

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX111623\  
Data File : VX038842.D  
Acq On : 16 Nov 2023 16:59  
Operator : JC/MD  
Sample : VX1116WBL01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
VX1116WBL01

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\82X111623W.M

Title : SW846 8260

Signal : TIC: VX038842.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         | 1.337       | 31            | 41          | 42           | rBV8     | 14711          | 44047         | 4.64%           | 0.838%        |
| 2         | 5.385       | 692           | 705         | 718          | rBV      | 102506         | 303164        | 31.97%          | 5.767%        |
| 3         | 5.550       | 721           | 732         | 745          | rVV      | 153945         | 436384        | 46.02%          | 8.301%        |
| 4         | 5.952       | 788           | 798         | 810          | rBV      | 110474         | 301256        | 31.77%          | 5.730%        |
| 5         | 6.757       | 921           | 930         | 946          | rBV      | 275952         | 670902        | 70.75%          | 12.761%       |
| 6         | 8.647       | 1234          | 1240        | 1250         | rBV      | 593177         | 948330        | 100.00%         | 18.038%       |
| 7         | 10.055      | 1465          | 1471        | 1483         | rBV      | 616116         | 889375        | 93.78%          | 16.917%       |
| 8         | 11.079      | 1632          | 1639        | 1653         | rBV      | 543252         | 707317        | 74.59%          | 13.454%       |
| 9         | 12.018      | 1788          | 1793        | 1808         | rVB      | 717540         | 946909        | 99.85%          | 18.011%       |
| 10        | 13.780      | 2076          | 2082        | 2091         | rVB3     | 5030           | 9636          | 1.02%           | 0.183%        |

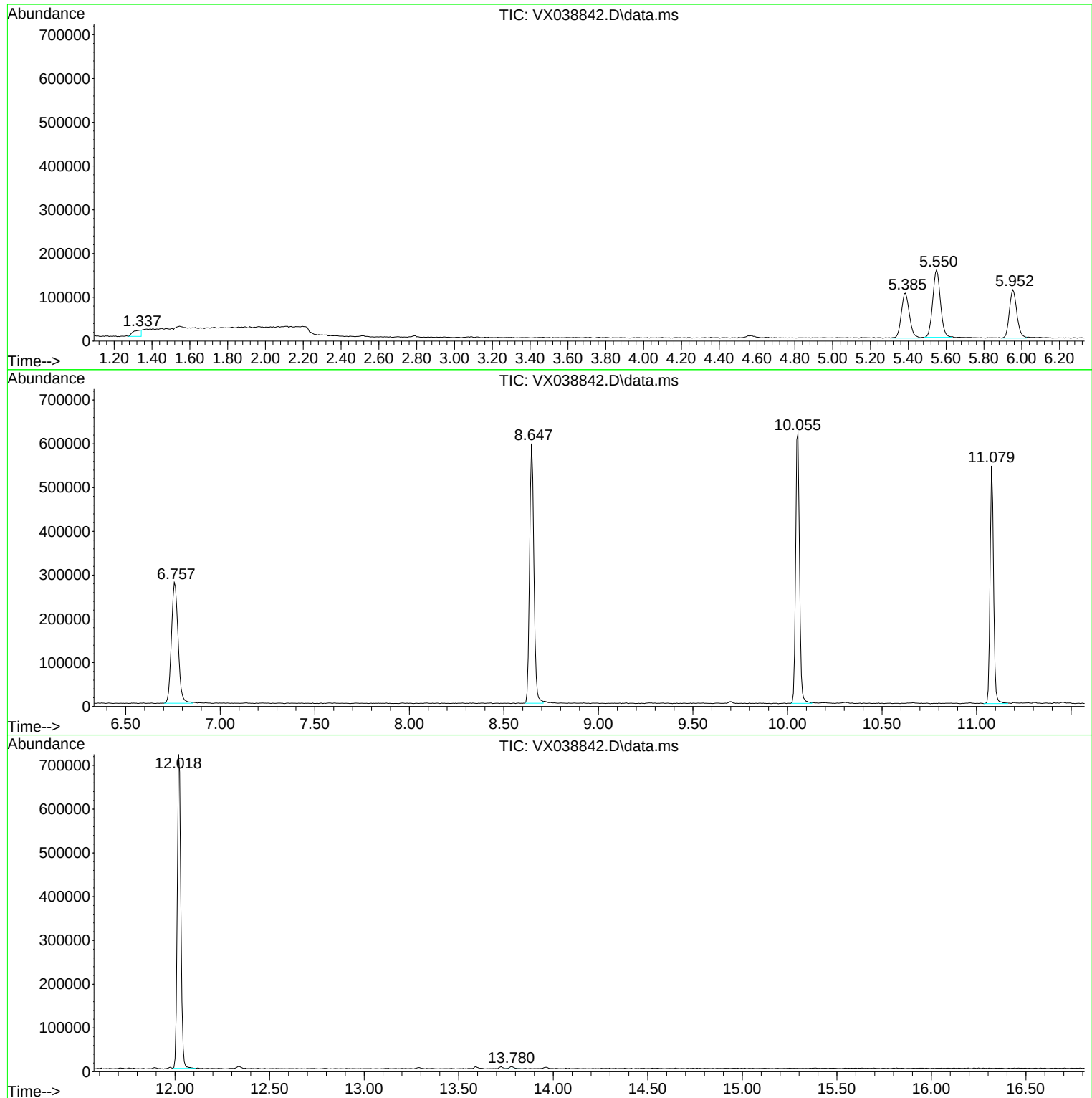
Sum of corrected areas: 5257320

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X111623W.M  
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

