LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027967.D
Acq On : 04 Apr 2022 18:54
Operator : JC/MD
Sample : PB143824ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
PB143824ZHE#04

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82X032922W.M
Title : SW846 8260

Signal : TIC: VX027967.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.239 | 22 | 25 | 41 | rVB | 21685 | 30722 | 2.24% | 0.481% |
| 2 | 2.788 | 272 | 279 | 294 | rBV | 147949 | 270068 | 19.70% | 4.232% |
| 3 | 3.574 | 402 | 408 | 418 | rBV2 | 6286 | 14157 | 1.03% | 0.222% |
| 4 | 5.391 | 693 | 706 | 723 | rBV | 54234 | 156140 | 11.39% | 2.447% |
| 5 | 5.556 | 723 | 733 | 754 | rVB | 97841 | 274280 | 20.01% | 4.299% |
| 6 | 5.958 | 788 | 799 | 815 | rBV | 58169 | 155790 | 11.36% | 2.442% |
| 7 | 6.348 | 855 | 863 | 873 | rBV2 | 5684 | 14901 | 1.09% | 0.234% |
| 8 | 6.763 | 923 | 931 | 946 | rVB | 145152 | 354512 | 25.86% | 5.556% |
| 9 | 7.799 | 1093 | 1101 | 1116 | rBV | 575222 | 973374 | 71.00% | 15.255% |
| 10 | 8.549 | 1218 | 1224 | 1234 | rBV | 90117 | 138185 | 10.08% | 2.166% |
| 11 | 8.653 | 1234 | 1241 | 1256 | rVB | 281410 | 456516 | 33.30% | 7.155% |
| 12 | 8.958 | 1285 | 1291 | 1298 | rVB | 10074 | 14379 | 1.05% | 0.225% |
| 13 | 9.244 | 1331 | 1338 | 1344 | rBV | 23833 | 34495 | 2.52% | 0.541% |
| 14 | 9.342 | 1350 | 1354 | 1359 | rBV | 61609 | 81302 | 5.93% | 1.274% |
| 15 | 9.482 | 1372 | 1377 | 1385 | rBV | 1013624 | 1370999 | 100.00% | 21.486% |
| 16 | 9.579 | 1388 | 1393 | 1403 | rVB | 119731 | 153043 | 11.16% | 2.398% |
| 17 | 9.915 | 1442 | 1448 | 1463 | rBV | 641018 | 805974 | 58.79% | 12.631% |
| 18 | 10.055 | 1463 | 1471 | 1479 | rBV | 299723 | 398488 | 29.07% | 6.245% |
| 19 | 10.640 | 1563 | 1567 | 1578 | rVB | 24690 | 30388 | 2.22% | 0.476% |
| 20 | 11.085 | 1634 | 1640 | 1652 | rVB | 256714 | 324054 | 23.64% | 5.079% |
| 21 | 12.024 | 1789 | 1794 | 1803 | rVB | 272486 | 329052 | 24.00% | 5.157% |

