

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX010224\  
Data File : VX039577.D  
Acq On : 02 Jan 2024 17:17  
Operator : JC/MD  
Sample : P1002-02 50X  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1210

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\_X\Method\82X121323W.M

Title : SW846 8260

Signal : TIC: VX039577.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         | 1.447       | 55            | 59          | 66           | rBV      | 950276         | 1167857       | 100.00%         | 24.344%       |
| 2         | 1.514       | 66            | 70          | 86           | rVB      | 73907          | 197659        | 16.92%          | 4.120%        |
| 3         | 2.099       | 158           | 166         | 174          | rVB      | 15714          | 31747         | 2.72%           | 0.662%        |
| 4         | 4.227       | 506           | 515         | 525          | rBV3     | 11921          | 34770         | 2.98%           | 0.725%        |
| 5         | 5.385       | 694           | 705         | 718          | rBV2     | 66635          | 194975        | 16.70%          | 4.064%        |
| 6         | 5.550       | 721           | 732         | 745          | rVV2     | 96265          | 278172        | 23.82%          | 5.799%        |
| 7         | 5.952       | 789           | 798         | 814          | rBV      | 78608          | 208918        | 17.89%          | 4.355%        |
| 8         | 6.757       | 921           | 930         | 948          | rBV      | 187189         | 445912        | 38.18%          | 9.295%        |
| 9         | 8.647       | 1233          | 1240        | 1252         | rBV      | 399290         | 627015        | 53.69%          | 13.070%       |
| 10        | 10.055      | 1465          | 1471        | 1485         | rBV      | 422739         | 603212        | 51.65%          | 12.574%       |
| 11        | 11.079      | 1634          | 1639        | 1652         | rBV      | 359456         | 458349        | 39.25%          | 9.554%        |
| 12        | 12.018      | 1789          | 1793        | 1808         | rVB      | 414527         | 548672        | 46.98%          | 11.437%       |

