LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076710.D
Acq On : 16 Feb 2023 14:39
Operator : JC\MD
Sample : 01563-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
AUD-1928

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\82N021323W.M
Title : SW846 8260

Signal : TIC: VN076710.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.096 | 22 | 27 | 40 | rVB | 138821 | 209759 | 1.33% | 0.519% |
| 2 | 2.672 | 117 | 125 | 146 | rBV | 8992504 | 15757284 | 100.00% | 38.985% |
| 3 | 3.802 | 306 | 317 | 334 | rBV | 193364 | 525420 | 3.33% | 1.300% |
| 4 | 4.301 | 391 | 402 | 417 | rBV | 450684 | 1291430 | 8.20% | 3.195% |
| 5 | 4.443 | 417 | 426 | 436 | rVV | 107435 | 315116 | 2.00% | 0.780% |
| 6 | 4.725 | 462 | 474 | 488 | rBV | 68874 | 225282 | 1.43% | 0.557% |
| 7 | 6.737 | 804 | 816 | 828 | rBV2 | 160818 | 510405 | 3.24% | 1.263% |
| 8 | 7.237 | 887 | 901 | 915 | rBV | 765491 | 2150711 | 13.65% | 5.321% |
| 9 | 7.566 | 949 | 957 | 973 | rVB2 | 501959 | 1236849 | 7.85% | 3.060% |
| 10 | 8.178 | 1049 | 1061 | 1065 | rBV | 298270 | 738880 | 4.69% | 1.828% |
| 11 | 8.231 | 1065 | 1070 | 1085 | rVB | 542324 | 1209117 | 7.67% | 2.991% |
| 12 | 8.589 | 1123 | 1131 | 1149 | rVB2 | 368906 | 1083214 | 6.87% | 2.680% |
| 13 | 9.107 | 1210 | 1219 | 1231 | rBV | 898253 | 1851183 | 11.75% | 4.580% |
| 14 | 9.266 | 1238 | 1246 | 1255 | rBV | 183877 | 408848 | 2.59% | 1.012% |
| 15 | 10.572 | 1458 | 1468 | 1474 | rBV | 1246812 | 2327859 | 14.77% | 5.759% |
| 16 | 10.631 | 1474 | 1478 | 1489 | rVB | 141718 | 265006 | 1.68% | 0.656% |
| 17 | 10.960 | 1525 | 1534 | 1545 | rBV2 | 95196 | 201389 | 1.28% | 0.498% |
| 18 | 11.866 | 1672 | 1688 | 1699 | rBV | 1075574 | 2031367 | 12.89% | 5.026% |
| 19 | 12.419 | 1772 | 1782 | 1791 | rBV3 | 87130 | 198944 | 1.26% | 0.492% |
| 20 | 12.854 | 1842 | 1856 | 1866 | rBV | 820107 | 1507913 | 9.57% | 3.731% |
| 21 | 13.342 | 1933 | 1939 | 1952 | rVB | 736820 | 1119801 | 7.11% | 2.770% |
| 22 | 13.689 | 1992 | 1998 | 2008 | rVB2 | 352268 | 592240 | 3.76% | 1.465% |
| 23 | 13.795 | 2008 | 2016 | 2023 | rBV | 1018235 | 1709060 | 10.85% | 4.228% |
| 24 | 13.877 | 2023 | 2030 | 2039 | rVV | 1547591 | 2448076 | 15.54% | 6.057% |
| 25 | 15.348 | 2271 | 2280 | 2290 | rBV2 | 158220 | 339118 | 2.15% | 0.839% |
| 26 | 15.660 | 2327 | 2333 | 2343 | rVB5 | 66117 | 164629 | 1.04% | 0.407% |

Sum of corrected areas: 40418900

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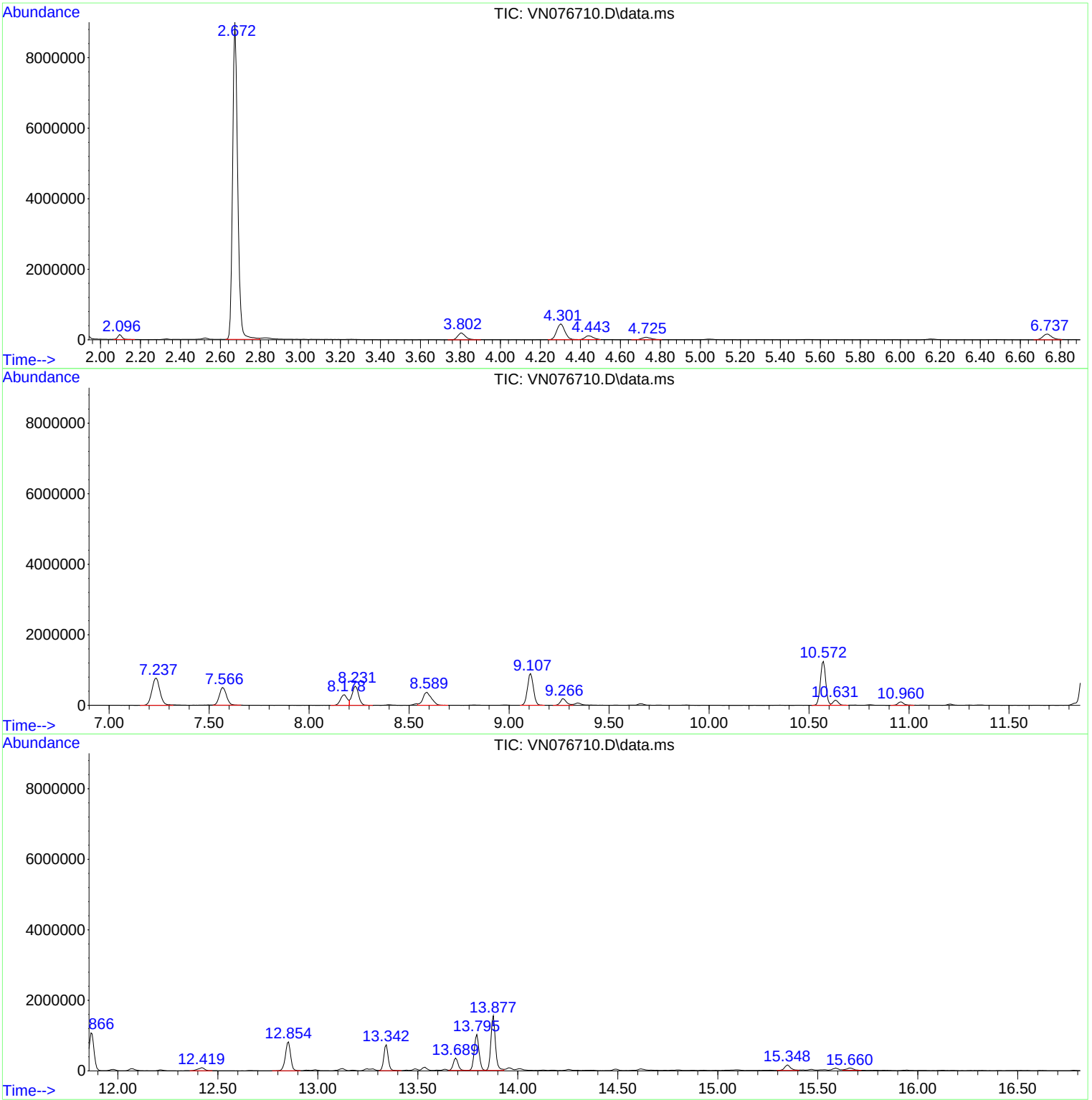
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
AUD-1928

