LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078054.D
Acq On : 05 Jun 2023 19:09
Operator : JC\MD
Sample : 03018-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
343

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 : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Title : SW846 8260

Signal : TIC: VN078054.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.830 | 142 | 149 | 157 | rVB3 | 34259 | 72759 | 2.32% | 0.371% |
| 2 | 4.447 | 416 | 424 | 434 | rBV4 | 11395 | 35607 | 1.13% | 0.181% |
| 3 | 7.577 | 947 | 956 | 964 | rBV2 | 32957 | 81422 | 2.60% | 0.415% |
| 4 | 8.171 | 1048 | 1057 | 1062 | rBV | 301933 | 720844 | 22.98% | 3.671% |
| 5 | 8.235 | 1062 | 1068 | 1079 | rVB | 505680 | 1151525 | 36.70% | 5.864% |
| 6 | 8.582 | 1117 | 1127 | 1138 | rBV | 302828 | 692128 | 22.06% | 3.525% |
| 7 | 8.700 | 1138 | 1147 | 1154 | rBV | 233509 | 594309 | 18.94% | 3.027% |
| 8 | 9.106 | 1206 | 1216 | 1230 | rBV | 772045 | 1593538 | 50.79% | 8.116% |
| 9 | 9.677 | 1304 | 1313 | 1318 | rBV | 89931 | 201179 | 6.41% | 1.025% |
| 10 | 9.747 | 1318 | 1325 | 1339 | rVB | 1719169 | 3137473 | 100.00% | 15.979% |
| 11 | 10.365 | 1421 | 1430 | 1440 | rBV | 372789 | 640724 | 20.42% | 3.263% |
| 12 | 10.571 | 1457 | 1465 | 1479 | rBV | 1156321 | 2213221 | 70.54% | 11.271% |
| 13 | 10.735 | 1486 | 1493 | 1507 | rVB | 381711 | 675722 | 21.54% | 3.441% |
| 14 | 10.994 | 1527 | 1537 | 1545 | rBV | 348199 | 590037 | 18.81% | 3.005% |
| 15 | 11.088 | 1547 | 1553 | 1560 | rVV4 | 69329 | 130758 | 4.17% | 0.666% |
| 16 | 11.176 | 1560 | 1568 | 1569 | rVV | 163816 | 227814 | 7.26% | 1.160% |
| 17 | 11.206 | 1569 | 1573 | 1582 | rVV | 472385 | 842377 | 26.85% | 4.290% |
| 18 | 11.294 | 1582 | 1588 | 1601 | rVB | 260685 | 441055 | 14.06% | 2.246% |
| 19 | 11.606 | 1633 | 1641 | 1652 | rBV | 706311 | 1123718 | 35.82% | 5.723% |
| 20 | 11.871 | 1679 | 1686 | 1698 | rBV | 1040930 | 1860993 | 59.32% | 9.478% |
| 21 | 12.312 | 1753 | 1761 | 1772 | rBV2 | 27597 | 49590 | 1.58% | 0.253% |
| 22 | 12.853 | 1844 | 1853 | 1864 | rBV | 755288 | 1352569 | 43.11% | 6.888% |
| 23 | 13.800 | 2005 | 2014 | 2022 | rBV | 686996 | 1206198 | 38.44% | 6.143% |

Sum of corrected areas: 19635560

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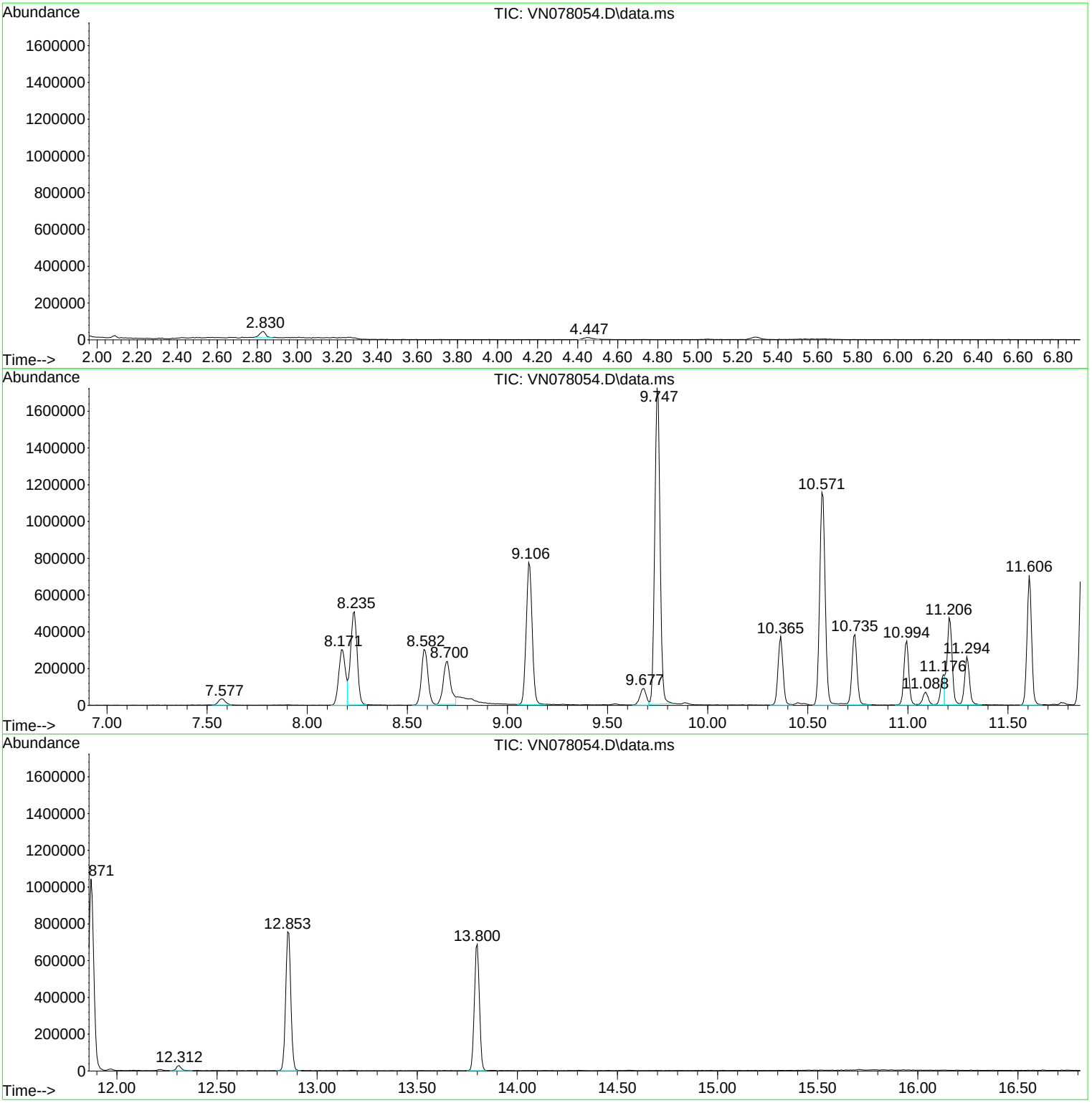
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
343

