

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN072224\  
Data File : VN083001.D  
Acq On : 22 Jul 2024 13:27  
Operator : JC\MD  
Sample : P3294-01  
Misc : 5.01g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
HR-1-071724

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\82N070824W.M

Title : SW846 8260

Signal : TIC: VN083001.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         | 2.818       | 135           | 147         | 148          | rBV6     | 12345          | 33388         | 7.70%           | 1.351%        |
| 2         | 8.165       | 1047          | 1056        | 1060         | rBV      | 64559          | 150539        | 34.73%          | 6.091%        |
| 3         | 8.218       | 1060          | 1065        | 1077         | rVB      | 104963         | 235135        | 54.25%          | 9.514%        |
| 4         | 8.577       | 1115          | 1126        | 1134         | rBV      | 70099          | 149106        | 34.40%          | 6.033%        |
| 5         | 9.100       | 1207          | 1215        | 1228         | rVB      | 166547         | 335713        | 77.45%          | 13.583%       |
| 6         | 10.565      | 1455          | 1464        | 1472         | rBV      | 230976         | 433449        | 100.00%         | 17.537%       |
| 7         | 11.865      | 1677          | 1685        | 1694         | rBV      | 243610         | 433368        | 99.98%          | 17.534%       |
| 8         | 12.853      | 1845          | 1853        | 1862         | rVB      | 181210         | 305522        | 70.49%          | 12.362%       |
| 9         | 13.794      | 2005          | 2013        | 2020         | rBV      | 245582         | 395340        | 91.21%          | 15.996%       |

