LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091124\
Data File : VN083794.D
Acq On : 11 Sep 2024 14:21
Operator : JC\MD
Sample : P3839-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
830

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\82N091024W.M
Title : SW846 8260

Signal : TIC: VN083794.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.077 | 17 | 21 | 41 | rVB | 68097 | 149295 | 1.73% | 0.788% |
| 2 | 3.824 | 309 | 318 | 333 | rBV | 97258 | 264792 | 3.06% | 1.397% |
| 3 | 4.742 | 460 | 474 | 495 | rBV | 79068 | 298514 | 3.45% | 1.575% |
| 4 | 5.577 | 599 | 616 | 629 | rBV3 | 26880 | 90503 | 1.05% | 0.477% |
| 5 | 6.765 | 788 | 818 | 846 | rBV | 2331742 | 8641097 | 100.00% | 45.581% |
| 6 | 7.218 | 887 | 895 | 907 | rBV4 | 34482 | 102743 | 1.19% | 0.542% |
| 7 | 7.977 | 1015 | 1024 | 1040 | rBV | 88864 | 207500 | 2.40% | 1.095% |
| 8 | 8.165 | 1045 | 1056 | 1060 | rBV | 117245 | 265186 | 3.07% | 1.399% |
| 9 | 8.224 | 1060 | 1066 | 1077 | rVB | 177074 | 400912 | 4.64% | 2.115% |
| 10 | 8.577 | 1112 | 1126 | 1133 | rBV | 123401 | 326794 | 3.78% | 1.724% |
| 11 | 8.783 | 1157 | 1161 | 1176 | rVB2 | 27308 | 91209 | 1.06% | 0.481% |
| 12 | 9.100 | 1206 | 1215 | 1226 | rVB | 307217 | 627798 | 7.27% | 3.312% |
| 13 | 9.271 | 1236 | 1244 | 1254 | rBV | 86797 | 190006 | 2.20% | 1.002% |
| 14 | 10.565 | 1457 | 1464 | 1471 | rBV | 459508 | 839353 | 9.71% | 4.427% |
| 15 | 10.959 | 1521 | 1531 | 1544 | rBV | 639685 | 1128679 | 13.06% | 5.954% |
| 16 | 11.200 | 1565 | 1572 | 1584 | rVB | 181394 | 298906 | 3.46% | 1.577% |
| 17 | 11.865 | 1669 | 1685 | 1694 | rBV | 538332 | 976546 | 11.30% | 5.151% |
| 18 | 12.847 | 1844 | 1852 | 1862 | rBV | 422684 | 721473 | 8.35% | 3.806% |
| 19 | 13.335 | 1931 | 1935 | 1942 | rVB | 84374 | 130409 | 1.51% | 0.688% |
| 20 | 13.547 | 1964 | 1971 | 1979 | rBV2 | 71785 | 139618 | 1.62% | 0.736% |
| 21 | 13.788 | 2005 | 2012 | 2020 | rBV | 597720 | 1032006 | 11.94% | 5.444% |
| 22 | 13.871 | 2020 | 2026 | 2033 | rVV | 1011547 | 1642879 | 19.01% | 8.666% |
| 23 | 13.941 | 2033 | 2038 | 2048 | rVV4 | 141078 | 391517 | 4.53% | 2.065% |

Sum of corrected areas: 18957735

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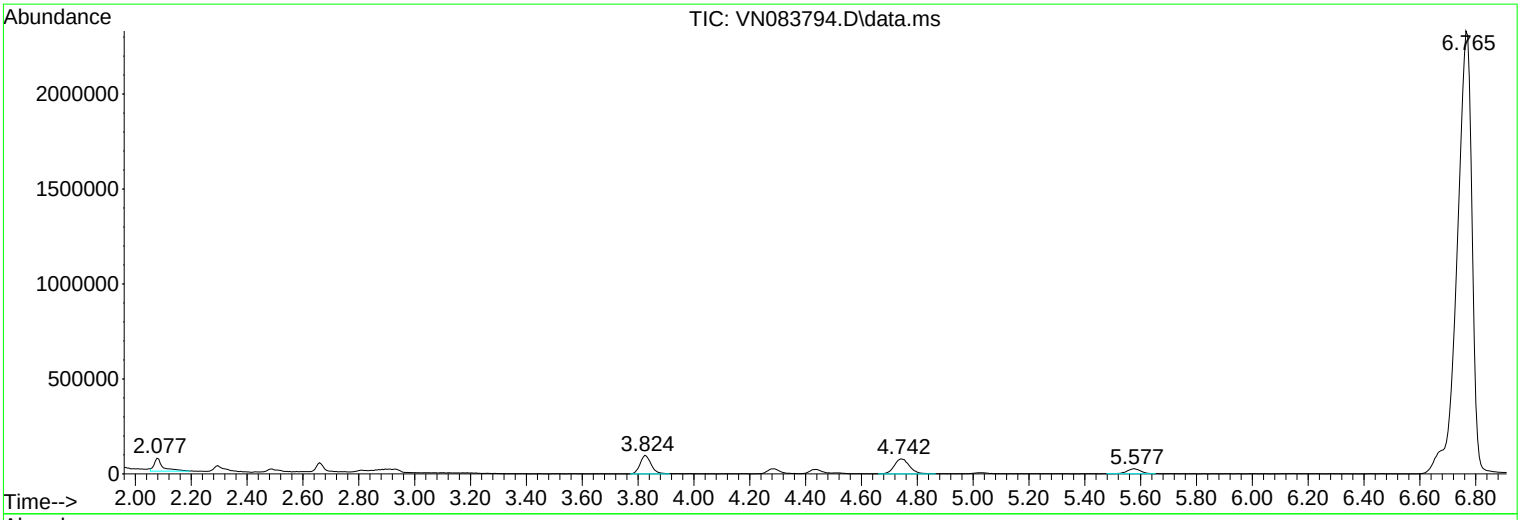
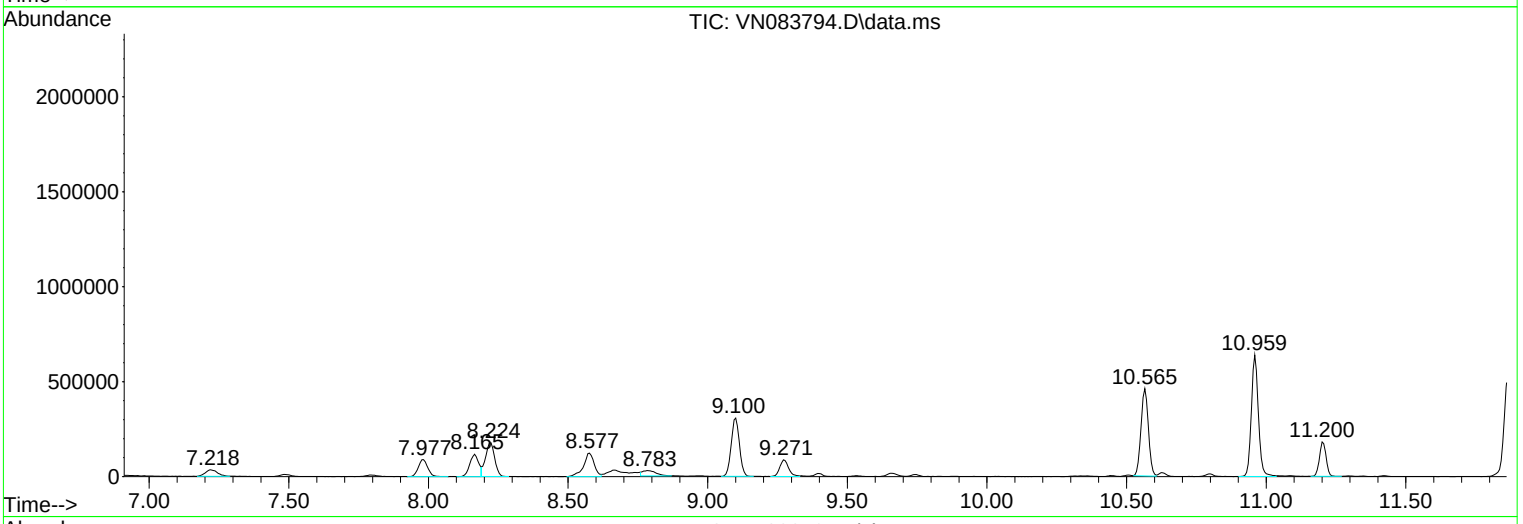
ALS Vial : 5 Sample Multiplier: 1