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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



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Data File : VN078054.D
Acq On : 05 Jun 2023 19:09
Operator : JC\MD
Sample : 03018-08
Misc : 5.0mL/MSVOA_N/WATER
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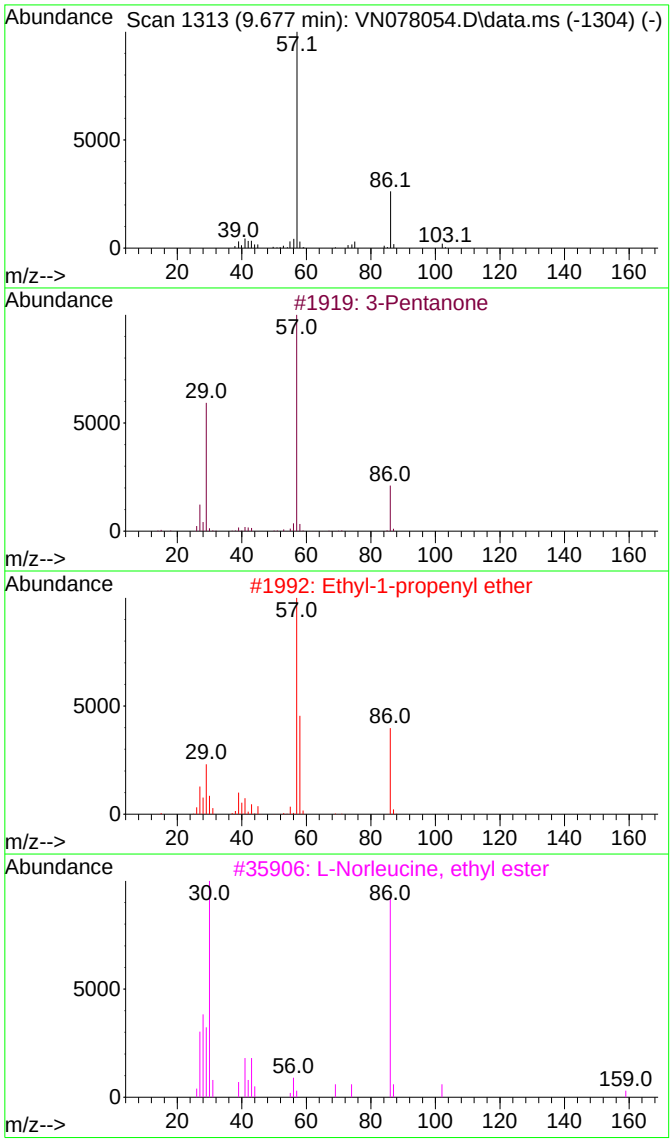
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

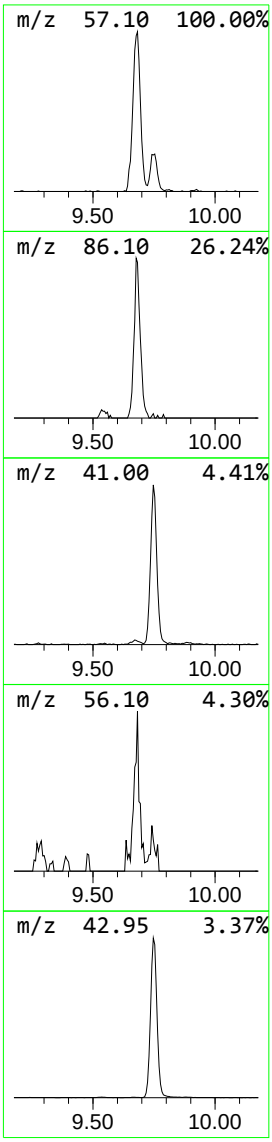
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 3-Pentanone Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.677 | 6.31 ug/l | 201179 | 1,4-Difluorobenzene | 9.106 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Pentanone | 86 | C5H10O | 000096-22-0 | 64 |
| 2 | Ethyl-1-propenyl ether | 86 | C5H10O | 000928-55-2 | 23 |
| 3 | L-Norleucine, ethyl ester | 159 | C8H17NO2 | 022628-26-8 | 17 |
| 4 | Propanoic acid, 2,2-dimethyl- | 102 | C5H10O2 | 000075-98-9 | 12 |
| 5 | Propanoic acid, 3-amino-2-methyl- | 103 | C4H9NO2 | 000144-90-1 | 9 |



