LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011322\
Data File : VU046754.D
Acq On : 13 Jan 2022 13:59
Operator : SY/MD
Sample : N1101-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
BFXX0

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\Method\SFAMUTR122121WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU046754.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.363 | 3 | 7 | 24 | rVB2 | 28138 | 29286 | 1.33% | 0.532% |
| 2 | 1.446 | 26 | 33 | 38 | rVV | 20860 | 22391 | 1.02% | 0.406% |
| 3 | 1.600 | 71 | 81 | 89 | rBV3 | 29416 | 40286 | 1.83% | 0.731% |
| 4 | 1.919 | 172 | 180 | 192 | rBV | 20821 | 27713 | 1.26% | 0.503% |
| 5 | 2.578 | 366 | 385 | 400 | rBV5 | 80351 | 165384 | 7.51% | 3.002% |
| 6 | 3.874 | 771 | 788 | 807 | rVB | 89295 | 212190 | 9.64% | 3.852% |
| 7 | 4.645 | 1013 | 1028 | 1074 | rBV2 | 40926 | 156014 | 7.09% | 2.832% |
| 8 | 5.070 | 1144 | 1160 | 1182 | rBV | 46002 | 108249 | 4.92% | 1.965% |
| 9 | 5.317 | 1224 | 1237 | 1251 | rVB2 | 12648 | 27493 | 1.25% | 0.499% |
| 10 | 5.729 | 1344 | 1365 | 1382 | rBV2 | 84130 | 224870 | 10.22% | 4.082% |
| 11 | 6.250 | 1514 | 1527 | 1544 | rBV | 82856 | 154963 | 7.04% | 2.813% |
| 12 | 6.546 | 1603 | 1619 | 1653 | rBV | 1164241 | 2200866 | 100.00% | 39.950% |
| 13 | 6.694 | 1653 | 1665 | 1679 | rVB2 | 55226 | 107651 | 4.89% | 1.954% |
| 14 | 6.883 | 1714 | 1724 | 1743 | rBV3 | 11619 | 23450 | 1.07% | 0.426% |
| 15 | 7.568 | 1925 | 1937 | 1954 | rVB | 28152 | 48841 | 2.22% | 0.887% |
| 16 | 7.899 | 2028 | 2040 | 2055 | rBV | 98793 | 167744 | 7.62% | 3.045% |
| 17 | 8.182 | 2117 | 2128 | 2141 | rBV | 18325 | 30651 | 1.39% | 0.556% |
| 18 | 8.555 | 2233 | 2244 | 2255 | rBV2 | 36754 | 59659 | 2.71% | 1.083% |
| 19 | 8.636 | 2257 | 2269 | 2293 | rBV | 202349 | 352761 | 16.03% | 6.403% |
| 20 | 8.787 | 2305 | 2316 | 2342 | rVB | 87553 | 158057 | 7.18% | 2.869% |
| 21 | 9.417 | 2501 | 2512 | 2529 | rBV | 126483 | 205832 | 9.35% | 3.736% |
| 22 | 10.343 | 2791 | 2800 | 2815 | rVB2 | 23881 | 37190 | 1.69% | 0.675% |
| 23 | 10.758 | 2917 | 2929 | 2944 | rVB | 57992 | 93244 | 4.24% | 1.693% |
| 24 | 11.687 | 3208 | 3218 | 3230 | rBV2 | 87089 | 130128 | 5.91% | 2.362% |
| 25 | 11.812 | 3246 | 3257 | 3275 | rVB | 154234 | 244052 | 11.09% | 4.430% |
| 26 | 12.195 | 3363 | 3376 | 3389 | rBV | 118051 | 189120 | 8.59% | 3.433% |
| 27 | 12.886 | 3580 | 3591 | 3609 | rBV | 196686 | 290991 | 13.22% | 5.282% |