Sum of corrected areas: 6380819

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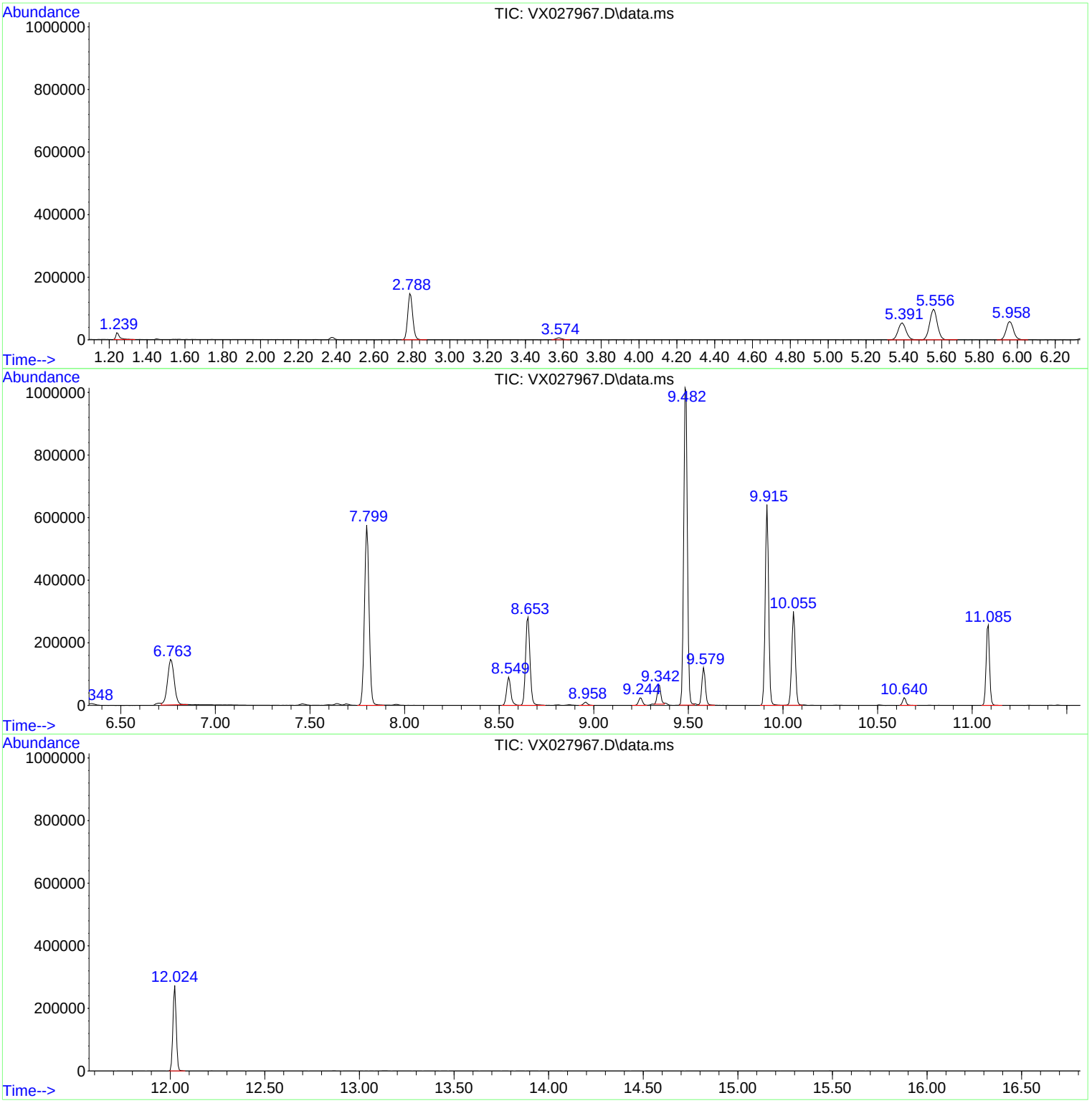
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
PB143824ZHE#04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027967.D
Acq On : 04 Apr 2022 18:54
Operator : JC/MD
Sample : PB143824ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
PB143824ZHE#04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

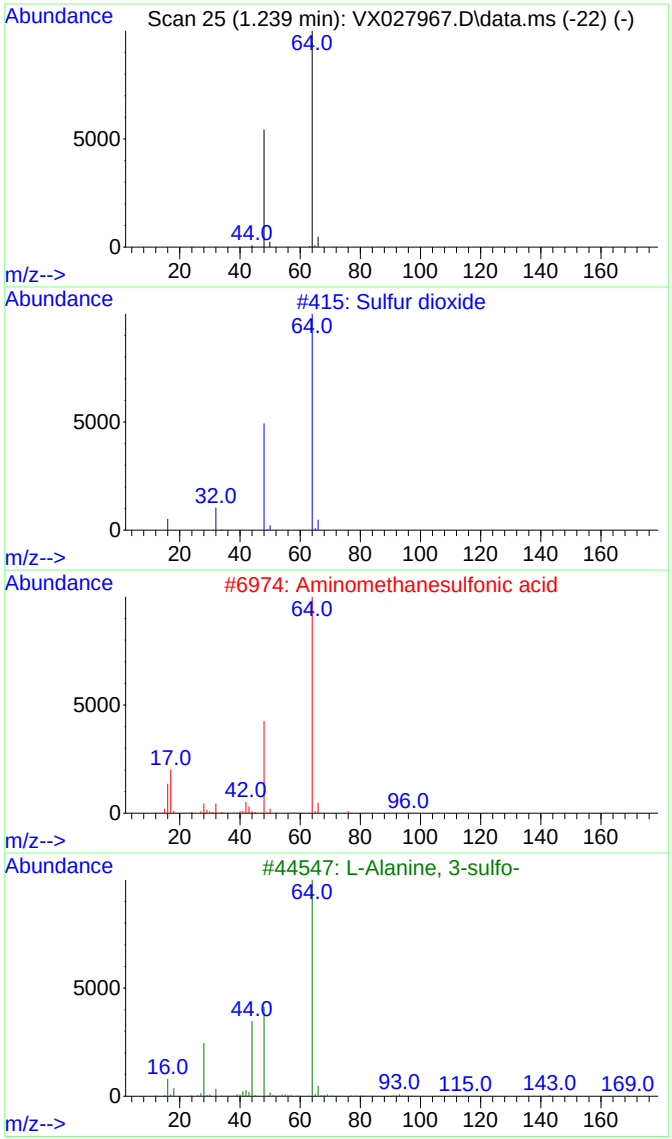
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