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Data File : VN078054.D
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Operator : JC\MD
Sample : 03018-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
343

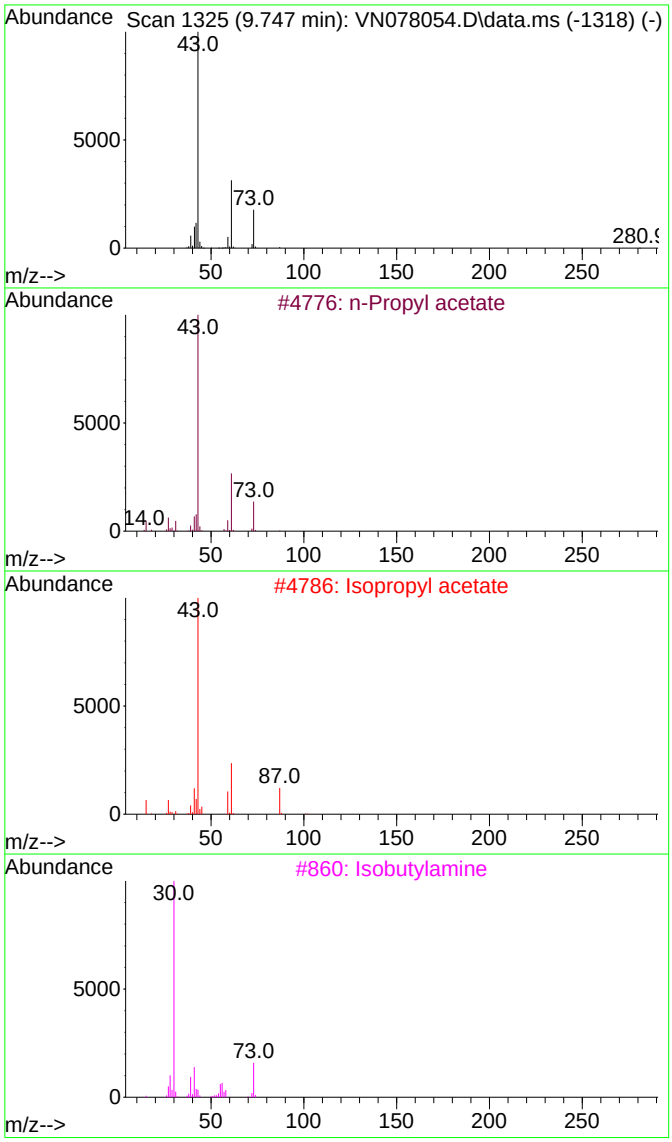
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

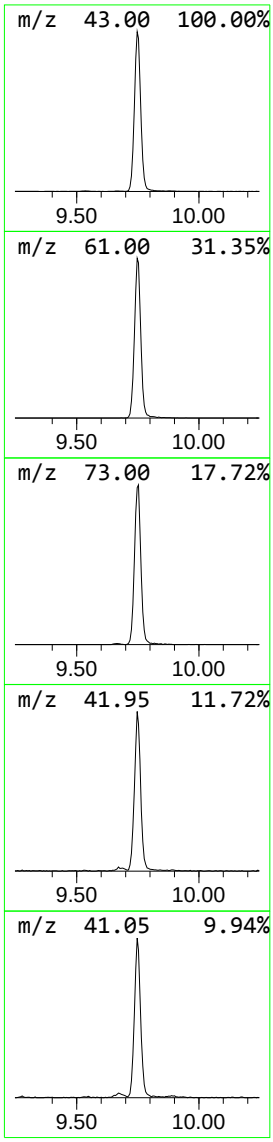
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 n-Propyl acetate Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.747 | 98.44 ug/l | 3137470 | 1,4-Difluorobenzene | 9.106 |

| 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 | 38 |
| 3 | Isobutylamine | 73 | C4H11N | 000078-81-9 | 9 |
| 4 | Propanal, 2,3-dihydroxy-, (S)- | 90 | C3H6O3 | 000497-09-6 | 9 |
| 5 | Isobutyl acetate | 116 | C6H12O2 | 000110-19-0 | 9 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078054.D
Acq On : 05 Jun 2023 19:09
Operator : JC\MD
Sample : 03018-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
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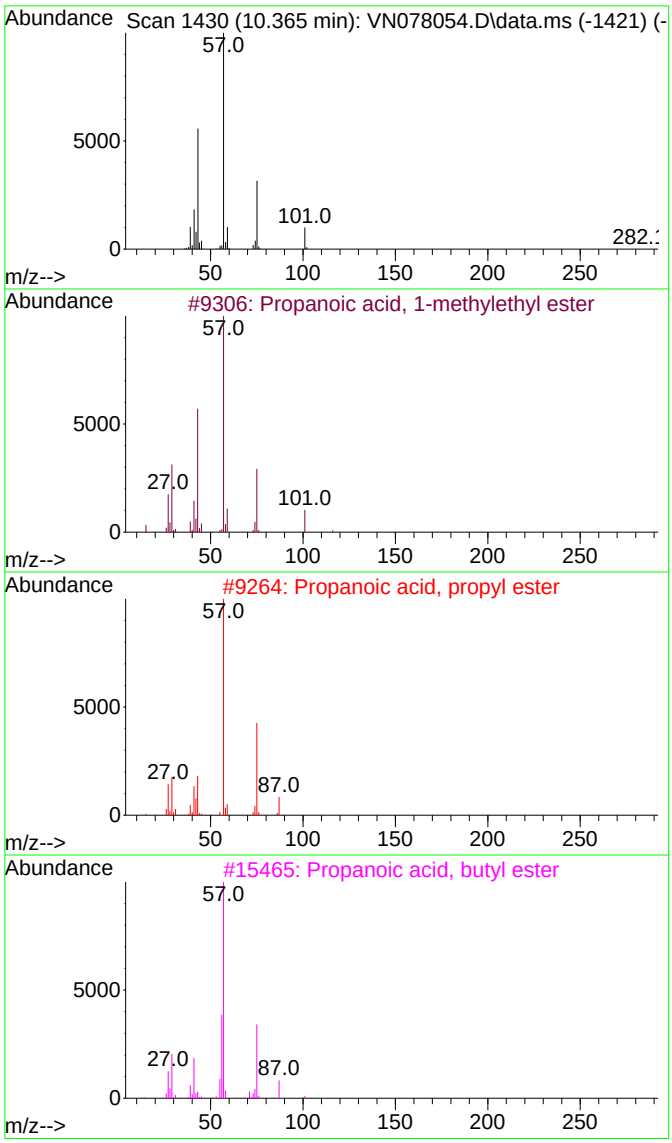
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