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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



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Data File : VN076710.D
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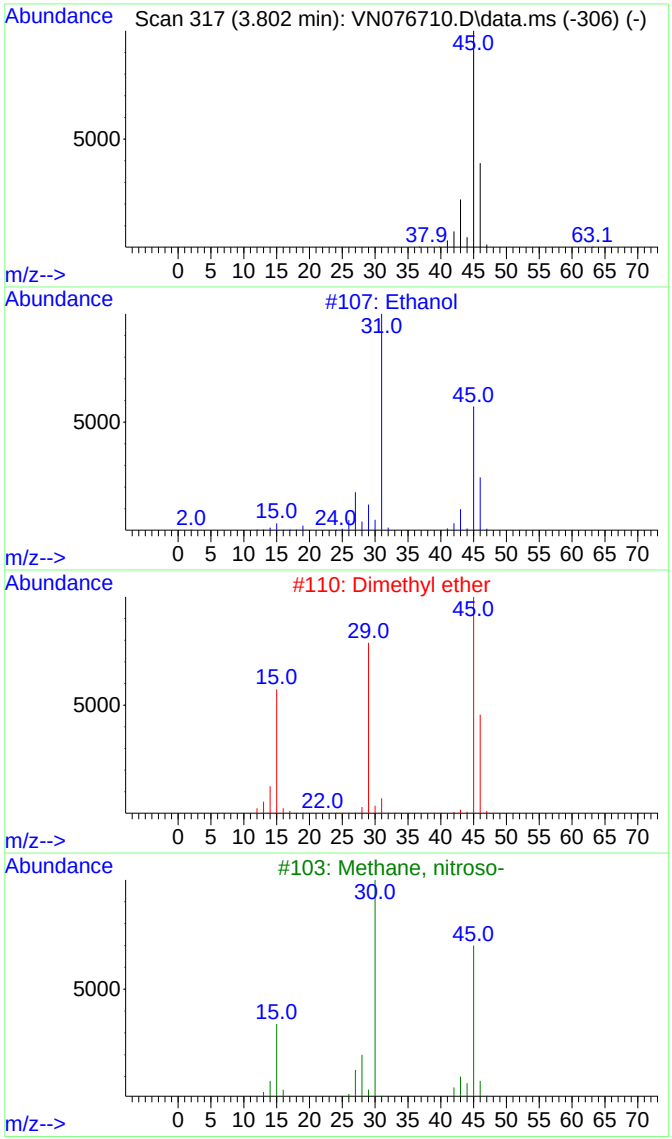
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

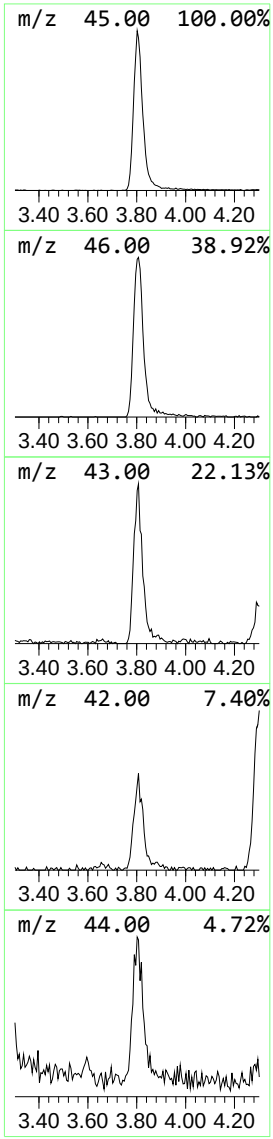
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 Ethanol Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.802 | 21.73 ug/l | 525420 | Pentafluorobenzene | 8.231 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol | 46 | C2H6O | 000064-17-5 | 74 |
| 2 | Dimethyl ether | 46 | C2H6O | 000115-10-6 | 9 |
| 3 | Methane, nitroso- | 45 | CH3NO | 000865-40-7 | 4 |
| 4 | Formic acid | 46 | CH2O2 | 000064-18-6 | 4 |
| 5 | Oxalic acid | 90 | C2H2O4 | 000144-62-7 | 4 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076710.D
Acq On : 16 Feb 2023 14:39
Operator : JC\MD
Sample : 01563-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
AUD-1928

