LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV051120\
Data File : VV015988.D
Acq On : 11 May 2020 14:38
Operator : SY/MD
Sample : L2520-13
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** MSVOA_V
**ClientSampleId :** H41Y5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_V\METHOD\SOMVTR050720WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.142 | 12 | 16 | 27 | rVB | 6859 | 8243 | 1.59% | 0.182% |
| 2 | 1.245 | 36 | 48 | 60 | rBV2 | 11281 | 38429 | 7.43% | 0.850% |
| 3 | 1.315 | 63 | 70 | 81 | rVB | 55471 | 62233 | 12.02% | 1.376% |
| 4 | 1.460 | 93 | 115 | 144 | rBV2 | 40452 | 210074 | 40.59% | 4.644% |
| 5 | 1.579 | 146 | 152 | 162 | rVB | 55822 | 65872 | 12.73% | 1.456% |
| 6 | 2.122 | 312 | 321 | 337 | rVB2 | 104225 | 170483 | 32.94% | 3.769% |
| 7 | 3.933 | 871 | 884 | 923 | rBV2 | 53896 | 190759 | 36.86% | 4.217% |
| 8 | 4.380 | 1005 | 1023 | 1050 | rBV | 78840 | 208761 | 40.34% | 4.615% |
| 9 | 4.637 | 1092 | 1103 | 1114 | rBV4 | 4776 | 10002 | 1.93% | 0.221% |
| 10 | 5.074 | 1223 | 1239 | 1270 | rBV2 | 183652 | 461169 | 89.10% | 10.195% |
| 11 | 5.643 | 1403 | 1416 | 1437 | rBV | 179880 | 364659 | 70.46% | 8.061% |
| 12 | 5.936 | 1497 | 1507 | 1509 | rBV6 | 5222 | 6919 | 1.34% | 0.153% |
| 13 | 6.096 | 1544 | 1557 | 1584 | rBV | 111266 | 231399 | 44.71% | 5.116% |
| 14 | 7.010 | 1830 | 1841 | 1860 | rBV2 | 49297 | 93410 | 18.05% | 2.065% |
| 15 | 7.338 | 1931 | 1943 | 1963 | rBV | 214152 | 379151 | 73.26% | 8.382% |
| 16 | 7.646 | 2028 | 2039 | 2063 | rBV2 | 29755 | 54737 | 10.58% | 1.210% |
| 17 | 7.997 | 2139 | 2148 | 2163 | rVB2 | 35801 | 63118 | 12.20% | 1.395% |
| 18 | 8.116 | 2172 | 2185 | 2224 | rBV2 | 247398 | 517557 | 100.00% | 11.442% |
| 19 | 8.874 | 2409 | 2421 | 2450 | rBV | 284010 | 464367 | 89.72% | 10.266% |
| 20 | 10.238 | 2833 | 2845 | 2859 | rBV | 77980 | 123272 | 23.82% | 2.725% |
| 21 | 10.405 | 2888 | 2897 | 2904 | rBV3 | 6274 | 9872 | 1.91% | 0.218% |
| 22 | 11.270 | 3155 | 3166 | 3185 | rBV | 277667 | 432034 | 83.48% | 9.551% |
| 23 | 11.646 | 3272 | 3283 | 3304 | rVB | 223297 | 356954 | 68.97% | 7.891% |