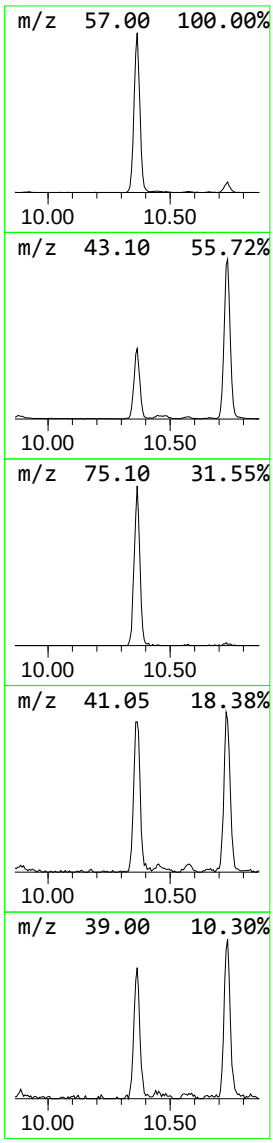
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.365 | 20.10 ug/l | 640724 | 1,4-Difluorobenzene | 9.106 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propanoic acid, 1-methylethyl ester | 116 | C6H12O2 | 000637-78-5 | 83 |
| 2 | Propanoic acid, propyl ester | 116 | C6H12O2 | 000106-36-5 | 53 |
| 3 | Propanoic acid, butyl ester | 130 | C7H14O2 | 000590-01-2 | 37 |
| 4 | Propane, 1-(1-methylethoxy)- | 102 | C6H14O | 000627-08-7 | 23 |
| 5 | Butanoic acid, methyl ester | 102 | C5H10O2 | 000623-42-7 | 14 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078054.D
Acq On : 05 Jun 2023 19:09
Operator : JC\MD
Sample : 03018-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
343

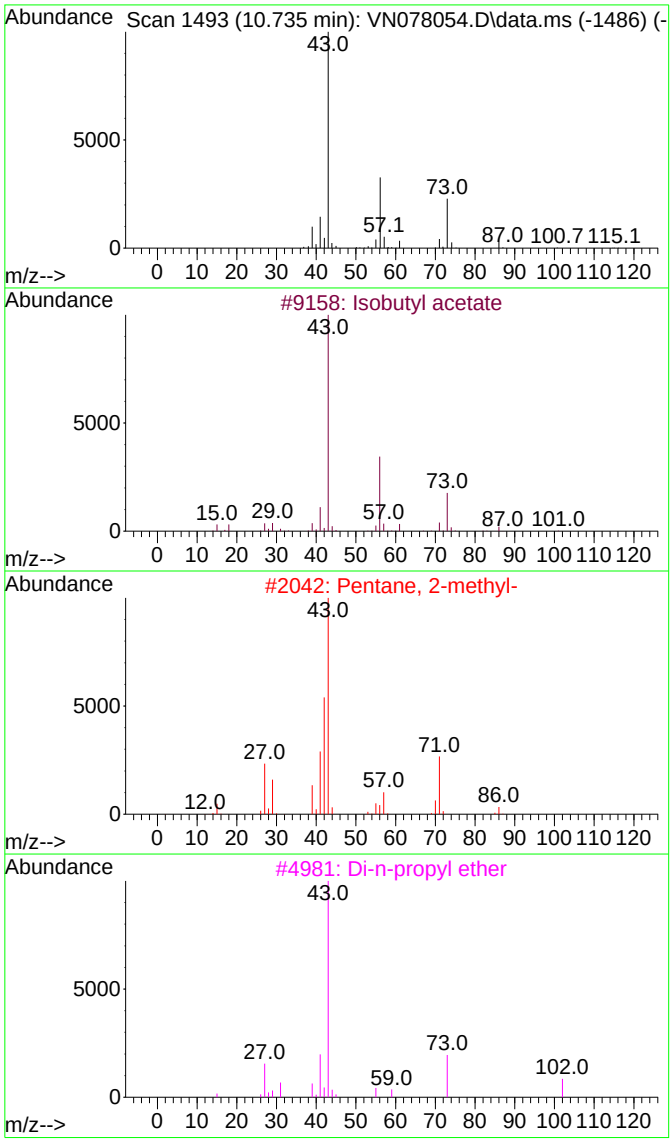
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