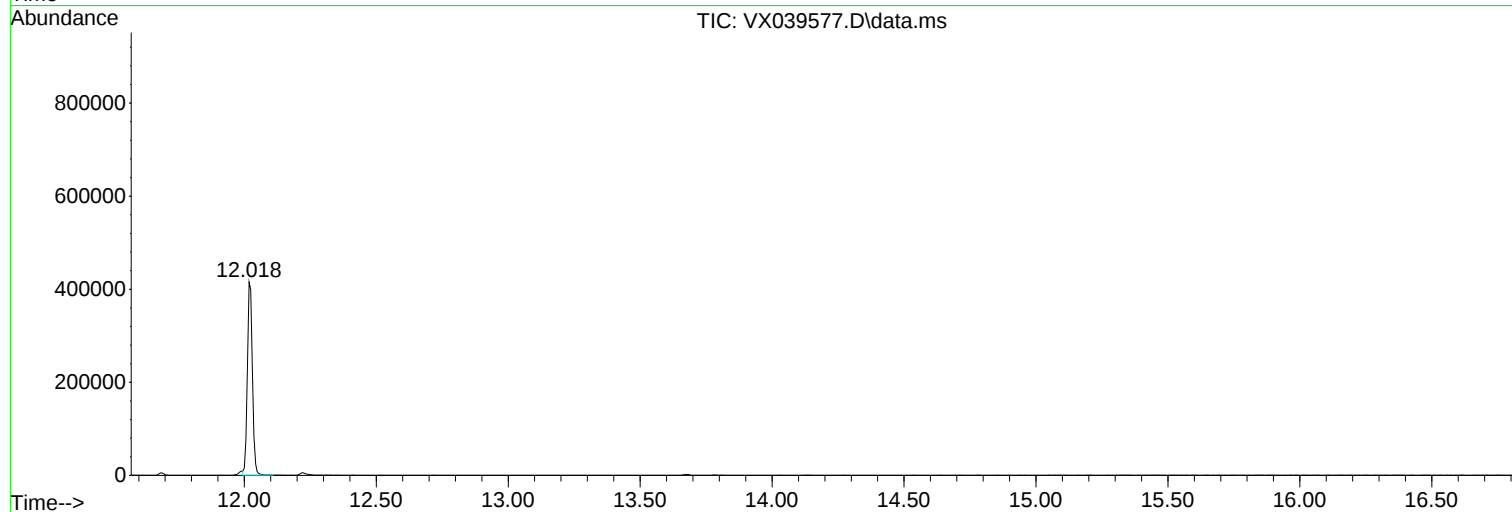
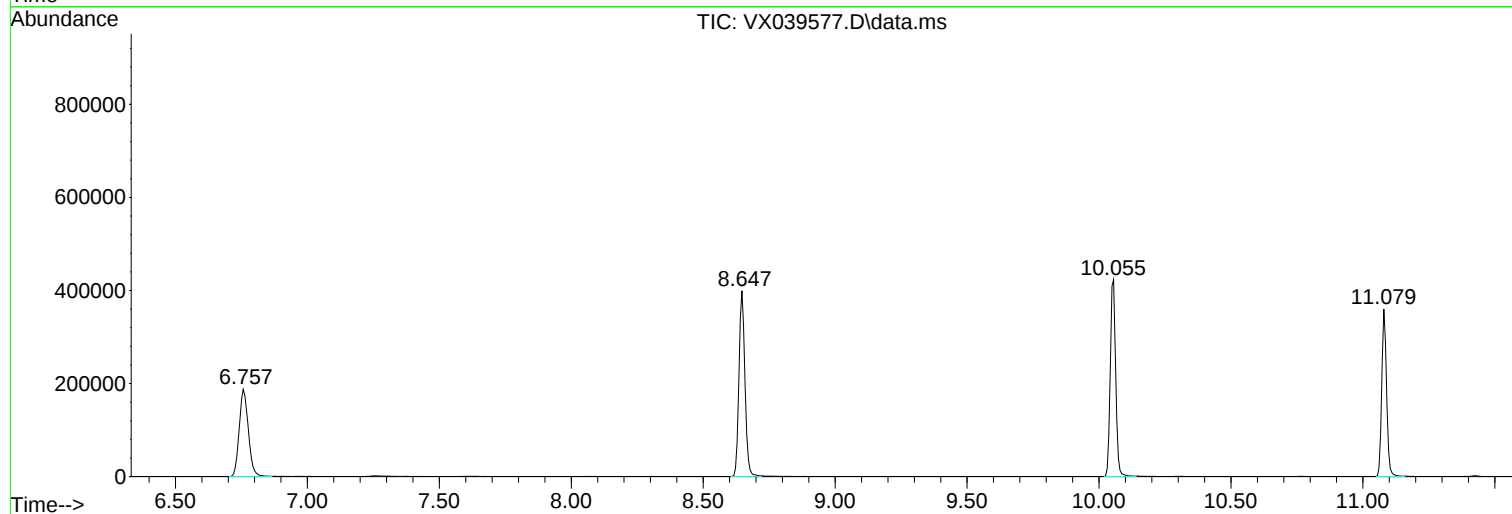