Sum of corrected areas: 5509076

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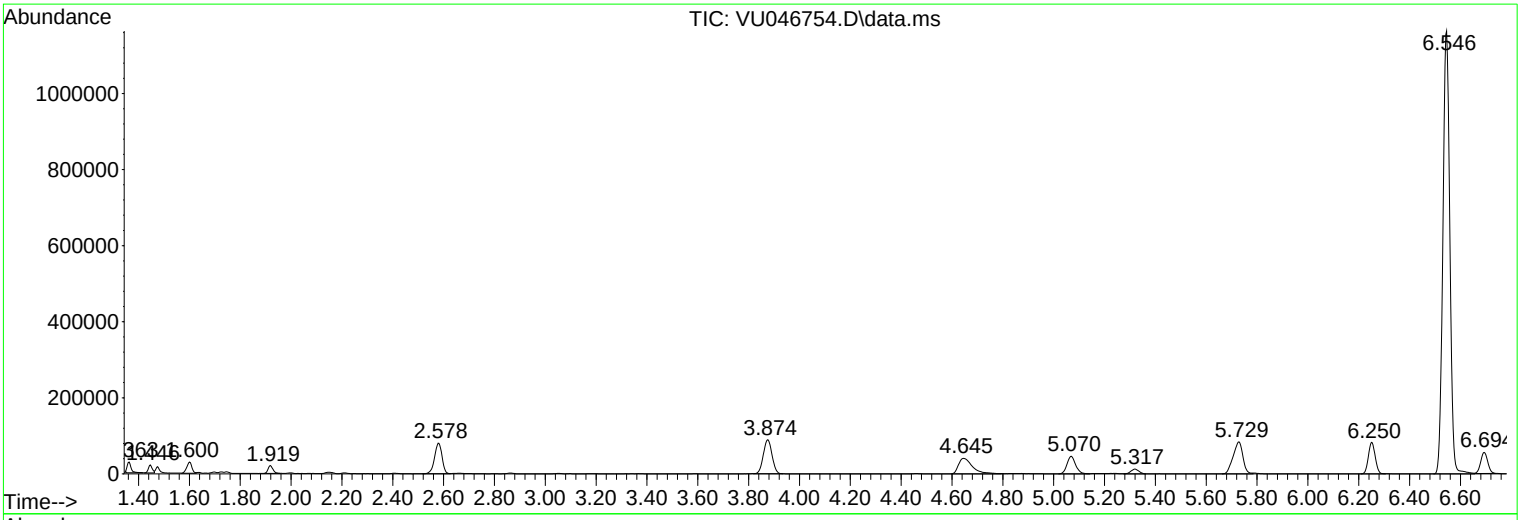
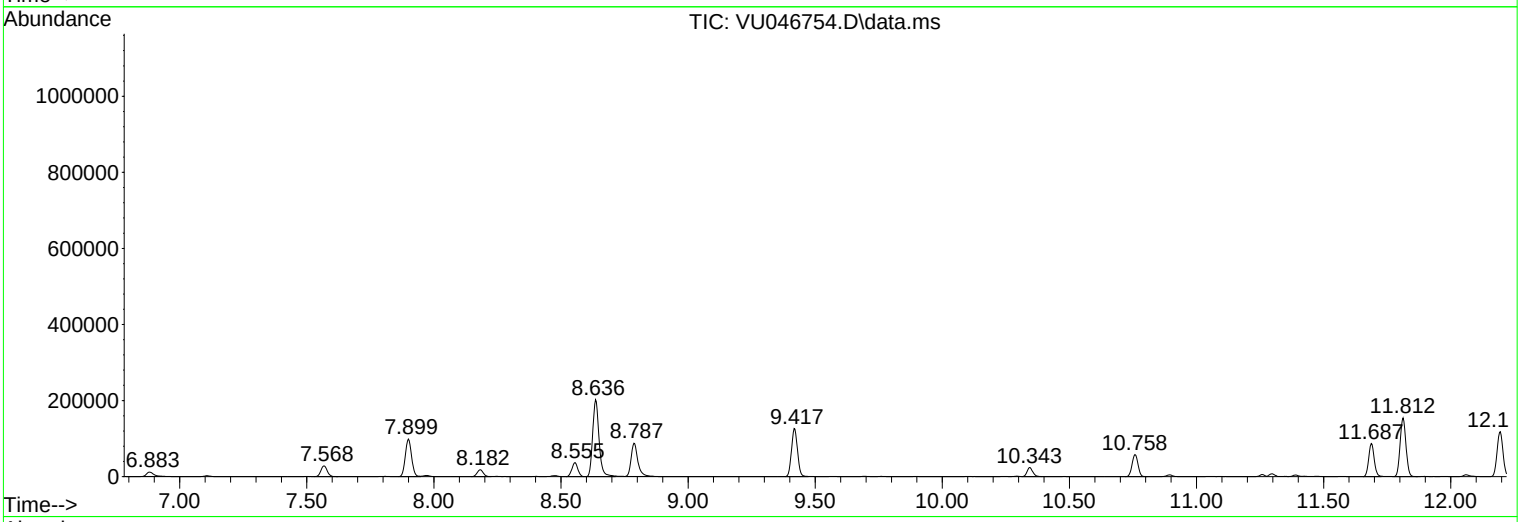
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

