

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN102621\  
 Data File : VN069166.D  
 Acq On : 25 Oct 2021 21:30  
 Operator : JC/MD  
 Sample : M4284-06  
 Misc : 5.00mL/MSVOA\_N/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 20878-WATER

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\82N101221W.M  
 Title : SW846 8260

Signal : TIC: VN069166.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         | 2.295       | 94            | 114         | 128          | rBV      | 318365         | 1080331       | 51.93%          | 6.770%        |
| 2         | 4.288       | 836           | 857         | 876          | rBV      | 161437         | 475280        | 22.85%          | 2.978%        |
| 3         | 4.540       | 926           | 951         | 987          | rBV      | 508404         | 1642486       | 78.96%          | 10.293%       |
| 4         | 7.313       | 1963          | 1985        | 2013         | rBV3     | 83974          | 270394        | 13.00%          | 1.695%        |
| 5         | 8.024       | 2227          | 2250        | 2261         | rBV2     | 256140         | 609387        | 29.29%          | 3.819%        |
| 6         | 8.088       | 2262          | 2274        | 2304         | rVB      | 490389         | 1118752       | 53.78%          | 7.011%        |
| 7         | 8.442       | 2384          | 2406        | 2430         | rBV      | 279495         | 664226        | 31.93%          | 4.163%        |
| 8         | 8.971       | 2583          | 2603        | 2636         | rBV      | 719826         | 1487862       | 71.52%          | 9.324%        |
| 9         | 10.443      | 3134          | 3152        | 3167         | rBV      | 1125354        | 2080209       | 100.00%         | 13.036%       |
| 10        | 10.507      | 3168          | 3176        | 3201         | rVB      | 77880          | 150354        | 7.23%           | 0.942%        |
| 11        | 11.746      | 3621          | 3638        | 3664         | rBV      | 1034783        | 1895524       | 91.12%          | 11.879%       |
| 12        | 11.846      | 3664          | 3675        | 3692         | rVB      | 38642          | 66179         | 3.18%           | 0.415%        |
| 13        | 11.950      | 3701          | 3714        | 3737         | rVB2     | 91829          | 178515        | 8.58%           | 1.119%        |
| 14        | 12.283      | 3823          | 3838        | 3854         | rBV      | 48685          | 84747         | 4.07%           | 0.531%        |
| 15        | 12.733      | 3990          | 4006        | 4029         | rBV      | 827239         | 1425728       | 68.54%          | 8.935%        |
| 16        | 12.986      | 4089          | 4100        | 4109         | rBV      | 40724          | 69679         | 3.35%           | 0.437%        |
| 17        | 13.063      | 4120          | 4129        | 4143         | rVB2     | 24066          | 38296         | 1.84%           | 0.240%        |
| 18        | 13.222      | 4170          | 4188        | 4203         | rBV      | 18815          | 34512         | 1.66%           | 0.216%        |
| 19        | 13.369      | 4232          | 4243        | 4257         | rBV      | 72029          | 112121        | 5.39%           | 0.703%        |
| 20        | 13.618      | 4325          | 4336        | 4343         | rBV2     | 18677          | 27900         | 1.34%           | 0.175%        |
| 21        | 13.677      | 4343          | 4358        | 4371         | rVV      | 929279         | 1598578       | 76.85%          | 10.018%       |
| 22        | 13.742      | 4372          | 4382        | 4411         | rVB      | 283868         | 513509        | 24.69%          | 3.218%        |
| 23        | 13.879      | 4421          | 4433        | 4441         | rBV4     | 19752          | 34973         | 1.68%           | 0.219%        |
| 24        | 14.536      | 4666          | 4678        | 4689         | rBV7     | 18203          | 38264         | 1.84%           | 0.240%        |
| 25        | 14.930      | 4811          | 4825        | 4840         | rBV5     | 14604          | 30667         | 1.47%           | 0.192%        |
| 26        | 15.204      | 4911          | 4927        | 4956         | rVB3     | 97240          | 201072        | 9.67%           | 1.260%        |
| 27        | 15.507      | 5027          | 5040        | 5054         | rBV2     | 14888          | 27528         | 1.32%           | 0.173%        |

