

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN111124\  
 Data File : VN084764.D  
 Acq On : 11 Nov 2024 12:06  
 Operator : JC\MD  
 Sample : VN1111MBL01  
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 VN1111MBL01

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\82N103024W.M  
 Title : SW846 8260

Signal : TIC: VN084764.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         | 2.283       | 51            | 56          | 65           | rBV2     | 14541          | 33794         | 4.39%           | 0.777%        |
| 2         | 2.912       | 153           | 163         | 168          | rVB7     | 17344          | 57021         | 7.41%           | 1.311%        |
| 3         | 7.218       | 888           | 895         | 903          | rBV      | 2947           | 8346          | 1.08%           | 0.192%        |
| 4         | 8.165       | 1046          | 1056        | 1060         | rBV      | 116519         | 272434        | 35.40%          | 6.265%        |
| 5         | 8.224       | 1060          | 1066        | 1077         | rVB      | 204015         | 453807        | 58.96%          | 10.436%       |
| 6         | 8.571       | 1117          | 1125        | 1137         | rBV      | 124123         | 276233        | 35.89%          | 6.352%        |
| 7         | 9.100       | 1206          | 1215        | 1225         | rBV      | 284923         | 583981        | 75.88%          | 13.430%       |
| 8         | 10.565      | 1456          | 1464        | 1472         | rBV      | 429629         | 769657        | 100.00%         | 17.700%       |
| 9         | 11.865      | 1677          | 1685        | 1697         | rBV      | 371539         | 660561        | 85.83%          | 15.191%       |
| 10        | 12.070      | 1714          | 1720        | 1725         | rVB2     | 5904           | 11563         | 1.50%           | 0.266%        |
| 11        | 12.400      | 1771          | 1776        | 1784         | rBB3     | 6272           | 11760         | 1.53%           | 0.270%        |
| 12        | 12.847      | 1844          | 1852        | 1863         | rBV      | 295953         | 490010        | 63.67%          | 11.269%       |
| 13        | 12.976      | 1869          | 1874        | 1879         | rVB3     | 7228           | 12285         | 1.60%           | 0.283%        |
| 14        | 13.035      | 1879          | 1884        | 1891         | rVB2     | 5776           | 8750          | 1.14%           | 0.201%        |
| 15        | 13.223      | 1911          | 1916        | 1924         | rVB3     | 8564           | 13477         | 1.75%           | 0.310%        |
| 16        | 13.735      | 1997          | 2003        | 2006         | rBV3     | 13286          | 21938         | 2.85%           | 0.505%        |
| 17        | 13.788      | 2006          | 2012        | 2023         | rVB      | 329672         | 580029        | 75.36%          | 13.339%       |
| 18        | 14.058      | 2052          | 2058        | 2062         | rBV      | 8403           | 13086         | 1.70%           | 0.301%        |
| 19        | 14.106      | 2062          | 2066        | 2071         | rVB3     | 7402           | 11890         | 1.54%           | 0.273%        |
| 20        | 15.394      | 2279          | 2285        | 2291         | rVB3     | 11152          | 17847         | 2.32%           | 0.410%        |
| 21        | 15.500      | 2297          | 2303        | 2310         | rBV3     | 5690           | 7986          | 1.04%           | 0.184%        |
| 22        | 15.635      | 2322          | 2326        | 2335         | rVB2     | 8685           | 15733         | 2.04%           | 0.362%        |
| 23        | 15.841      | 2353          | 2361        | 2368         | rBV5     | 7596           | 16239         | 2.11%           | 0.373%        |

