

Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR080718\  
 Data File : VR025584.D  
 Acq On : 7 Aug 2018 19:23  
 Operator : SY/MD  
 Sample : J4358-18  
 Misc : 25mL/MSVOA R/WATER  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 MSVOA\_R  
 ClientSampleId :  
 ESWY2

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\_R\METHODS\SOMRTR073018WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

| 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         | 1.621       | 40            | 48          | 70           | rBV      | 6359236        | 27644838      | 100.00%         | 52.534%       |
| 2         | 1.791       | 70            | 76          | 101          | rVB2     | 592331         | 2239704       | 8.10%           | 4.256%        |
| 3         | 2.156       | 127           | 136         | 146          | rBV4     | 111345         | 409131        | 1.48%           | 0.777%        |
| 4         | 3.635       | 366           | 379         | 392          | rBV3     | 189245         | 612521        | 2.22%           | 1.164%        |
| 5         | 4.888       | 573           | 585         | 598          | rBV      | 134887         | 425568        | 1.54%           | 0.809%        |
| 6         | 6.683       | 870           | 880         | 899          | rVB      | 4656638        | 12827624      | 46.40%          | 24.376%       |
| 7         | 7.206       | 956           | 966         | 978          | rVB2     | 244014         | 605321        | 2.19%           | 1.150%        |
| 8         | 7.857       | 1063          | 1073        | 1091         | rBV2     | 487410         | 1343846       | 4.86%           | 2.554%        |
| 9         | 8.465       | 1163          | 1173        | 1182         | rBV      | 581184         | 1080347       | 3.91%           | 2.053%        |
| 10        | 8.903       | 1235          | 1245        | 1257         | rBV      | 313867         | 612430        | 2.22%           | 1.164%        |
| 11        | 9.974       | 1413          | 1421        | 1428         | rBV      | 769298         | 1187058       | 4.29%           | 2.256%        |
| 12        | 10.594      | 1516          | 1523        | 1530         | rBV      | 525919         | 801115        | 2.90%           | 1.522%        |
| 13        | 11.288      | 1631          | 1637        | 1646         | rBV      | 794154         | 1171909       | 4.24%           | 2.227%        |
| 14        | 13.222      | 1948          | 1955        | 1963         | rBV      | 633990         | 868495        | 3.14%           | 1.650%        |
| 15        | 13.514      | 1997          | 2003        | 2011         | rBV      | 563533         | 793121        | 2.87%           | 1.507%        |