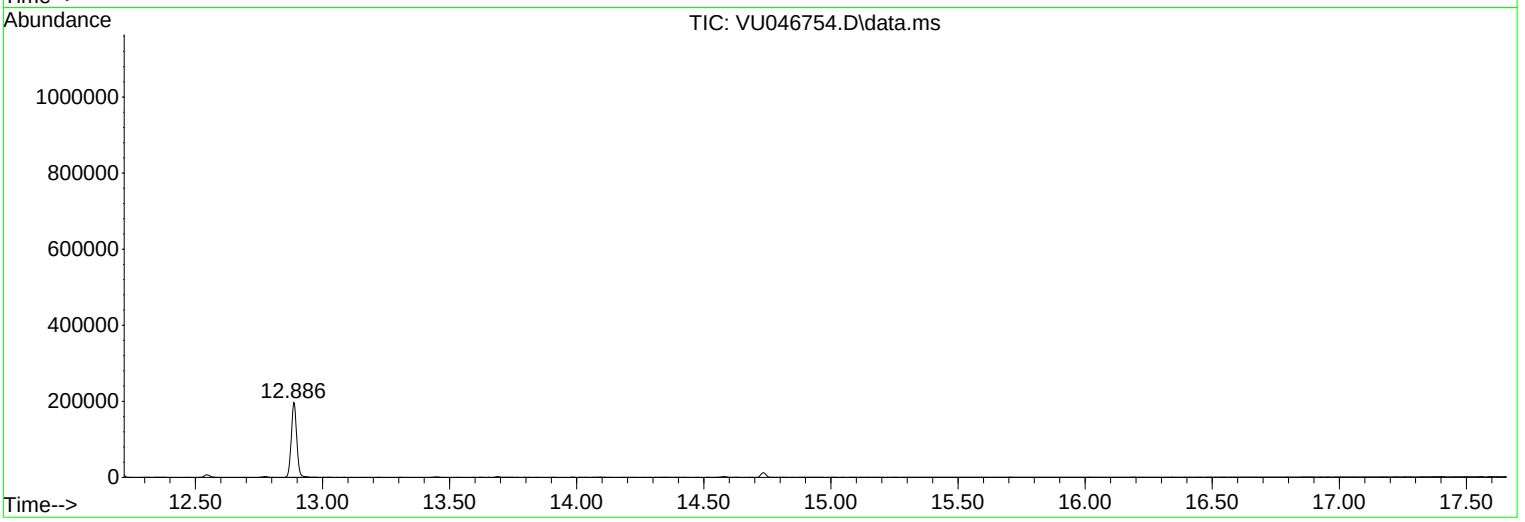
**Instrument :**
MSVOA_U
**ClientSampleId :**
BFXX0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011322\
Data File : VU046754.D
Acq On : 13 Jan 2022 13:59
Operator : SY/MD
Sample : N1101-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
BFXX0

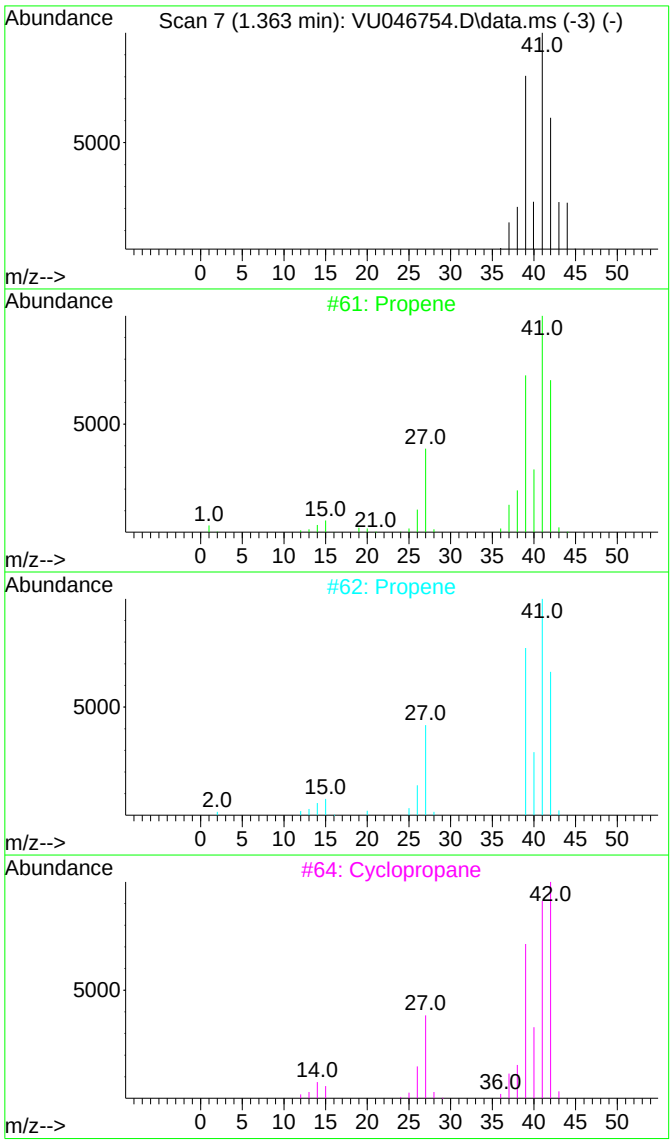
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

