

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX121224\  
Data File : VX044256.D  
Acq On : 12 Dec 2024 16:42  
Operator : JC/MD  
Sample : P5261-06  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
RE103D3-20241209

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\82X121124W.M

Title : SW846 8260

Signal : TIC: VX044256.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         | 1.587       | 69            | 82          | 83           | rBV2     | 18243          | 52261         | 5.88%           | 1.120%        |
| 2         | 5.379       | 692           | 704         | 719          | rBV      | 80909          | 240981        | 27.13%          | 5.163%        |
| 3         | 5.550       | 721           | 732         | 745          | rVV2     | 126021         | 365837        | 41.18%          | 7.839%        |
| 4         | 5.952       | 786           | 798         | 815          | rBV      | 103782         | 276134        | 31.08%          | 5.917%        |
| 5         | 6.757       | 920           | 930         | 943          | rBV      | 217942         | 523519        | 58.93%          | 11.217%       |
| 6         | 7.116       | 980           | 989         | 1007         | rBV      | 395003         | 888366        | 100.00%         | 19.035%       |
| 7         | 8.647       | 1234          | 1240        | 1251         | rBV      | 453883         | 713287        | 80.29%          | 15.284%       |
| 8         | 10.049      | 1465          | 1470        | 1480         | rBV      | 433351         | 619671        | 69.75%          | 13.278%       |
| 9         | 11.079      | 1634          | 1639        | 1652         | rBV      | 350315         | 450038        | 50.66%          | 9.643%        |
| 10        | 12.018      | 1788          | 1793        | 1806         | rBV      | 416252         | 536945        | 60.44%          | 11.505%       |

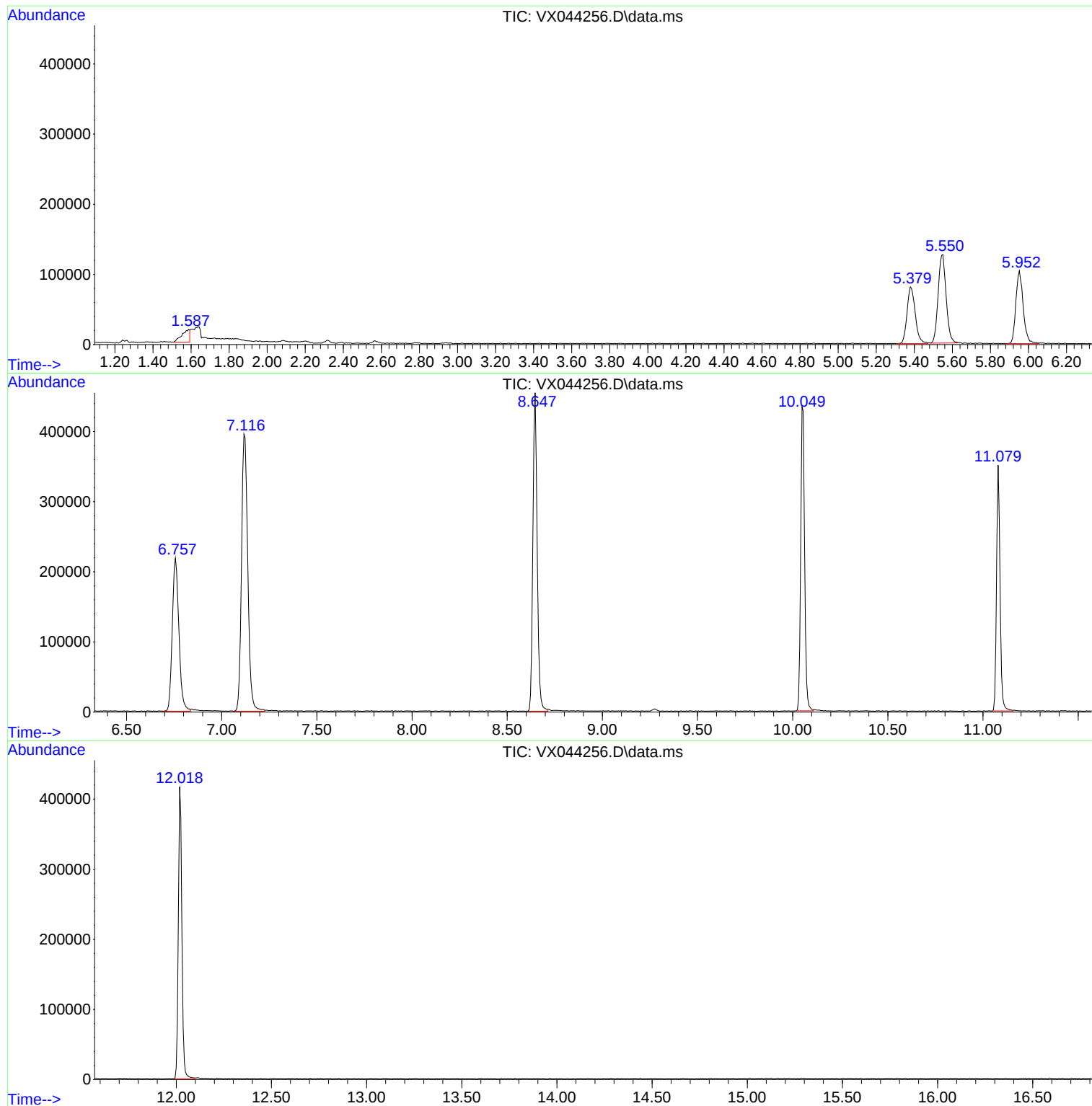
Sum of corrected areas: 4667039

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X121124W.M  
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