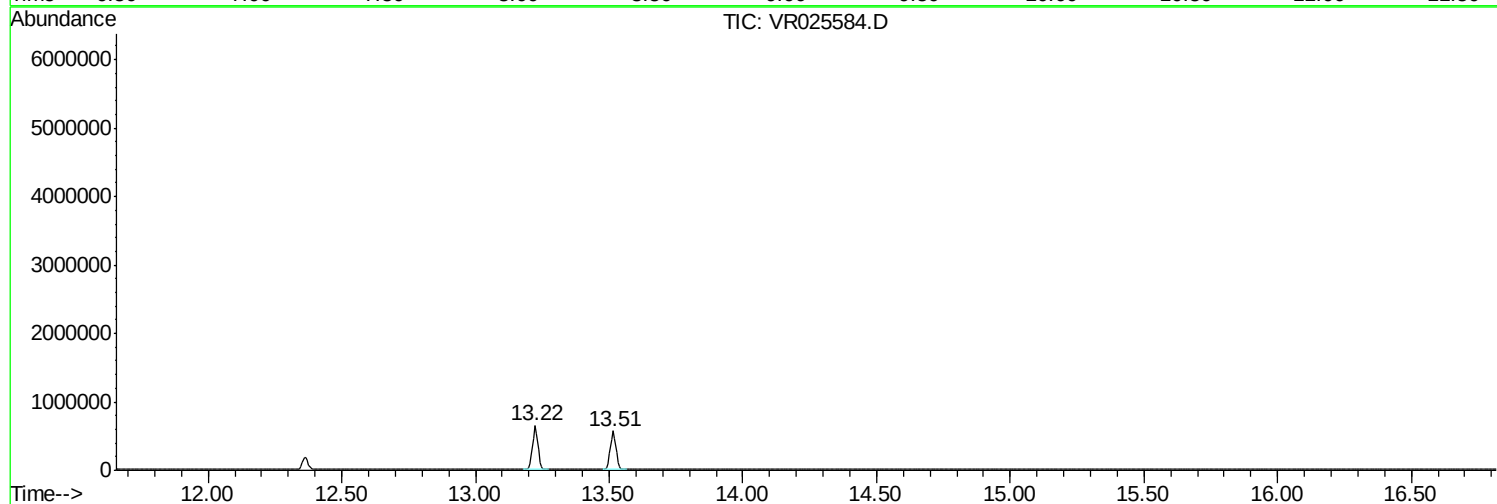
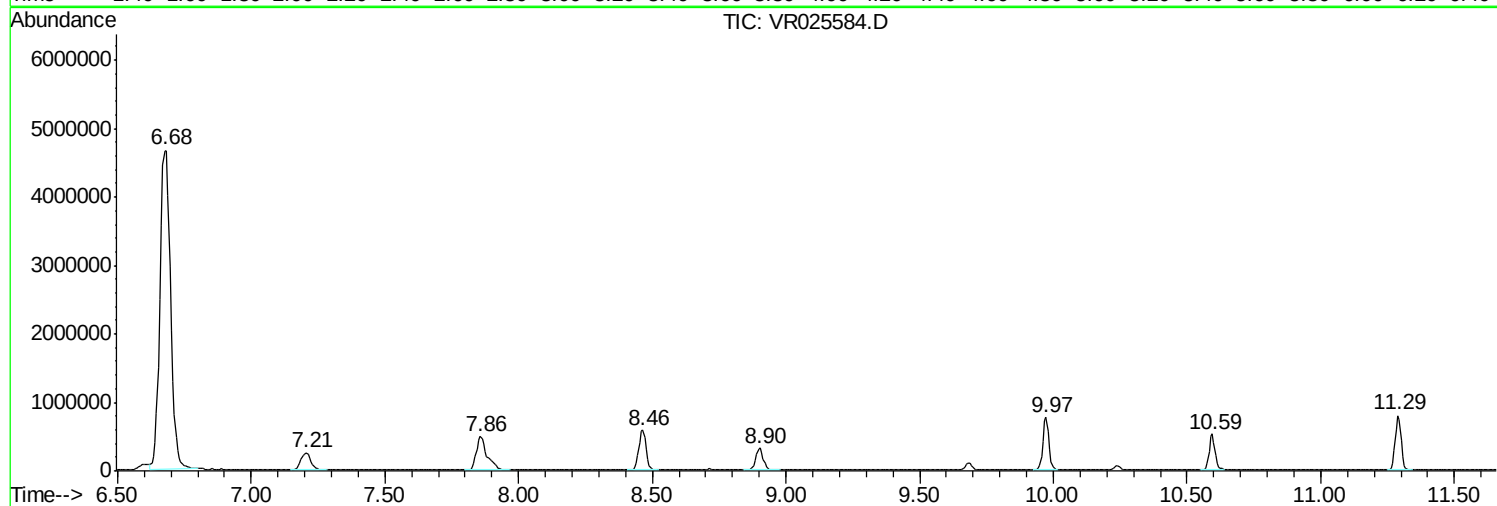
