LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX032218\
Data File : VX000417.D
Acq On : 22 Mar 2018 19:53
Operator : JC/MD
Sample : J2005-12
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** BR-3-031918

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\82X032018W.M
Title : SW846 8260

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.075 | 76 | 80 | 94 | rBV | 265750 | 317719 | 62.55% | 9.584% |
| 2 | 1.276 | 108 | 113 | 123 | rBV | 58068 | 79839 | 15.72% | 2.408% |
| 3 | 1.593 | 159 | 165 | 170 | rBV3 | 4230 | 7017 | 1.38% | 0.212% |
| 4 | 2.623 | 328 | 334 | 342 | rVB | 17975 | 32284 | 6.36% | 0.974% |
| 5 | 3.215 | 421 | 431 | 445 | rVB | 93536 | 226093 | 44.51% | 6.820% |
| 6 | 5.513 | 798 | 808 | 822 | rBV | 63056 | 177579 | 34.96% | 5.357% |
| 7 | 5.678 | 824 | 835 | 850 | rVV | 92295 | 256057 | 50.41% | 7.724% |
| 8 | 6.080 | 891 | 901 | 916 | rBV2 | 68000 | 180190 | 35.47% | 5.436% |
| 9 | 6.873 | 1020 | 1031 | 1043 | rBV | 154498 | 361008 | 71.07% | 10.890% |
| 10 | 8.726 | 1328 | 1335 | 1345 | rBV | 326080 | 507940 | 100.00% | 15.322% |
| 11 | 10.122 | 1558 | 1564 | 1572 | rBV | 325227 | 441991 | 87.02% | 13.333% |
| 12 | 11.146 | 1726 | 1732 | 1741 | rBV | 266759 | 329280 | 64.83% | 9.933% |
| 13 | 12.085 | 1881 | 1886 | 1894 | rVB | 328345 | 398008 | 78.36% | 12.006% |

Sum of corrected areas: 3315005

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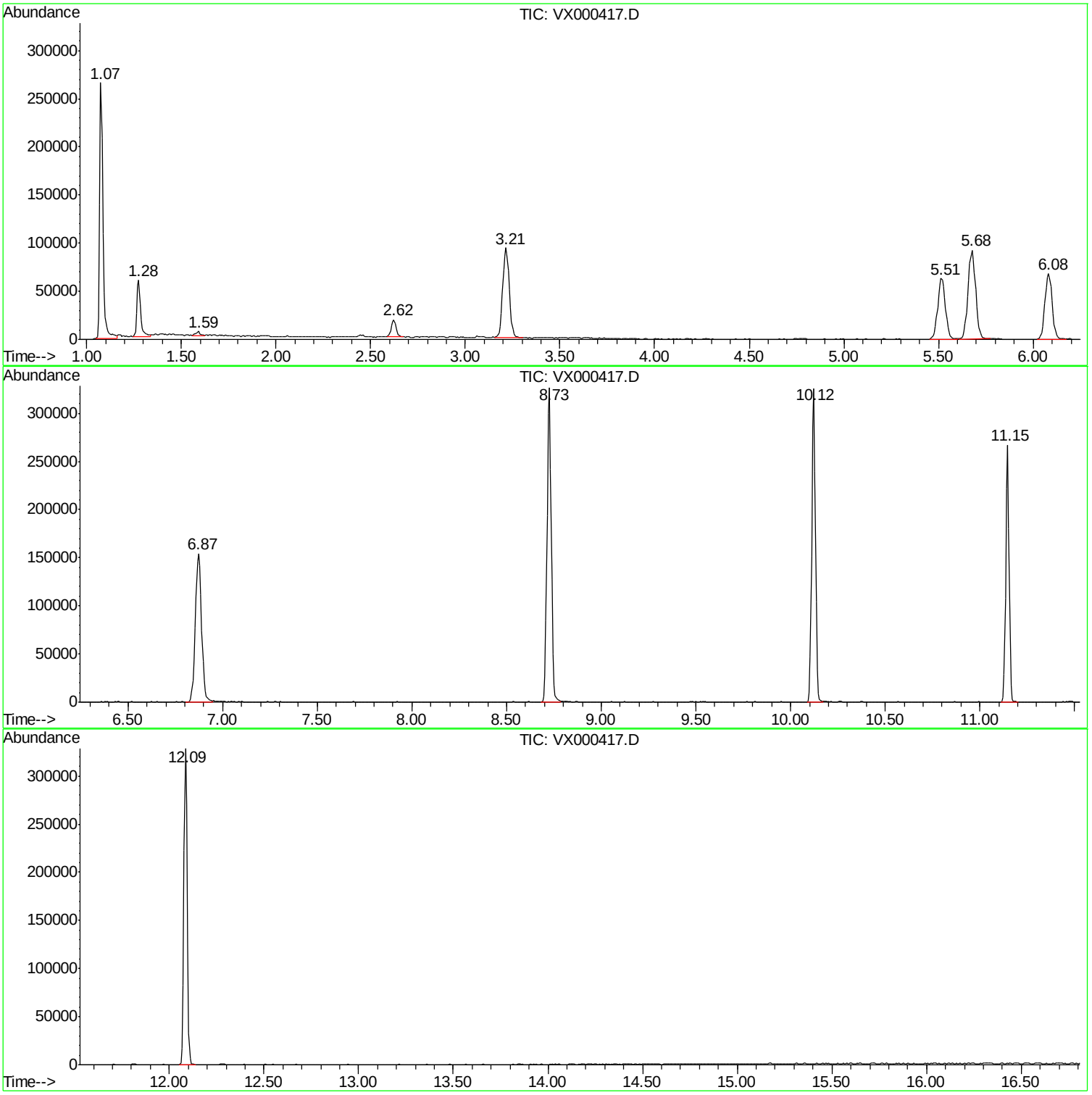
MSVOA_X
**ClientSampleId :**
BR-3-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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



# Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX032218\
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ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** BR-3-031918

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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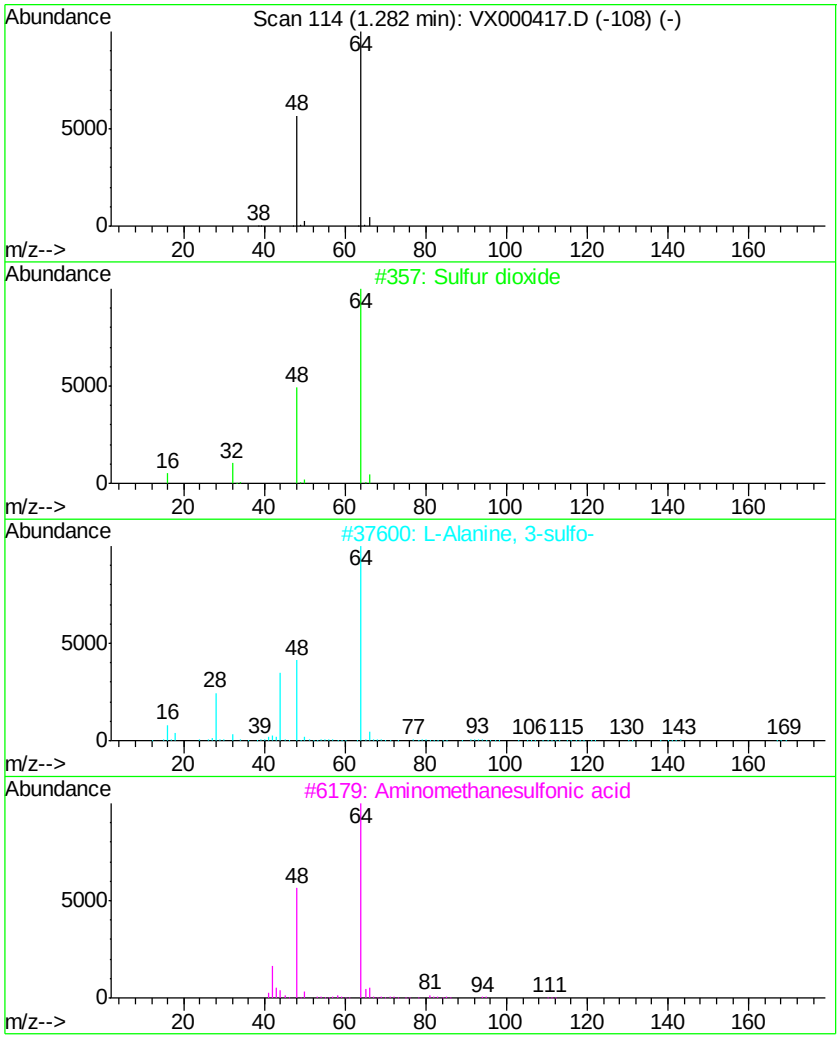
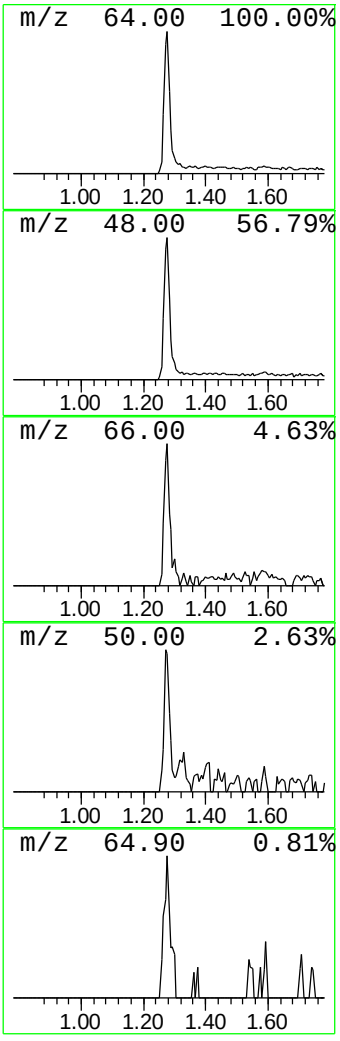
Peak Number 2 Sulfur dioxide Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.28 | 15.59 ug/l | 79839 | Pentafluorobenzene | 5.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 83 |
| 2 | L-Alanine, 3-sulfo- | 169 | C3H7NO5S | 000498-40-8 | 9 |
| 3 | Aminomethanesulfonic acid | 111 | CH5NO3S | 013881-91-9 | 9 |
| 4 | Ethene, 1,1-difluoro- | 64 | C2H2F2 | 000075-38-7 | 4 |
| 5 | Ethyl Chloride | 64 | C2H5Cl | 000075-00-3 | 3 |