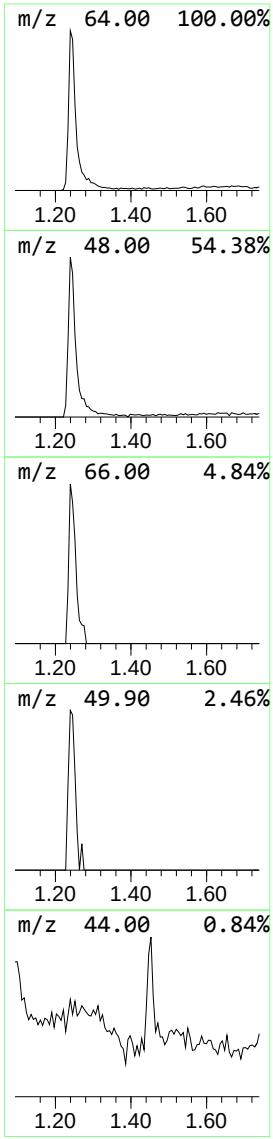
**********

Peak Number 1 Sulfur dioxide Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.239 | 5.60 ug/l | 30722 | Pentafluorobenzene | 5.556 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 90 |
| 2 | Aminomethanesulfonic acid | 111 | CH5NO3S | 013881-91-9 | 64 |
| 3 | L-Alanine, 3-sulfo- | 169 | C3H7NO5S | 000498-40-8 | 9 |
| 4 | Ethene, 1,1-difluoro- | 64 | C2H2F2 | 000075-38-7 | 4 |
| 5 | Ethyl Chloride | 64 | C2H5Cl | 000075-00-3 | 4 |



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Data File : VX027967.D
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Operator : JC/MD
Sample : PB143824ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
PB143824ZHE#04

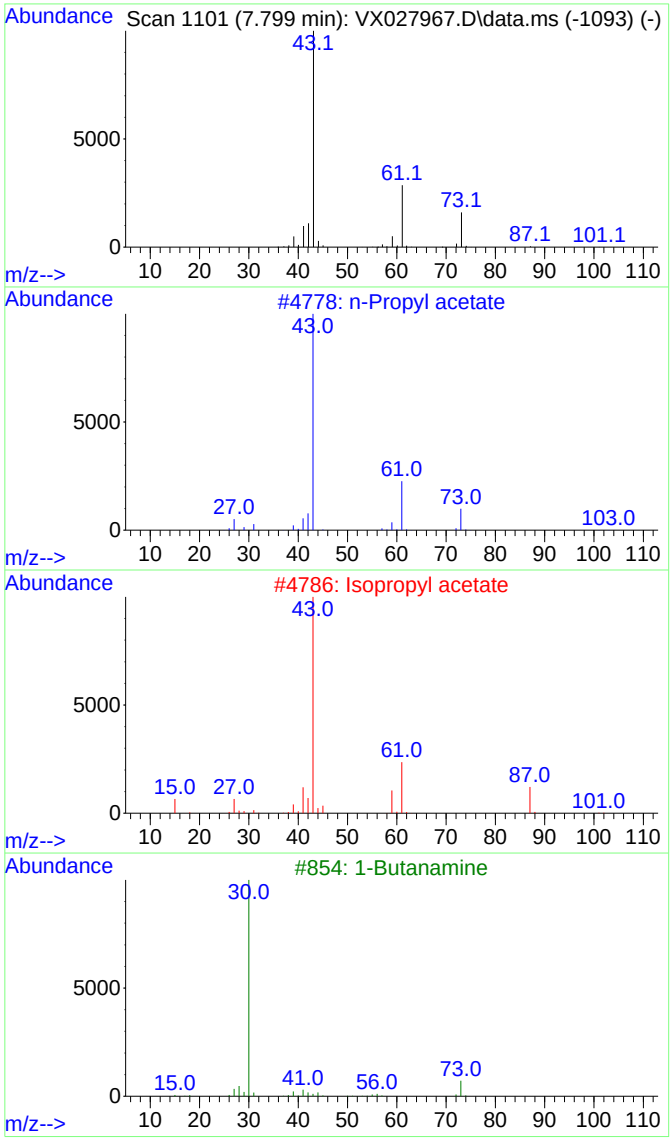
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