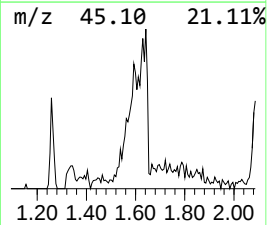
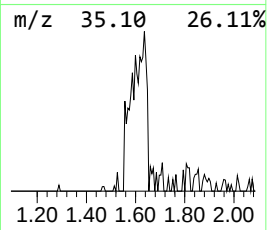
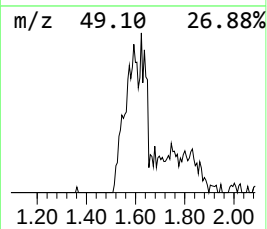
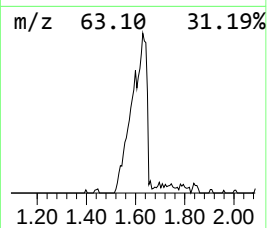
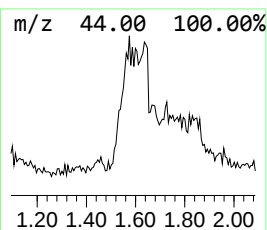
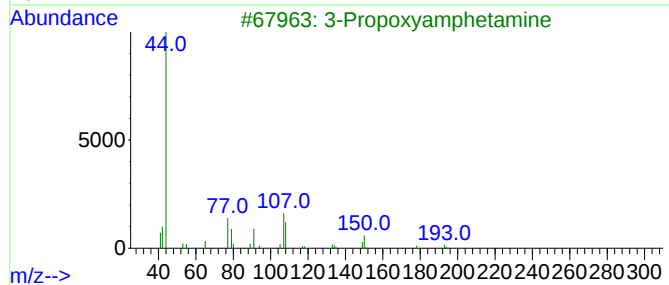
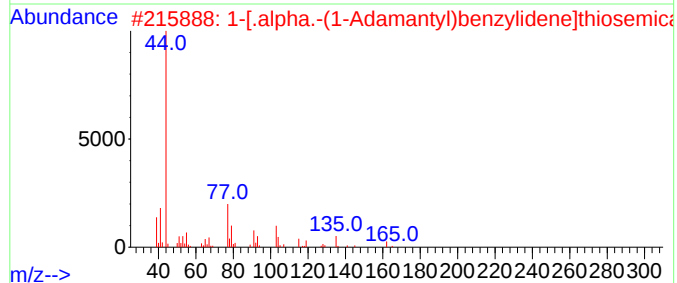
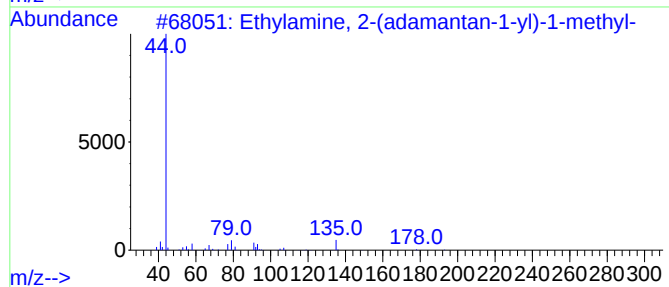
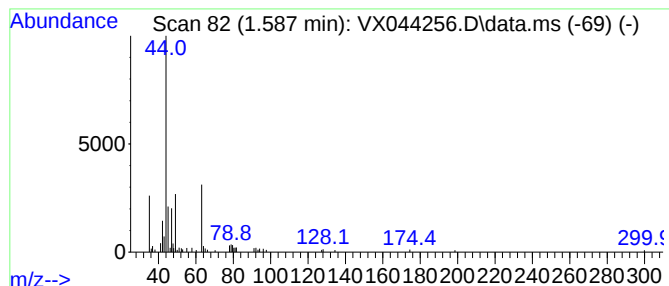
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown1.587 Concentration Rank 1

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 1.587 | 7.14 ug/l | 52261 | Pentafluorobenzene | 5.550 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | Ethylamine, 2-(adamantan-1-yl)-1... | 193 | C13H23N      | 1000310-59-0 | 10      |      |      |
| 2    | 1-[.alpha.-(1-Adamantyl)benzylid... | 313 | C18H23N3S    | 1000222-83-3 | 10      |      |      |
| 3    | 3-Propoxyamphetamine                | 193 | C12H19NO     | 1000124-04-4 | 10      |      |      |
| 4    | 2-Chloro-N-(hydroxymethyl)acetamide | 123 | C3H6ClNO2    | 002832-19-1  | 9       |      |      |
| 5    | Alanine                             | 89  | C3H7NO2      | 000056-41-7  | 9       |      |      |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown1.587     | 1.587 | 7.1     | ug/l  | 52261    | 1                     | 5.550 | 365837 | 50.0 |