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Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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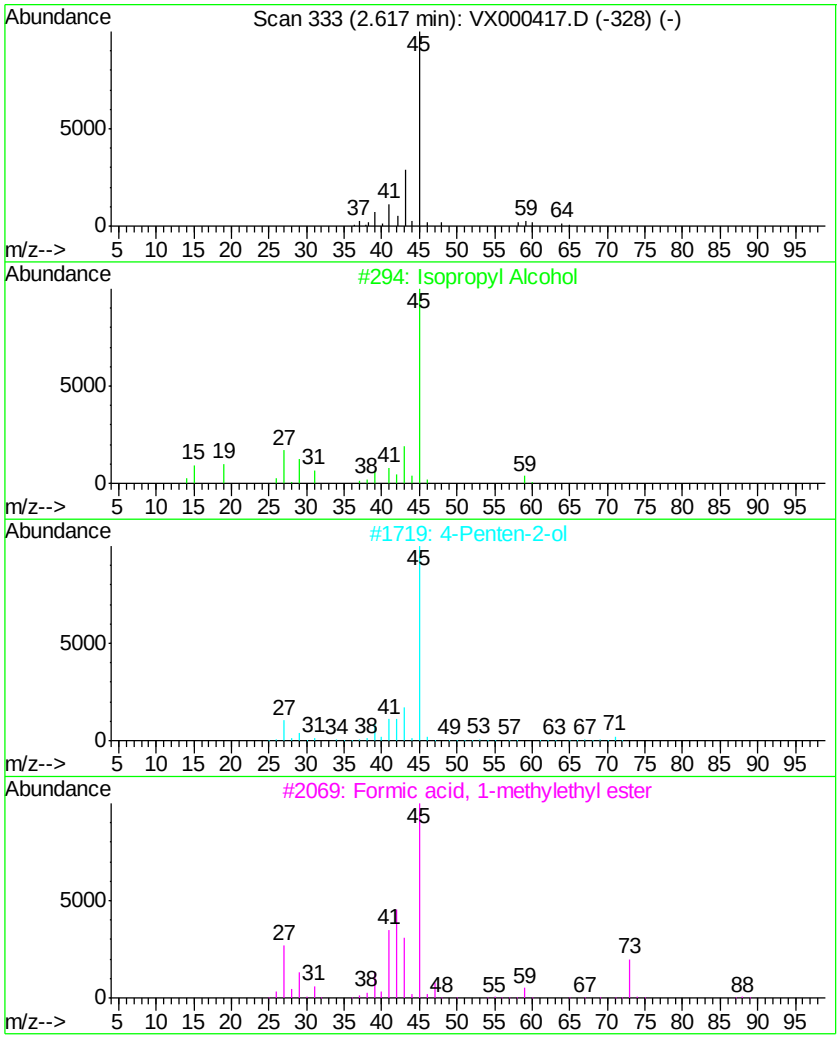
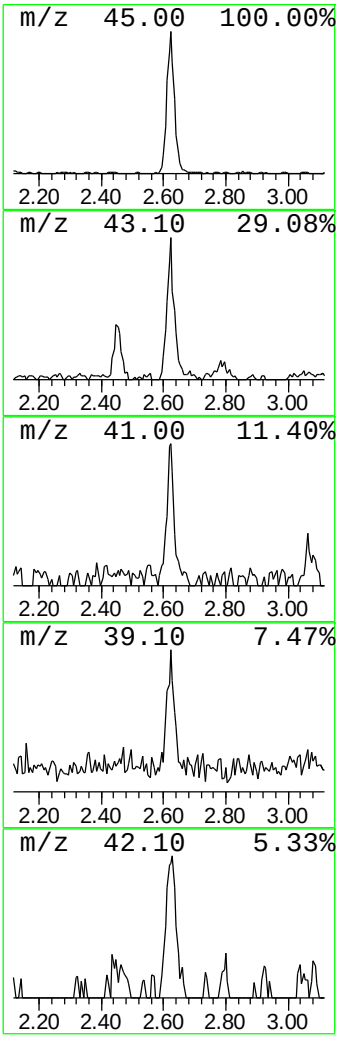
Peak Number 3 Isopropyl Alcohol Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.62 | 6.30 ug/l | 32284 | Pentafluorobenzene | 5.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Isopropyl Alcohol | 60 | C3H8O | 000067-63-0 | 56 |
| 2 | 4-Penten-2-ol | 86 | C5H10O | 000625-31-0 | 9 |
| 3 | Formic acid, 1-methylethyl ester | 88 | C4H8O2 | 000625-55-8 | 9 |
| 4 | (S)-(+)-2-Pentanol | 88 | C5H12O | 026184-62-3 | 9 |
| 5 | Propane, 2-ethoxy- | 88 | C5H12O | 000625-54-7 | 9 |



Tentatively Identified Compound (LSC) summary

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Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Sulfur dioxide | 1.28 | 15.6 | ug/l | 79839 | 1 | 5.68 | 256057 | 50.0 |
| Isopropyl Alcohol | 2.62 | 6.3 | ug/l | 32284 | 1 | 5.68 | 256057 | 50.0 |