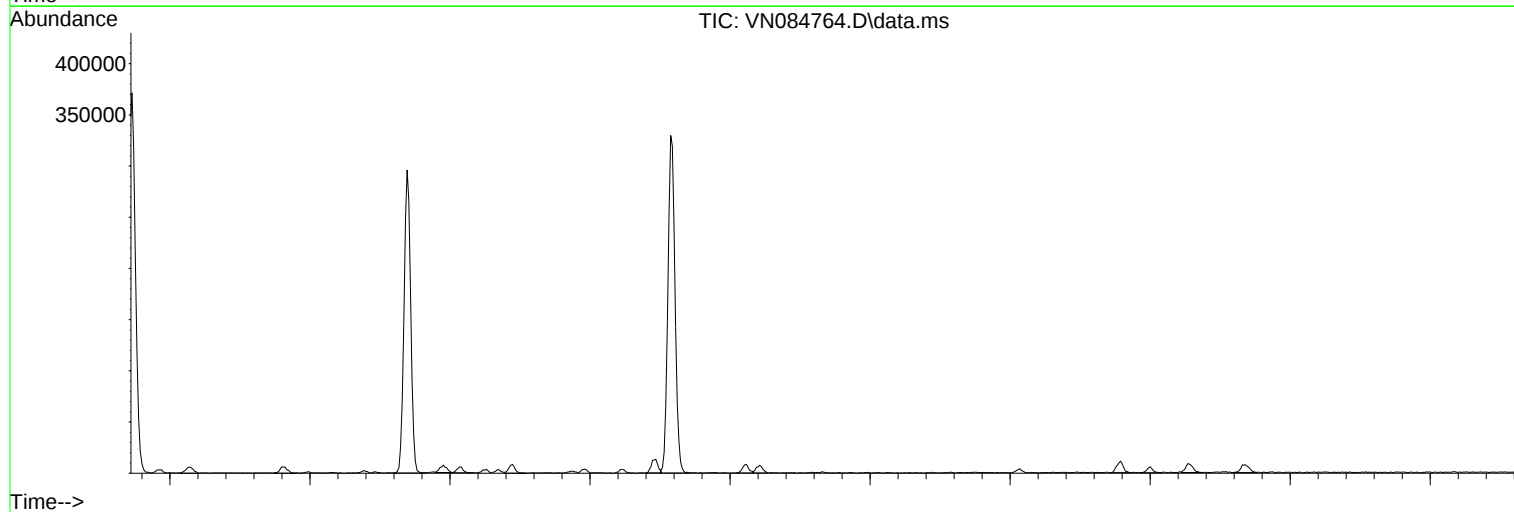
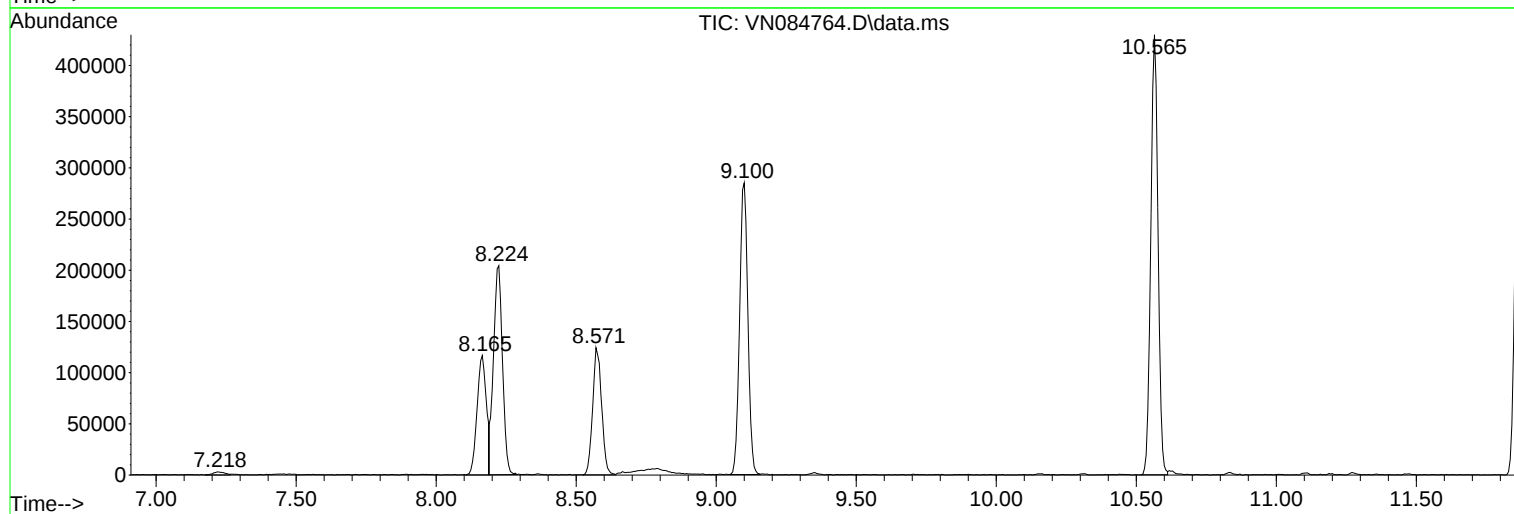
