

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN091124\  
 Data File : VN083812.D  
 Acq On : 11 Sep 2024 21:57  
 Operator : JC\MD  
 Sample : P3912-01  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 282-COMPOSITE-1

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\82N091024W.M  
 Title : SW846 8260

Signal : TIC: VN083812.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       | 53            | 58          | 74           | rVB3     | 21858          | 63957         | 3.02%           | 0.690%        |
| 2         | 8.165       | 1044          | 1056        | 1061         | rBV      | 101541         | 251980        | 11.91%          | 2.719%        |
| 3         | 8.224       | 1061          | 1066        | 1075         | rVB      | 166131         | 355241        | 16.79%          | 3.834%        |
| 4         | 8.577       | 1117          | 1126        | 1132         | rBV      | 104912         | 239246        | 11.31%          | 2.582%        |
| 5         | 8.665       | 1132          | 1141        | 1148         | rBV4     | 32213          | 136219        | 6.44%           | 1.470%        |
| 6         | 9.100       | 1206          | 1215        | 1226         | rVB      | 290343         | 587655        | 27.78%          | 6.342%        |
| 7         | 10.565      | 1456          | 1464        | 1479         | rVB      | 396949         | 717810        | 33.93%          | 7.746%        |
| 8         | 11.865      | 1677          | 1685        | 1696         | rBV      | 494322         | 869076        | 41.08%          | 9.379%        |
| 9         | 12.847      | 1845          | 1852        | 1863         | rVB      | 383990         | 631044        | 29.83%          | 6.810%        |
| 10        | 13.788      | 2005          | 2012        | 2022         | rVB      | 559850         | 939044        | 44.39%          | 10.134%       |
| 11        | 14.923      | 2200          | 2205        | 2212         | rBV2     | 15969          | 25813         | 1.22%           | 0.279%        |
| 12        | 15.053      | 2217          | 2227        | 2234         | rBV3     | 44734          | 81410         | 3.85%           | 0.879%        |
| 13        | 15.429      | 2282          | 2291        | 2299         | rVB5     | 7179           | 21951         | 1.04%           | 0.237%        |
| 14        | 15.553      | 2306          | 2312        | 2319         | rBV6     | 11242          | 31102         | 1.47%           | 0.336%        |
| 15        | 15.635      | 2319          | 2326        | 2335         | rVV      | 997806         | 1987908       | 93.96%          | 21.452%       |
| 16        | 15.747      | 2335          | 2345        | 2351         | rVV3     | 39825          | 98885         | 4.67%           | 1.067%        |
| 17        | 15.941      | 2372          | 2378        | 2385         | rBV2     | 23741          | 42071         | 1.99%           | 0.454%        |
| 18        | 16.123      | 2399          | 2409        | 2418         | rBV5     | 16734          | 43068         | 2.04%           | 0.465%        |
| 19        | 16.711      | 2503          | 2509        | 2512         | rBV2     | 12854          | 27548         | 1.30%           | 0.297%        |
| 20        | 16.776      | 2512          | 2520        | 2522         | rBV      | 1197155        | 2115633       | 100.00%         | 22.831%       |