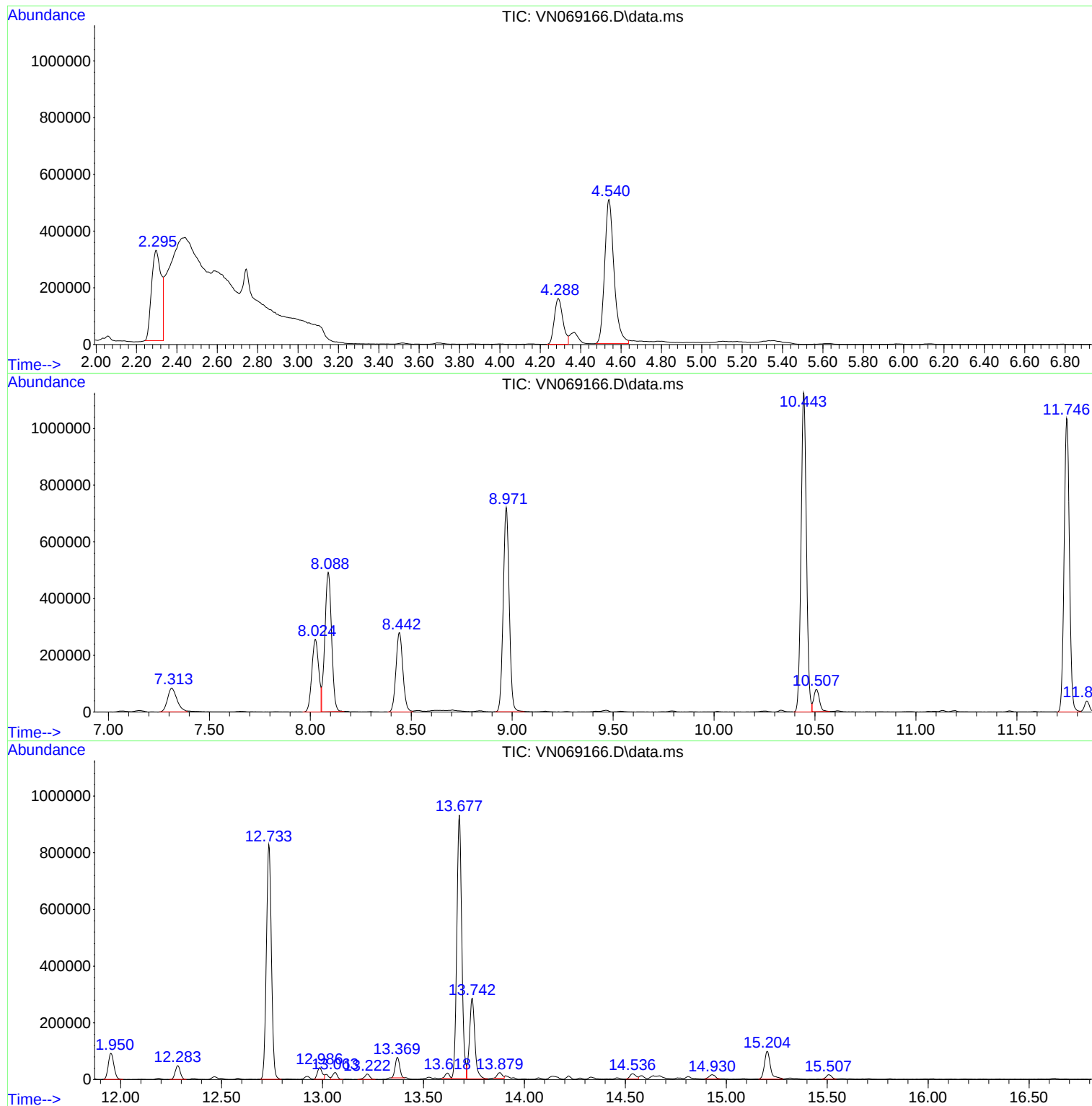
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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
20878-WATER

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N101221W.M  
Quant Title : SW846 8260

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



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ClientSampleId :  
20878-WATER