Sum of corrected areas: 4523474

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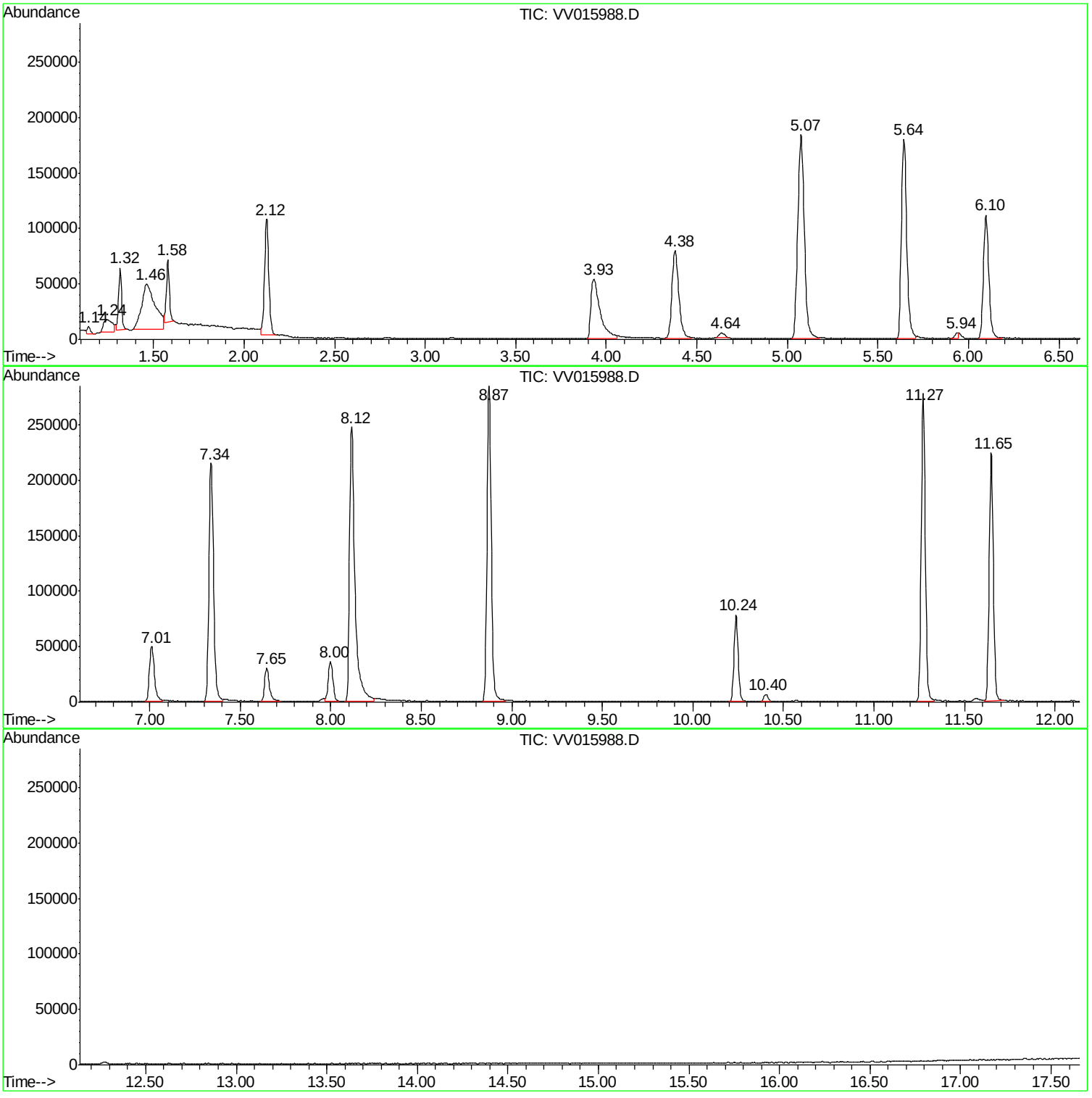
**Instrument :** MSVOA_V
**ClientSampleId :** H41Y5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