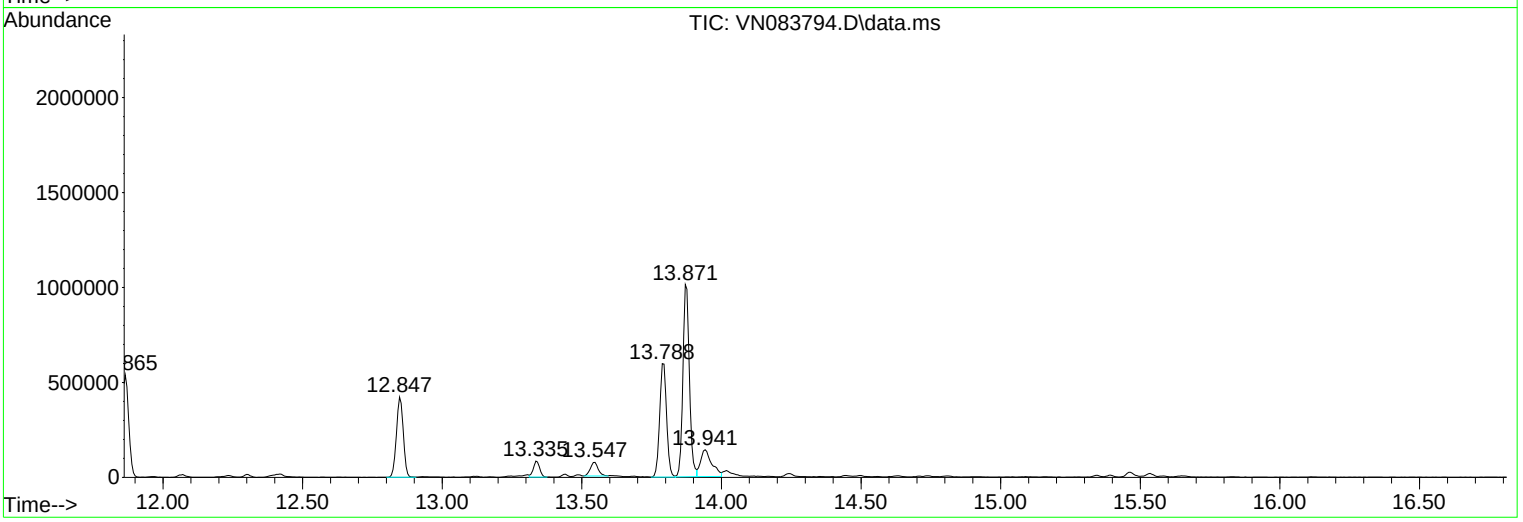
**Instrument :**
MSVOA_N
**ClientSampleId :**
830

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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



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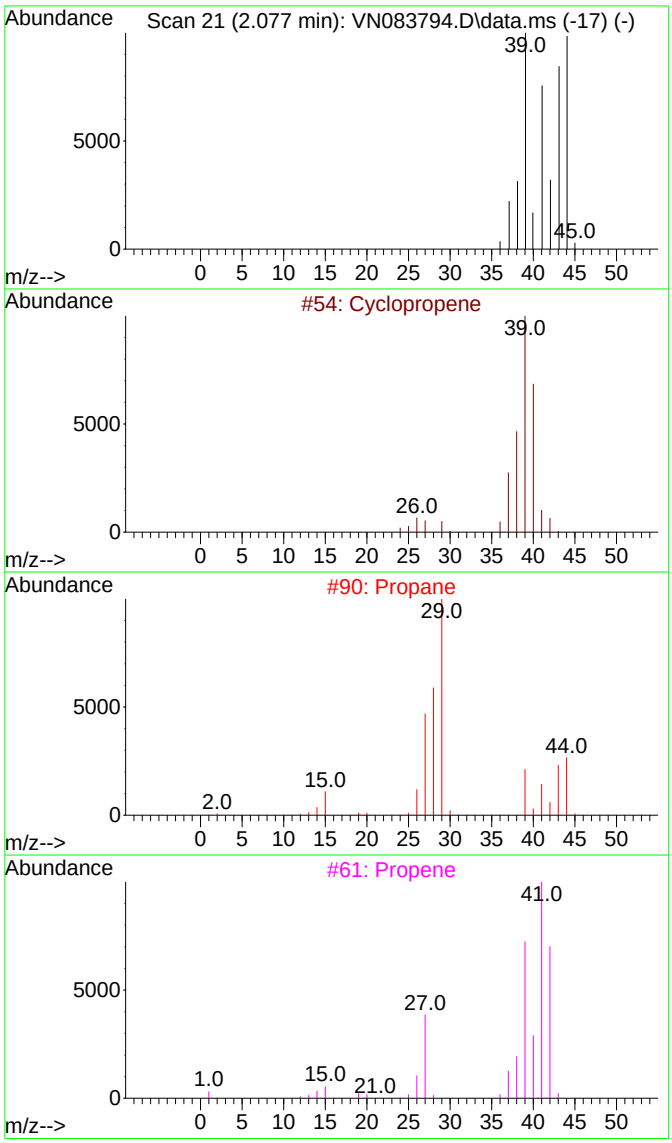
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