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

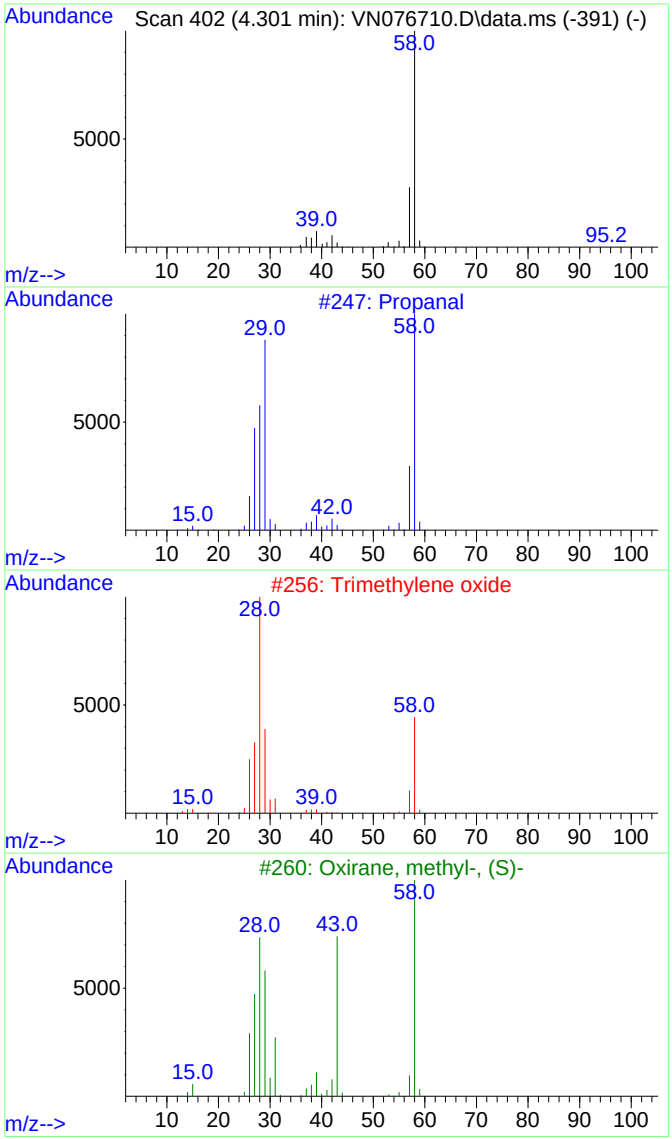
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

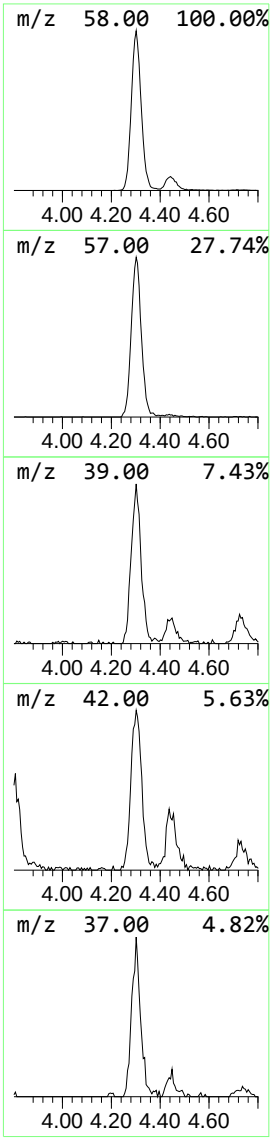
**********

Peak Number 3 Propanal Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.301 | 53.40 ug/l | 1291430 | Pentafluorobenzene | 8.231 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propanal | 58 | C3H6O | 000123-38-6 | 78 |
| 2 | Trimethylene oxide | 58 | C3H6O | 000503-30-0 | 9 |
| 3 | Oxirane, methyl-, (S)- | 58 | C3H6O | 016088-62-3 | 7 |
| 4 | Propylene oxide | 58 | C3H6O | 000075-56-9 | 7 |
| 5 | Borane, compd. with dimethylamin... | 59 | C2H10BN | 000074-94-2 | 4 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076710.D
Acq On : 16 Feb 2023 14:39
Operator : JC\MD
Sample : 01563-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
AUD-1928

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

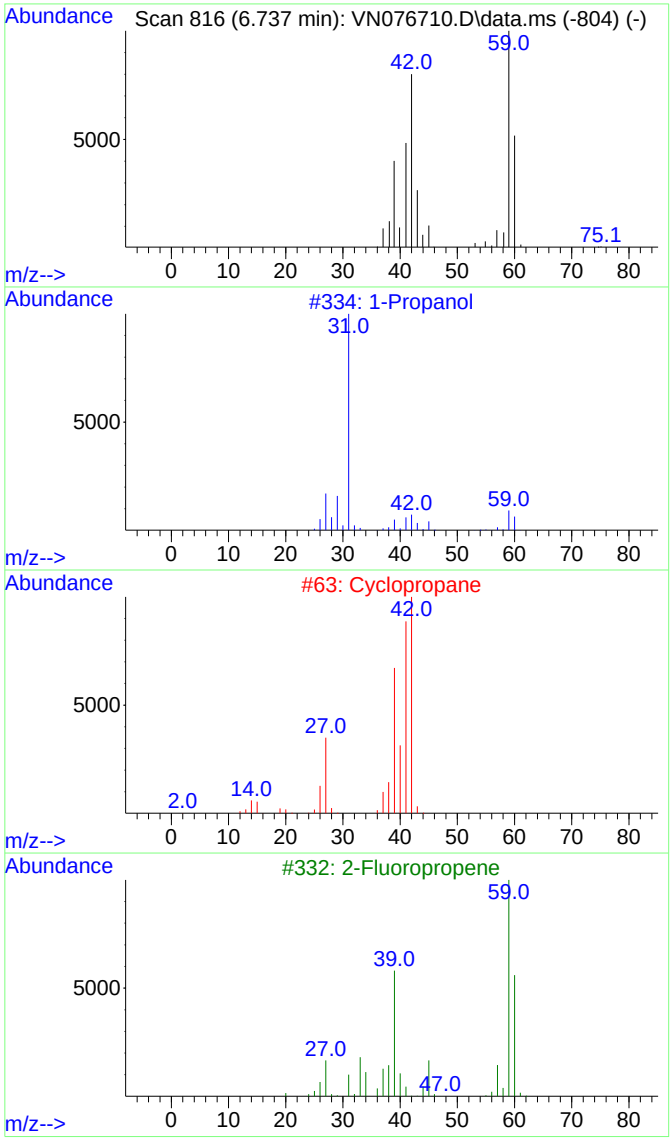
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