# Library Search Compound Report

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**Instrument :** MSVOA_V
**ClientSampleId :** H41Y5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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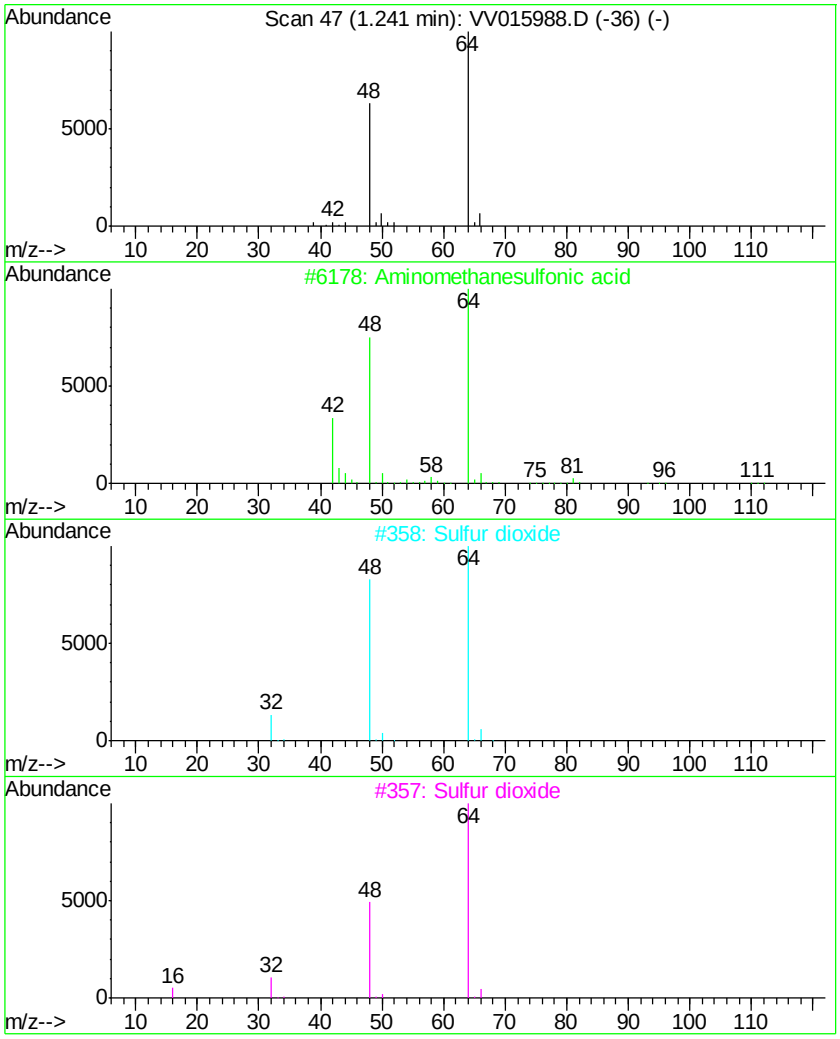
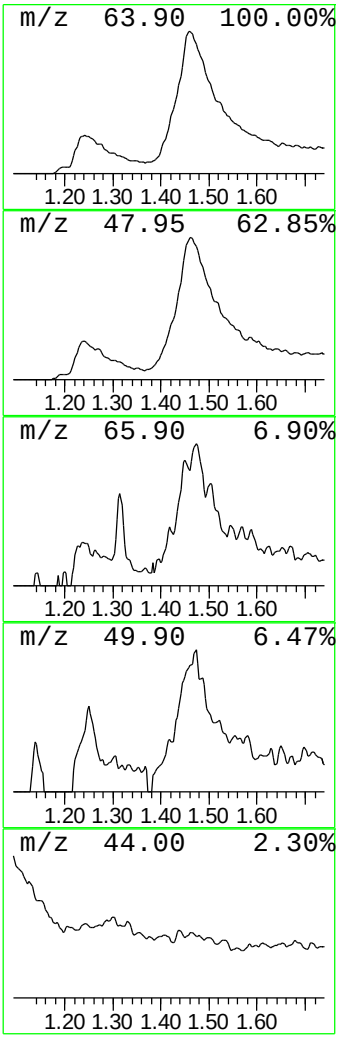
Peak Number 1 Aminomethanesulfonic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.24 | 0.53 ug/L | 38429 | 1,4-Difluorobenzene | 5.64 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Aminomethanesulfonic acid | 111 | CH5NO3S | 013881-91-9 | 74 |
| 2 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 74 |
| 3 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 74 |
| 4 | L-Alanine, 3-sulfo- | 169 | C3H7NO5S | 000498-40-8 | 64 |
| 5 | L-Alanine, 3-sulfo- | 169 | C3H7NO5S | 000498-40-8 | 9 |



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ALS Vial : 11 Sample Multiplier: 1

