3    |    |   | Aminomethanesulfonic acid     | 111 | CH5N03S  | 013881-91-9 | 64   |
| 4    |    |   | L-Alanine, 3-sulfo-           | 169 | C3H7N05S | 000498-40-8 | 9    |
| 5    |    |   | Ethene, 1,2-difluoro-         | 64  | C2H2F2   | 001691-13-0 | 5    |



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Instrument :  
MSVOA\_N  
ClientSampleId :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N122721W.M  
Quant Title : SW846 8260

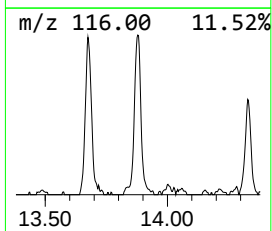
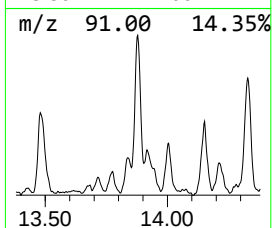
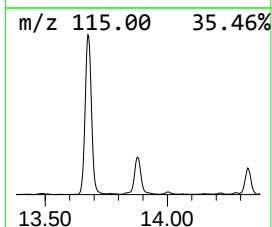
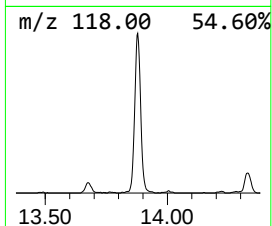
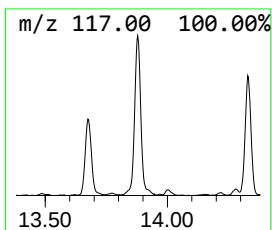
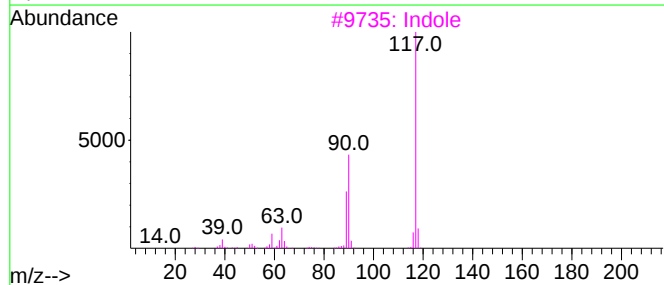
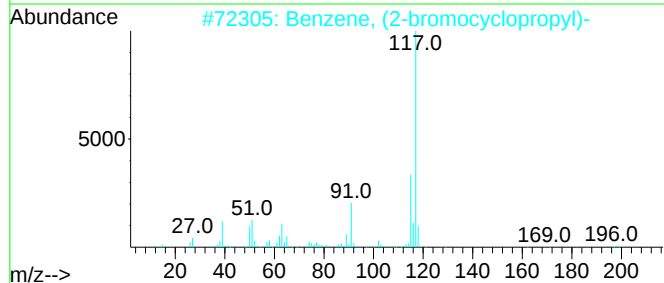
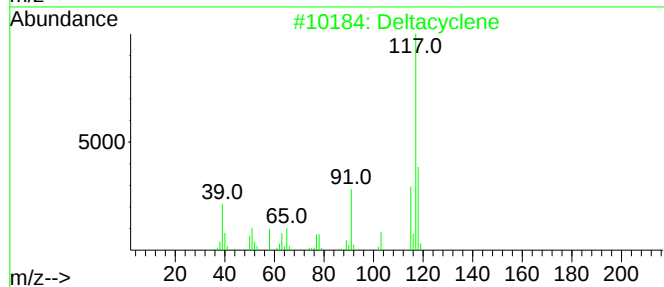
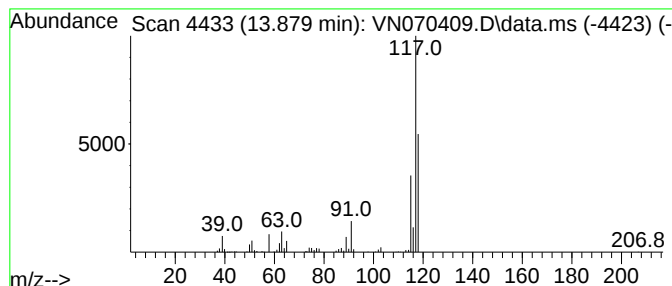
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Benzene, (2-bromocyclopropyl)- Concentration Rank 1

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 13.879 | 6.84 ug/l | 408673 | 1,4-Dichlorobenzene-d4 | 13.675 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|-----|---------|-------------|------|
| 1    |    |   | Deltacyclene                   | 118 | C9H10   | 007785-10-6 | 59   |
| 2    |    |   | Benzene, (2-bromocyclopropyl)- | 196 | C9H9Br  | 036617-02-4 | 50   |
| 3    |    |   | Indole                         | 117 | C8H7N   | 000120-72-9 | 47   |
| 4    |    |   | Benzonitrile, 2-methyl-        | 117 | C8H7N   | 000529-19-1 | 43   |
| 5    |    |   | trans-Cinnamyl bromide         | 196 | C9H9Br  | 026146-77-0 | 42   |