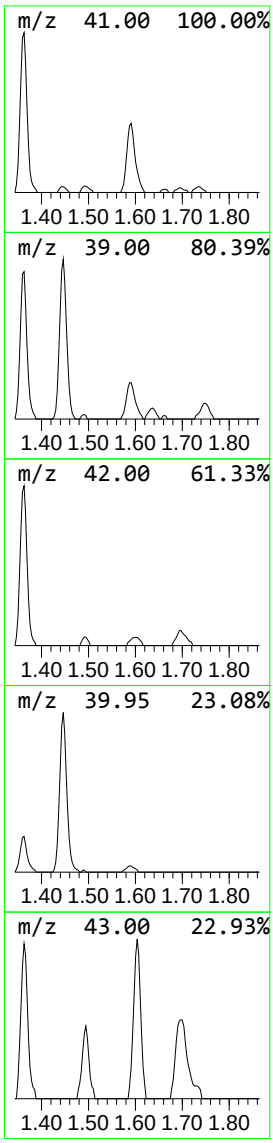
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.363 | 0.94 ug/L | 29286 | 1,4-Difluorobenzene | 6.250 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propene | 42 | C3H6 | 000115-07-1 | 90 |
| 2 | Propene | 42 | C3H6 | 000115-07-1 | 42 |
| 3 | Cyclopropane | 42 | C3H6 | 000075-19-4 | 9 |
| 4 | Cyclopropene | 40 | C3H4 | 002781-85-3 | 9 |
| 5 | Cyclopropane | 42 | C3H6 | 000075-19-4 | 7 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011322\
Data File : VU046754.D
Acq On : 13 Jan 2022 13:59
Operator : SY/MD
Sample : N1101-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
BFXX0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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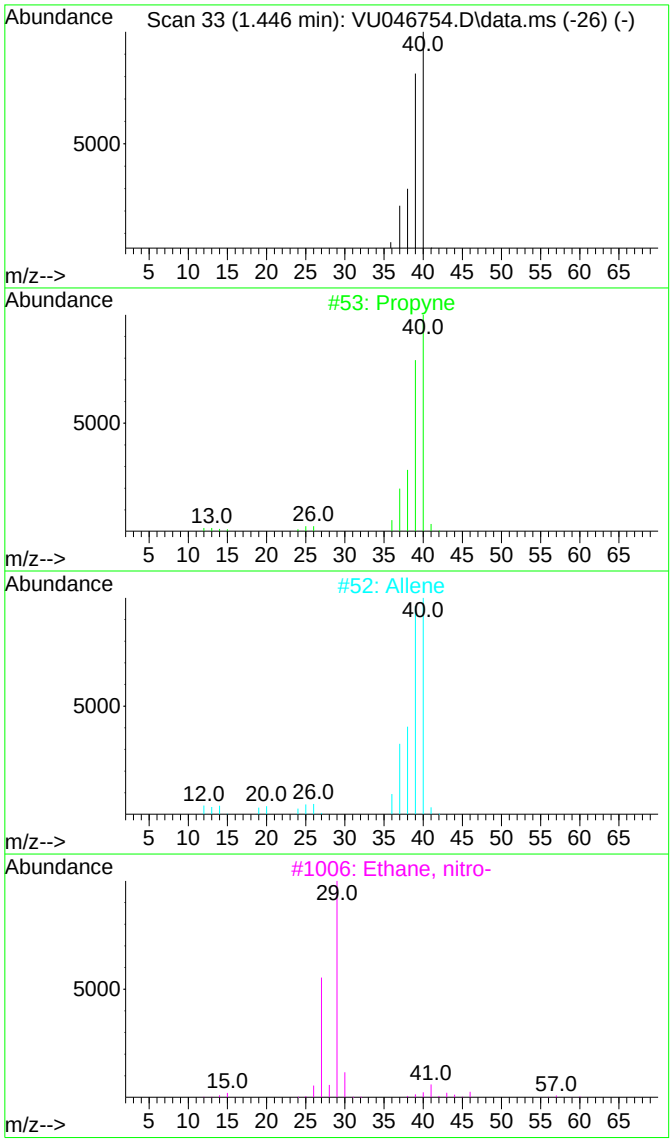
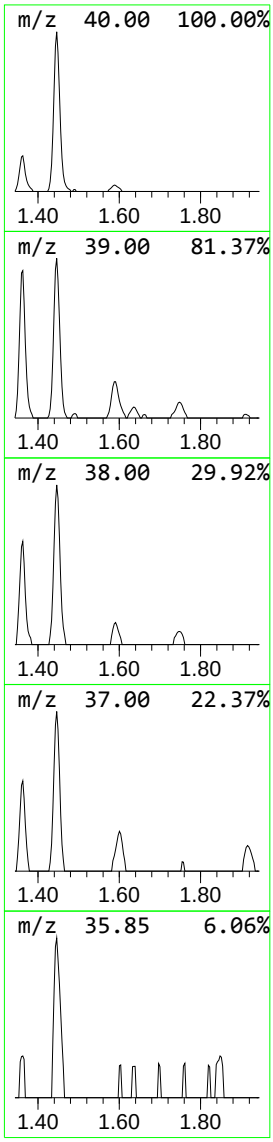
Peak Number 2 Propyne Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.446 | 0.72 ug/L | 22391 | 1,4-Difluorobenzene | 6.250 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propyne | 40 | C3H4 | 000074-99-7 | 90 |
| 2 | Allene | 40 | C3H4 | 000463-49-0 | 83 |
| 3 | Ethane, nitro- | 75 | C2H5NO2 | 000079-24-3 | 1 |
| 4 | 3-Methyl-1,2-diazirine | 56 | C2H4N2 | 1000305-83-7 | 1 |
| 5 | 1-Butanamine, 2-methyl- | 87 | C5H13N | 000096-15-1 | 1 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011322\
Data File : VU046754.D
Acq On : 13 Jan 2022 13:59
Operator : SY/MD
Sample : N1101-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
BFXX0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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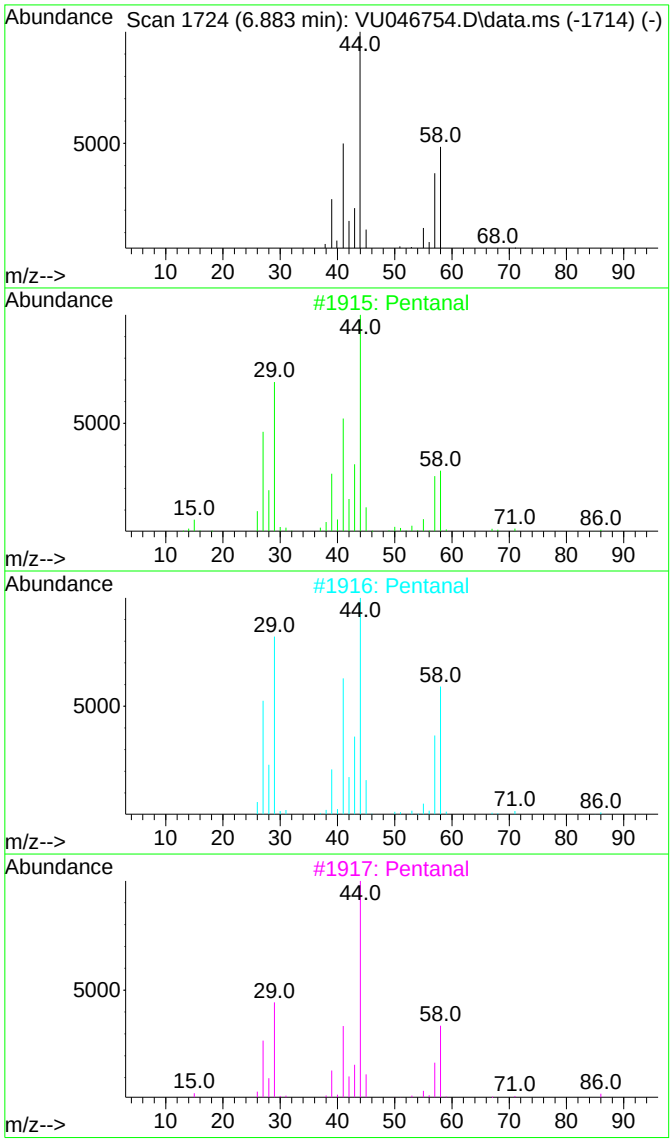
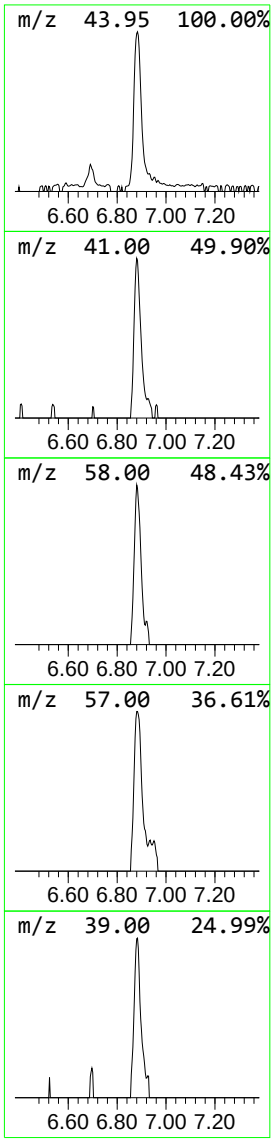
Peak Number 3 Pentanal Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.883 | 0.76 ug/L | 23450 | 1,4-Difluorobenzene | 6.250 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentanal | 86 | C5H10O | 000110-62-3 | 64 |
| 2 | Pentanal | 86 | C5H10O | 000110-62-3 | 56 |
| 3 | Pentanal | 86 | C5H10O | 000110-62-3 | 56 |
| 4 | Cyclopropyl carbinol | 72 | C4H8O | 002516-33-8 | 33 |
| 5 | 1-Octadecanamine, N-methyl- | 283 | C19H41N | 002439-55-6 | 9 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011322\
Data File : VU046754.D
Acq On : 13 Jan 2022 13:59
Operator : SY/MD
Sample : N1101-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
BFXX0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