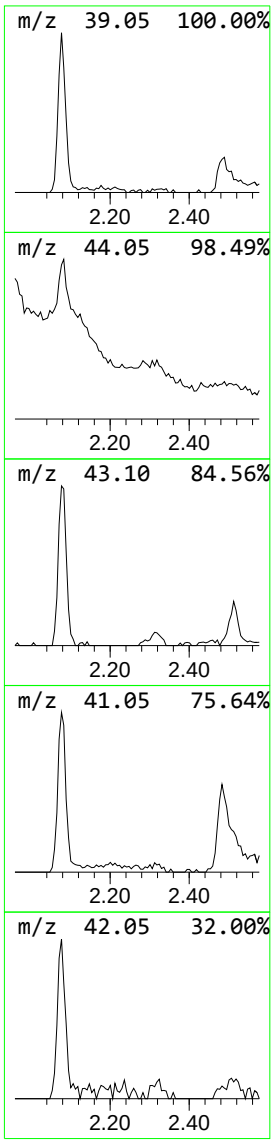
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 unknown2.077 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.077 | 18.62 ug/l | 149295 | Pentafluorobenzene | 8.224 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopropene | 40 | C3H4 | 002781-85-3 | 39 |
| 2 | Propane | 44 | C3H8 | 000074-98-6 | 9 |
| 3 | Propene | 42 | C3H6 | 000115-07-1 | 9 |
| 4 | Butanenitrile | 69 | C4H7N | 000109-74-0 | 2 |
| 5 | Ethanamine, 2-propoxy- | 103 | C5H13NO | 042185-03-5 | 2 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091124\
Data File : VN083794.D
Acq On : 11 Sep 2024 14:21
Operator : JC\MD
Sample : P3839-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
830

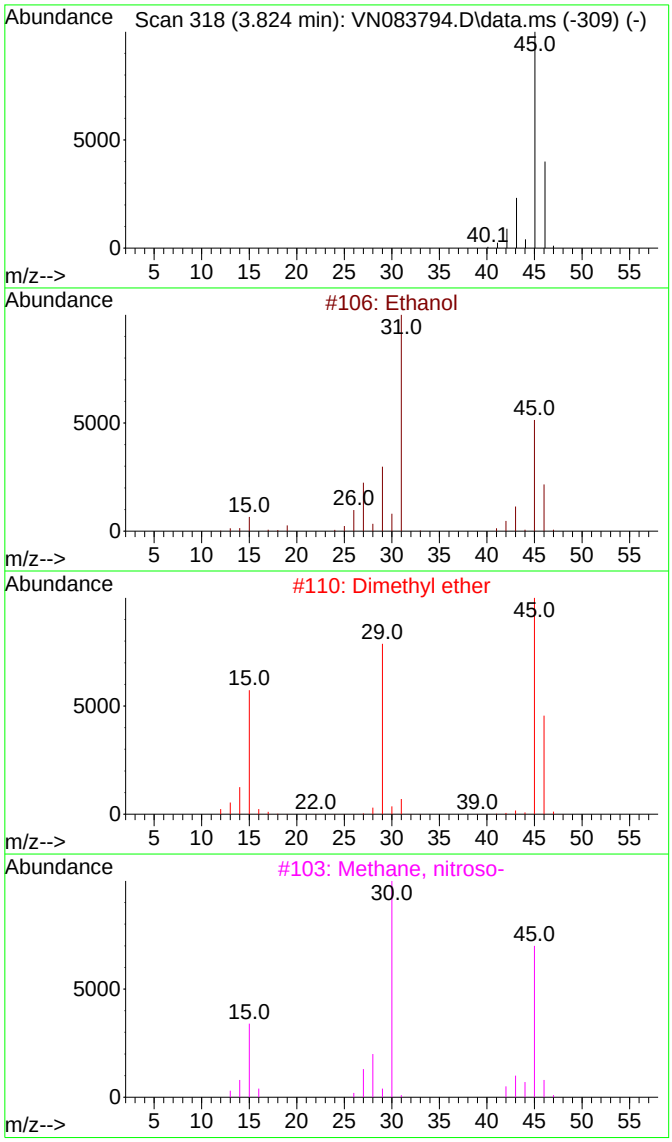
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

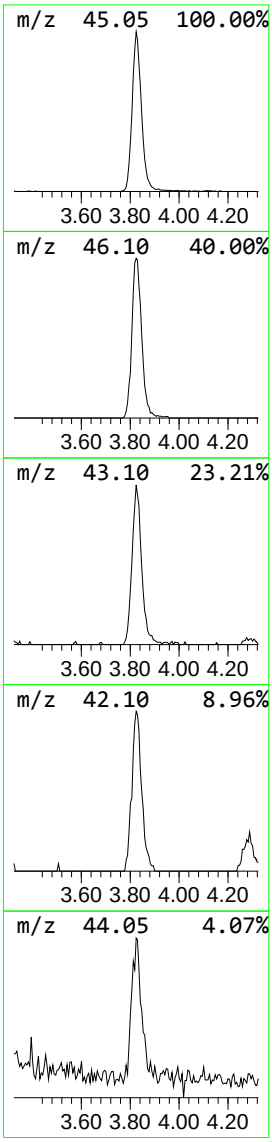
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 Ethanol Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.824 | 33.02 ug/l | 264792 | Pentafluorobenzene | 8.224 |

| 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\VN091124\
Data File : VN083794.D
Acq On : 11 Sep 2024 14:21
Operator : JC\MD
Sample : P3839-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
830

