

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX112524\  
Data File : VX043986.D  
Acq On : 25 Nov 2024 15:03  
Operator : JC/MD  
Sample : P4886-03  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
Storage-Blank-WATER-REF-4

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X112124W.M  
Title : SW846 8260

Signal : TIC: VX043986.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         | 1.239       | 22            | 25          | 33           | rBV3     | 6734           | 11662         | 1.63%           | 0.311%        |
| 2         | 1.587       | 68            | 82          | 83           | rBV5     | 15135          | 47950         | 6.68%           | 1.280%        |
| 3         | 5.379       | 693           | 704         | 721          | rBV      | 82716          | 246694        | 34.38%          | 6.585%        |
| 4         | 5.544       | 721           | 731         | 744          | rBV      | 124199         | 363968        | 50.72%          | 9.716%        |
| 5         | 5.946       | 785           | 797         | 814          | rBV      | 102175         | 276670        | 38.55%          | 7.385%        |
| 6         | 6.757       | 922           | 930         | 948          | rBV      | 214795         | 525102        | 73.17%          | 14.017%       |
| 7         | 8.647       | 1233          | 1240        | 1258         | rBV      | 434451         | 717635        | 100.00%         | 19.157%       |
| 8         | 10.055      | 1465          | 1471        | 1482         | rBV      | 413142         | 609652        | 84.95%          | 16.274%       |
| 9         | 11.079      | 1634          | 1639        | 1652         | rBV      | 328069         | 439406        | 61.23%          | 11.729%       |
| 10        | 12.018      | 1788          | 1793        | 1806         | rBV      | 393413         | 507428        | 70.71%          | 13.545%       |