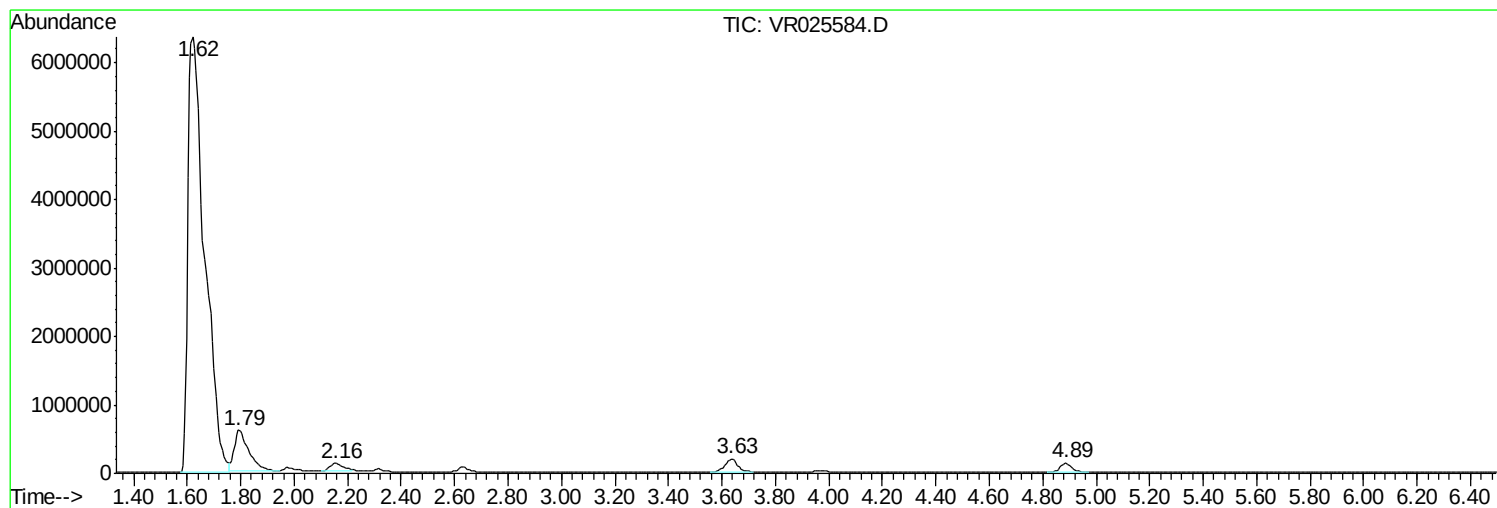
Sum of corrected areas: 52623028