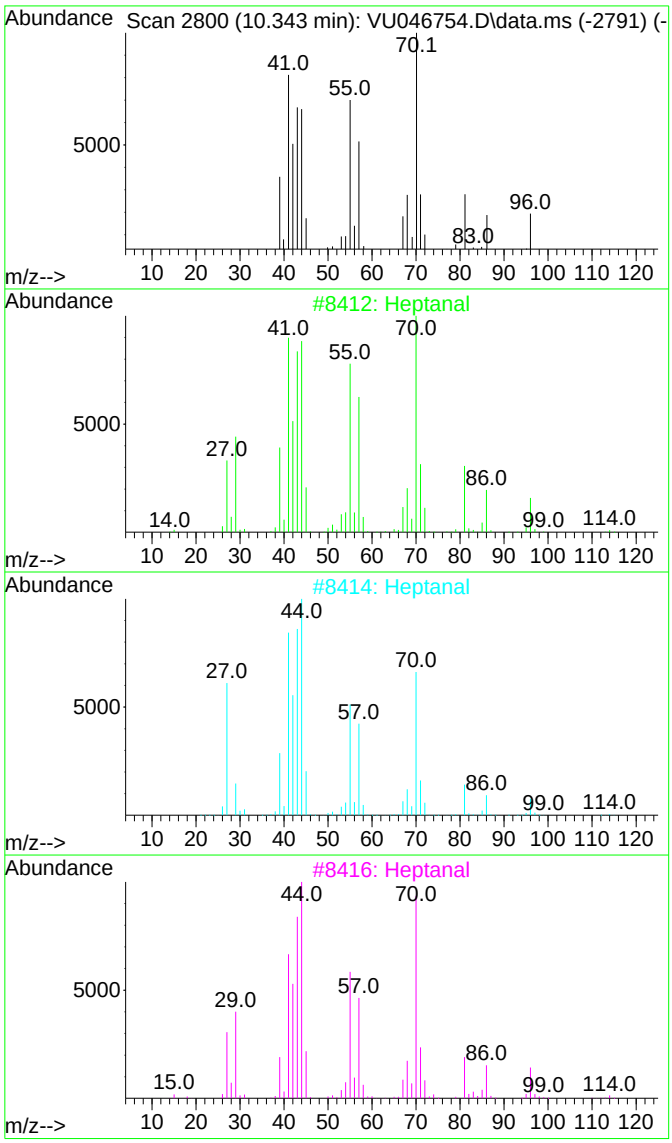
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

