

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX041418\  
 Data File : VX000885.D  
 Acq On : 14 Apr 2018 19:44  
 Operator : JC/MD  
 Sample : J2353-13  
 Misc : 5.0mL/MSVOA X/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 LF012MW029-180410

## 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 : W:\HPCHEM1\MSVOA\_X\METHOD\82X041018W.M  
 Title : SW846 8260

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         | 1.075       | 76            | 80          | 93           | rBV      | 1051819        | 1155301       | 99.96%          | 15.521%       |
| 2         | 1.343       | 117           | 124         | 128          | rBV      | 26573          | 85255         | 7.38%           | 1.145%        |
| 3         | 2.398       | 290           | 297         | 302          | rBV3     | 10997          | 24305         | 2.10%           | 0.327%        |
| 4         | 2.453       | 302           | 306         | 311          | rVB      | 11528          | 19297         | 1.67%           | 0.259%        |
| 5         | 5.513       | 793           | 808         | 821          | rBV2     | 137142         | 386747        | 33.46%          | 5.196%        |
| 6         | 5.672       | 823           | 834         | 855          | rBV      | 216623         | 615848        | 53.29%          | 8.273%        |
| 7         | 6.080       | 890           | 901         | 915          | rBV      | 145967         | 374335        | 32.39%          | 5.029%        |
| 8         | 6.873       | 1020          | 1031        | 1048         | rBV      | 301120         | 715185        | 61.88%          | 9.608%        |
| 9         | 8.726       | 1327          | 1335        | 1357         | rBV      | 685844         | 1155715       | 100.00%         | 15.526%       |
| 10        | 10.122      | 1558          | 1564        | 1581         | rBV      | 624679         | 874546        | 75.67%          | 11.749%       |
| 11        | 11.146      | 1726          | 1732        | 1747         | rBV      | 692218         | 901923        | 78.04%          | 12.117%       |
| 12        | 12.085      | 1880          | 1886        | 1897         | rBV      | 937212         | 1135178       | 98.22%          | 15.250%       |