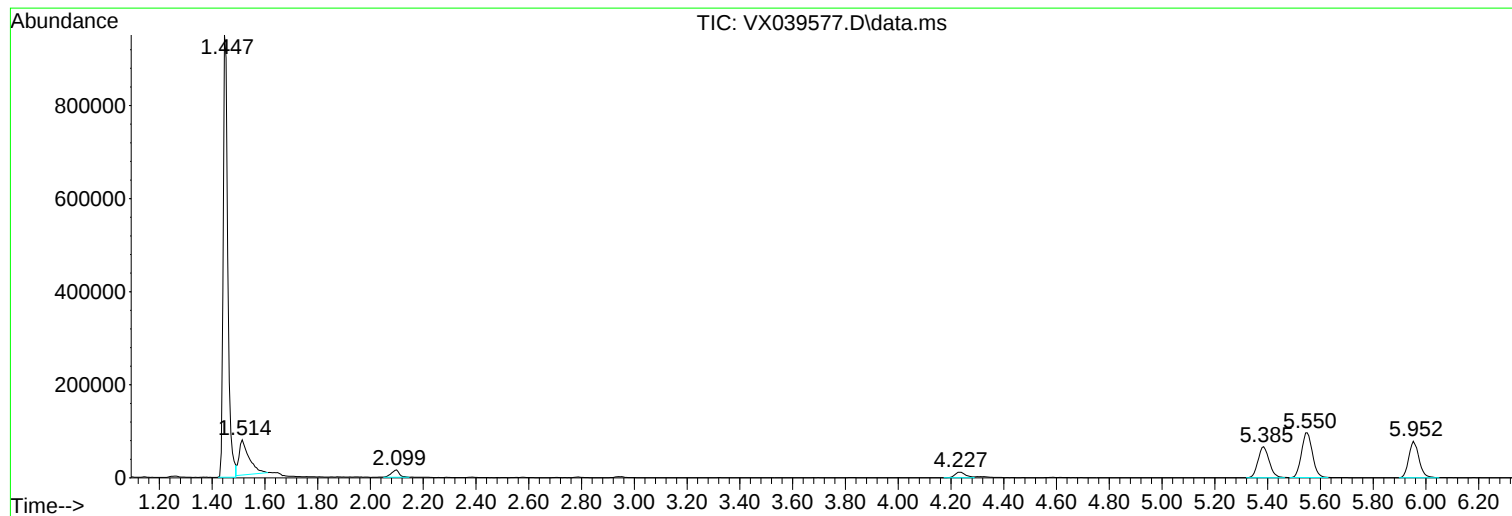
Sum of corrected areas: 4797258