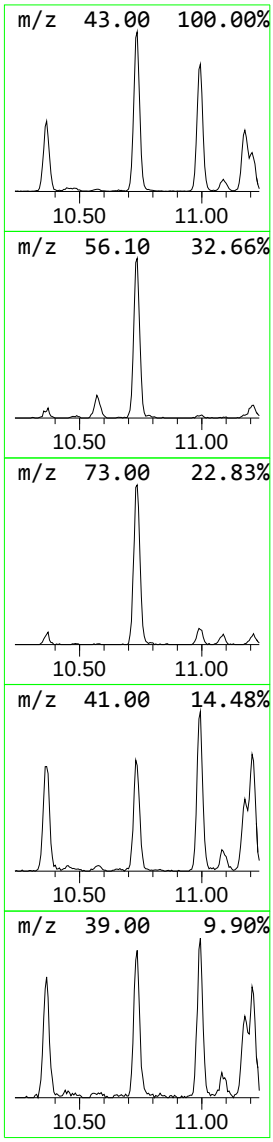
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 Isobutyl acetate Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.735 | 18.15 ug/l | 675722 | Chlorobenzene-d5 | 11.871 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Isobutyl acetate | 116 | C6H12O2 | 000110-19-0 | 83 |
| 2 | Pentane, 2-methyl- | 86 | C6H14 | 000107-83-5 | 9 |
| 3 | Di-n-propyl ether | 102 | C6H14O | 000111-43-3 | 9 |
| 4 | 2-Butanone, 3-methyl- | 86 | C5H10O | 000563-80-4 | 9 |
| 5 | 2-Pentanone, 3-methyl- | 100 | C6H12O | 000565-61-7 | 9 |



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Operator : JC\MD
Sample : 03018-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
343

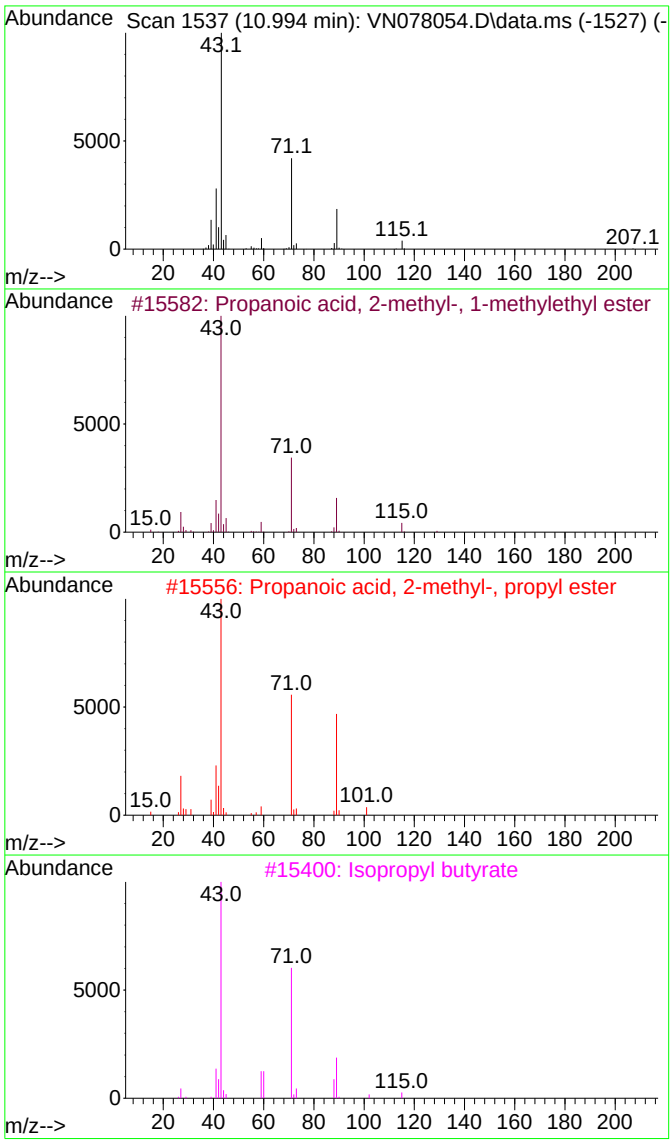
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

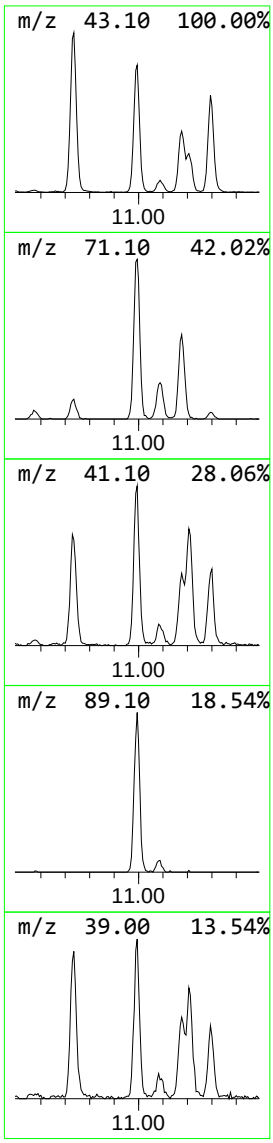
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.994 | 15.85 ug/l | 590037 | Chlorobenzene-d5 | 11.871 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propanoic acid, 2-methyl-, 1-met... | 130 | C7H14O2 | 000617-50-5 | 83 |
| 2 | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5 | 78 |
| 3 | Isopropyl butyrate | 130 | C7H14O2 | 000638-11-9 | 64 |
| 4 | 3-Pentanone, 2,4-dimethyl- | 114 | C7H14O | 000565-80-0 | 53 |
| 5 | 2,3-Hexanedione | 114 | C6H10O2 | 003848-24-6 | 42 |