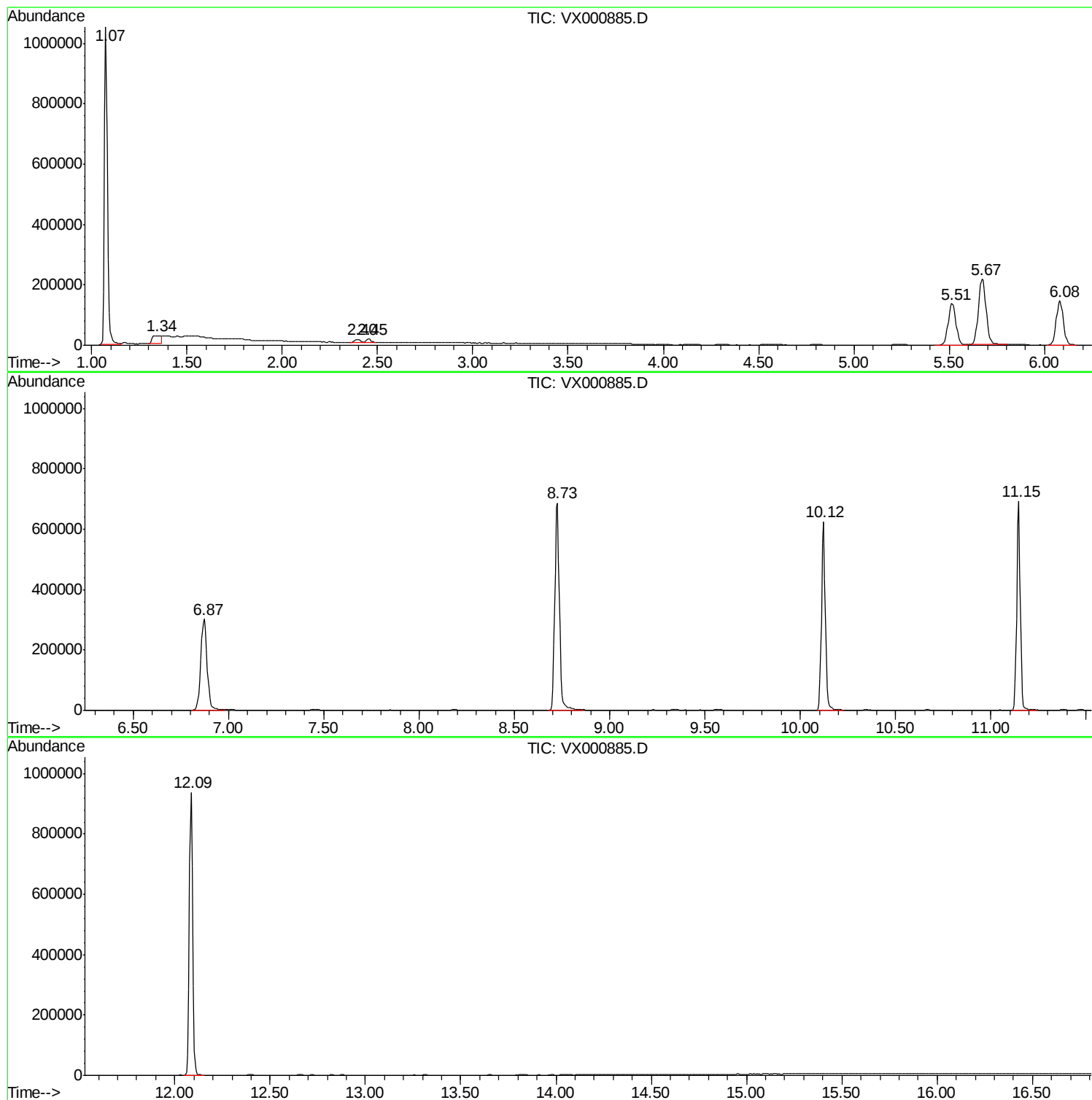
Sum of corrected areas: 7443635

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Quant Method : W:\HPCHEM1\MSVOA\_X\METHOD\82X041018W.M  
Quant Title : SW846 8260