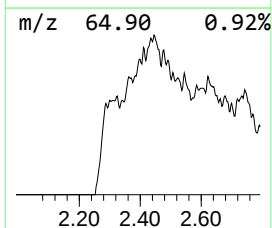
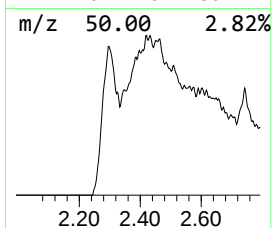
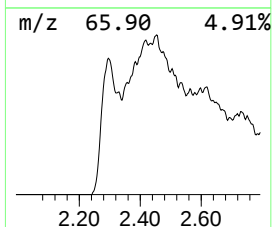
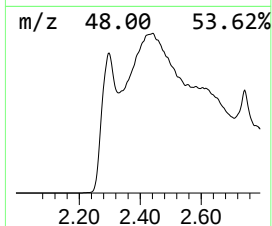
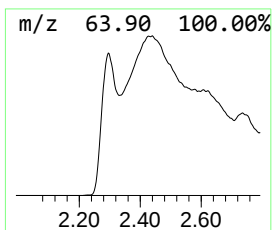
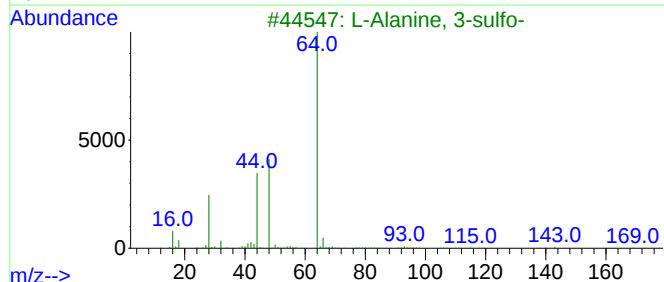
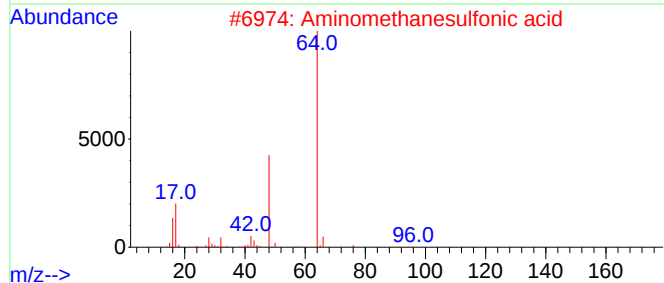
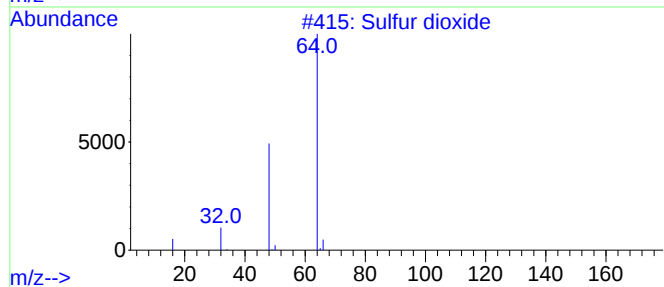
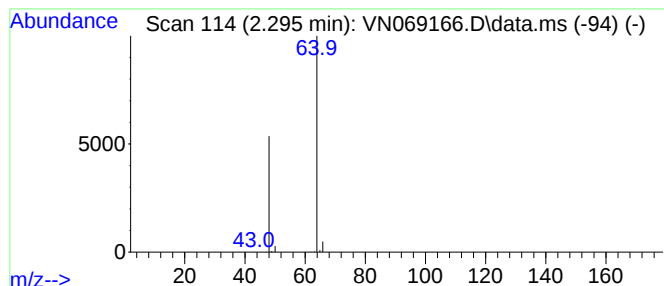
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N101221W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Sulfur dioxide Concentration Rank 1

| R.T.  | EstConc    | Area    | Relative to ISTD   | R.T.  |
|-------|------------|---------|--------------------|-------|
| 2.295 | 48.28 ug/l | 1080330 | Pentafluorobenzene | 8.088 |

| 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    |    |   | Ethene, 1,1-difluoro-     | 64  | C2H2F2   | 000075-38-7 | 4    |
| 5    |    |   | Ethyl Chloride            | 64  | C2H5Cl   | 000075-00-3 | 3    |



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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
20878-WATER