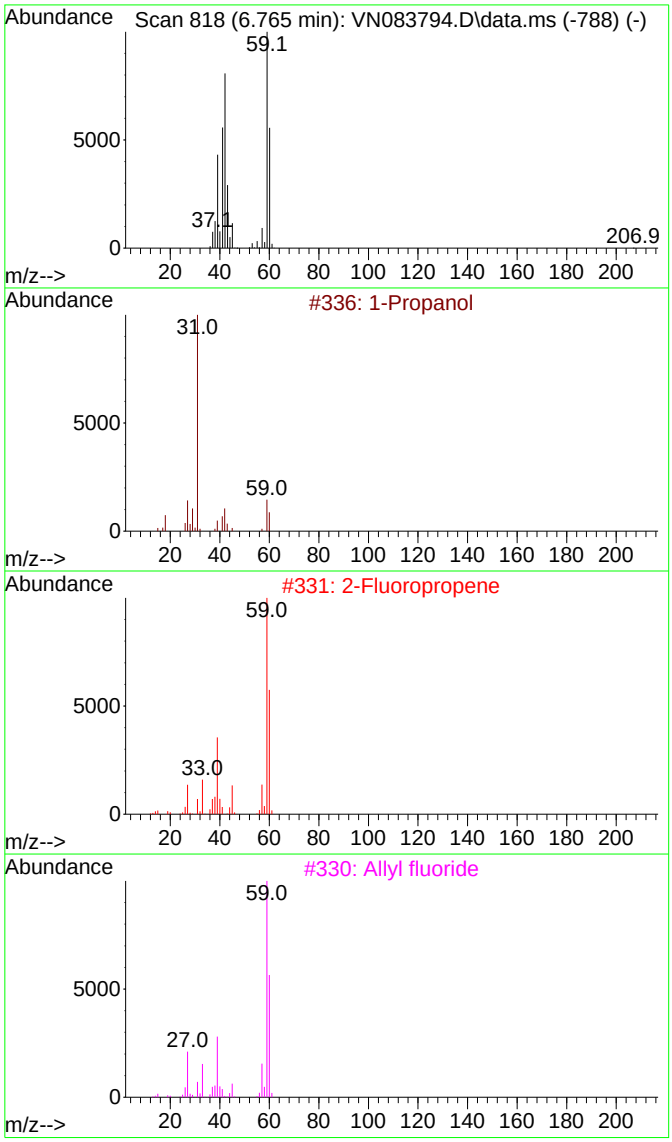
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

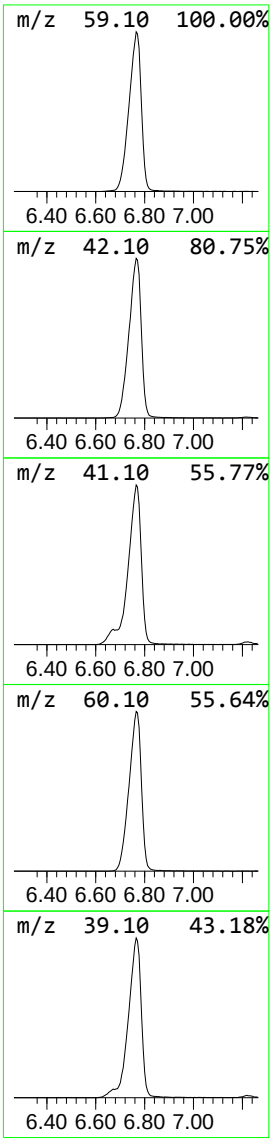
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 1-Propanol Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.765 | 1077.68 ug/l | 8641100 | Pentafluorobenzene | 8.224 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Propanol | 60 | C3H8O | 000071-23-8 | 59 |
| 2 | 2-Fluoropropene | 60 | C3H5F | 001184-60-7 | 50 |
| 3 | Allyl fluoride | 60 | C3H5F | 000818-92-8 | 32 |
| 4 | Cyclopropane | 42 | C3H6 | 000075-19-4 | 25 |
| 5 | Formamidoxime | 60 | CH4N2O | 000624-82-8 | 9 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091124\
Data File : VN083794.D
Acq On : 11 Sep 2024 14:21
Operator : JC\MD
Sample : P3839-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
830

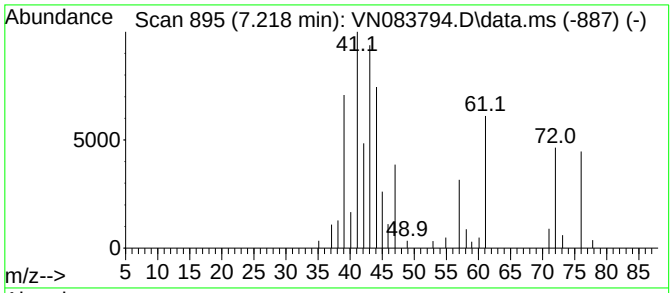
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

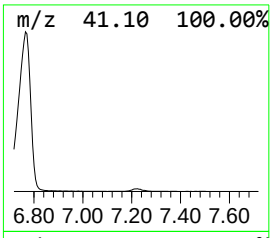
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

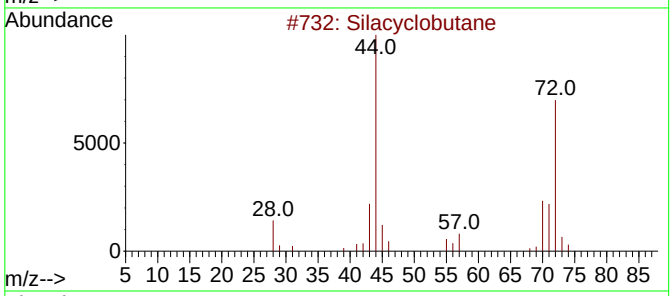
**********
Peak Number 5 unknown7.218 Concentration Rank 10