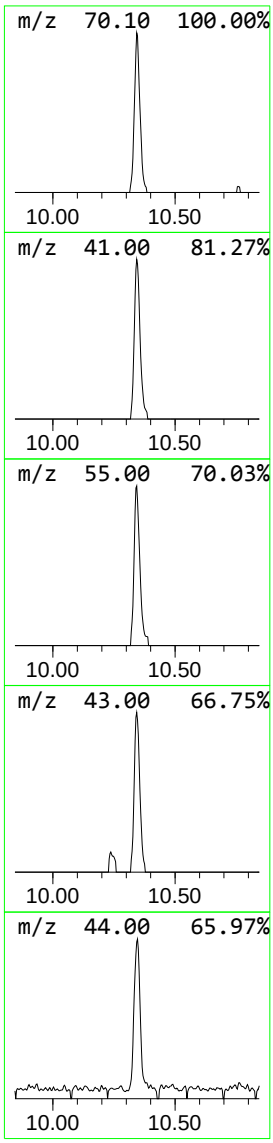
**********

Peak Number 5 Heptanal Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.343 | 0.90 ug/L | 37190 | Chlorobenzene-d5 | 9.417 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptanal | 114 | C7H14O | 000111-71-7 | 86 |
| 2 | Heptanal | 114 | C7H14O | 000111-71-7 | 64 |
| 3 | Heptanal | 114 | C7H14O | 000111-71-7 | 64 |
| 4 | Heptanal | 114 | C7H14O | 000111-71-7 | 64 |
| 5 | Heptanal | 114 | C7H14O | 000111-71-7 | 50 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011322\
Data File : VU046754.D
Acq On : 13 Jan 2022 13:59
Operator : SY/MD
Sample : N1101-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
BFXX0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