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



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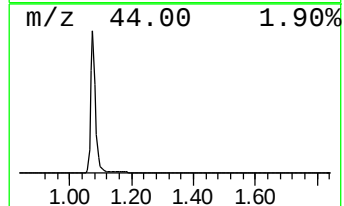
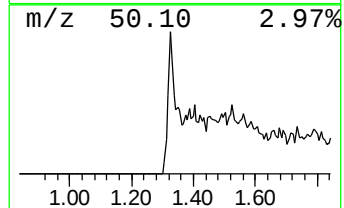
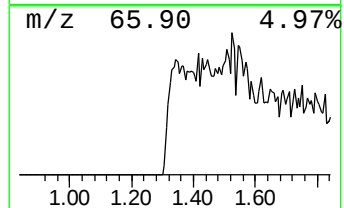
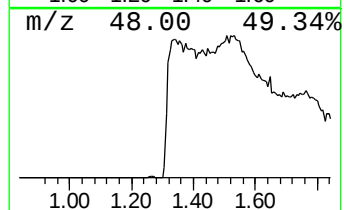
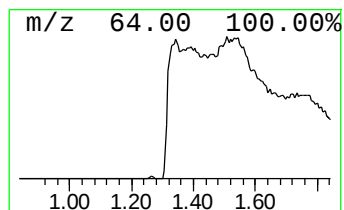
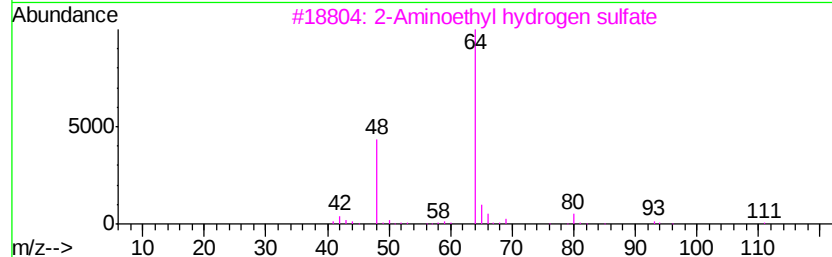
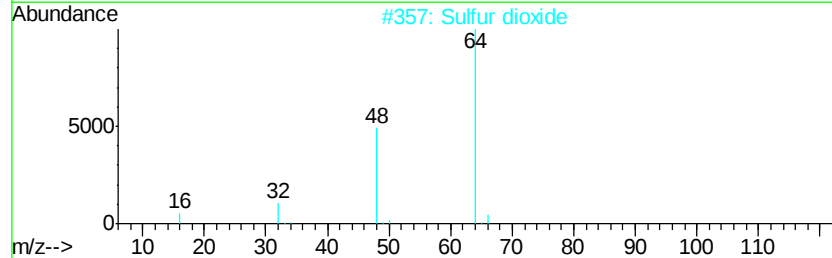
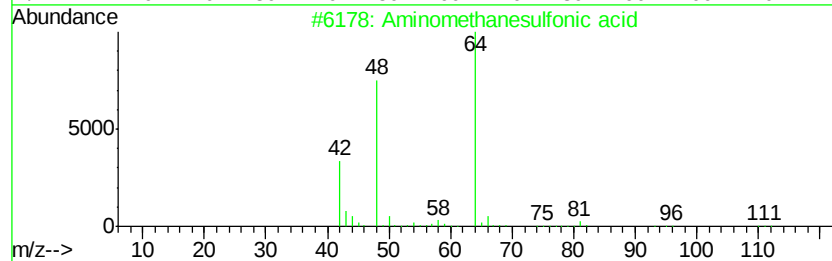
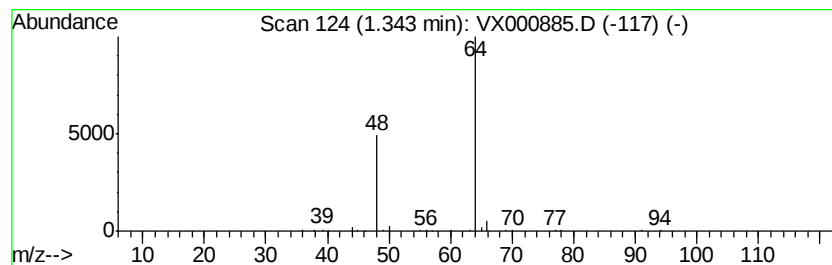
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Peak Number 2 Aminomethanesulfonic acid Concentration Rank 2

| R.T. | EstConc   | Area  | Relative to ISTD   | R.T. |
|------|-----------|-------|--------------------|------|
| 1.34 | 6.92 ug/l | 85255 | Pentafluorobenzene | 5.68 |

| Hit# | of | Tentative ID                  | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------|-----|----------|-------------|------|
| 1    | 5  | Aminomethanesulfonic acid     | 111 | CH5NO3S  | 013881-91-9 | 83   |
| 2    |    | Sulfur dioxide                | 64  | O2S      | 007446-09-5 | 83   |
| 3    |    | 2-Aminoethyl hydrogen sulfate | 141 | C2H7NO4S | 000926-39-6 | 83   |
| 4    |    | L-Alanine, 3-sulfo-           | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 5    |    | Ethene, 1,1-difluoro-         | 64  | C2H2F2   | 000075-38-7 | 5    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| Aminomethanesulfo... | 1.34 | 6.9     | ug/l  | 85255    | 1                     | 5.68 | 615848 | 50.0 |