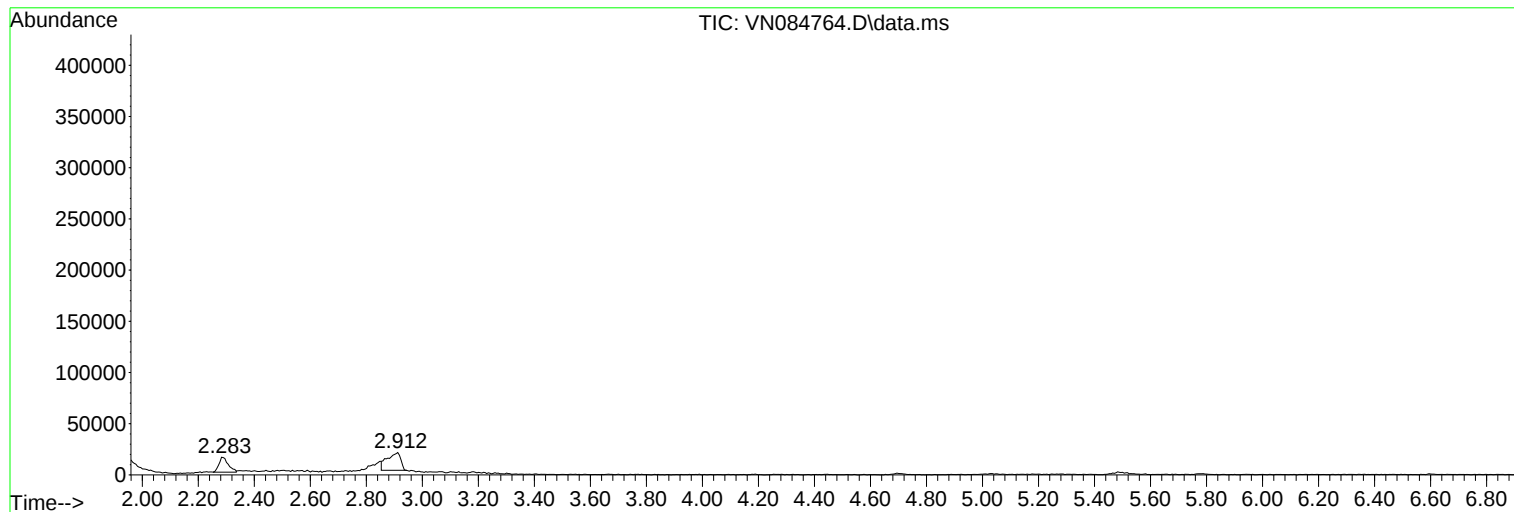
Sum of corrected areas: 4348427