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ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
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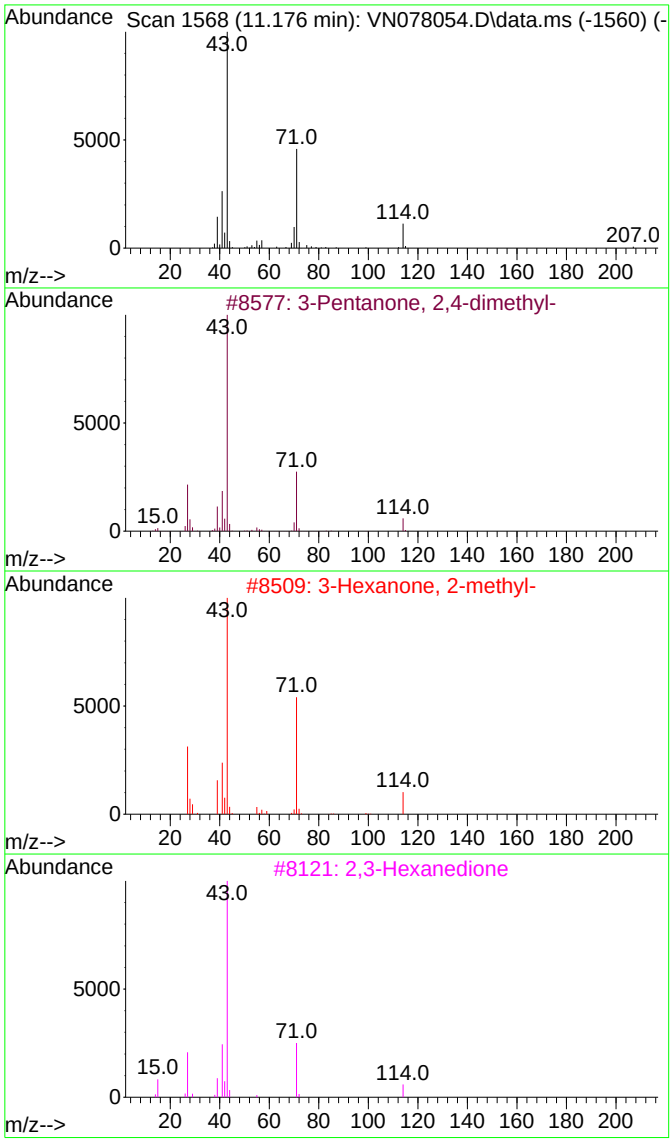
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

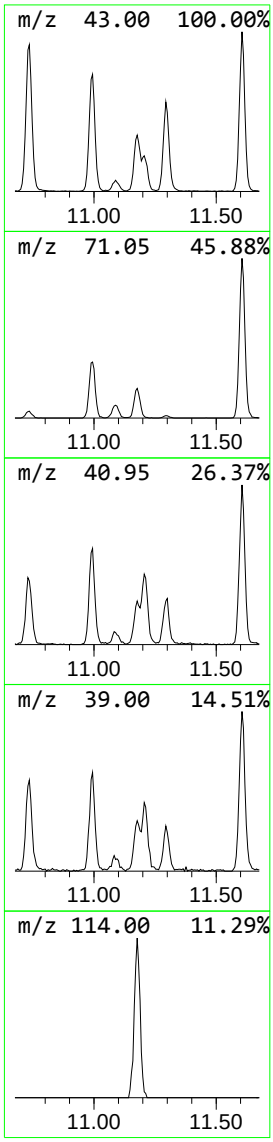
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.177 | 6.12 ug/l | 227814 | Chlorobenzene-d5 | 11.871 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Pentanone, 2,4-dimethyl- | 114 | C7H14O | 000565-80-0 | 86 |
| 2 | 3-Hexanone, 2-methyl- | 114 | C7H14O | 007379-12-6 | 80 |
| 3 | 2,3-Hexanedione | 114 | C6H10O2 | 003848-24-6 | 59 |
| 4 | 2,5-Octanedione | 142 | C8H14O2 | 003214-41-3 | 56 |
| 5 | 4-Heptanone | 114 | C7H14O | 000123-19-3 | 53 |



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Sample : 03018-08
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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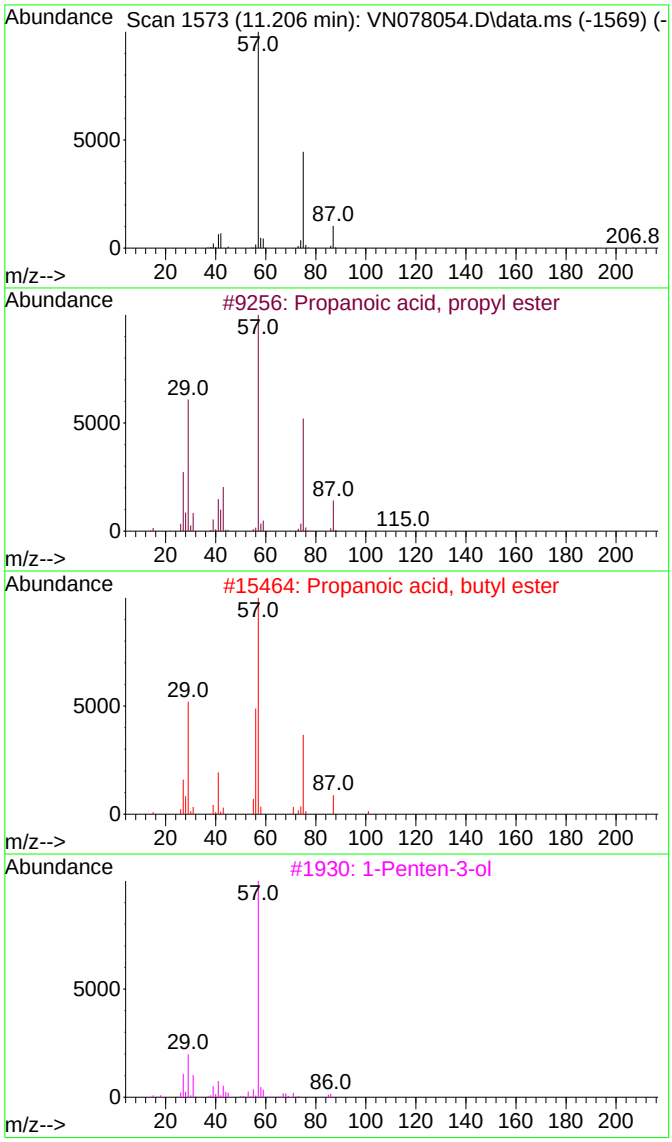
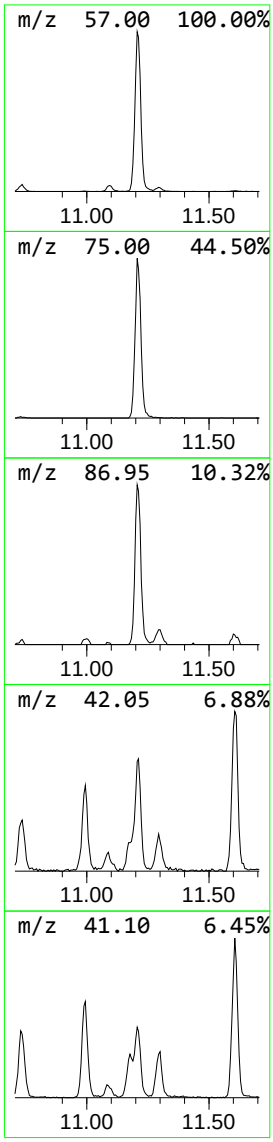
**********
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.206 | 22.63 ug/l | 842377 | Chlorobenzene-d5 | 11.871 |