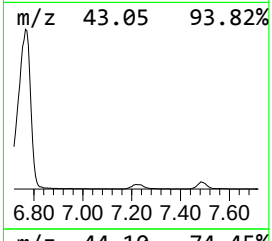
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.218 | 12.81 ug/l | 102743 | Pentafluorobenzene | 8.224 |

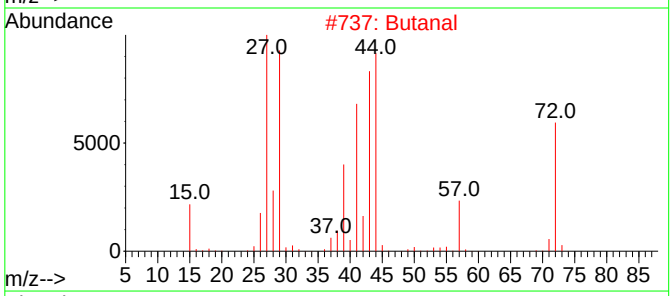
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Silacyclobutane | 72 | C3H8Si | 1000434-34-1 | 22 |
| 2 | Butanal | 72 | C4H8O | 000123-72-8 | 22 |
| 3 | Trimethylphosphine | 76 | C3H9P | 000594-09-2 | 20 |
| 4 | Allyl chloride | 76 | C3H5Cl | 000107-05-1 | 10 |
| 5 | Propene | 42 | C3H6 | 000115-07-1 | 10 |

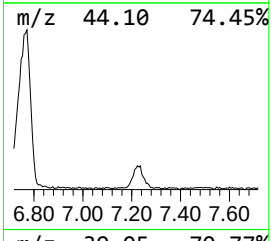


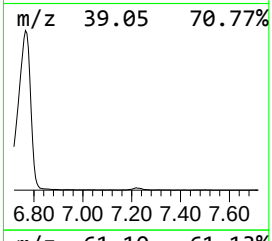



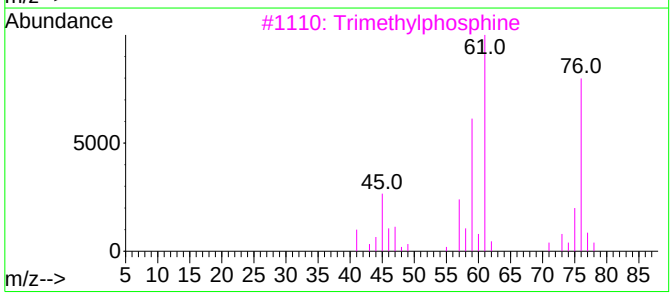



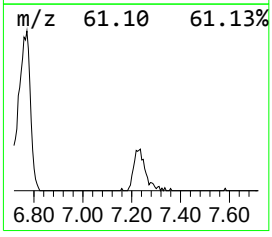



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ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
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**ClientSampleId :**
830

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

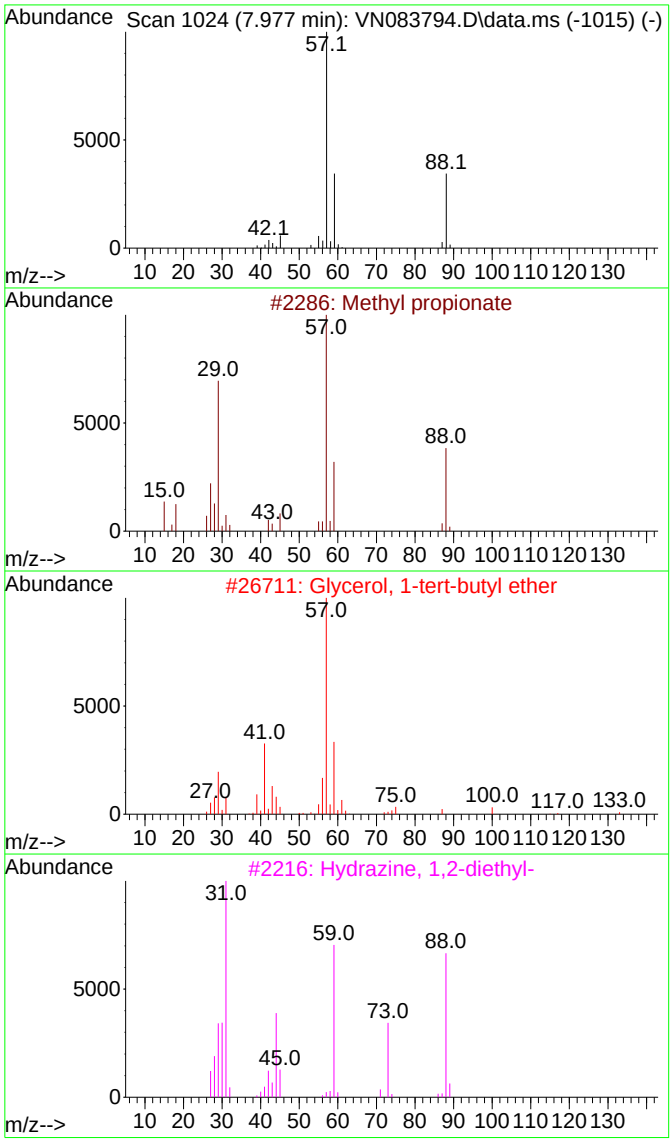
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

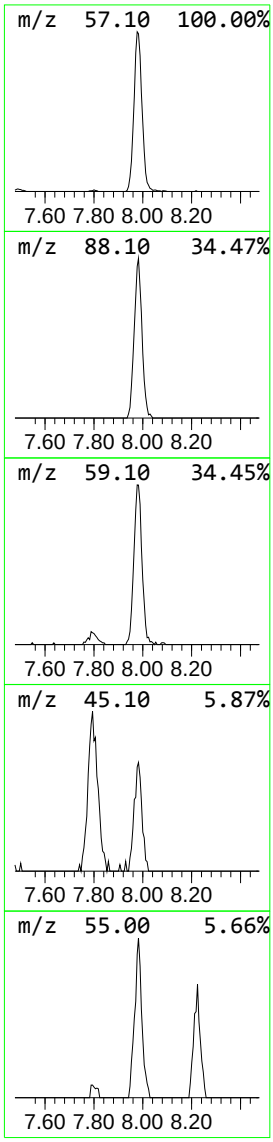
**********

Peak Number 6 Methyl propionate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.977 | 25.88 ug/l | 207500 | Pentafluorobenzene | 8.224 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl propionate | 88 | C4H8O2 | 000554-12-1 | 90 |
| 2 | Glycerol, 1-tert-butyl ether | 148 | C7H16O3 | 1010381-75-8 | 25 |
| 3 | Hydrazine, 1,2-diethyl- | 88 | C4H12N2 | 001615-80-1 | 9 |
| 4 | Propanoic acid, 2,2-dimethyl- | 102 | C5H10O2 | 000075-98-9 | 9 |
| 5 | Propane, 2-bromo-2-methyl- | 136 | C4H9Br | 000507-19-7 | 9 |



