

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX051623\  
 Data File : VX035692.D  
 Acq On : 16 May 2023 15:39  
 Operator : JC/MD  
 Sample : 02751-03  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 FSND-PRO-01-99-05062023

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\82X051123W.M

Title : SW846 8260

Signal : TIC: VX035692.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         | 1.142       | 6             | 9           | 20           | rVB      | 33007          | 37299         | 3.34%           | 0.585%        |
| 2         | 2.294       | 192           | 198         | 200          | rBV      | 14162          | 23542         | 2.11%           | 0.369%        |
| 3         | 2.319       | 200           | 202         | 208          | rVB      | 14875          | 19045         | 1.70%           | 0.299%        |
| 4         | 5.385       | 692           | 705         | 720          | rBV2     | 122017         | 360579        | 32.26%          | 5.654%        |
| 5         | 5.550       | 720           | 732         | 753          | rVB      | 212169         | 598545        | 53.54%          | 9.386%        |
| 6         | 5.952       | 787           | 798         | 814          | rBV      | 151603         | 405475        | 36.27%          | 6.358%        |
| 7         | 6.763       | 920           | 931         | 953          | rBV      | 347629         | 833606        | 74.57%          | 13.072%       |
| 8         | 7.580       | 1059          | 1065        | 1073         | rBV2     | 7983           | 16089         | 1.44%           | 0.252%        |
| 9         | 8.647       | 1233          | 1240        | 1253         | rBV      | 722054         | 1117847       | 100.00%         | 17.529%       |
| 10        | 9.519       | 1377          | 1383        | 1396         | rBV      | 84582          | 118892        | 10.64%          | 1.864%        |
| 11        | 10.055      | 1465          | 1471        | 1484         | rBV      | 739813         | 1014319       | 90.74%          | 15.906%       |
| 12        | 11.079      | 1634          | 1639        | 1648         | rBV      | 644023         | 803245        | 71.86%          | 12.596%       |
| 13        | 11.927      | 1774          | 1778        | 1783         | rBV2     | 9740           | 12661         | 1.13%           | 0.199%        |
| 14        | 12.024      | 1788          | 1794        | 1805         | rBV      | 738733         | 968564        | 86.65%          | 15.188%       |
| 15        | 15.542      | 2366          | 2371        | 2379         | rBV3     | 15174          | 25569         | 2.29%           | 0.401%        |
| 16        | 16.469      | 2518          | 2523        | 2534         | rBV4     | 10425          | 21781         | 1.95%           | 0.342%        |

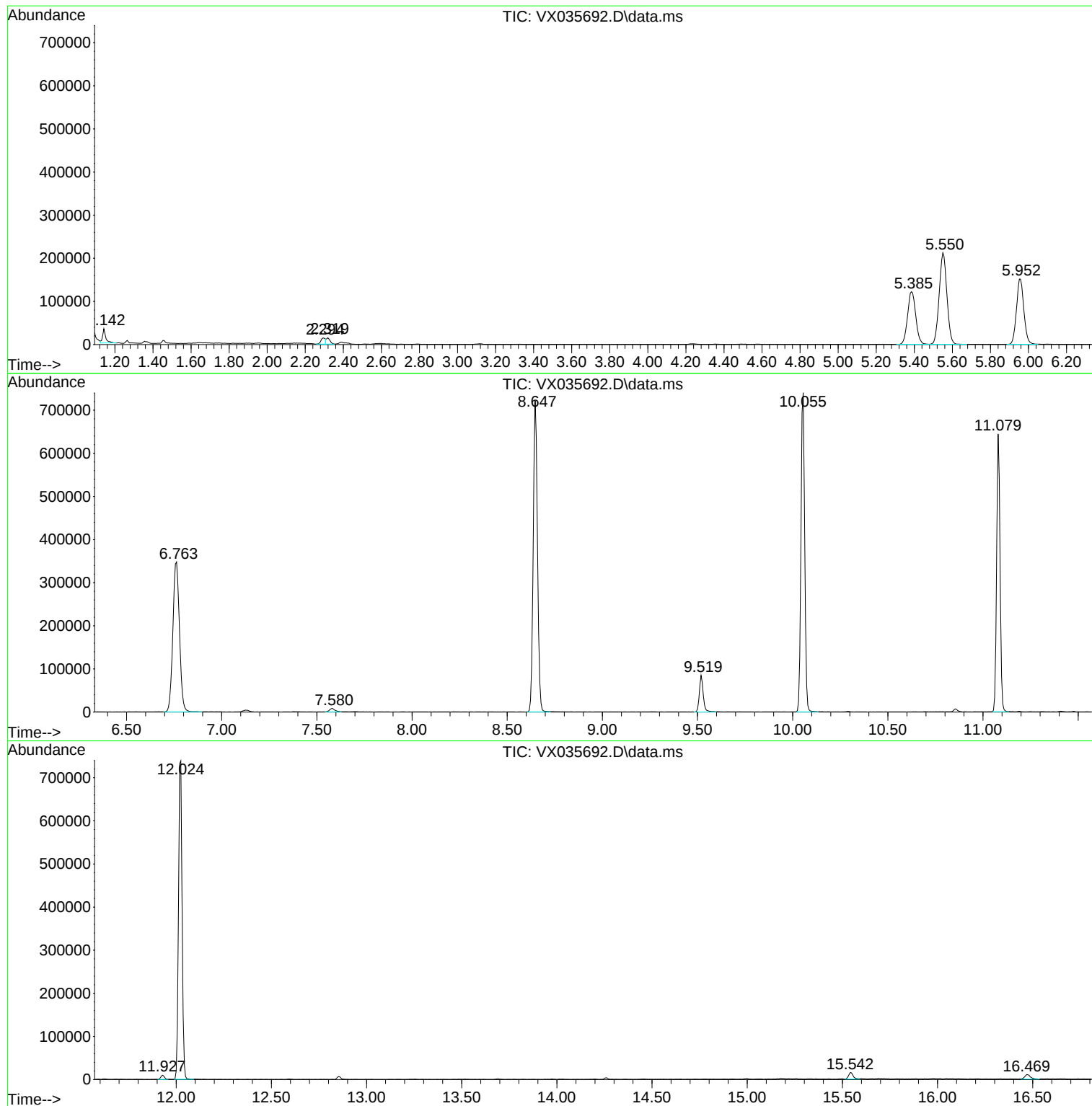
Sum of corrected areas: 6377058

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X051123W.M  
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