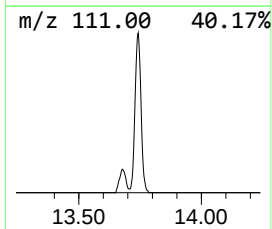
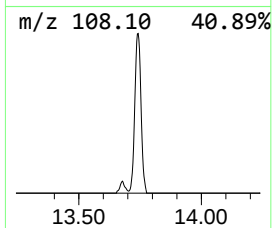
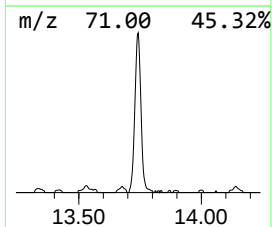
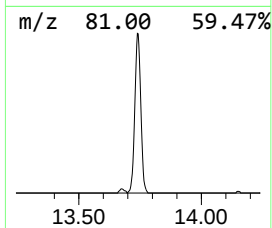
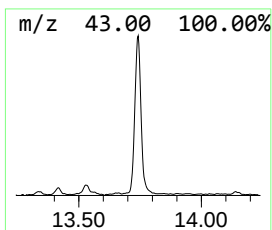
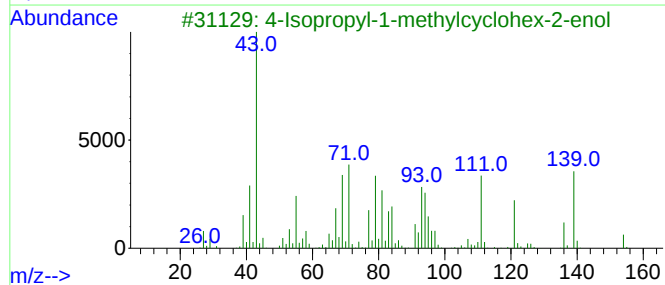
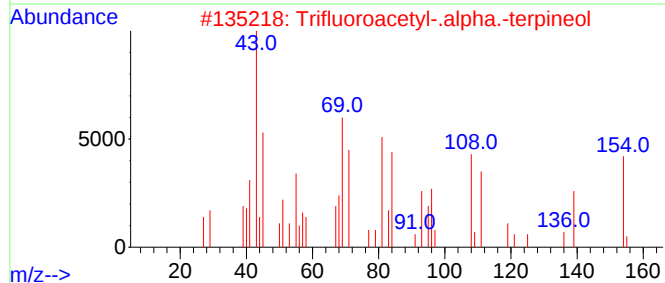
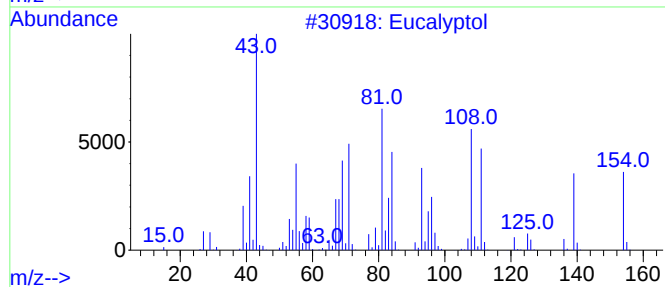
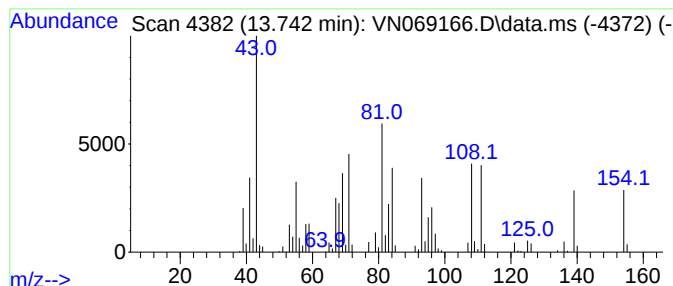
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Quant Title : SW846 8260

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

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Peak Number 2 Eucalyptol Concentration Rank 2

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 13.742 | 16.06 ug/l | 513509 | 1,4-Dichlorobenzene-d4 | 13.678 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Eucalyptol                          | 154 | C10H18O    | 000470-82-6  | 99   |
| 2    |    |   | Trifluoroacetyl-.alpha.-terpineol   | 250 | C12H17F3O2 | 1000058-17-6 | 68   |
| 3    |    |   | 4-Isopropyl-1-methylcyclohex-2-enol | 154 | C10H18O    | 000619-62-5  | 35   |
| 4    |    |   | 1-Hepten-6-one, 2-methyl-           | 126 | C8H14O     | 010408-15-8  | 27   |
| 5    |    |   | 2-Isopropyl-5-methylhex-2-enal      | 154 | C10H18O    | 035158-25-9  | 27   |



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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
20878-WATER