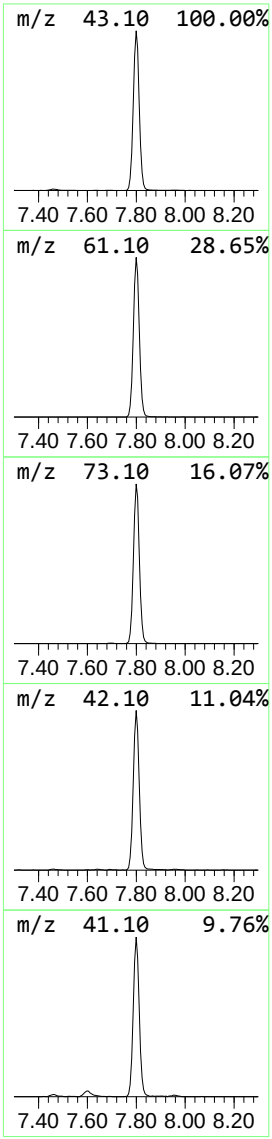
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 n-Propyl acetate Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.799 | 137.28 ug/l | 973374 | 1,4-Difluorobenzene | 6.763 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Propyl acetate | 102 | C5H10O2 | 000109-60-4 | 83 |
| 2 | Isopropyl acetate | 102 | C5H10O2 | 000108-21-4 | 36 |
| 3 | 1-Butanamine | 73 | C4H11N | 000109-73-9 | 9 |
| 4 | Isobutyl acetate | 116 | C6H12O2 | 000110-19-0 | 9 |
| 5 | Isobutylamine | 73 | C4H11N | 000078-81-9 | 7 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027967.D
Acq On : 04 Apr 2022 18:54
Operator : JC/MD
Sample : PB143824ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
PB143824ZHE#04

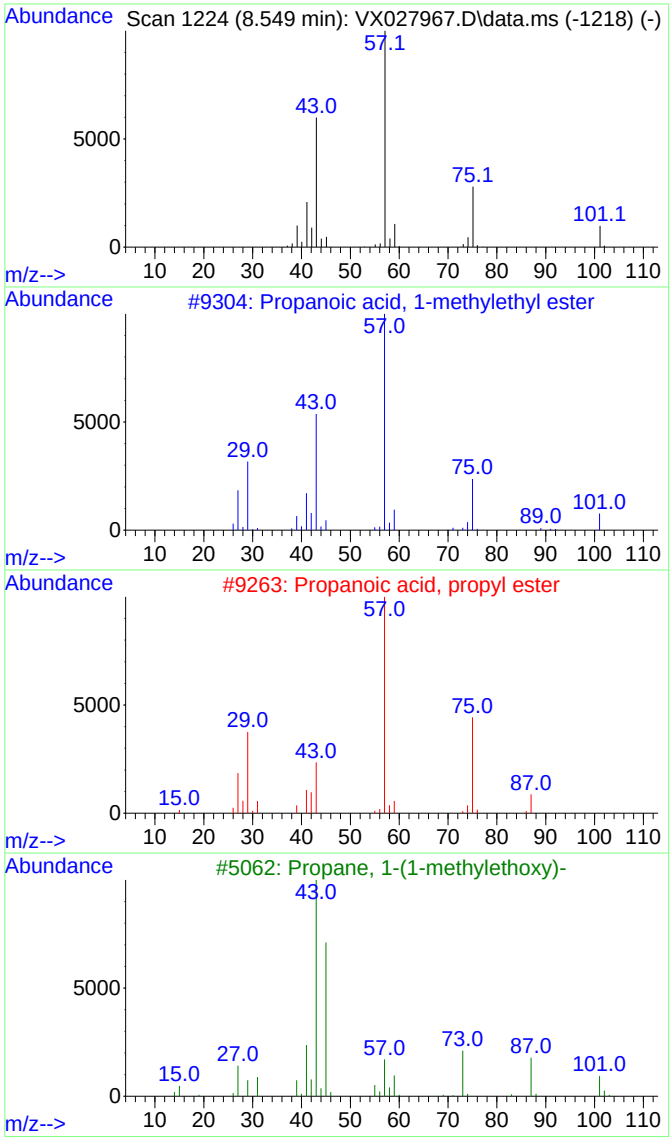
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

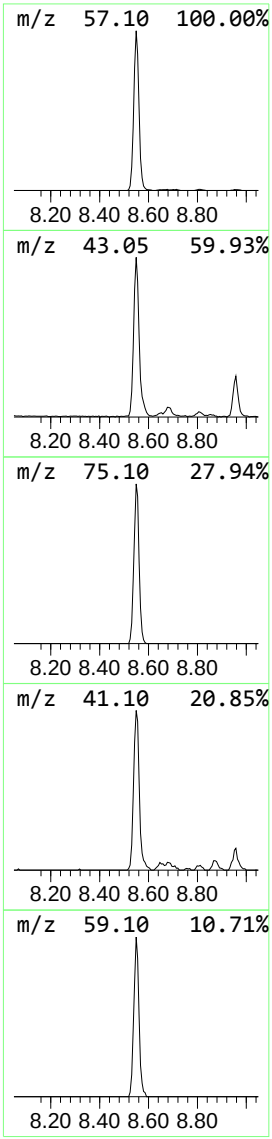
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.549 | 17.34 ug/l | 138185 | Chlorobenzene-d5 | 10.055 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propanoic acid, 1-methylethyl ester | 116 | C6H12O2 | 000637-78-5 | 90 |
| 2 | Propanoic acid, propyl ester | 116 | C6H12O2 | 000106-36-5 | 33 |
| 3 | Propane, 1-(1-methylethoxy)- | 102 | C6H14O | 000627-08-7 | 25 |
| 4 | o-Isopropylhydroxylamine | 75 | C3H9NO | 1000322-42-6 | 25 |
| 5 | Butanoic acid, methyl ester | 102 | C5H10O2 | 000623-42-7 | 10 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027967.D
Acq On : 04 Apr 2022 18:54
Operator : JC/MD
Sample : PB143824ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
PB143824ZHE#04