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ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
MW-62

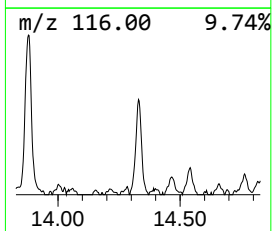
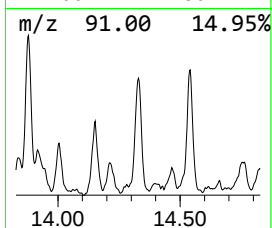
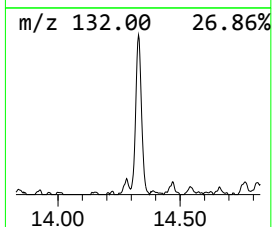
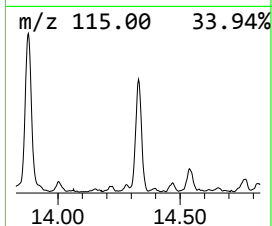
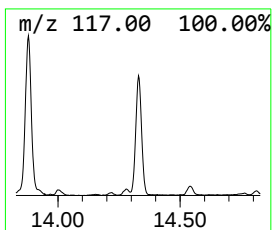
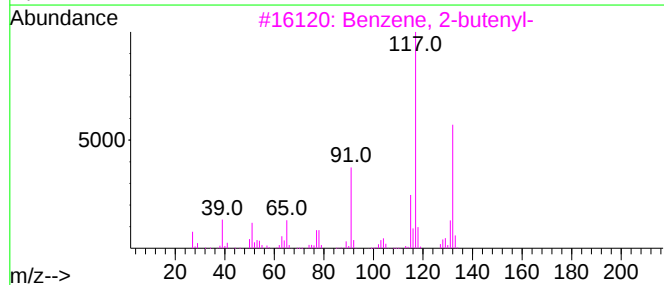
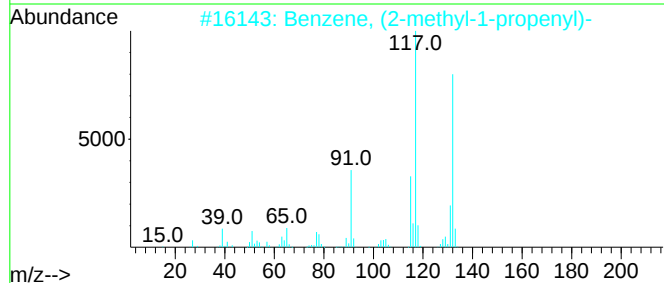
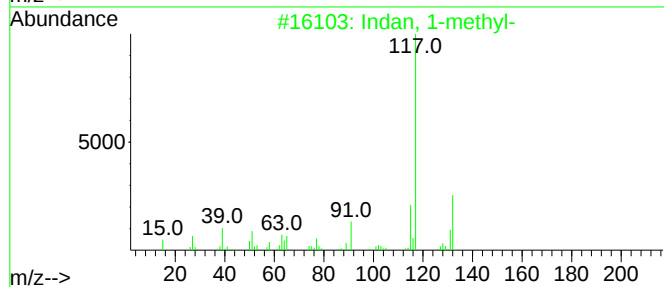
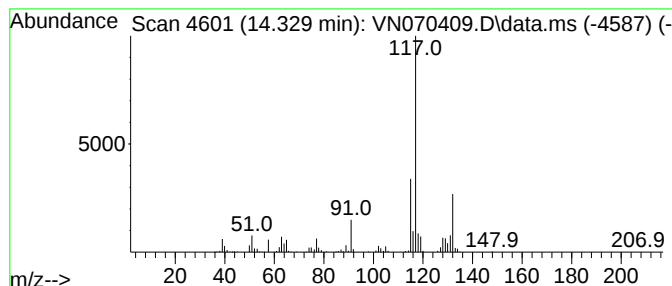
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N122721W.M  
Quant Title : SW846 8260

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

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

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 14.329 | 6.73 ug/l | 402148 | 1,4-Dichlorobenzene-d4 | 13.675 |

| Hit# | of 5 | Tentative ID                    | MW  | MolForm | CAS#        | Qual |
|------|------|---------------------------------|-----|---------|-------------|------|
| 1    |      | Indan, 1-methyl-                | 132 | C10H12  | 000767-58-8 | 81   |
| 2    |      | Benzene, (2-methyl-1-propenyl)- | 132 | C10H12  | 000768-49-0 | 78   |
| 3    |      | Benzene, 2-butenyl-             | 132 | C10H12  | 001560-06-1 | 78   |
| 4    |      | 3-Phenylbut-1-ene               | 132 | C10H12  | 000934-10-1 | 72   |
| 5    |      | Benzene, 1-ethenyl-4-ethyl-     | 132 | C10H12  | 003454-07-7 | 72   |