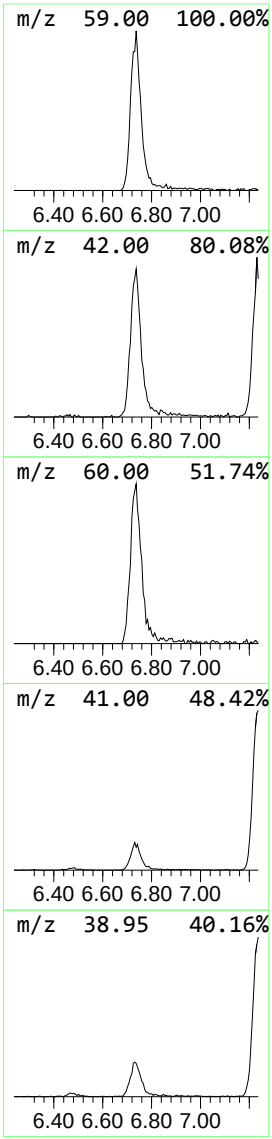
**********

Peak Number 4 1-Propanol Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.737 | 21.11 ug/l | 510405 | Pentafluorobenzene | 8.231 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Propanol | 60 | C3H8O | 000071-23-8 | 59 |
| 2 | Cyclopropane | 42 | C3H6 | 000075-19-4 | 43 |
| 3 | 2-Fluoropropene | 60 | C3H5F | 001184-60-7 | 37 |
| 4 | Allyl fluoride | 60 | C3H5F | 000818-92-8 | 35 |
| 5 | 3-Buten-1-ol | 72 | C4H8O | 000627-27-0 | 27 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076710.D
Acq On : 16 Feb 2023 14:39
Operator : JC\MD
Sample : 01563-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
AUD-1928

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

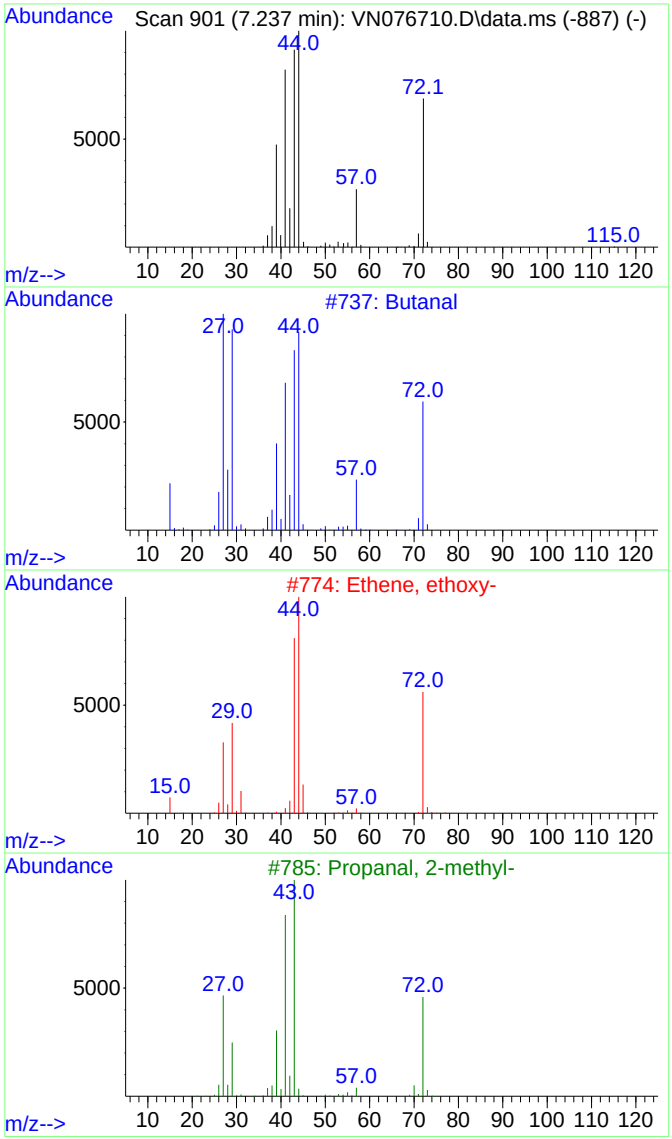
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