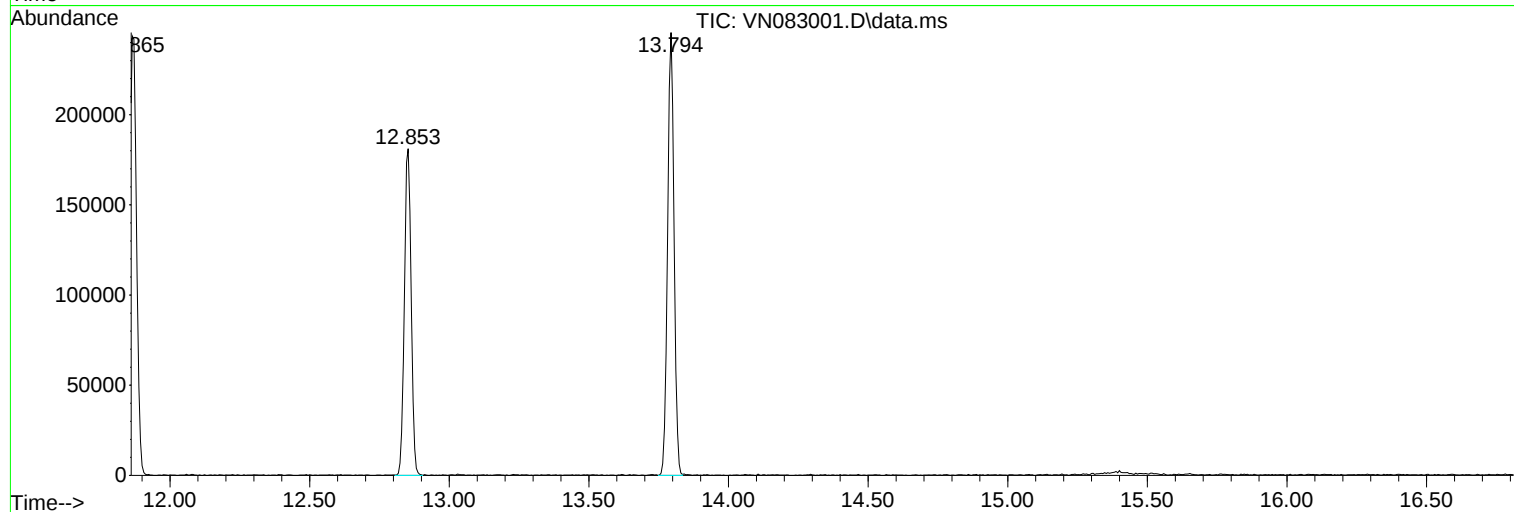
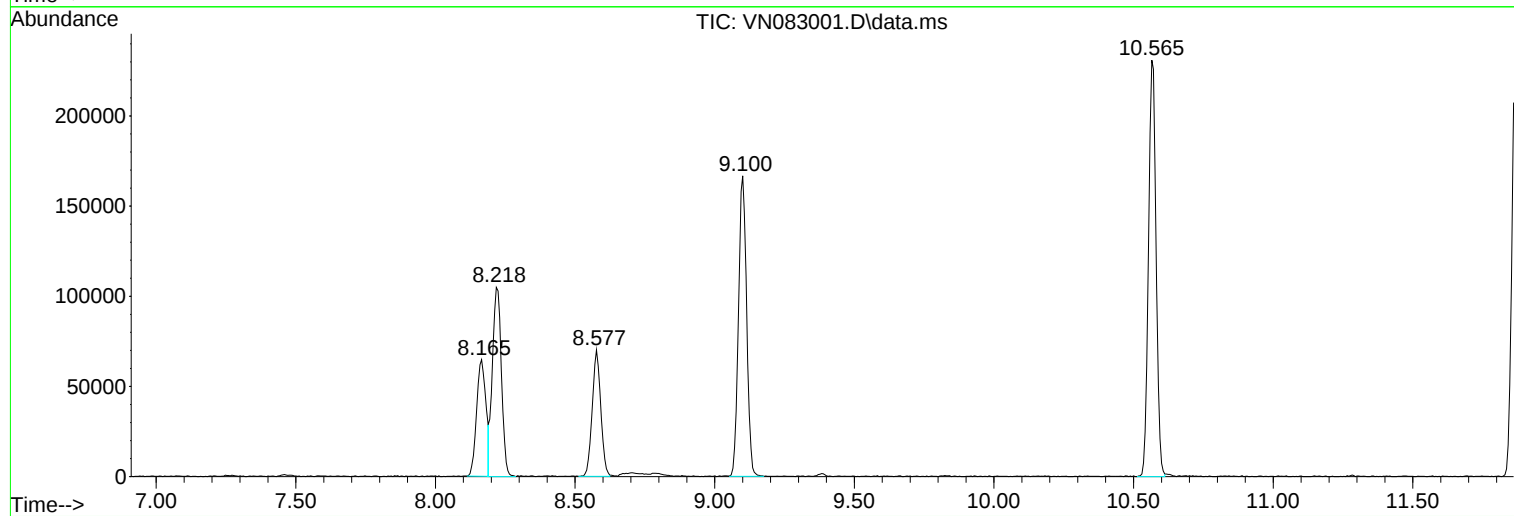
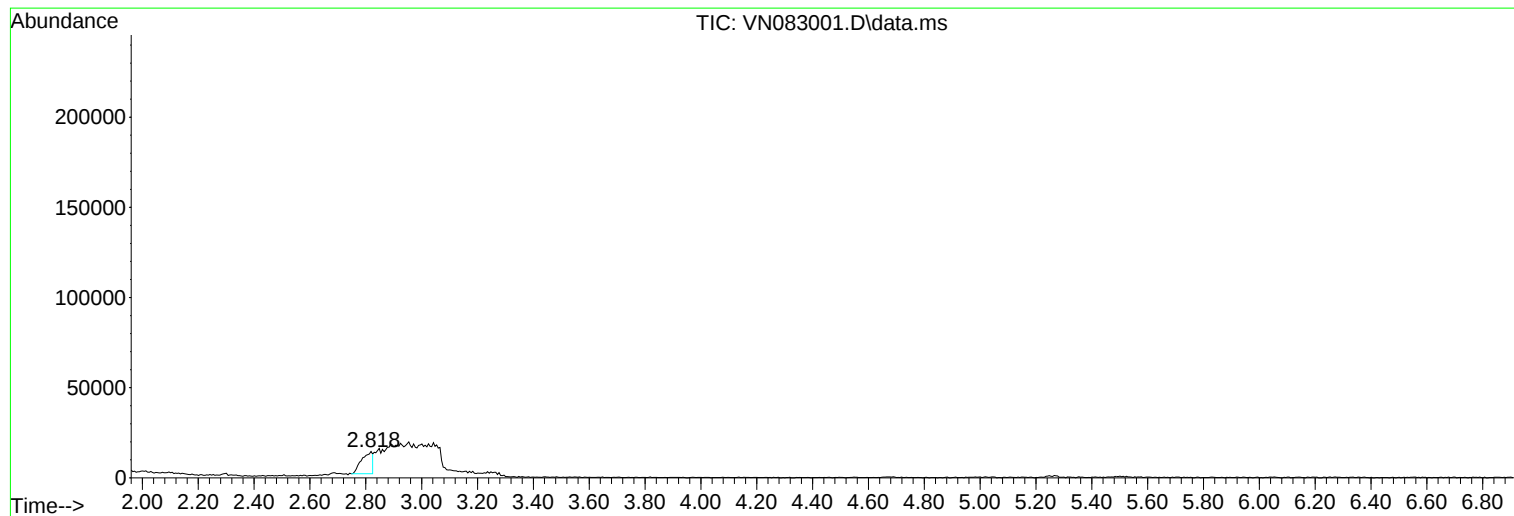
Sum of corrected areas: 2471560

