LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

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\SOMUTR081920WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

| 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 | 17 | rVB2 | 24674 | 24605 | 6.15% | 0.670% |
| 2 | 1.494 | 43 | 48 | 56 | rVB | 6791 | 6670 | 1.67% | 0.182% |
| 3 | 1.604 | 71 | 82 | 90 | rBV3 | 51635 | 67629 | 16.90% | 1.840% |
| 4 | 1.668 | 96 | 102 | 108 | rBV3 | 3826 | 6376 | 1.59% | 0.174% |
| 5 | 1.922 | 172 | 181 | 191 | rVB | 40278 | 54057 | 13.51% | 1.471% |
| 6 | 2.002 | 199 | 206 | 216 | rVB2 | 14128 | 19430 | 4.86% | 0.529% |
| 7 | 2.256 | 276 | 285 | 293 | rVB2 | 13996 | 19221 | 4.80% | 0.523% |
| 8 | 2.578 | 375 | 385 | 398 | rBV | 59139 | 97207 | 24.29% | 2.645% |
| 9 | 2.658 | 398 | 410 | 437 | rVB2 | 20810 | 53349 | 13.33% | 1.452% |
| 10 | 2.845 | 442 | 468 | 520 | rBV2 | 51339 | 363577 | 90.86% | 9.894% |
| 11 | 3.150 | 554 | 563 | 575 | rVB4 | 5141 | 11262 | 2.81% | 0.306% |
| 12 | 3.385 | 625 | 636 | 651 | rVB4 | 5109 | 12638 | 3.16% | 0.344% |
| 13 | 3.890 | 772 | 793 | 811 | rBV | 59254 | 144379 | 36.08% | 3.929% |
| 14 | 4.526 | 975 | 991 | 1005 | rVB3 | 4937 | 13210 | 3.30% | 0.359% |
| 15 | 4.652 | 1015 | 1030 | 1053 | rBV | 61457 | 163370 | 40.83% | 4.446% |
| 16 | 4.825 | 1070 | 1084 | 1100 | rVV2 | 24798 | 54528 | 13.63% | 1.484% |
| 17 | 5.086 | 1148 | 1165 | 1179 | rBV2 | 66037 | 144104 | 36.01% | 3.921% |
| 18 | 5.591 | 1313 | 1322 | 1338 | rVB4 | 2528 | 5554 | 1.39% | 0.151% |
| 19 | 5.742 | 1348 | 1369 | 1398 | rBV2 | 126678 | 340771 | 85.16% | 9.273% |
| 20 | 6.263 | 1517 | 1531 | 1552 | rVB | 96490 | 180833 | 45.19% | 4.921% |
| 21 | 6.510 | 1595 | 1608 | 1625 | rBV2 | 23526 | 47292 | 11.82% | 1.287% |
| 22 | 6.703 | 1655 | 1668 | 1683 | rVB2 | 78915 | 151373 | 37.83% | 4.119% |
| 23 | 7.468 | 1897 | 1906 | 1918 | rVB3 | 6289 | 10873 | 2.72% | 0.296% |
| 24 | 7.575 | 1923 | 1939 | 1952 | rBV2 | 41493 | 71415 | 17.85% | 1.943% |
| 25 | 7.722 | 1974 | 1985 | 1999 | rVB2 | 19137 | 34245 | 8.56% | 0.932% |
| 26 | 7.906 | 2030 | 2042 | 2057 | rVV | 145233 | 244166 | 61.02% | 6.644% |
| 27 | 8.185 | 2119 | 2129 | 2144 | rBV3 | 27765 | 47811 | 11.95% | 1.301% |
| 28 | 8.639 | 2257 | 2270 | 2294 | rBV | 231719 | 400151 | 100.00% | 10.889% |
| 29 | 8.931 | 2348 | 2361 | 2375 | rBV6 | 2562 | 5929 | 1.48% | 0.161% |
| 30 | 9.420 | 2499 | 2513 | 2531 | rBV | 153034 | 249744 | 62.41% | 6.796% |
| 31 | 10.754 | 2916 | 2928 | 2942 | rBV3 | 62103 | 101864 | 25.46% | 2.772% |
| 32 | 11.468 | 3139 | 3150 | 3160 | rVB3 | 4395 | 7125 | 1.78% | 0.194% |
| 33 | 11.806 | 3243 | 3255 | 3270 | rVB | 148262 | 226515 | 56.61% | 6.164% |
| 34 | 12.050 | 3322 | 3331 | 3345 | rBV | 22237 | 35666 | 8.91% | 0.971% |