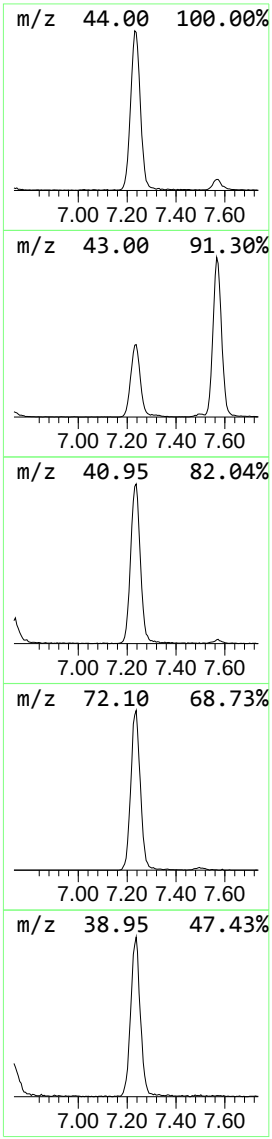
**********

Peak Number 5 Butanal Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.237 | 88.94 ug/l | 2150710 | Pentafluorobenzene | 8.231 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butanal | 72 | C4H8O | 000123-72-8 | 91 |
| 2 | Ethene, ethoxy- | 72 | C4H8O | 000109-92-2 | 38 |
| 3 | Propanal, 2-methyl- | 72 | C4H8O | 000078-84-2 | 35 |
| 4 | 2-Propen-1-ol, 2-methyl-, acetate | 114 | C6H10O2 | 000820-71-3 | 23 |
| 5 | Methacrolein | 70 | C4H6O | 000078-85-3 | 22 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076710.D
Acq On : 16 Feb 2023 14:39
Operator : JC\MD
Sample : 01563-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
AUD-1928

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

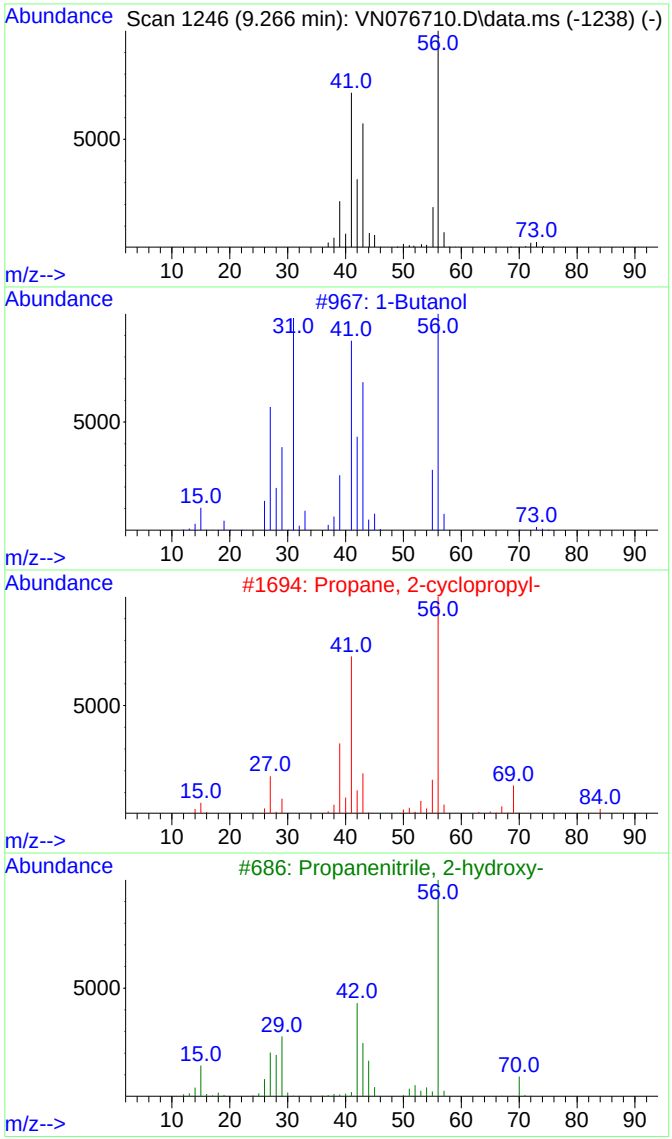
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

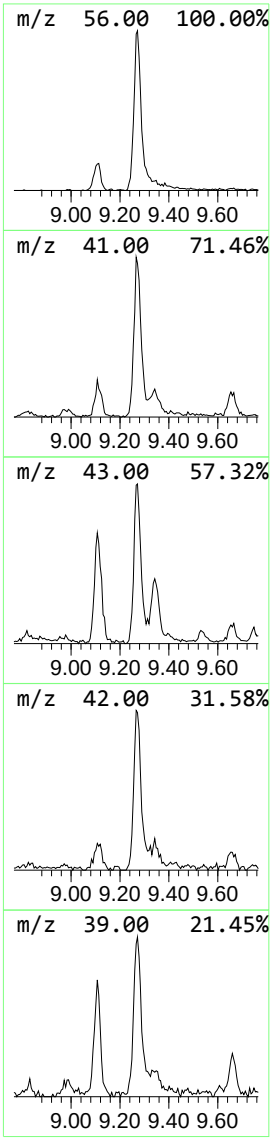
**********

Peak Number 6 1-Butanol Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.266 | 11.04 ug/l | 408848 | 1,4-Difluorobenzene | 9.107 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Butanol | 74 | C4H10O | 000071-36-3 | 90 |
| 2 | Propane, 2-cyclopropyl- | 84 | C6H12 | 003638-35-5 | 36 |
| 3 | Propanenitrile, 2-hydroxy- | 71 | C3H5NO | 000078-97-7 | 9 |
| 4 | Diaziridine,3,3-dimethyl- | 72 | C3H8N2 | 004901-76-2 | 9 |
| 5 | 1-Propanol, 2-methyl- | 74 | C4H10O | 000078-83-1 | 9 |