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N070824W.M  
Quant Title : SW846 8260

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



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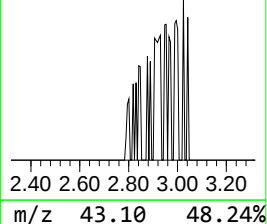
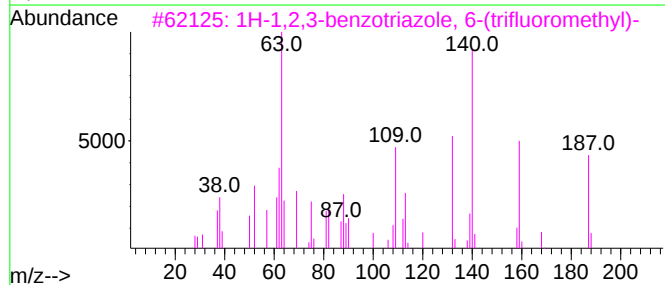
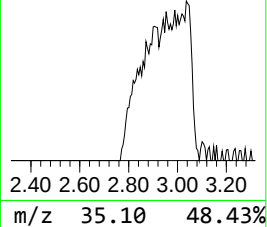
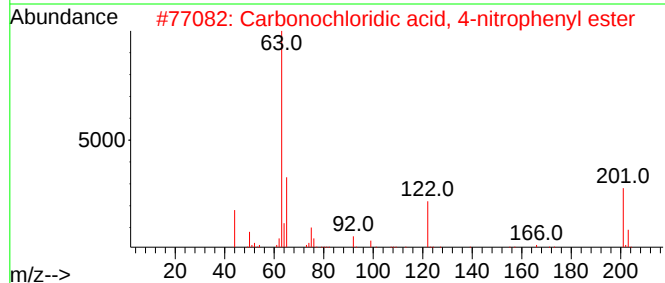
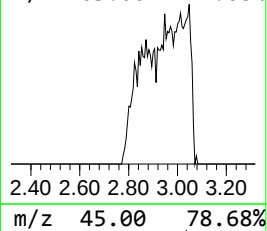
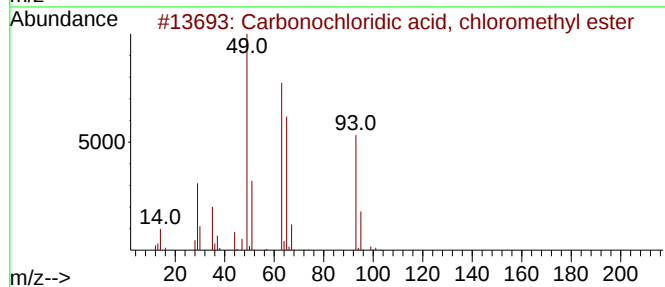
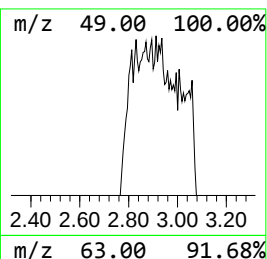
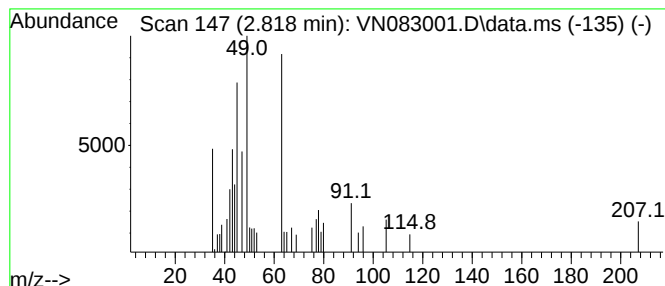
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Peak Number 1 unknown2.818 Concentration Rank 1

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 2.818 | 7.10 ug/l | 33388 | Pentafluorobenzene | 8.218 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Carbonochloridic acid, chloromet... | 128 | C2H2Cl2O2 | 022128-62-7  | 38   |
| 2    |    |   | Carbonochloridic acid, 4-nitroph... | 201 | C7H4ClNO4 | 007693-46-1  | 9    |
| 3    |    |   | 1H-1,2,3-benzotriazole, 6-(trifl... | 187 | C7H4F3N3  | 1000400-13-8 | 9    |
| 4    |    |   | 2-Chloroethyl methyl sulfone        | 142 | C3H7ClO2S | 050890-51-2  | 9    |
| 5    |    |   | 6-Methoxybenzofuroxan               | 166 | C7H6N2O3  | 003524-06-9  | 9    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown2.818     | 2.818 | 7.1     | ug/l  | 33388    | 1                     | 8.218 | 235135 | 50.0 |