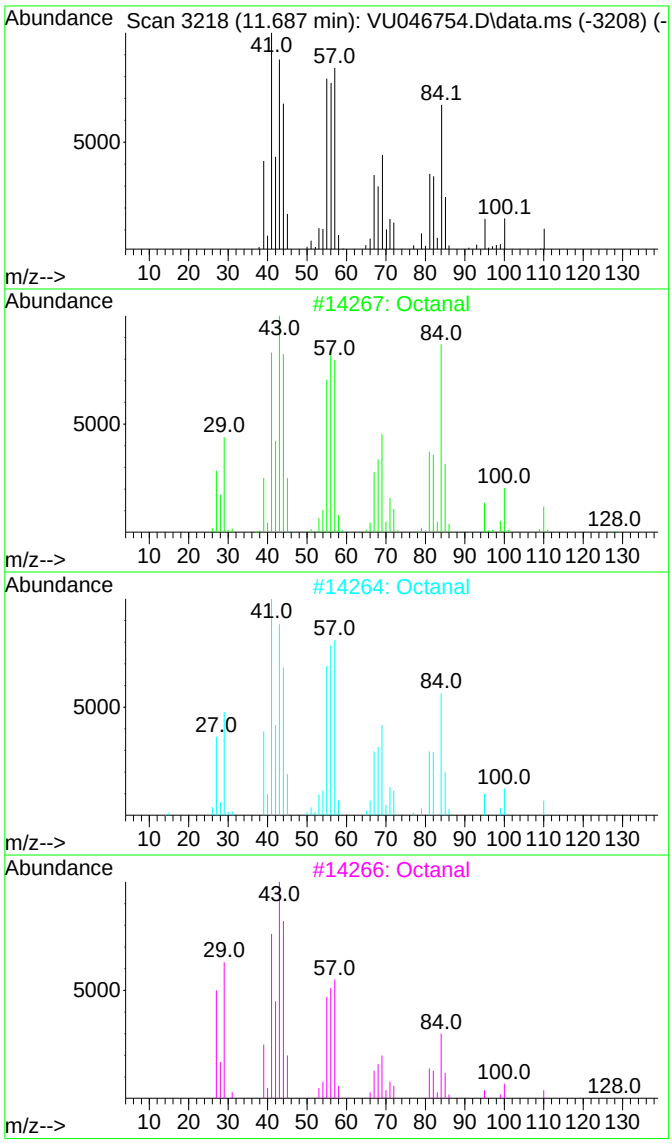
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

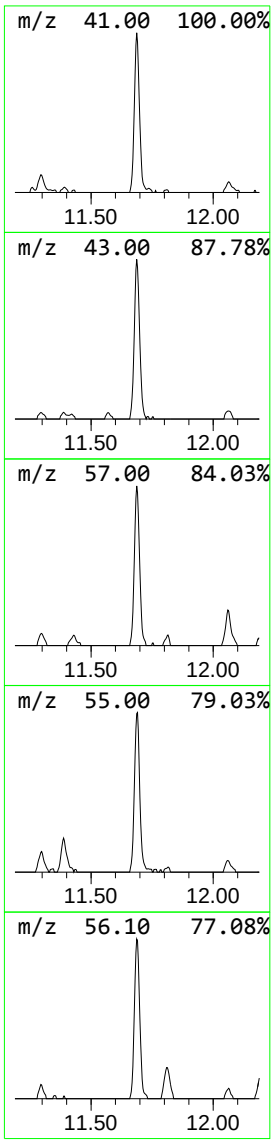
**********

Peak Number 6 Octanal Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.687 | 2.67 ug/L | 130128 | 1,4-Dichlorobenzene-d4 | 11.812 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octanal | 128 | C8H16O | 000124-13-0 | 91 |
| 2 | Octanal | 128 | C8H16O | 000124-13-0 | 91 |
| 3 | Octanal | 128 | C8H16O | 000124-13-0 | 90 |
| 4 | Octanal | 128 | C8H16O | 000124-13-0 | 78 |
| 5 | 1-Hexene | 84 | C6H12 | 000592-41-6 | 43 |



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Data File : VU046754.D
Acq On : 13 Jan 2022 13:59
Operator : SY/MD
Sample : N1101-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
BFXX0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