| 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 | 40 |
| 3 | 1-Penten-3-ol | 86 | C5H10O | 000616-25-1 | 7 |
| 4 | 1-Butanamine, 3-methyl- | 87 | C5H13N | 000107-85-7 | 5 |
| 5 | 1-Butanamine, 2-methyl- | 87 | C5H13N | 000096-15-1 | 4 |



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**Instrument :**
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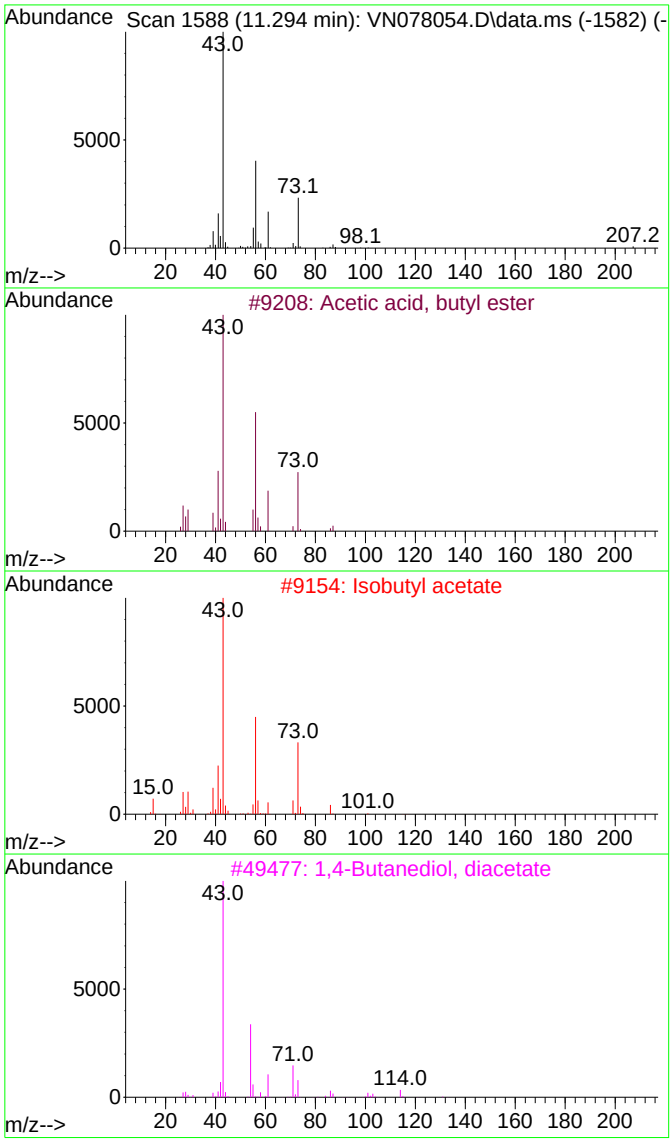
Quant Title : SW846 8260

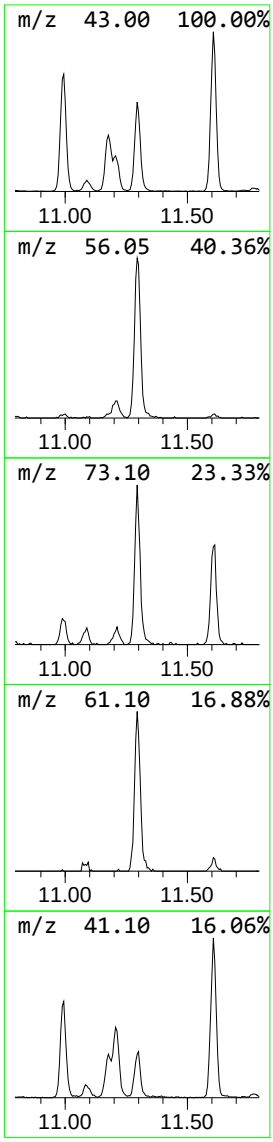
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 8 Acetic acid, butyl ester Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.294 | 11.85 ug/l | 441055 | Chlorobenzene-d5 | 11.871 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetic acid, butyl ester | 116 | C6H12O2 | 000123-86-4 | 64 |
| 2 | Isobutyl acetate | 116 | C6H12O2 | 000110-19-0 | 39 |
| 3 | 1,4-Butanediol, diacetate | 174 | C8H14O4 | 000628-67-1 | 12 |
| 4 | Isopropyl acetate | 102 | C5H10O2 | 000108-21-4 | 10 |
| 5 | Isobutylamine | 73 | C4H11N | 000078-81-9 | 9 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
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Sample : 03018-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
343