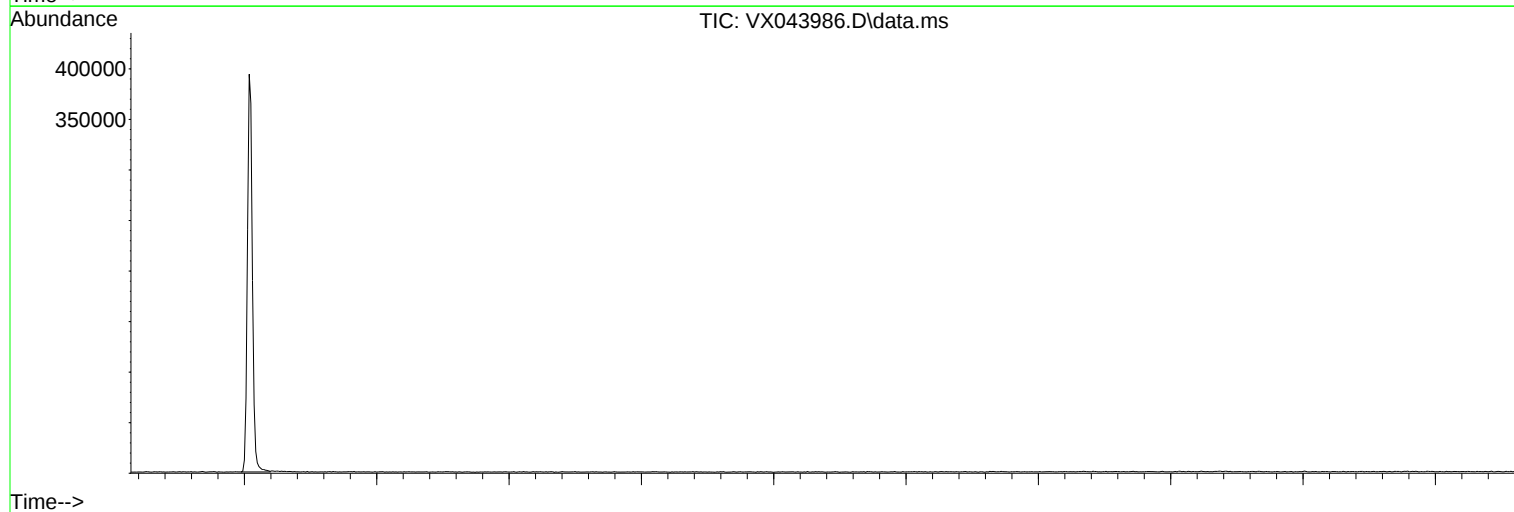
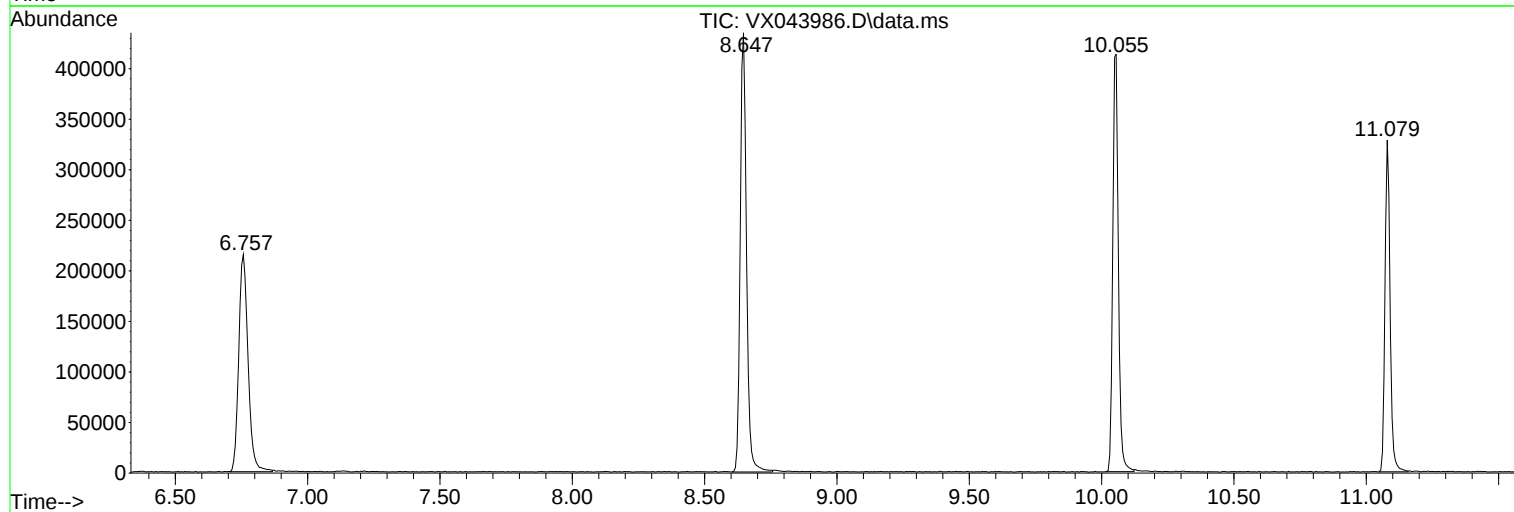
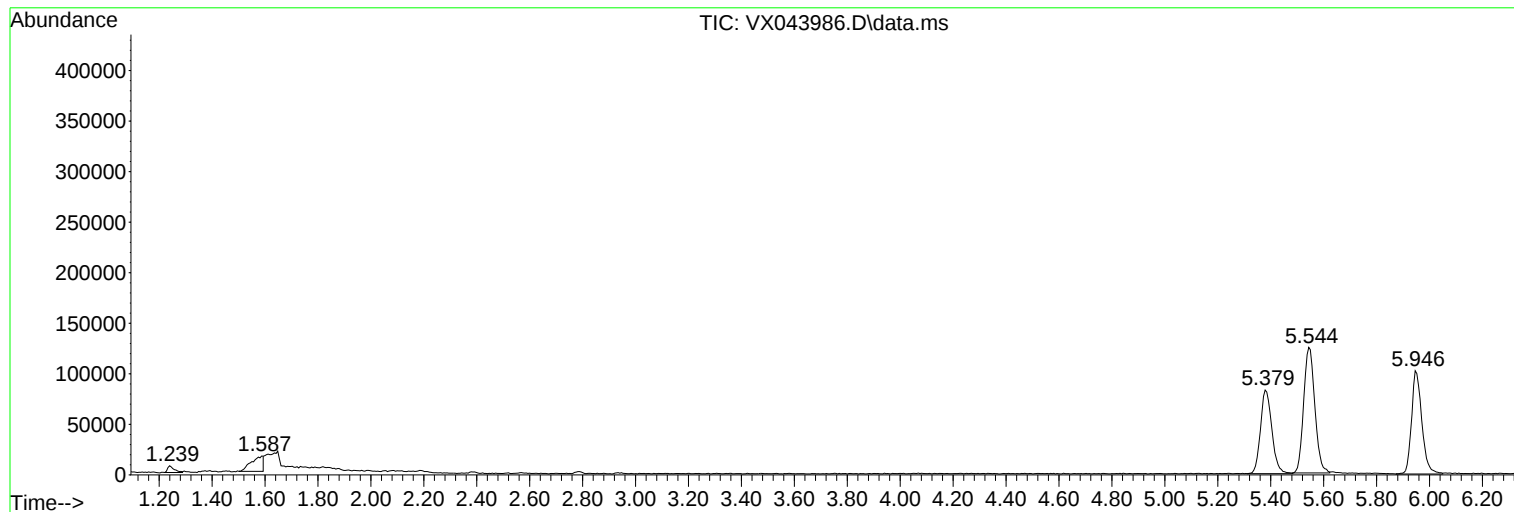
Sum of corrected areas: 3746167

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ClientSampleId :  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X112124W.M  
Quant Title : SW846 8260