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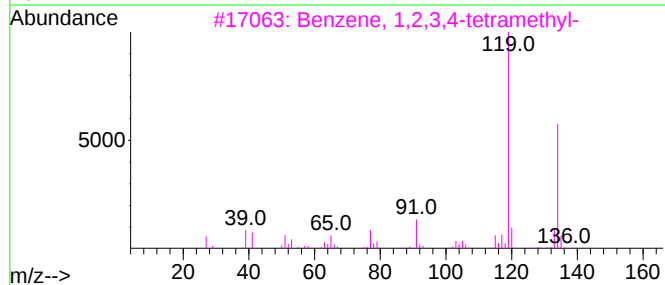
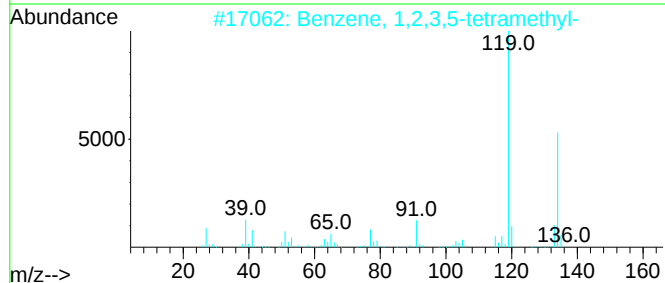
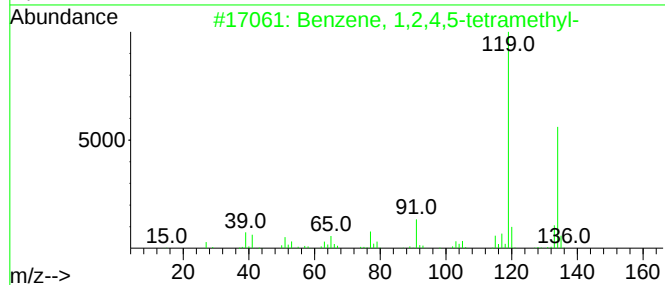
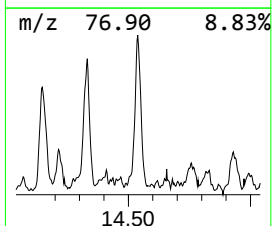
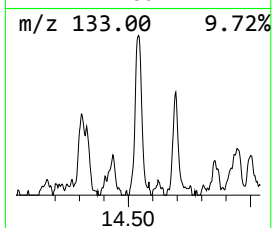
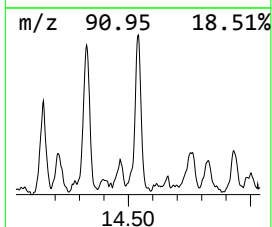
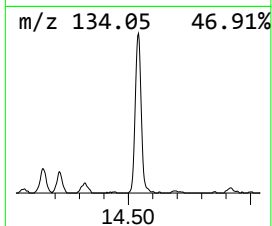
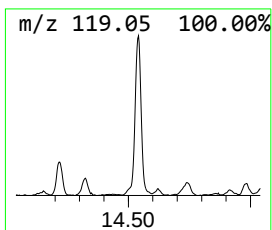
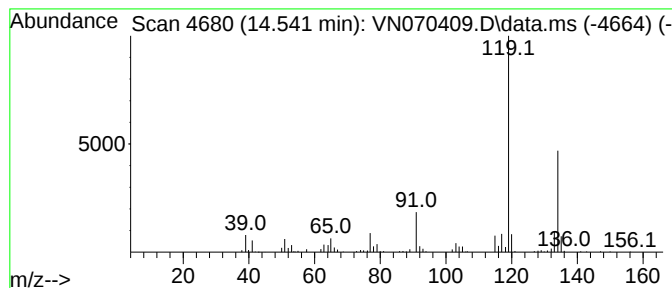
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 4

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 14.541 | 5.42 ug/l | 323855 | 1,4-Dichlorobenzene-d4 | 13.675 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|-----|---------|-------------|------|
| 1    |    |   | Benzene, 1,2,4,5-tetramethyl-  | 134 | C10H14  | 000095-93-2 | 96   |
| 2    |    |   | Benzene, 1,2,3,5-tetramethyl-  | 134 | C10H14  | 000527-53-7 | 94   |
| 3    |    |   | Benzene, 1,2,3,4-tetramethyl-  | 134 | C10H14  | 000488-23-3 | 94   |
| 4    |    |   | Benzene, 1-ethyl-2,3-dimethyl- | 134 | C10H14  | 000933-98-2 | 91   |
| 5    |    |   | Benzene, 2-ethyl-1,4-dimethyl- | 134 | C10H14  | 001758-88-9 | 90   |



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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     | 2.236  | 5.8     | ug/l  | 288572   | 1                     | 8.088  | 2485330 | 50.0 |
| Benzene, (2-bro... | 13.879 | 6.8     | ug/l  | 408673   | 4                     | 13.675 | 2987660 | 50.0 |
| Indan, 1-methyl-   | 14.329 | 6.7     | ug/l  | 402148   | 4                     | 13.675 | 2987660 | 50.0 |
| Benzene, 1,2,4,... | 14.541 | 5.4     | ug/l  | 323855   | 4                     | 13.675 | 2987660 | 50.0 |