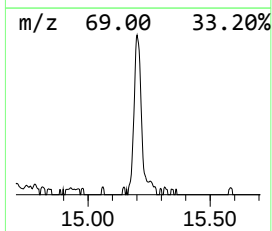
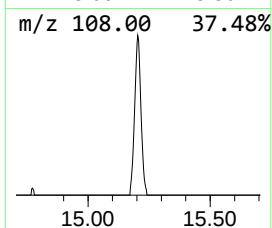
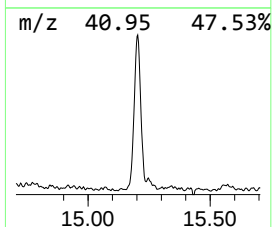
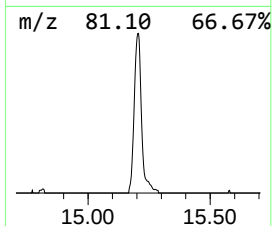
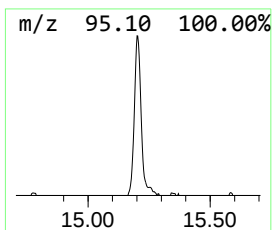
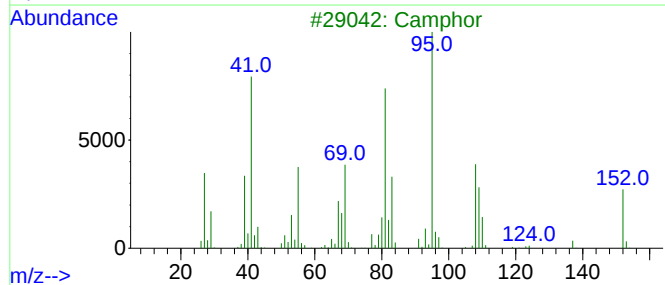
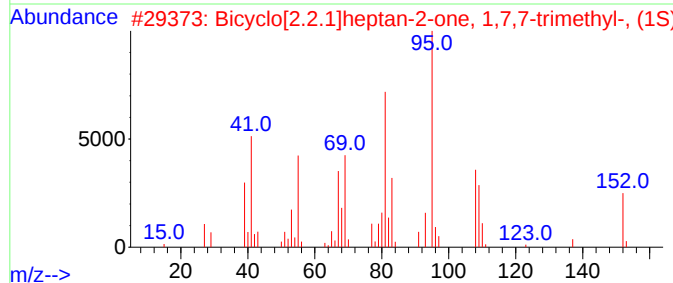
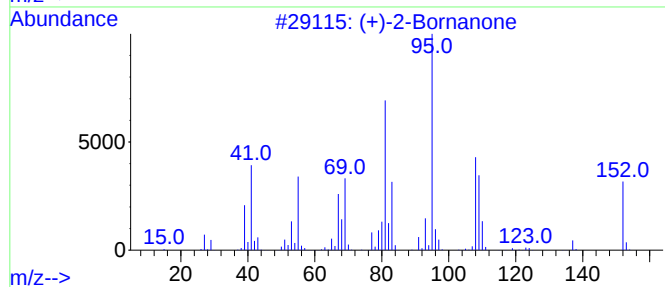
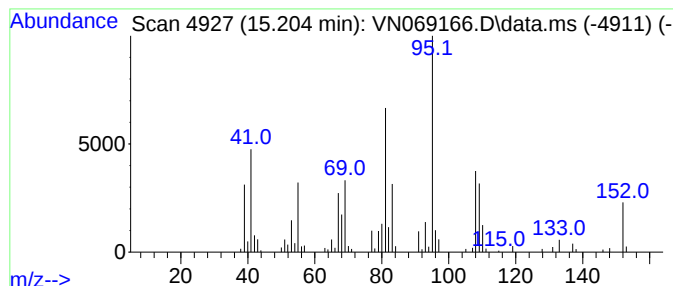
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Quant Title : SW846 8260

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

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Peak Number 3 (+)-2-Bornanone Concentration Rank 3

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 15.204 | 6.29 ug/l | 201072 | 1,4-Dichlorobenzene-d4 | 13.678 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | (+)-2-Bornanone                     | 152 | C10H16O | 000464-49-3 | 98   |
| 2    |    |   | Bicyclo[2.2.1]heptan-2-one, 1,7,... | 152 | C10H16O | 000464-48-2 | 98   |
| 3    |    |   | Camphor                             | 152 | C10H16O | 000076-22-2 | 98   |
| 4    |    |   | 1-(1-Propynyl)cyclohexanol          | 138 | C9H14O  | 000697-37-0 | 49   |
| 5    |    |   | 2-Butanone, 4-(5-methyl-2-furanyl)- | 152 | C9H12O2 | 013679-56-6 | 49   |



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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
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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   | 2.295  | 48.3    | ug/l  | 1080330  | 1                     | 8.088  | 1118750 | 50.0 |
| Eucalyptol       | 13.742 | 16.1    | ug/l  | 513509   | 4                     | 13.678 | 1598580 | 50.0 |
| (+)-2-Bornanone  | 15.204 | 6.3     | ug/l  | 201072   | 4                     | 13.678 | 1598580 | 50.0 |