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**Instrument :**
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
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TIC Library : C:\Database\NIST20.L
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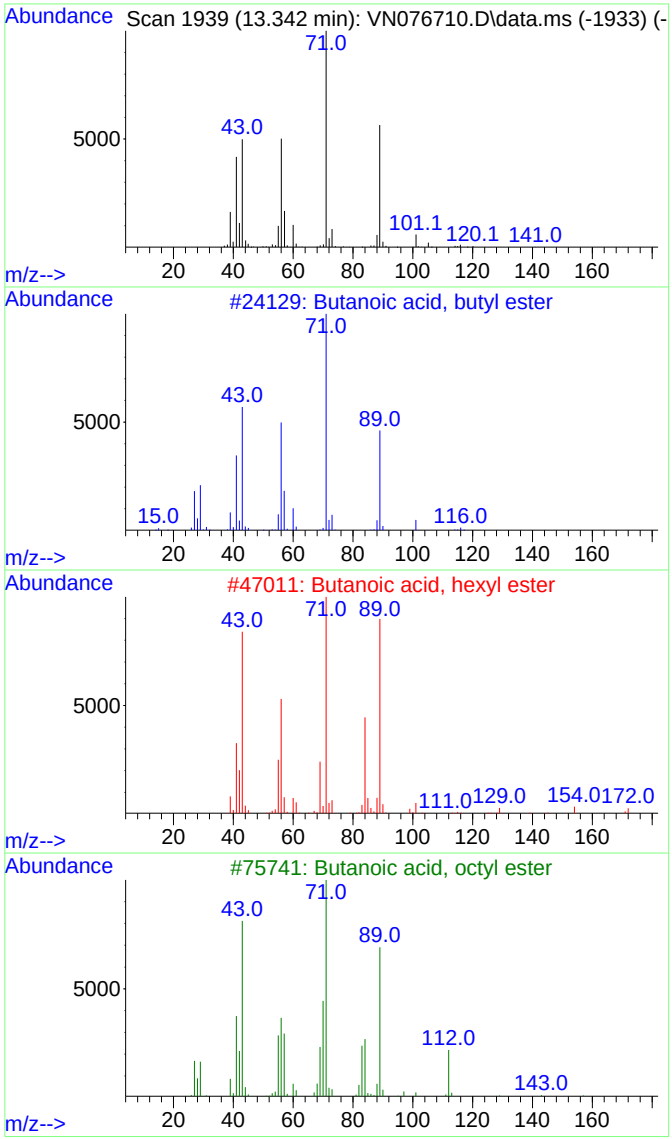
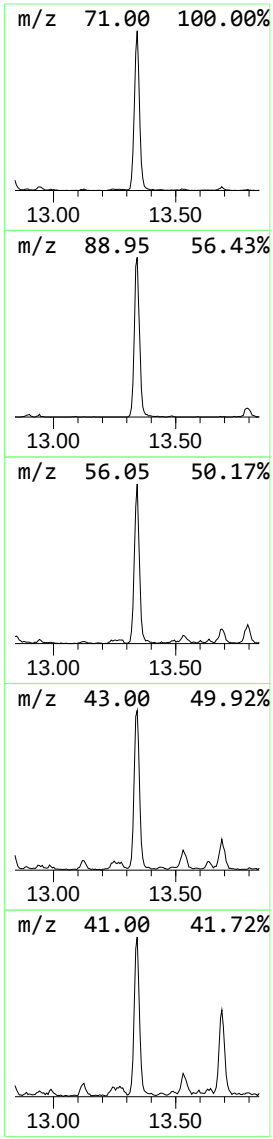
**********
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.342 | 32.76 ug/l | 1119800 | 1,4-Dichlorobenzene-d4 | 13.795 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butanoic acid, butyl ester | 144 | C8H16O2 | 000109-21-7 | 90 |
| 2 | Butanoic acid, hexyl ester | 172 | C10H20O2 | 002639-63-6 | 74 |
| 3 | Butanoic acid, octyl ester | 200 | C12H24O2 | 000110-39-4 | 64 |
| 4 | Butanoic acid, propyl ester | 130 | C7H14O2 | 000105-66-8 | 59 |
| 5 | Butanoic acid, heptyl ester | 186 | C11H22O2 | 005870-93-9 | 56 |



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ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
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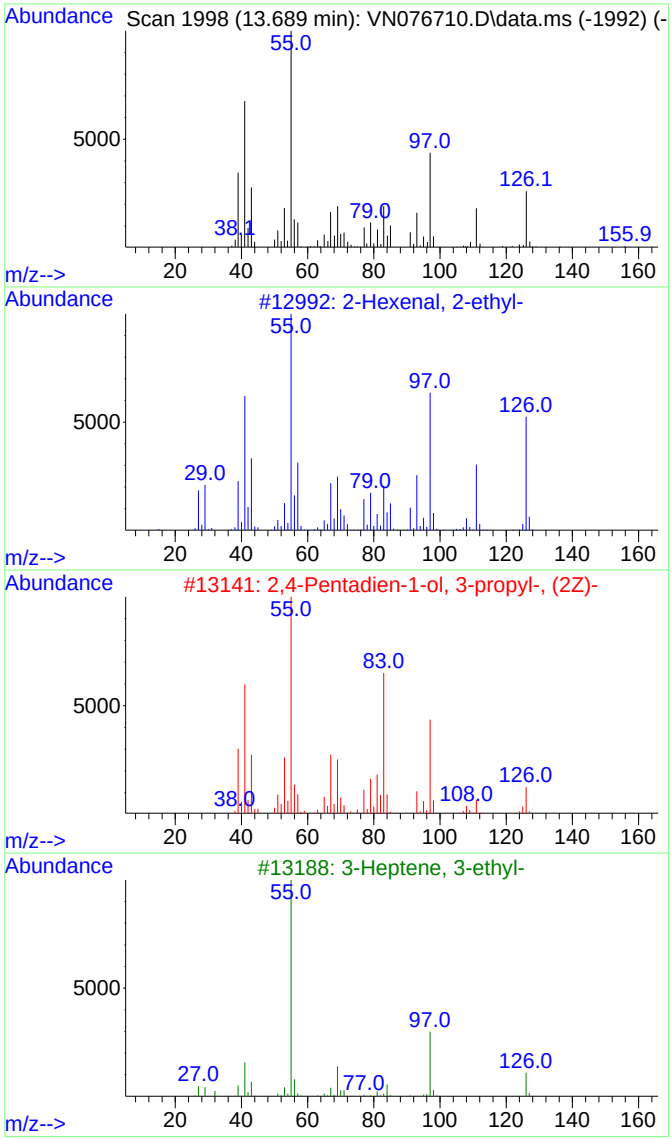
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