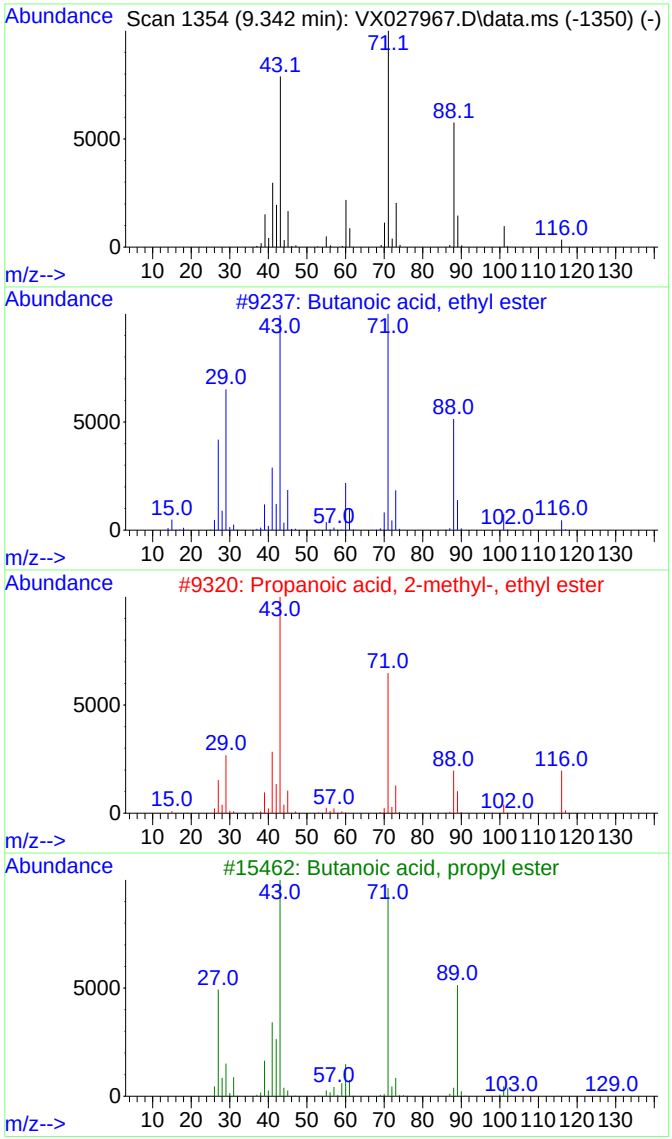
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

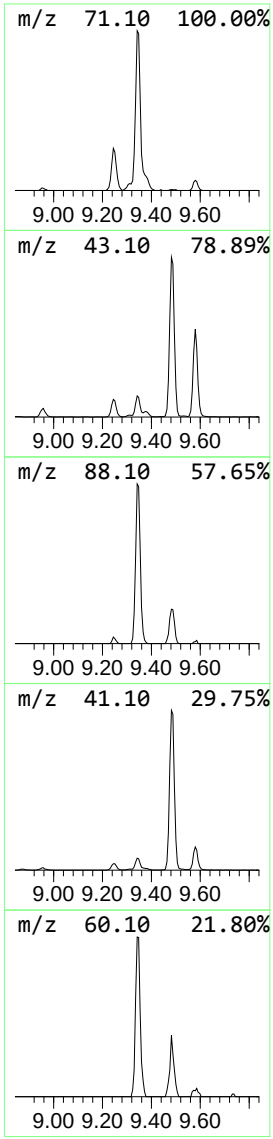
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.342 | 10.20 ug/l | 81302 | Chlorobenzene-d5 | 10.055 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butanoic acid, ethyl ester | 116 | C6H12O2 | 000105-54-4 | 97 |
| 2 | Propanoic acid, 2-methyl-, ethyl... | 116 | C6H12O2 | 000097-62-1 | 59 |
| 3 | Butanoic acid, propyl ester | 130 | C7H14O2 | 000105-66-8 | 47 |
| 4 | 3-Methyl-6-(methylthio)hexa-1,5-... | 158 | C8H14OS | 1000191-74-2 | 40 |
| 5 | 4-Butoxy-2-butanone | 144 | C8H16O2 | 030536-44-8 | 38 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027967.D
Acq On : 04 Apr 2022 18:54
Operator : JC/MD
Sample : PB143824ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
PB143824ZHE#04