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Instrument :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N103024W.M  
Quant Title : SW846 8260

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



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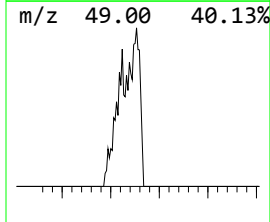
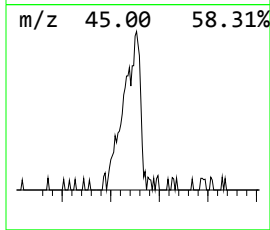
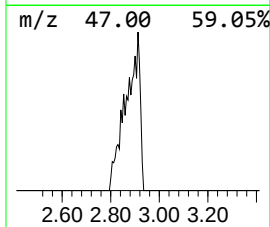
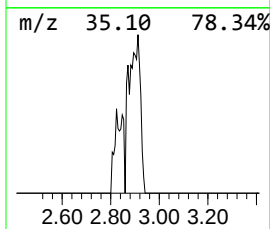
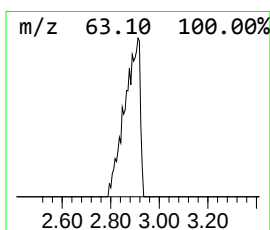
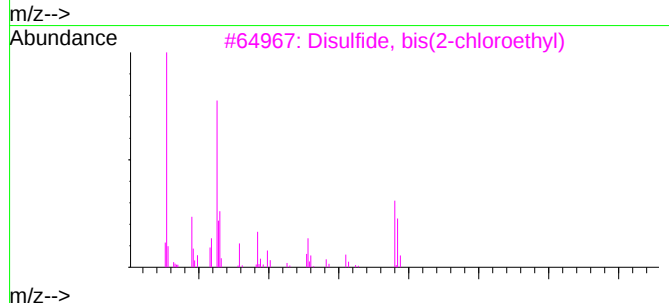
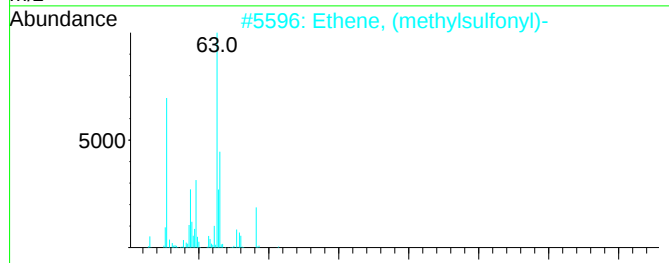
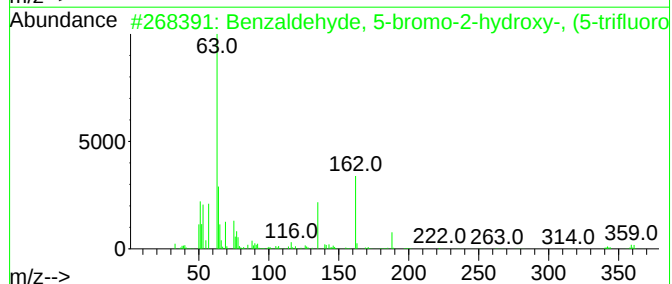
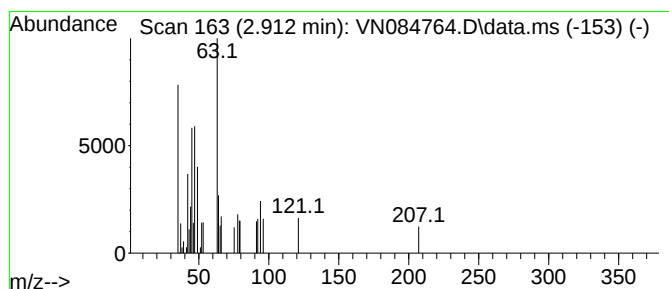
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Peak Number 1 unknown2.912 Concentration Rank 1

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 2.912 | 6.28 ug/l | 57021 | Pentafluorobenzene | 8.224 |

| Hit# of 5 | Tentative ID                        | MW  | MolForm      | CAS#         | Qual |
|-----------|-------------------------------------|-----|--------------|--------------|------|
| 1         | Benzaldehyde, 5-bromo-2-hydroxy-... | 359 | C13H9BrF3N3O | 1000276-33-1 | 12   |
| 2         | Ethene, (methylsulfonyl)-           | 106 | C3H6O2S      | 003680-02-2  | 10   |
| 3         | Disulfide, bis(2-chloroethyl)       | 190 | C4H8Cl2S2    | 001002-41-1  | 10   |
| 4         | 1H-Benzotriazole, 5-nitro-          | 164 | C6H4N4O2     | 002338-12-7  | 9    |
| 5         | 2-Chloroethyl methyl sulfoxide      | 126 | C3H7ClOS     | 005331-57-7  | 9    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown2.912     | 2.912 | 6.3     | ug/l  | 57021    | 1                     | 8.224 | 453807 | 50.0 |