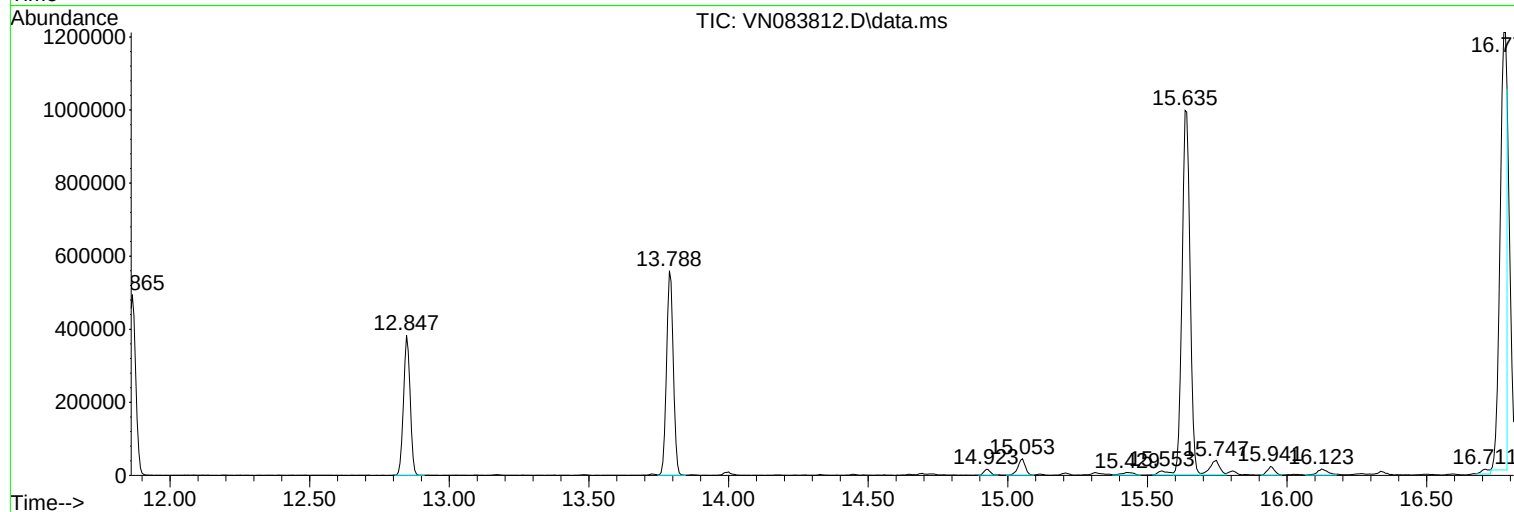
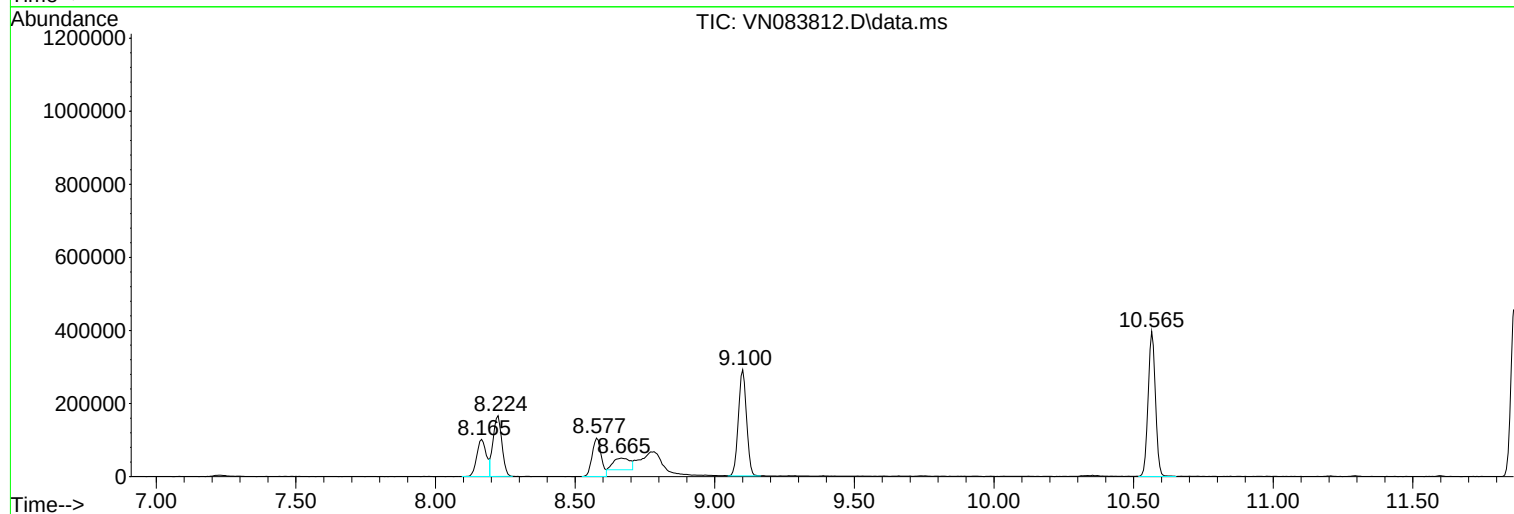