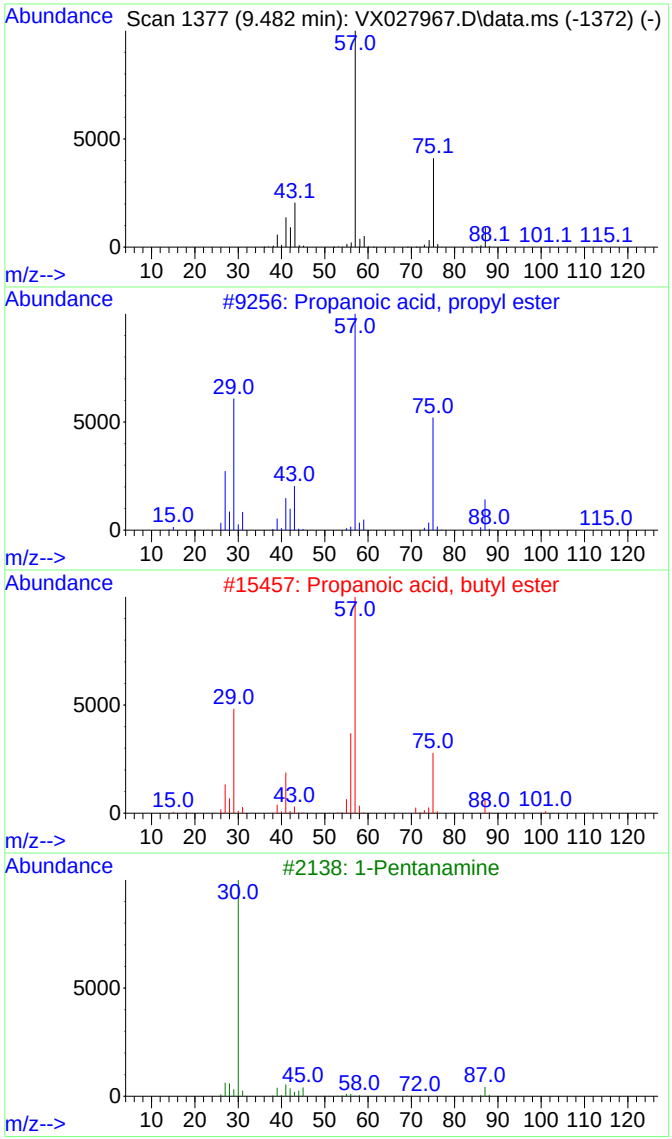
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

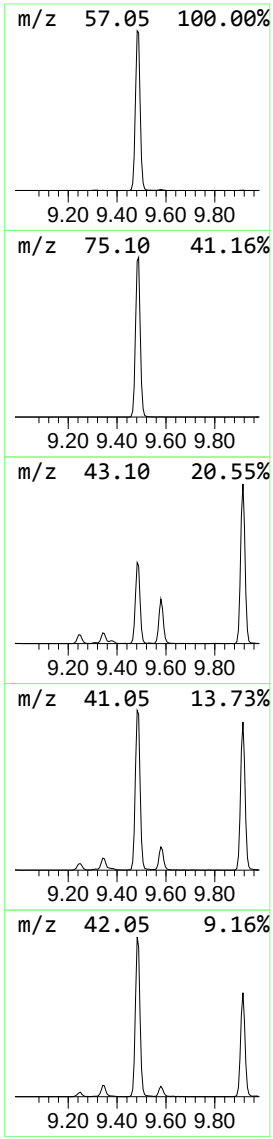
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.482 | 172.03 ug/l | 1371000 | Chlorobenzene-d5 | 10.055 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propanoic acid, propyl ester | 116 | C6H12O2 | 000106-36-5 | 83 |
| 2 | Propanoic acid, butyl ester | 130 | C7H14O2 | 000590-01-2 | 38 |
| 3 | 1-Pentanamine | 87 | C5H13N | 000110-58-7 | 10 |
| 4 | Azetidine | 57 | C3H7N | 000503-29-7 | 9 |
| 5 | 2-(Isobutoxymethyl)oxirane | 130 | C7H14O2 | 003814-55-9 | 9 |



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Operator : JC/MD
Sample : PB143824ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
PB143824ZHE#04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