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX010224\  
Data File : VX039577.D  
Acq On : 02 Jan 2024 17:17  
Operator : JC/MD  
Sample : P1002-02 50X  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1210

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X121323W.M  
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX010224\  
Data File : VX039577.D  
Acq On : 02 Jan 2024 17:17  
Operator : JC/MD  
Sample : P1002-02 50X  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1210

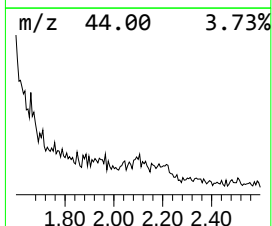
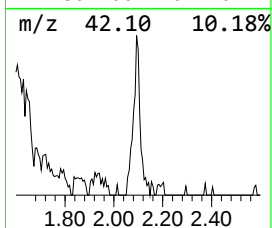
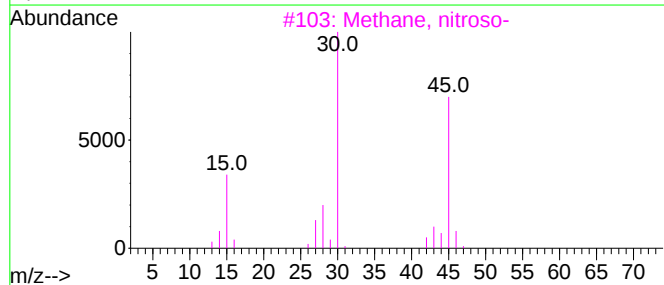
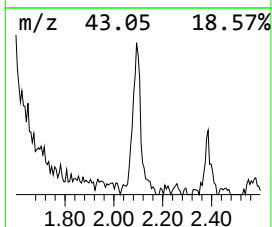
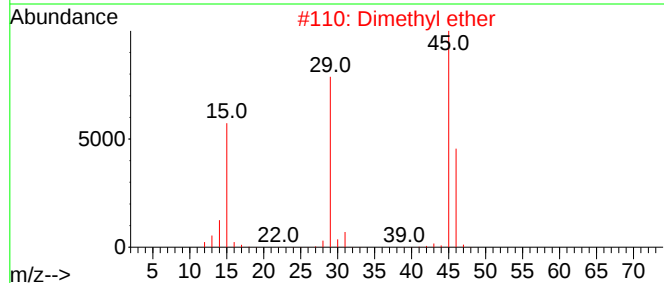
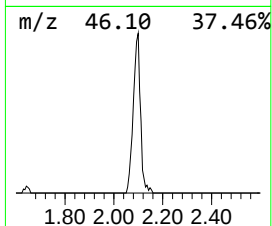
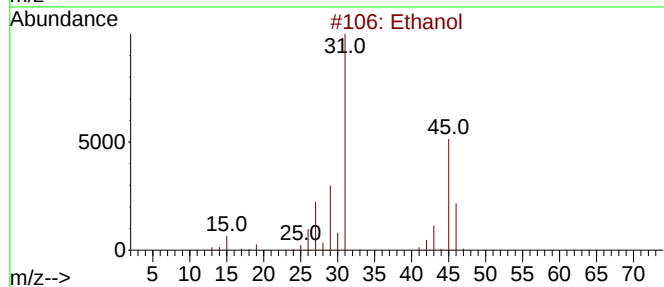
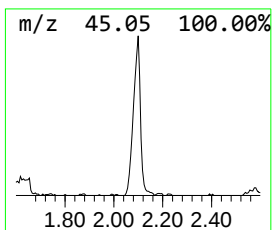
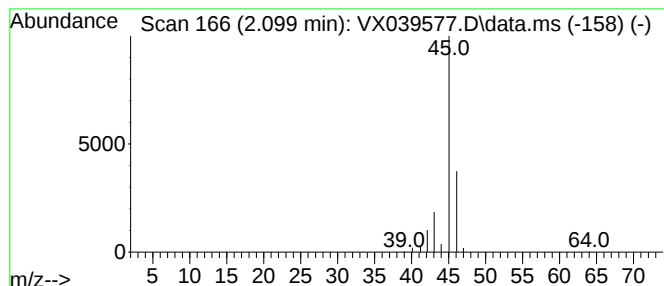
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X121323W.M  
Quant Title : SW846 8260