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ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
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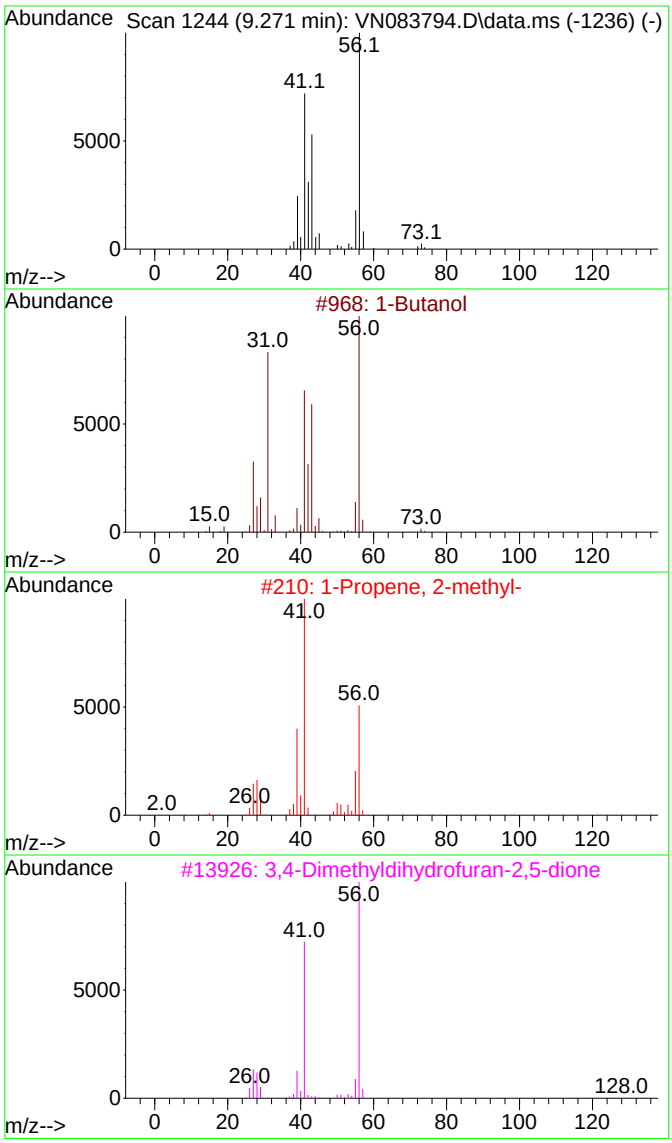
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

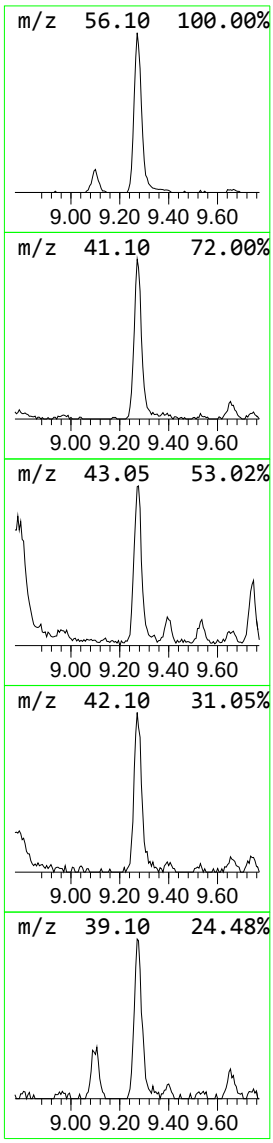
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 1-Butanol Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.271 | 15.13 ug/l | 190006 | 1,4-Difluorobenzene | 9.100 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Butanol | 74 | C4H10O | 000071-36-3 | 90 |
| 2 | 1-Propene, 2-methyl- | 56 | C4H8 | 000115-11-7 | 42 |
| 3 | 3,4-Dimethyldihydrofuran-2,5-dione | 128 | C6H8O3 | 007475-92-5 | 40 |
| 4 | Propane, 2-cyclopropyl- | 84 | C6H12 | 003638-35-5 | 36 |
| 5 | 3-Butenoic acid, 2-amino- | 101 | C4H7NO2 | 056512-51-7 | 9 |



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

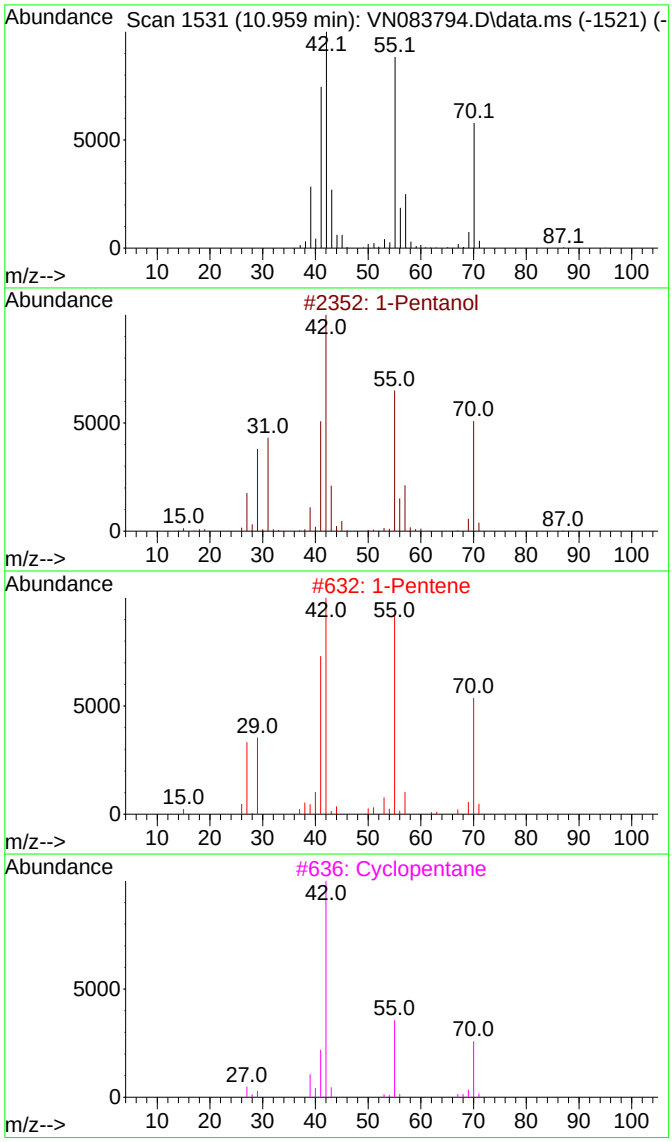
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