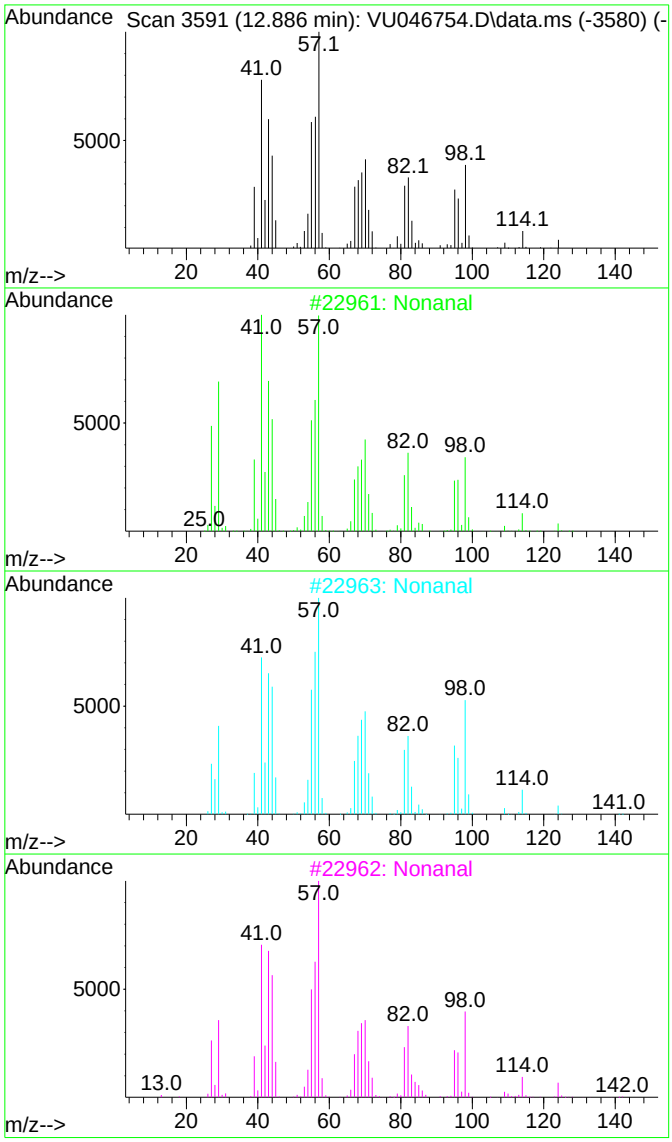
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

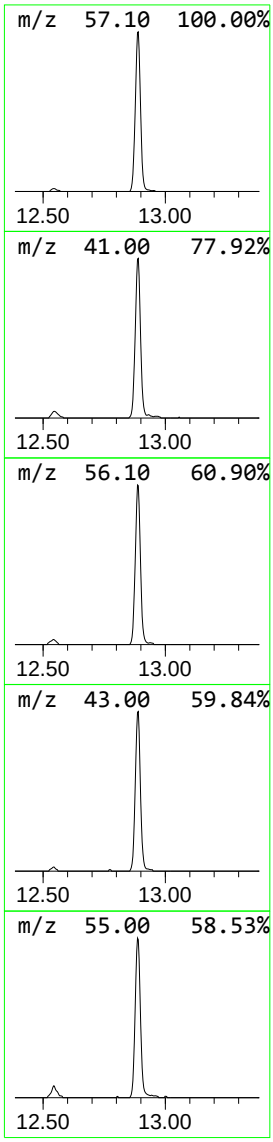
**********

Peak Number 7 Nonanal Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.886 | 5.96 ug/L | 290991 | 1,4-Dichlorobenzene-d4 | 11.812 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Nonanal | 142 | C9H18O | 000124-19-6 | 91 |
| 2 | Nonanal | 142 | C9H18O | 000124-19-6 | 91 |
| 3 | Nonanal | 142 | C9H18O | 000124-19-6 | 80 |
| 4 | Heptane, 2-chloro- | 134 | C7H15Cl | 001001-89-4 | 35 |
| 5 | 2-Hexene, 5-methyl-, (E)- | 98 | C7H14 | 007385-82-2 | 27 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011322\
Data File : VU046754.D
Acq On : 13 Jan 2022 13:59
Operator : SY/MD
Sample : N1101-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
BFXX0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| (DEL) Alkane: S... | 1.363 | 0.9 | ug/L | 29286 | 1 | 6.250 | 154963 | 5.0 |
| Propyne | 1.446 | 0.7 | ug/L | 22391 | 1 | 6.250 | 154963 | 5.0 |
| Pentanal | 6.883 | 0.8 | ug/L | 23450 | 1 | 6.250 | 154963 | 5.0 |
| Heptanal | 10.343 | 0.9 | ug/L | 37190 | 2 | 9.417 | 205832 | 5.0 |
| Octanal | 11.687 | 2.7 | ug/L | 130128 | 3 | 11.812 | 244052 | 5.0 |
| Nonanal | 12.886 | 6.0 | ug/L | 290991 | 3 | 11.812 | 244052 | 5.0 |