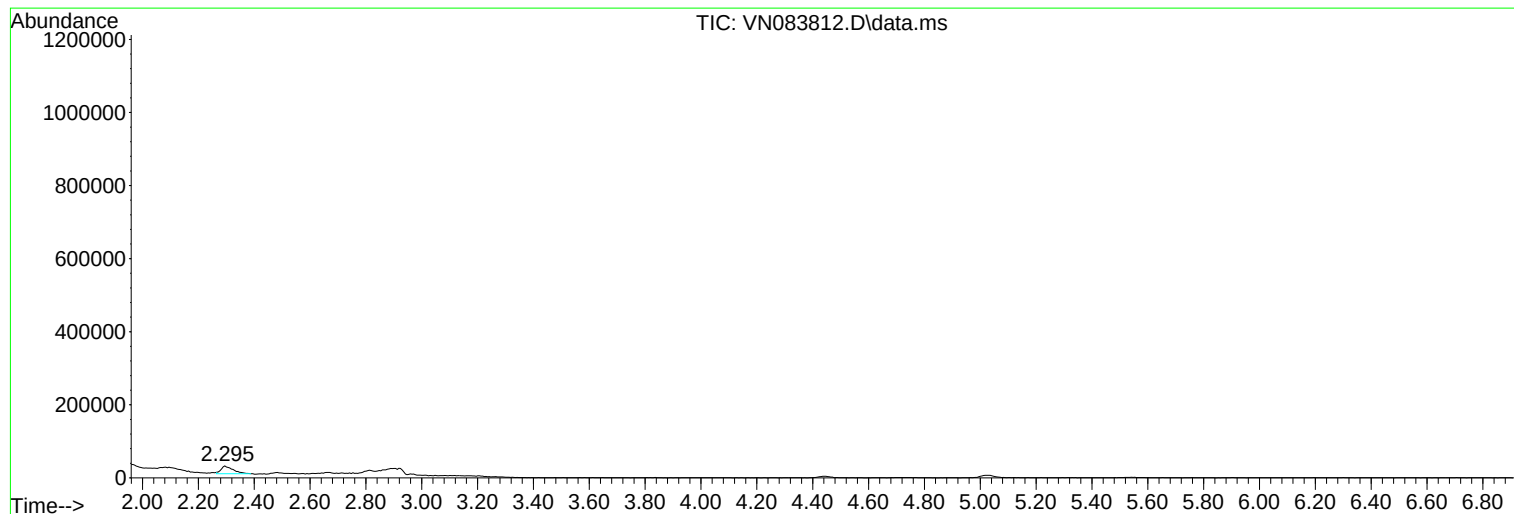
Sum of corrected areas: 9266661