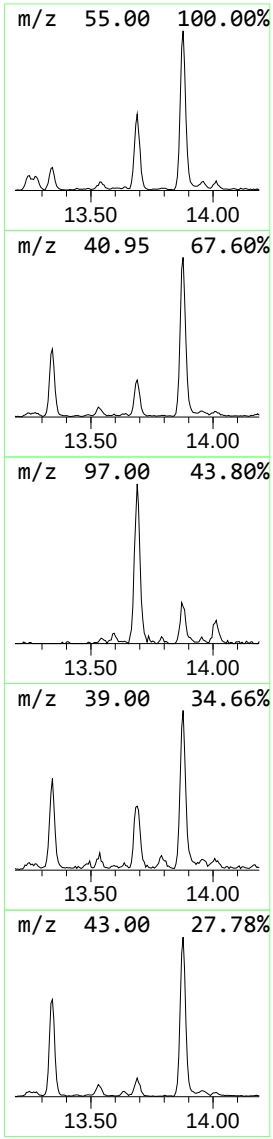
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 8 2-Hexenal, 2-ethyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.689 | 17.33 ug/l | 592240 | 1,4-Dichlorobenzene-d4 | 13.795 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Hexenal, 2-ethyl- | 126 | C8H14O | 000645-62-5 | 93 |
| 2 | 2,4-Pentadien-1-ol, 3-propyl-, (... | 126 | C8H14O | 1000142-17-9 | 50 |
| 3 | 3-Heptene, 3-ethyl- | 126 | C9H18 | 074764-46-8 | 47 |
| 4 | 4-Nonene | 126 | C9H18 | 002198-23-4 | 43 |
| 5 | 3-Nonene | 126 | C9H18 | 020063-77-8 | 38 |



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ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
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**ClientSampleId :**
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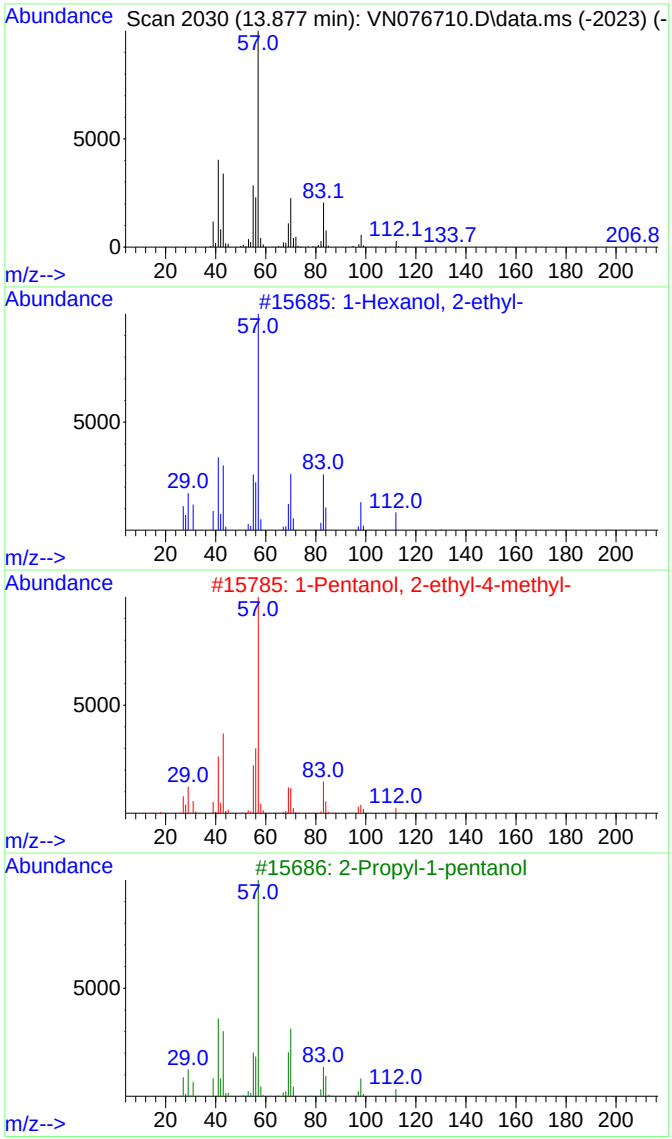
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

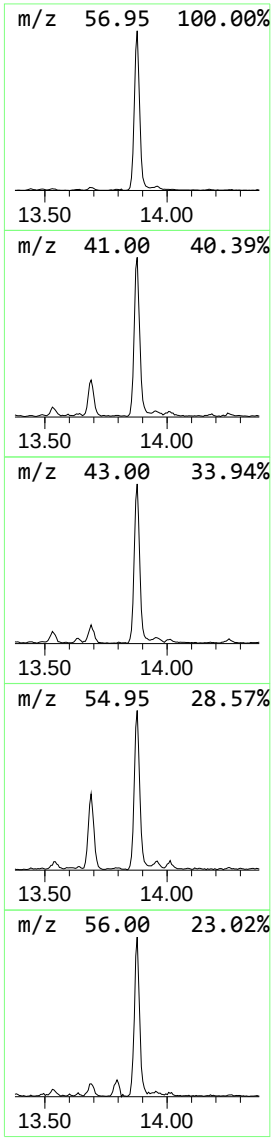
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.877 | 71.62 ug/l | 2448080 | 1,4-Dichlorobenzene-d4 | 13.795 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 78 |
| 2 | 1-Pentanol, 2-ethyl-4-methyl- | 130 | C8H18O | 000106-67-2 | 56 |
| 3 | 2-Propyl-1-pentanol | 130 | C8H18O | 058175-57-8 | 47 |
| 4 | Carbonic acid, isobutyl 2-ethylh... | 230 | C13H26O3 | 1000383-13-3 | 42 |
| 5 | Heptane, 1,1'-oxybis- | 214 | C14H30O | 000629-64-1 | 42 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076710.D
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Sample : 01563-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
AUD-1928