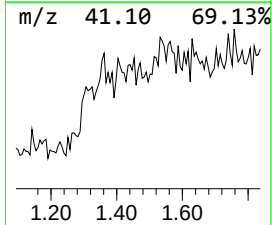
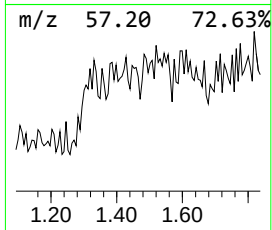
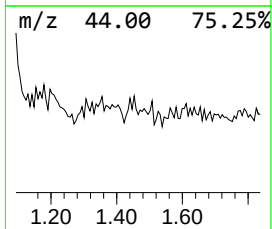
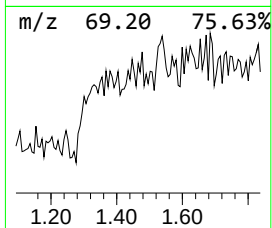
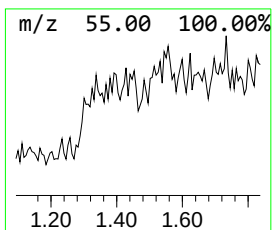
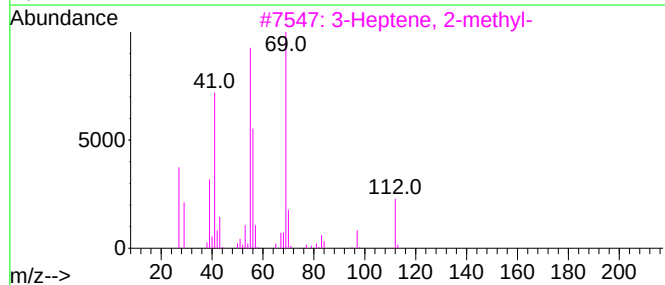
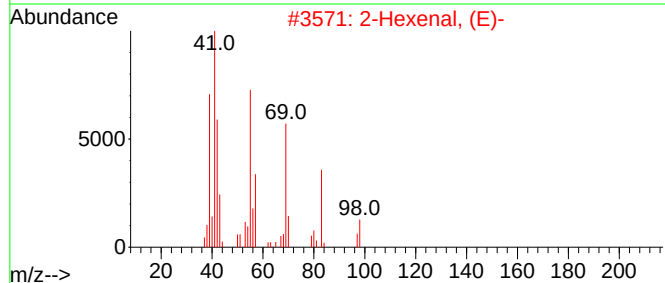
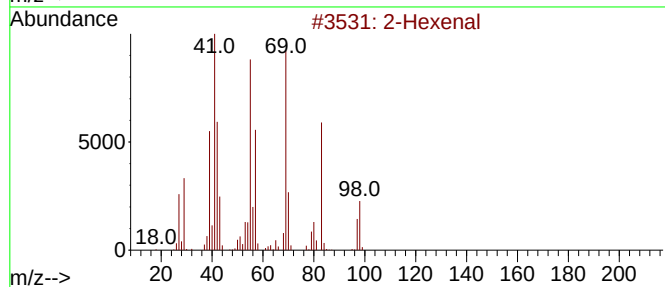
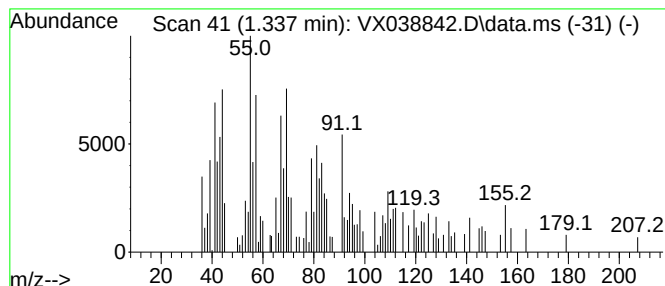
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Hexenal Concentration Rank 1

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 1.337 | 5.05 ug/l | 44047 | Pentafluorobenzene | 5.550 |

| Hit# | of                             | 5 | Tentative ID | MW  | MolForm | CAS#         | Qual |
|------|--------------------------------|---|--------------|-----|---------|--------------|------|
| 1    | 2-Hexenal                      |   |              | 98  | C6H10O  | 000505-57-7  | 60   |
| 2    | 2-Hexenal, (E)-                |   |              | 98  | C6H10O  | 006728-26-3  | 30   |
| 3    | 3-Heptene, 2-methyl-           |   |              | 112 | C8H16   | 017618-76-7  | 18   |
| 4    | Allylhydrazon acetaldehyde     |   |              | 98  | C5H10N2 | 1010423-20-0 | 18   |
| 5    | Cyclohexanone, 3-methyl-, (R)- |   |              | 112 | C7H12O  | 013368-65-5  | 18   |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Hexenal        | 1.337 | 5.0     | ug/l  | 44047    | 1                     | 5.550 | 436384 | 50.0 |