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Instrument :  
MSVOA\_N  
ClientSampleId :  
282-COMPOSITE-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.M  
Quant Title : SW846 8260

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



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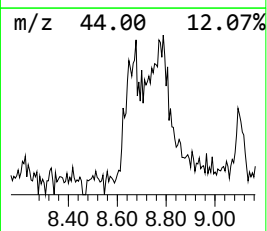
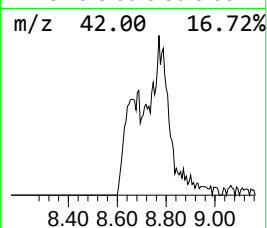
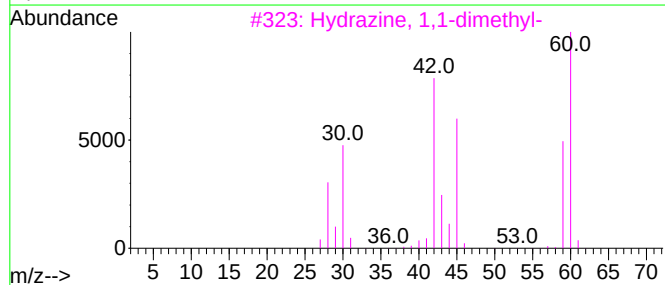
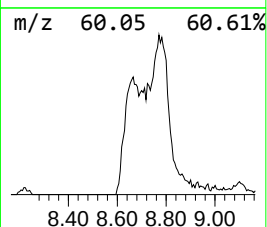
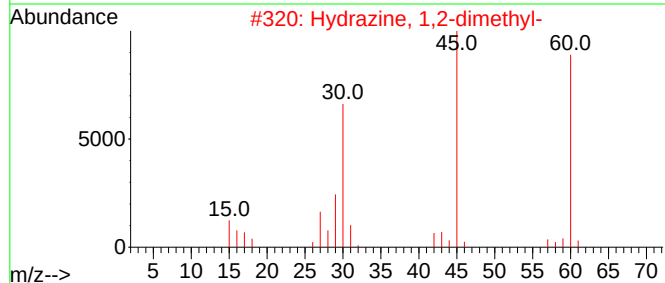
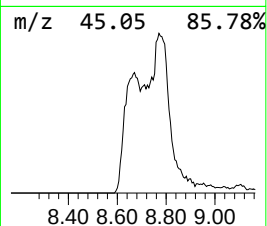
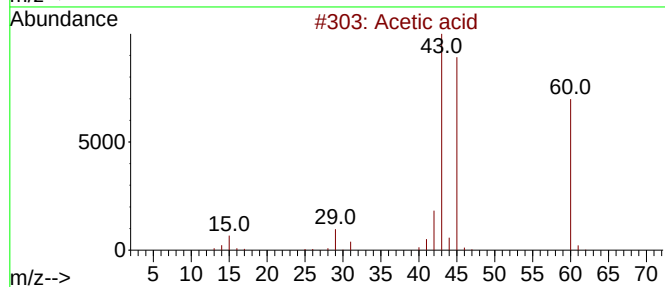
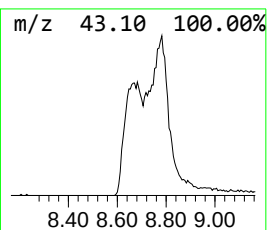
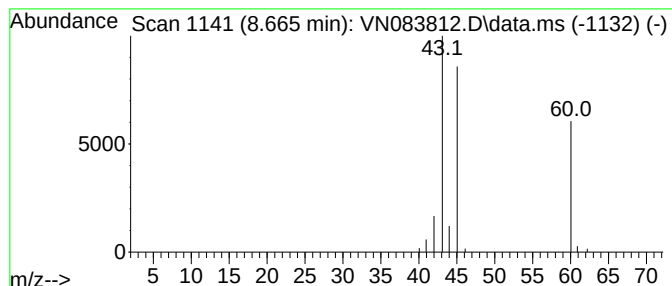
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N091024W.M  
Quant Title : SW846 8260

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

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Peak Number 2 Acetic acid Concentration Rank 2

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 8.665 | 11.59 ug/l | 136219 | 1,4-Difluorobenzene | 9.100 |

| Hit# | of | 5 | Tentative ID             | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------|----|---------|-------------|------|
| 1    |    |   | Acetic acid              | 60 | C2H4O2  | 000064-19-7 | 90   |
| 2    |    |   | Hydrazine, 1,2-dimethyl- | 60 | C2H8N2  | 000540-73-8 | 50   |
| 3    |    |   | Hydrazine, 1,1-dimethyl- | 60 | C2H8N2  | 000057-14-7 | 25   |
| 4    |    |   | Ammonium acetate         | 77 | C2H7NO2 | 000631-61-8 | 9    |
| 5    |    |   | Propanal, 3-methoxy-     | 88 | C4H8O2  | 002806-84-0 | 9    |