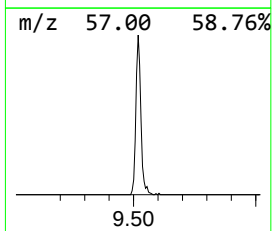
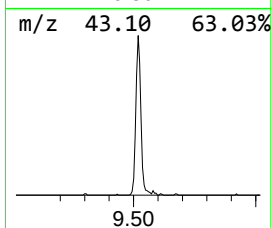
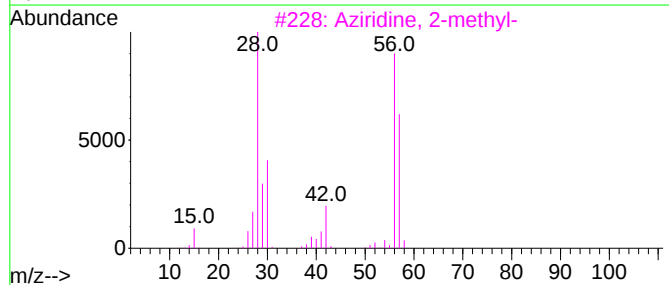
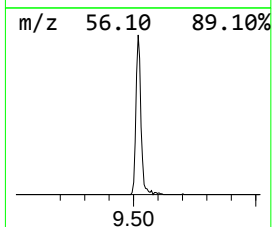
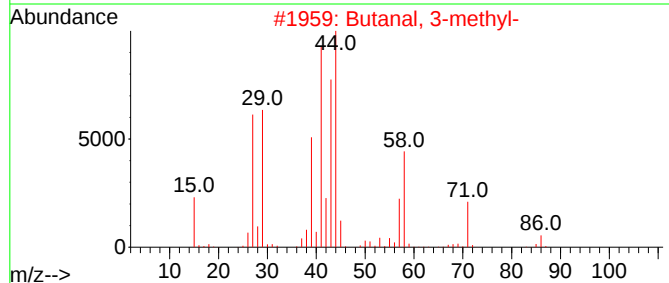
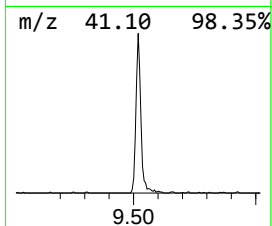
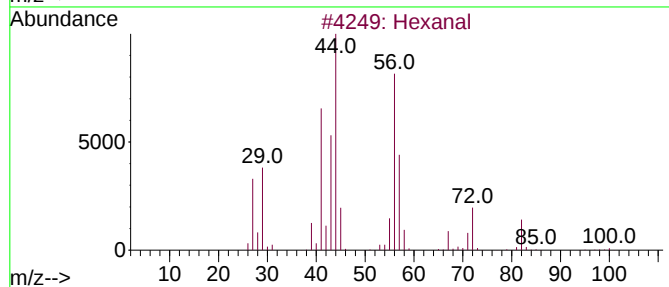
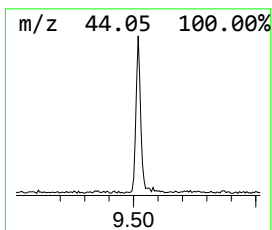
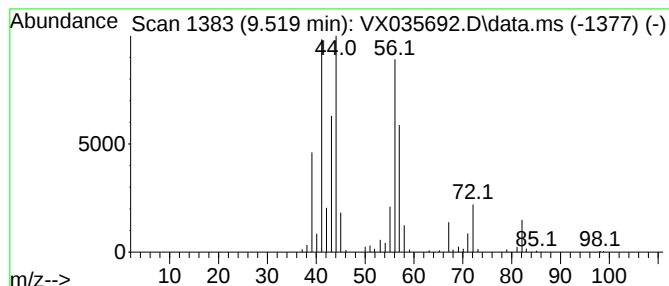
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Hexanal Concentration Rank 1

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.   |
|-------|-----------|--------|------------------|--------|
| 9.519 | 5.86 ug/l | 118892 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Hexanal                             | 100 | C6H12O  | 000066-25-1  | 72   |
| 2    |    |   | Butanal, 3-methyl-                  | 86  | C5H10O  | 000590-86-3  | 37   |
| 3    |    |   | Aziridine, 2-methyl-                | 57  | C3H7N   | 000075-55-8  | 27   |
| 4    |    |   | 2,2-Dimethyl-3-hydroxypropionald... | 102 | C5H10O2 | 000597-31-9  | 25   |
| 5    |    |   | (S)-3,4-Dimethylpentanol            | 116 | C7H16O  | 1000143-83-9 | 23   |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|------------------|-------|---------|-------|----------|-----------------------|--------|---------|------|
|                  |       |         |       |          | #                     | RT     | Resp    | Conc |
| Hexanal          | 9.519 | 5.9     | ug/l  | 118892   | 3                     | 10.055 | 1014320 | 50.0 |