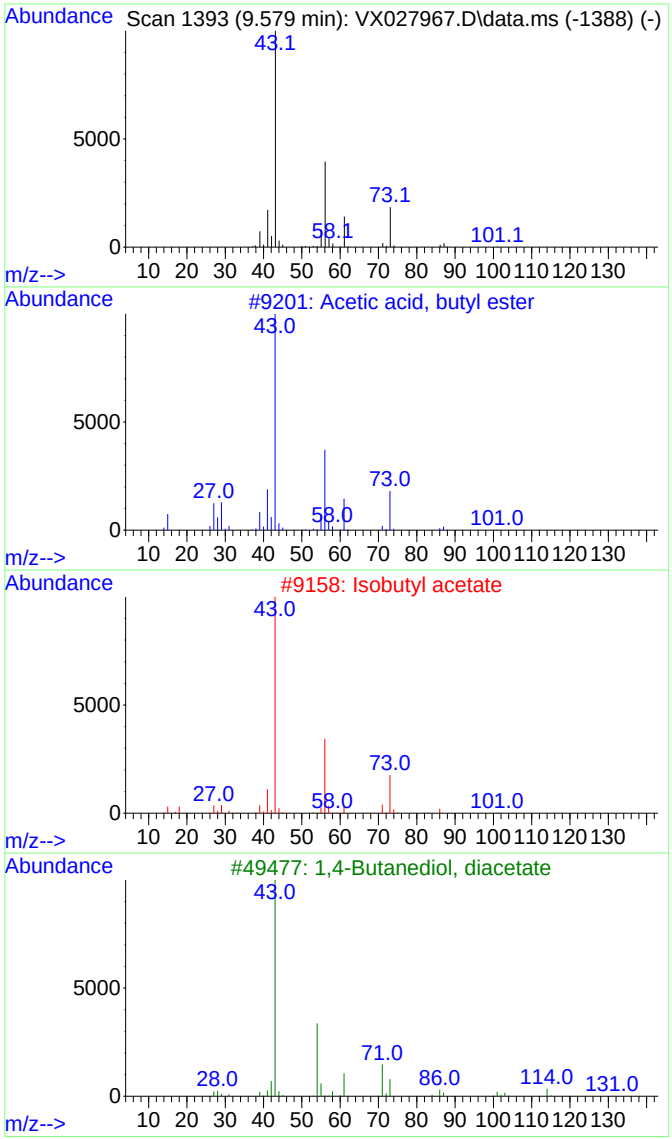
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

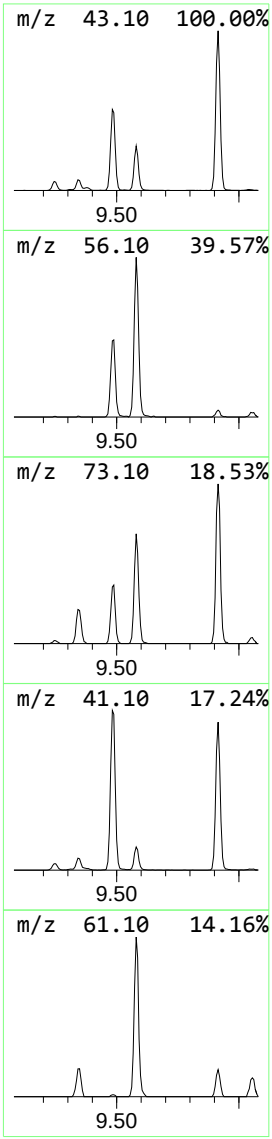
**********

Peak Number 6 Acetic acid, butyl ester Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.579 | 19.20 ug/l | 153043 | Chlorobenzene-d5 | 10.055 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetic acid, butyl ester | 116 | C6H12O2 | 000123-86-4 | 83 |
| 2 | Isobutyl acetate | 116 | C6H12O2 | 000110-19-0 | 40 |
| 3 | 1,4-Butanediol, diacetate | 174 | C8H14O4 | 000628-67-1 | 17 |
| 4 | Isobutylamine | 73 | C4H11N | 000078-81-9 | 9 |
| 5 | 2-Butanone, 3-methyl- | 86 | C5H10O | 000563-80-4 | 9 |



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Data File : VX027967.D
Acq On : 04 Apr 2022 18:54
Operator : JC/MD
Sample : PB143824ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
PB143824ZHE#04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

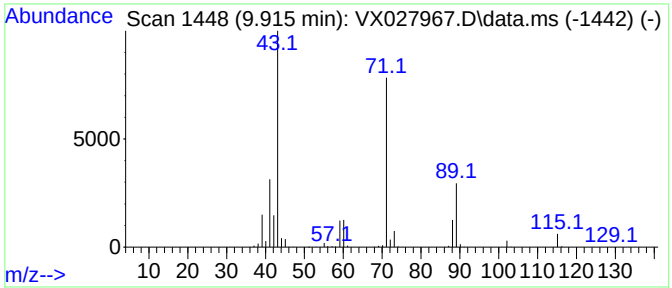
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