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



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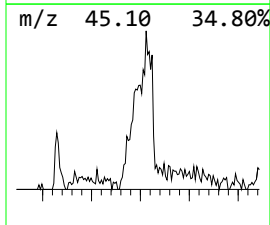
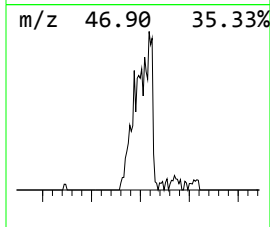
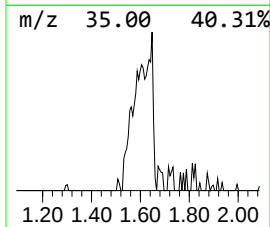
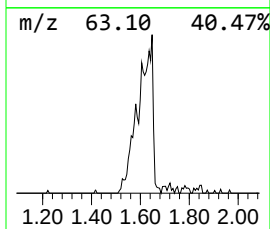
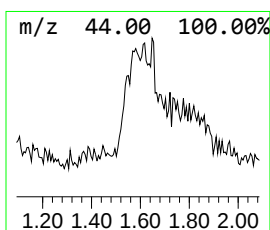
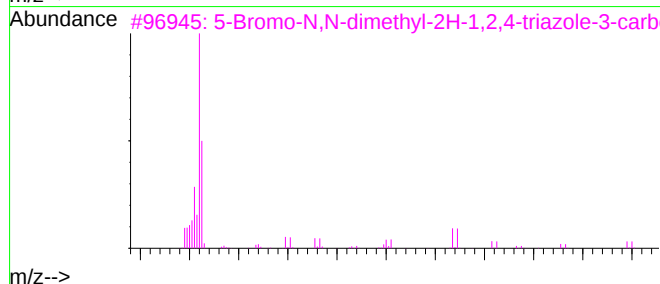
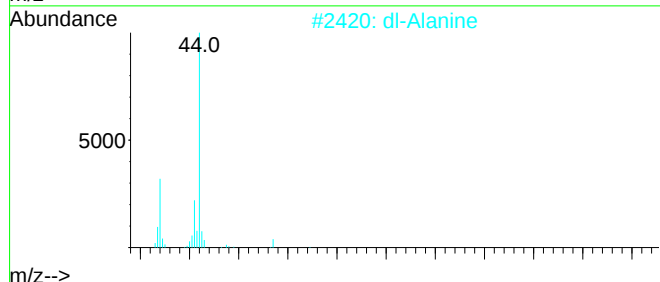
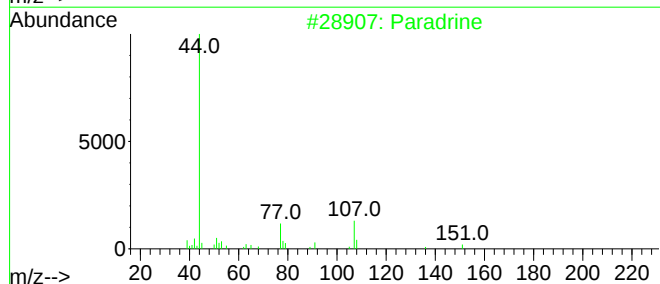
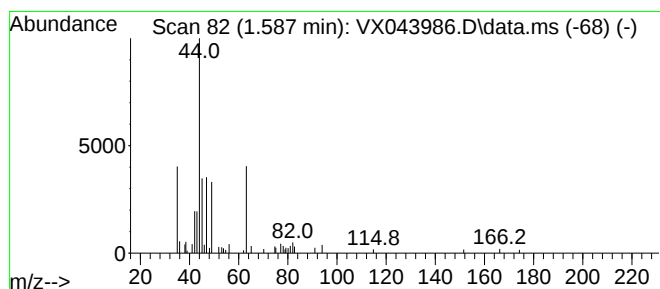
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Peak Number 1 unknown1.587 Concentration Rank 1

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 1.587 | 6.59 ug/l | 47950 | Pentafluorobenzene | 5.550 |

| Hit# of 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|-----------|-------------------------------------|-----|-------------|--------------|------|
| 1         | Paradrine                           | 151 | C9H13NO     | 000103-86-6  | 10   |
| 2         | dL-Alanine                          | 89  | C3H7NO2     | 000302-72-7  | 9    |
| 3         | 5-Bromo-N,N-dimethyl-2H-1,2,4-tr... | 218 | C5H7BrN4O   | 1000387-99-1 | 9    |
| 4         | Ethyl 2-(2-chloroacetamido)-3,3,... | 263 | C7H9ClF3NO4 | 1000224-74-2 | 9    |
| 5         | Cystamine                           | 152 | C4H12N2S2   | 000051-85-4  | 9    |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown1.587     | 1.587 | 6.6     | ug/l  | 47950    | 1                     | 5.550 | 363968 | 50.0 |