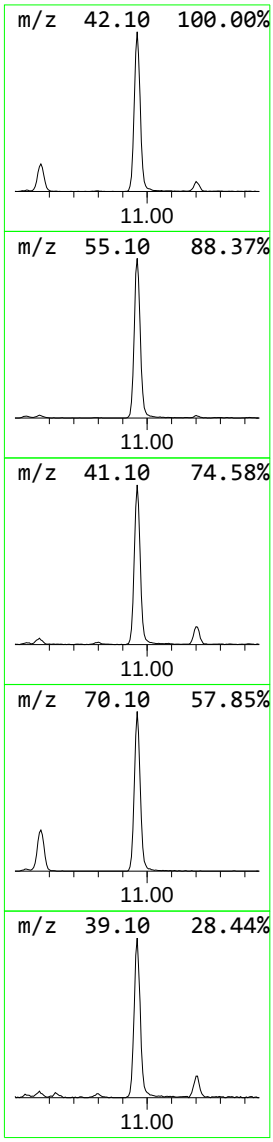
**********

Peak Number 8 1-Pentanol Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.959 | 57.79 ug/l | 1128680 | Chlorobenzene-d5 | 11.865 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Pentanol | 88 | C5H12O | 000071-41-0 | 86 |
| 2 | 1-Pentene | 70 | C5H10 | 000109-67-1 | 72 |
| 3 | Cyclopentane | 70 | C5H10 | 000287-92-3 | 64 |
| 4 | 3,3-Dimethyl-1,2-epoxybutane | 100 | C6H12O | 002245-30-9 | 53 |
| 5 | 1-Butanol, 3-methyl- | 88 | C5H12O | 000123-51-3 | 50 |



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Data File : VN083794.D
Acq On : 11 Sep 2024 14:21
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Sample : P3839-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
830

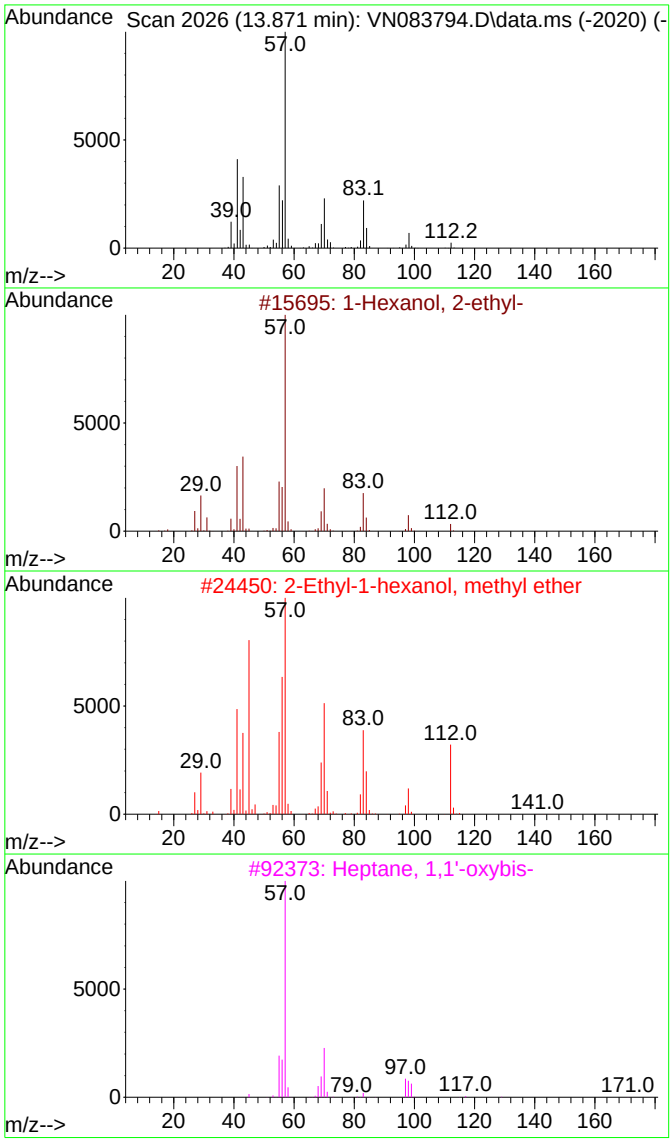
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

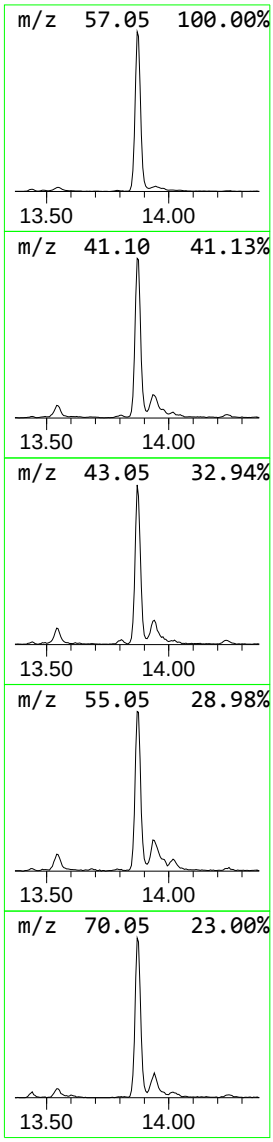
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.871 | 79.60 ug/l | 1642880 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 83 |
| 2 | 2-Ethyl-1-hexanol, methyl ether | 144 | C9H20O | 1000365-10-2 | 50 |
| 3 | Heptane, 1,1'-oxybis- | 214 | C14H30O | 000629-64-1 | 50 |
| 4 | 2-Propyl-1-pentanol | 130 | C8H18O | 058175-57-8 | 50 |
| 5 | Pentadecafluorooctanoic acid, 2-... | 526 | C16H17F15O2 | 1000406-80-9 | 38 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091124\
Data File : VN083794.D
Acq On : 11 Sep 2024 14:21
Operator : JC\MD
Sample : P3839-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
830