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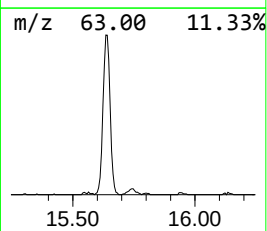
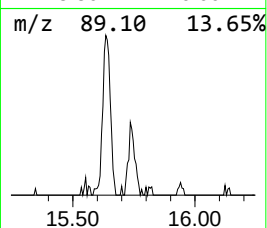
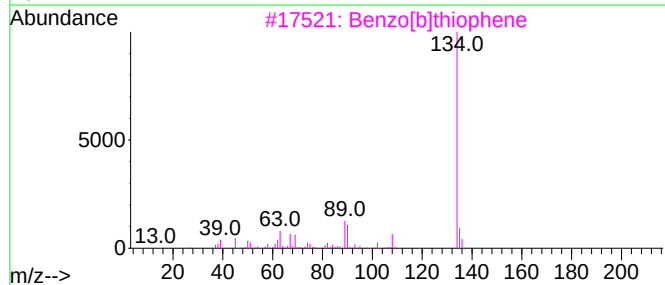
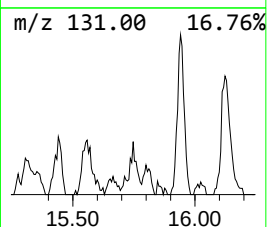
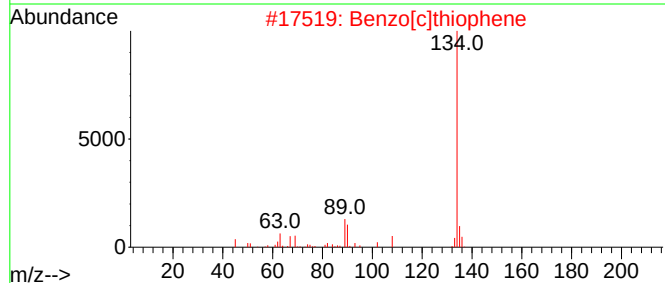
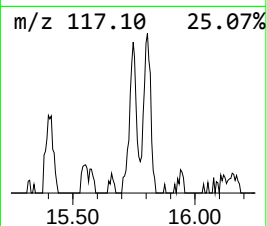
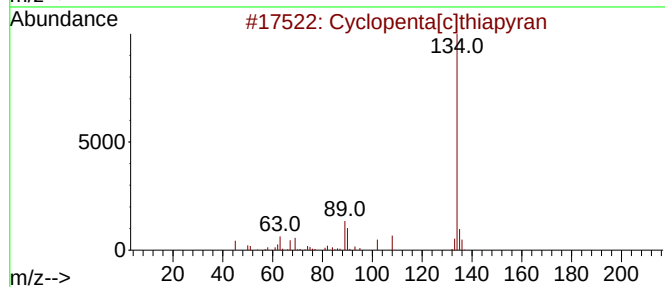
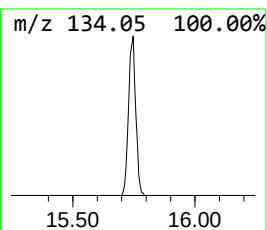
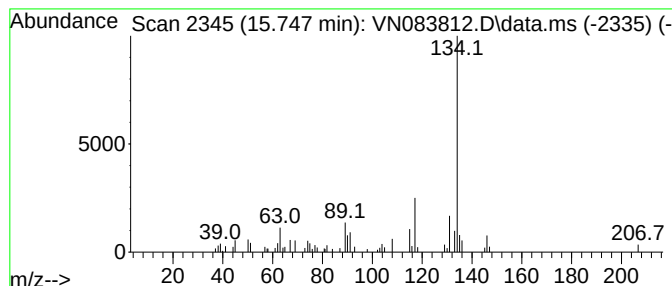
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Peak Number 3 Cyclopenta[c]thiapyran Concentration Rank 4

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 15.747 | 5.27 ug/l | 98885 | 1,4-Dichlorobenzene-d4 | 13.788 |

| Hit# | of | 5 | Tentative ID                 | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclopenta[c]thiapyran       | 134 | C8H6S   | 000270-63-3 | 64   |
| 2    |    |   | Benzo[c]thiophene            | 134 | C8H6S   | 000270-82-6 | 64   |
| 3    |    |   | Benzo[b]thiophene            | 134 | C8H6S   | 000095-15-8 | 64   |
| 4    |    |   | Thiazole, 2-methyl-4-phenyl- | 175 | C10H9NS | 001826-16-0 | 50   |
| 5    |    |   | 3-Deazaadenine               | 134 | C6H6N4  | 006811-77-4 | 47   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Acetic acid        | 8.665  | 11.6    | ug/l  | 136219   | 2                     | 9.100  | 587655 | 50.0 |
| Cyclopenta[c]th... | 15.747 | 5.3     | ug/l  | 98885    | 4                     | 13.788 | 939044 | 50.0 |