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

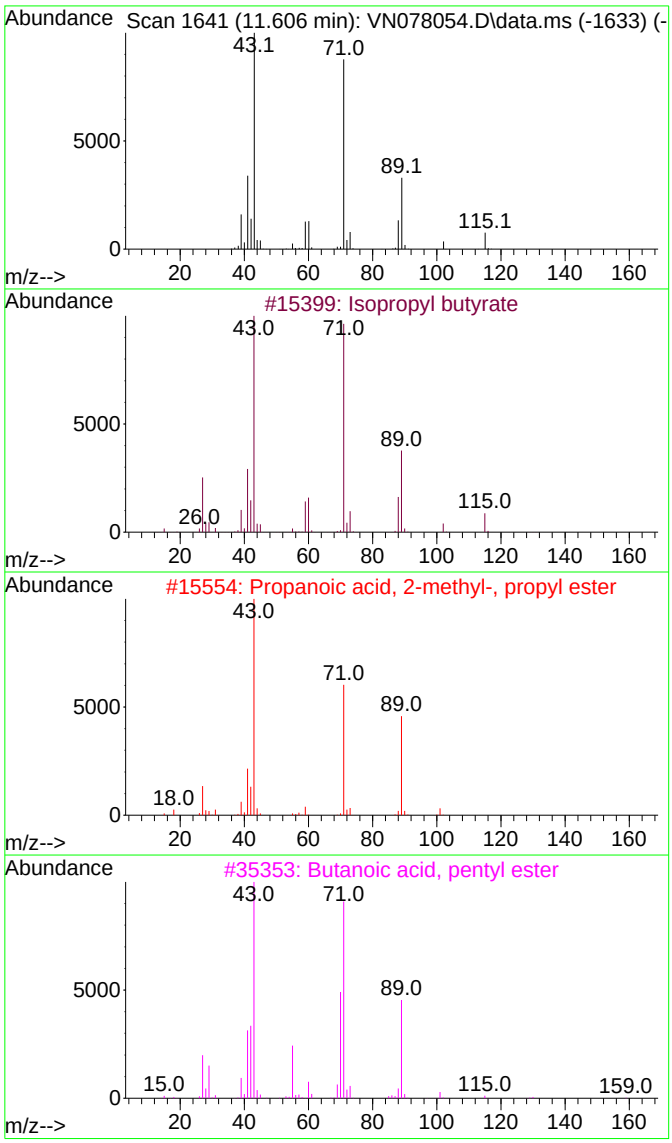
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

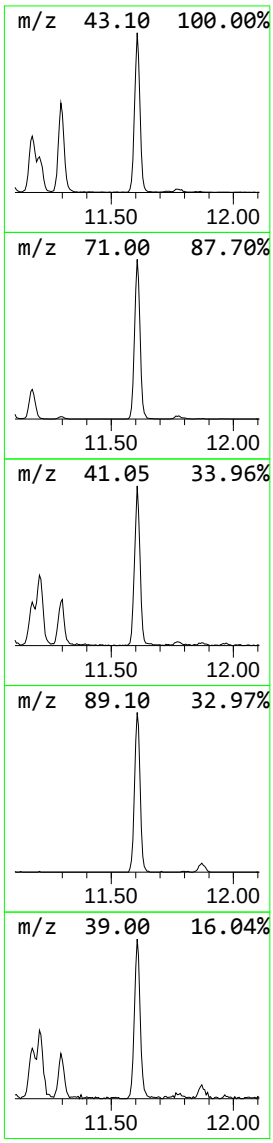
**********

Peak Number 9 Isopropyl butyrate Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.606 | 30.19 ug/l | 1123720 | Chlorobenzene-d5 | 11.871 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Isopropyl butyrate | 130 | C7H14O2 | 000638-11-9 | 91 |
| 2 | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5 | 72 |
| 3 | Butanoic acid, pentyl ester | 158 | C9H18O2 | 000540-18-1 | 64 |
| 4 | Propanoic acid, 2-methyl-, penty... | 158 | C9H18O2 | 002445-72-9 | 64 |
| 5 | Butanoic acid, hexyl ester | 172 | C10H20O2 | 002639-63-6 | 64 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078054.D
Acq On : 05 Jun 2023 19:09
Operator : JC\MD
Sample : 03018-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
343

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.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 |
| 3-Pentanone | 9.677 | 6.3 | ug/l | 201179 | 2 | 9.106 | 1593540 | 50.0 |
| n-Propyl acetate | 9.747 | 98.4 | ug/l | 3137470 | 2 | 9.106 | 1593540 | 50.0 |
| Propanoic acid,... | 10.365 | 20.1 | ug/l | 640724 | 2 | 9.106 | 1593540 | 50.0 |
| Isobutyl acetate | 10.735 | 18.1 | ug/l | 675722 | 3 | 11.871 | 1860990 | 50.0 |
| Propanoic acid,... | 10.994 | 15.9 | ug/l | 590037 | 3 | 11.871 | 1860990 | 50.0 |
| 3-Pentanone, 2,... | 11.177 | 6.1 | ug/l | 227814 | 3 | 11.871 | 1860990 | 50.0 |
| Propanoic acid,... | 11.206 | 22.6 | ug/l | 842377 | 3 | 11.871 | 1860990 | 50.0 |
| Acetic acid, bu... | 11.294 | 11.9 | ug/l | 441055 | 3 | 11.871 | 1860990 | 50.0 |
| Isopropyl butyrate | 11.606 | 30.2 | ug/l | 1123720 | 3 | 11.871 | 1860990 | 50.0 |