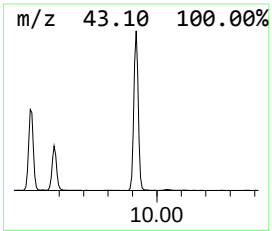
**********

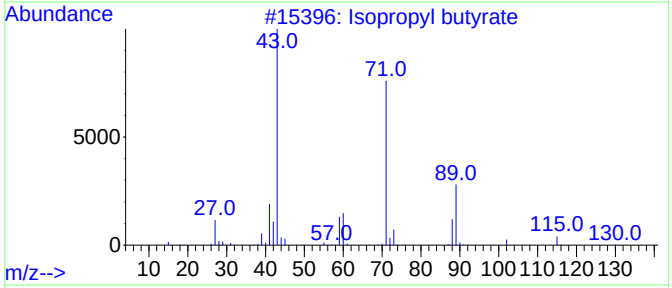
Peak Number 7 Isopropyl butyrate Concentration Rank 3

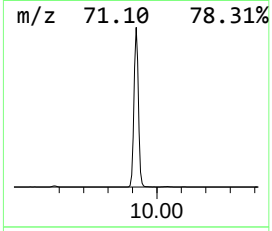
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.915 | 101.13 ug/l | 805974 | Chlorobenzene-d5 | 10.055 |

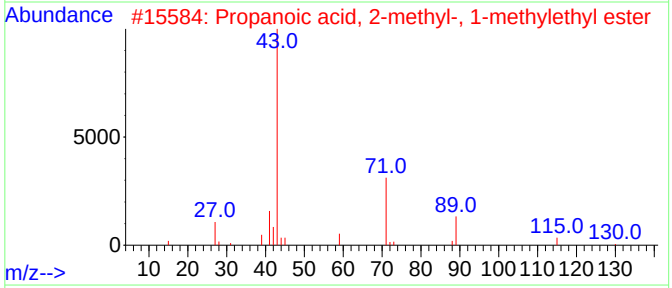
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Isopropyl butyrate | 130 | C7H14O2 | 000638-11-9 | 94 |
| 2 | Propanoic acid, 2-methyl-, 1-met... | 130 | C7H14O2 | 000617-50-5 | 78 |
| 3 | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5 | 72 |
| 4 | Ethylene glycol Formate Isobutyrate | 160 | C7H12O4 | 1000458-48-0 | 64 |
| 5 | Butanoic acid, propyl ester | 130 | C7H14O2 | 000105-66-8 | 64 |

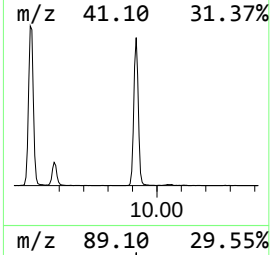


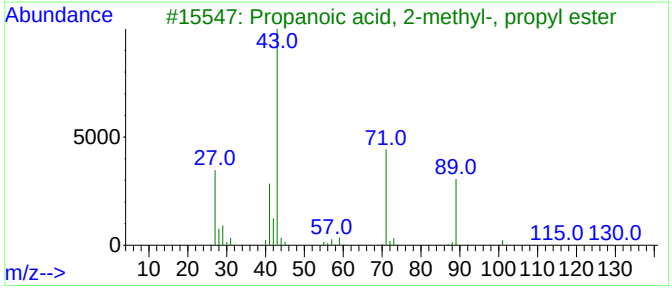



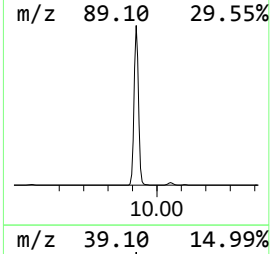



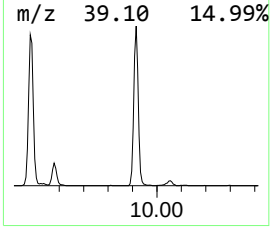



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027967.D
Acq On : 04 Apr 2022 18:54
Operator : JC/MD
Sample : PB143824ZHE#04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
PB143824ZHE#04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Sulfur dioxide | 1.239 | 5.6 | ug/l | 30722 | 1 | 5.556 | 274280 | 50.0 |
| n-Propyl acetate | 7.799 | 137.3 | ug/l | 973374 | 2 | 6.763 | 354512 | 50.0 |
| Propanoic acid,... | 8.549 | 17.3 | ug/l | 138185 | 3 | 10.055 | 398488 | 50.0 |
| Butanoic acid, ... | 9.342 | 10.2 | ug/l | 81302 | 3 | 10.055 | 398488 | 50.0 |
| Propanoic acid,... | 9.482 | 172.0 | ug/l | 1371000 | 3 | 10.055 | 398488 | 50.0 |
| Acetic acid, bu... | 9.579 | 19.2 | ug/l | 153043 | 3 | 10.055 | 398488 | 50.0 |
| Isopropyl butyrate | 9.915 | 101.1 | ug/l | 805974 | 3 | 10.055 | 398488 | 50.0 |