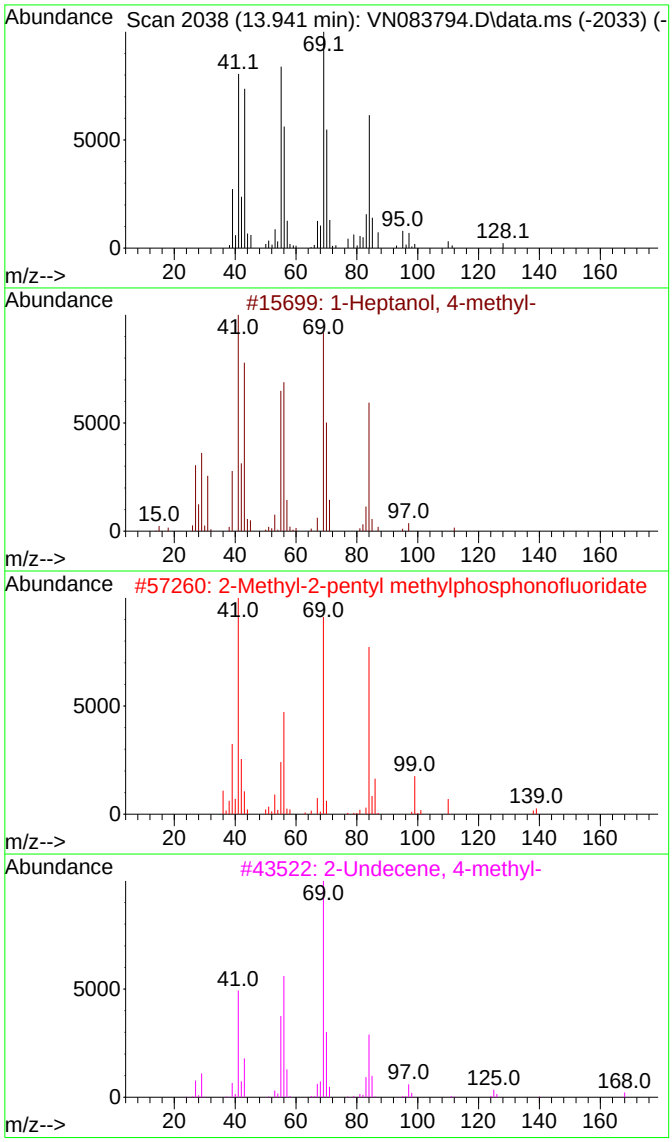
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

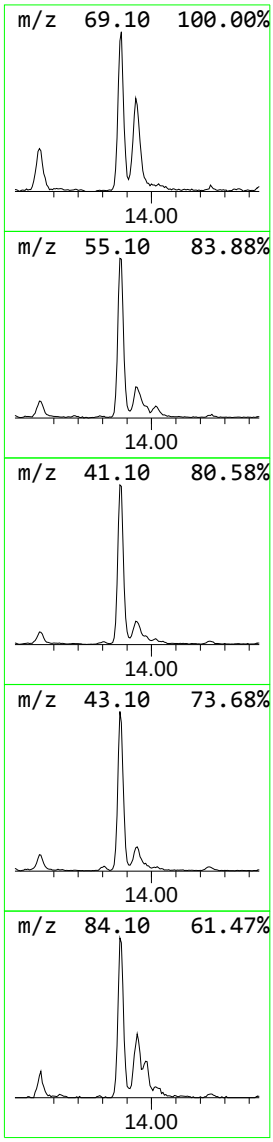
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 1-Heptanol, 4-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.941 | 18.97 ug/l | 391517 | 1,4-Dichlorobenzene-d4 | 13.794 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heptanol, 4-methyl- | 130 | C8H18O | 000817-91-4 | 86 |
| 2 | 2-Methyl-2-pentyl methylphosphon... | 182 | C7H16FO2P | 1000216-67-8 | 53 |
| 3 | 2-Undecene, 4-methyl- | 168 | C12H24 | 091695-32-8 | 50 |
| 4 | 1-Hexene, 3,3-dimethyl- | 112 | C8H16 | 003404-77-1 | 50 |
| 5 | Cetene | 224 | C16H32 | 000629-73-2 | 47 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091124\
Data File : VN083794.D
Acq On : 11 Sep 2024 14:21
Operator : JC\MD
Sample : P3839-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
MSVOA_N
**ClientSampleId :**
830

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.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 |
| unknown2.077 | 2.077 | 18.6 | ug/l | 149295 | 1 | 8.224 | 400912 | 50.0 |
| Ethanol | 3.824 | 33.0 | ug/l | 264792 | 1 | 8.224 | 400912 | 50.0 |
| 1-Propanol | 6.765 | 1077.7 | ug/l | 8641100 | 1 | 8.224 | 400912 | 50.0 |
| unknown7.218 | 7.218 | 12.8 | ug/l | 102743 | 1 | 8.224 | 400912 | 50.0 |
| Methyl propionate | 7.977 | 25.9 | ug/l | 207500 | 1 | 8.224 | 400912 | 50.0 |
| 1-Butanol | 9.271 | 15.1 | ug/l | 190006 | 2 | 9.100 | 627798 | 50.0 |
| 1-Pentanol | 10.959 | 57.8 | ug/l | 1128680 | 3 | 11.865 | 976546 | 50.0 |
| 1-Hexanol, 2-et... | 13.871 | 79.6 | ug/l | 1642880 | 4 | 13.794 | 1032010 | 50.0 |
| 1-Heptanol, 4-m... | 13.941 | 19.0 | ug/l | 391517 | 4 | 13.794 | 1032010 | 50.0 |