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA R\DATA\VR080718\  
Data File : VR025584.D  
Acq On : 7 Aug 2018 19:23  
Operator : SY/MD  
Sample : J4358-18  
Misc : 25mL/MSVOA R/WATER  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_R  
ClientSampleId :  
ESWY2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_R\METHODS\SOMRTR073018WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR080718\  
Data File : VR025584.D  
Acq On : 7 Aug 2018 19:23  
Operator : SY/MD  
Sample : J4358-18  
Misc : 25mL/MSVOA R/WATER  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_R  
ClientSampleId :  
ESWY2

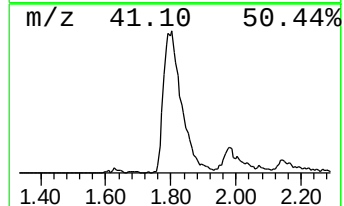
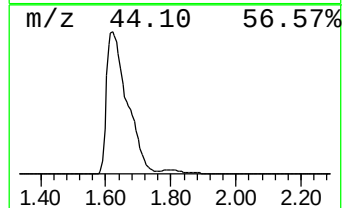
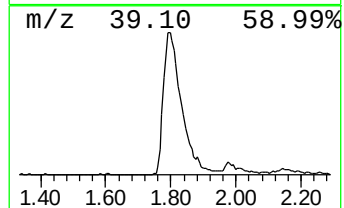
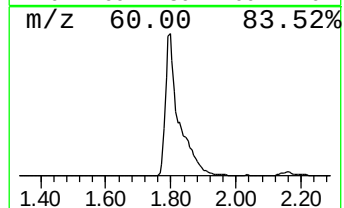
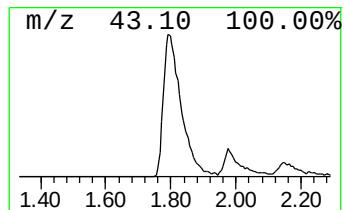
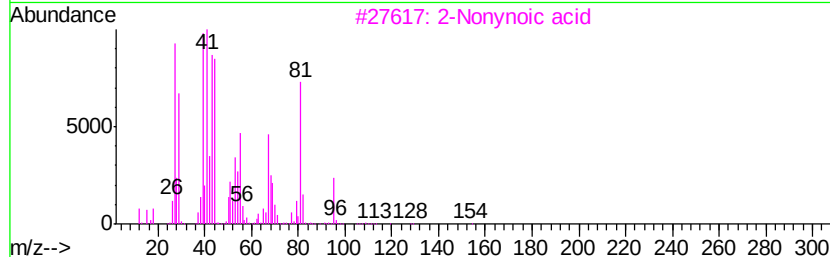
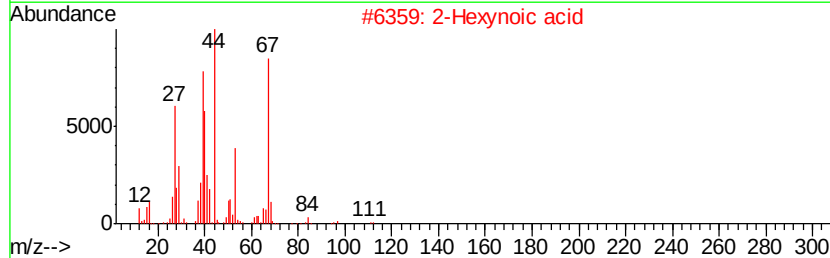
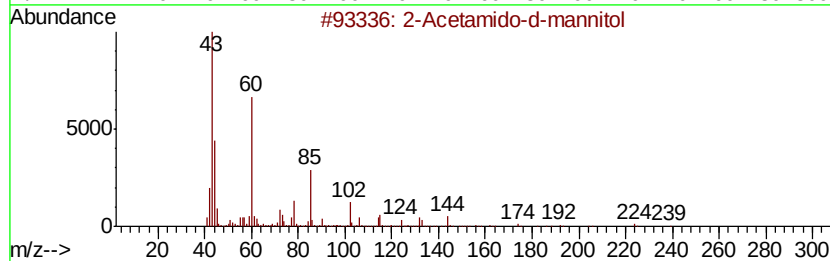
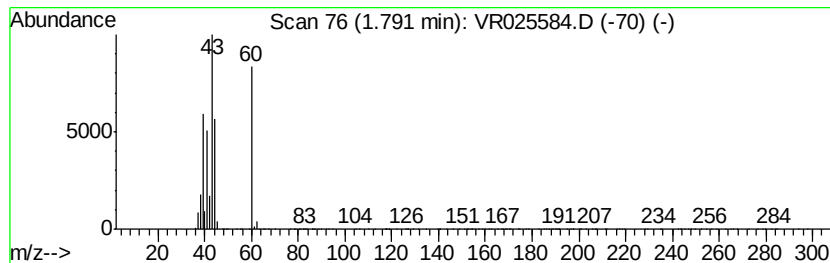
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_R\METHODS\SOMRTR073018WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 2-Acetamido-d-mannitol Concentration Rank 2

| R.T. | EstConc    | Area    | Relative to ISTD    | R.T. |
|------|------------|---------|---------------------|------|
| 1.79 | 10.37 ug/L | 2239700 | 1,4-Difluorobenzene | 8.46 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | 2-Acetamido-d-mannitol              | 239 | C8H17NO7   | 1000124-70-1 | 64   |
| 2    |    | 2-Hexynoic acid                     | 112 | C6H8O2     | 000764-33-0  | 25   |
| 3    |    | 2-Nonynoic acid                     | 154 | C9H14O2    | 001846-70-4  | 16   |
| 4    |    | Bis(3-methylbutyl) fluorene-2,7-... | 466 | C23H30O6S2 | 253664-95-8  | 14   |
| 5    |    | (E)-1-Propene-1,2,3-tricarboxyli... | 174 | C6H6O6     | 004023-65-8  | 12   |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA\_R\DATA\VR080718\  
Data File : VR025584.D  
Acq On : 7 Aug 2018 19:23  
Operator : SY/MD  
Sample : J4358-18  
Misc : 25mL/MSVOA\_R/WATER  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
MSVOA\_R  
ClientSampleId :  
ESWY2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_R\METHODS\SOMRTR073018WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |         |      |
|----------------------|------|---------|-------|----------|-----------------------|------|---------|------|
|                      |      |         |       |          | #                     | RT   | Resp    | Conc |
| 2-Acetamido-d-man... | 1.79 | 10.4    | ug/L  | 2239700  | 1                     | 8.46 | 1080350 | 5.0  |