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

\*\*\*\*\*  
Peak Number 3 Ethanol Concentration Rank 4

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 2.099 | 5.71 ug/l | 31747 | Pentafluorobenzene | 5.550 |

| Hit# | of                | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|-------------------|---|--------------|----|---------|-------------|------|
| 1    | Ethanol           |   |              | 46 | C2H6O   | 000064-17-5 | 86   |
| 2    | Dimethyl ether    |   |              | 46 | C2H6O   | 000115-10-6 | 9    |
| 3    | Methane, nitroso- |   |              | 45 | CH3NO   | 000865-40-7 | 7    |
| 4    | Formic acid       |   |              | 46 | CH2O2   | 000064-18-6 | 4    |
| 5    | Formamide         |   |              | 45 | CH3NO   | 000075-12-7 | 3    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX010224\  
Data File : VX039577.D  
Acq On : 02 Jan 2024 17:17  
Operator : JC/MD  
Sample : P1002-02 50X  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1210

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X121323W.M  
Quant Title : SW846 8260

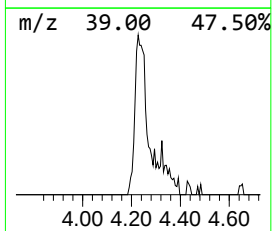
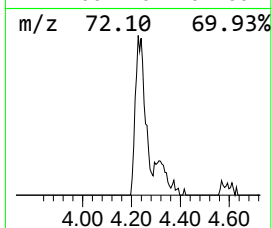
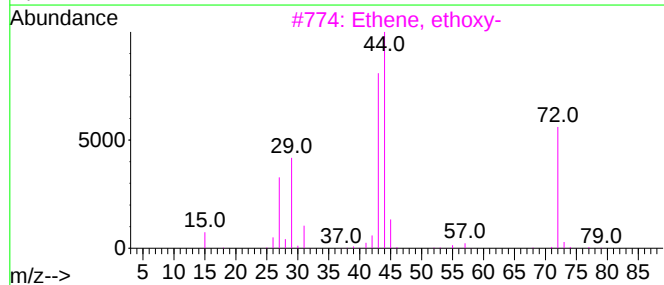
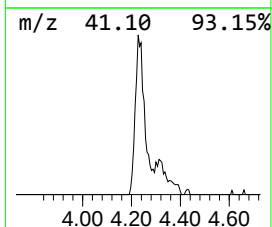
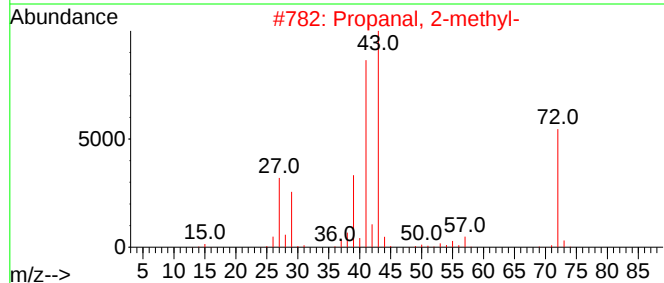
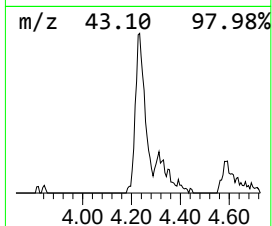
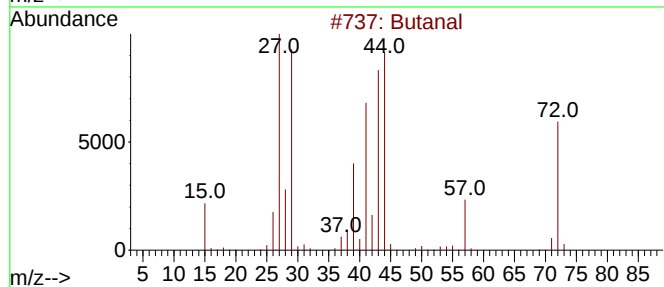
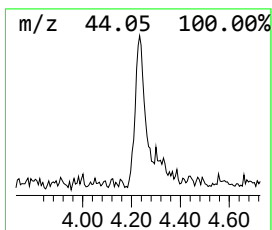
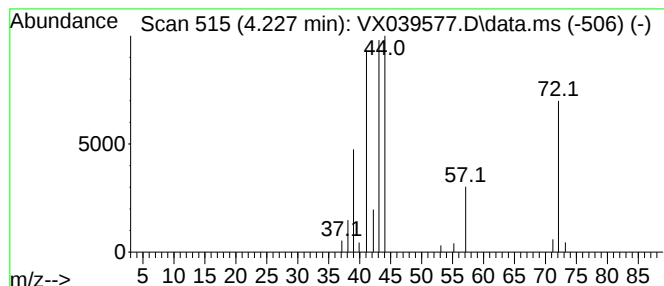
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 4 Butanal Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 4.227 | 6.25 ug/l | 34770 | Pentafluorobenzene | 5.550 |

| Hit# | of | 5 | Tentative ID           | MW | MolForm | CAS#        | Qual |
|------|----|---|------------------------|----|---------|-------------|------|
| 1    |    |   | Butanal                | 72 | C4H8O   | 000123-72-8 | 91   |
| 2    |    |   | Propanal, 2-methyl-    | 72 | C4H8O   | 000078-84-2 | 49   |
| 3    |    |   | Ethene, ethoxy-        | 72 | C4H8O   | 000109-92-2 | 38   |
| 4    |    |   | 1-Propene, 3-methoxy-  | 72 | C4H8O   | 000627-40-7 | 32   |
| 5    |    |   | 2-Propanone, hydrazone | 72 | C3H8N2  | 005281-20-9 | 27   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX010224\  
Data File : VX039577.D  
Acq On : 02 Jan 2024 17:17  
Operator : JC/MD  
Sample : P1002-02 50X  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1210

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X121323W.M  
Quant Title : SW846 8260

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

| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Ethanol          | 2.099 | 5.7     | ug/l  | 31747    | 1                     | 5.550 | 278172 | 50.0 |
| Butanal          | 4.227 | 6.3     | ug/l  | 34770    | 1                     | 5.550 | 278172 | 50.0 |