**Instrument :** MSVOA_V
**ClientSampleId :** H41Y5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

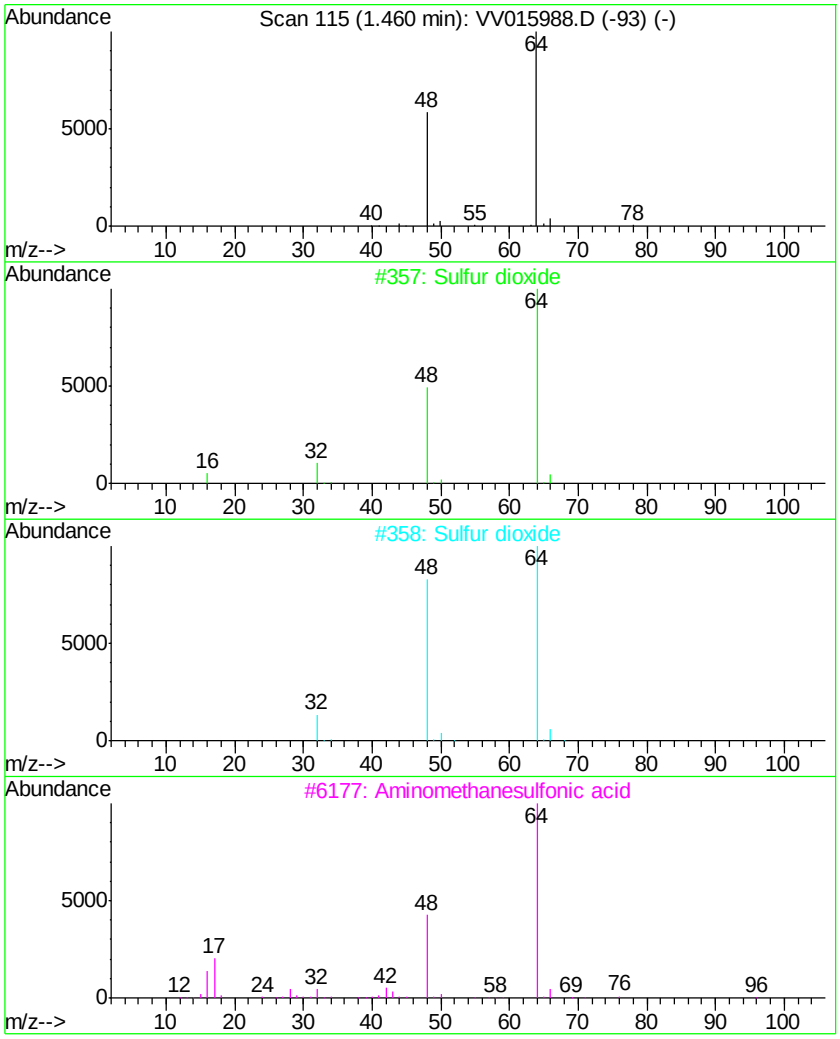
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

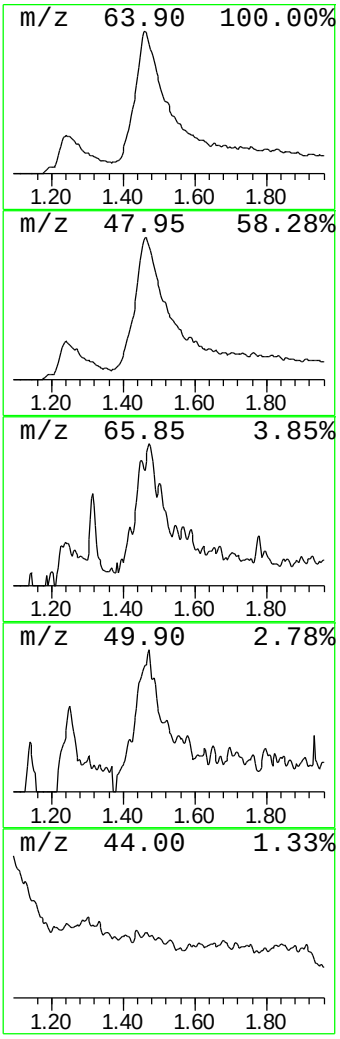
**********

Peak Number 2 Sulfur dioxide Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.46 | 2.88 ug/L | 210074 | 1,4-Difluorobenzene | 5.64 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 90 |
| 2 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 74 |
| 3 | Aminomethanesulfonic acid | 111 | CH5NO3S | 013881-91-9 | 9 |
| 4 | Ethene, 1,1-difluoro- | 64 | C2H2F2 | 000075-38-7 | 5 |
| 5 | L-Alanine, 3-sulfo- | 169 | C3H7NO5S | 000498-40-8 | 4 |



Tentatively Identified Compound (LSC) summary

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ALS Vial : 11 Sample Multiplier: 1

**Instrument :** MSVOA_V
**ClientSampleId :** H41Y5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Aminomethanesulfo... | 1.24 | 0.5 | ug/L | 38429 | 1 | 5.64 | 364659 | 5.0 |
| Sulfur dioxide | 1.46 | 2.9 | ug/L | 210074 | 1 | 5.64 | 364659 | 5.0 |