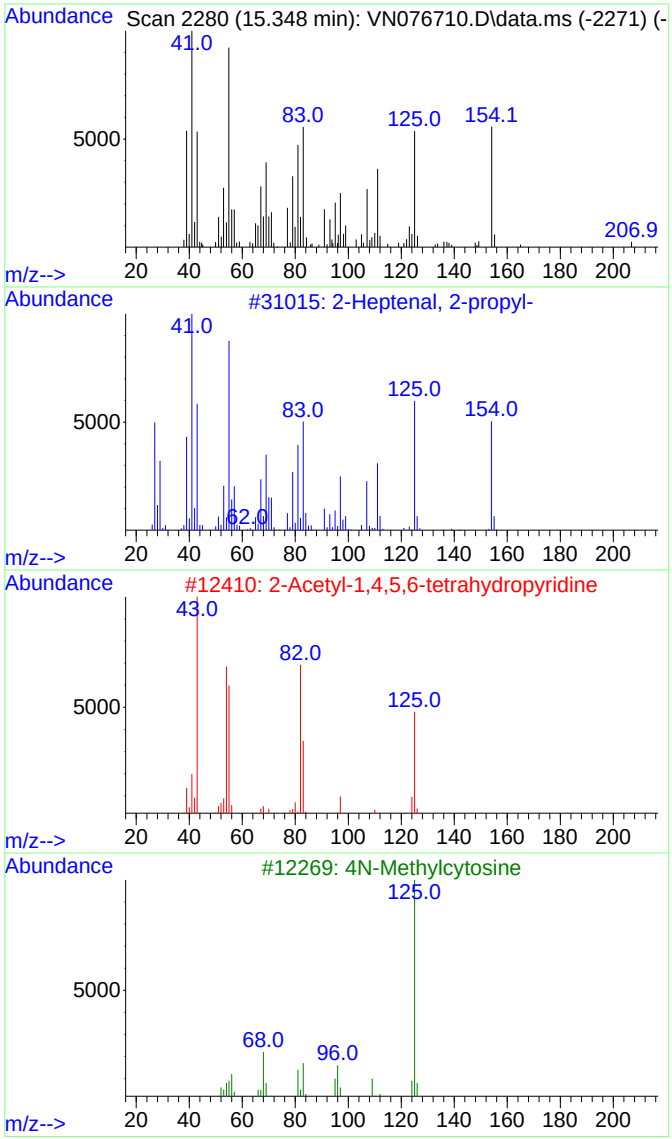
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

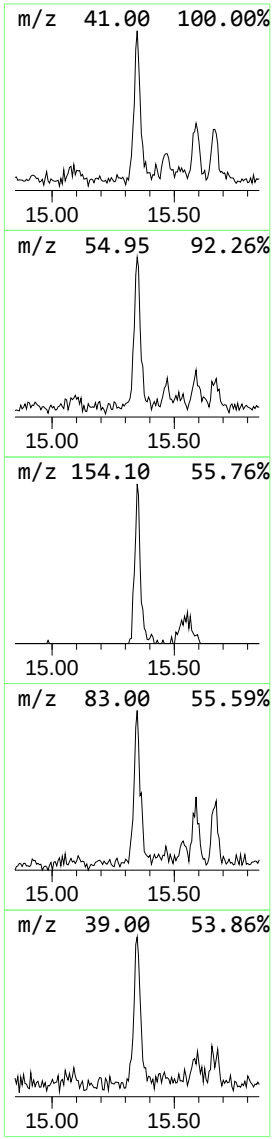
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 2-Heptenal, 2-propyl- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.348 | 9.92 ug/l | 339118 | 1,4-Dichlorobenzene-d4 | 13.795 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Heptenal, 2-propyl- | 154 | C10H18O | 034880-43-8 | 95 |
| 2 | 2-Acetyl-1,4,5,6-tetrahydropyridine | 125 | C7H11NO | 025343-57-1 | 30 |
| 3 | 4N-Methylcytosine | 125 | C5H7N3O | 006220-47-9 | 22 |
| 4 | 6-Acetoxy-4-methyl-hept-4-enoic ... | 200 | C10H16O4 | 1000193-37-1 | 22 |
| 5 | Cyclohexane, (1-methylbutyl)- | 154 | C11H22 | 061208-94-4 | 22 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
Data File : VN076710.D
Acq On : 16 Feb 2023 14:39
Operator : JC\MD
Sample : 01563-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
AUD-1928

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.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 |
| Ethanol | 3.802 | 21.7 | ug/l | 525420 | 1 | 8.231 | 1209120 | 50.0 |
| Propanal | 4.301 | 53.4 | ug/l | 1291430 | 1 | 8.231 | 1209120 | 50.0 |
| 1-Propanol | 6.737 | 21.1 | ug/l | 510405 | 1 | 8.231 | 1209120 | 50.0 |
| Butanal | 7.237 | 88.9 | ug/l | 2150710 | 1 | 8.231 | 1209120 | 50.0 |
| 1-Butanol | 9.266 | 11.0 | ug/l | 408848 | 2 | 9.107 | 1851180 | 50.0 |
| Butanoic acid, ... | 13.342 | 32.8 | ug/l | 1119800 | 4 | 13.795 | 1709060 | 50.0 |
| 2-Hexenal, 2-et... | 13.689 | 17.3 | ug/l | 592240 | 4 | 13.795 | 1709060 | 50.0 |
| 1-Hexanol, 2-et... | 13.877 | 71.6 | ug/l | 2448080 | 4 | 13.795 | 1709060 | 50.0 |
| 2-Heptenal, 2-p... | 15.348 | 9.9 | ug/l | 339118 | 4 | 13.795 | 1709060 | 50.0 |