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

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\SOMUTR081920WMA.M
Title : TRACE VOA SOM01.0

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 12.185 | 3361 | 3373 | 3386 | rBV | 152035 | 241915 | 60.46% | 6.583% |
| 36 | 13.201 | 3682 | 3689 | 3696 | rVB6 | 4222 | 5989 | 1.50% | 0.163% |
| 37 | 15.465 | 4384 | 4393 | 4401 | rBV4 | 6640 | 9977 | 2.49% | 0.271% |

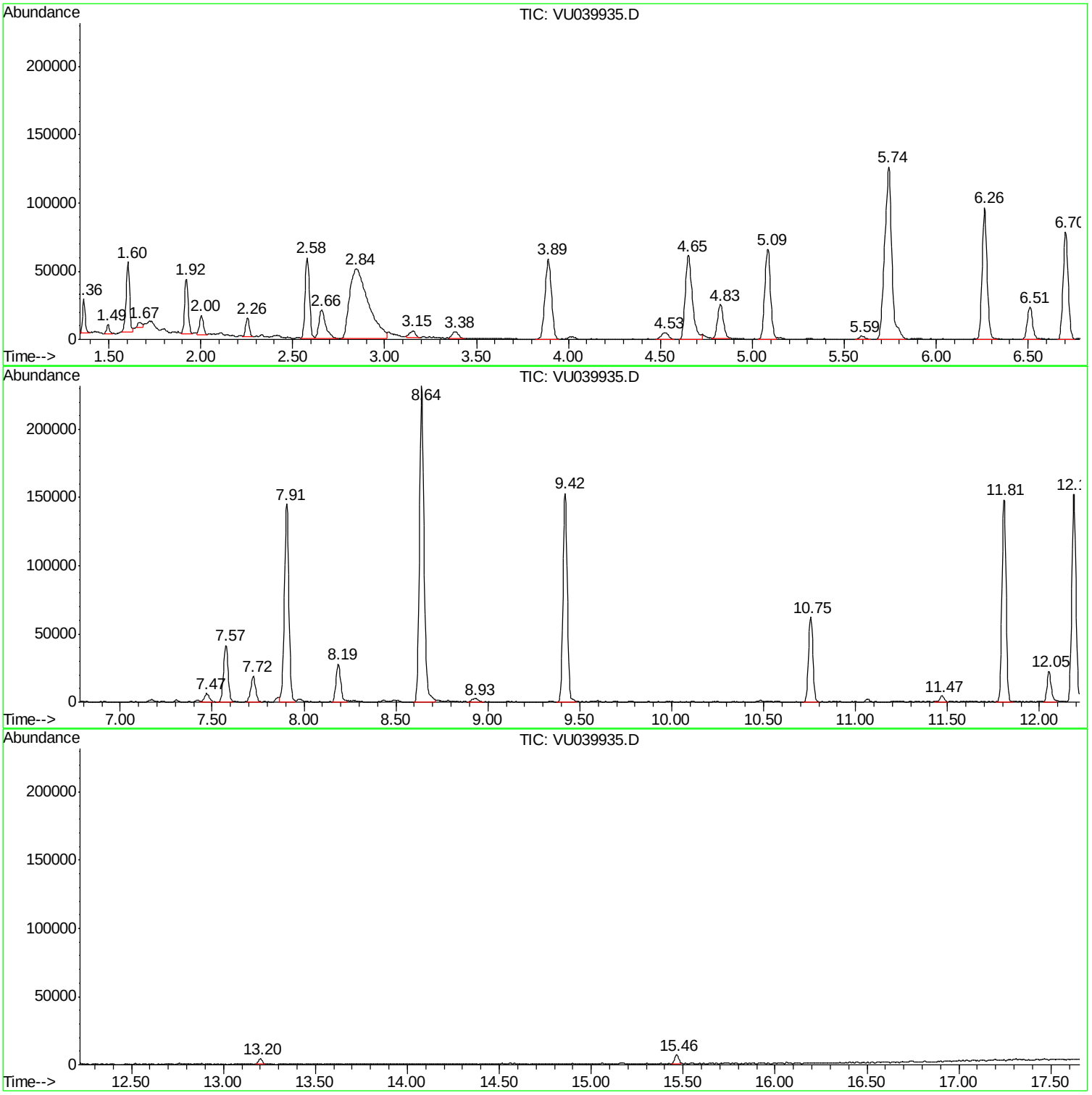
Sum of corrected areas: 3674820

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

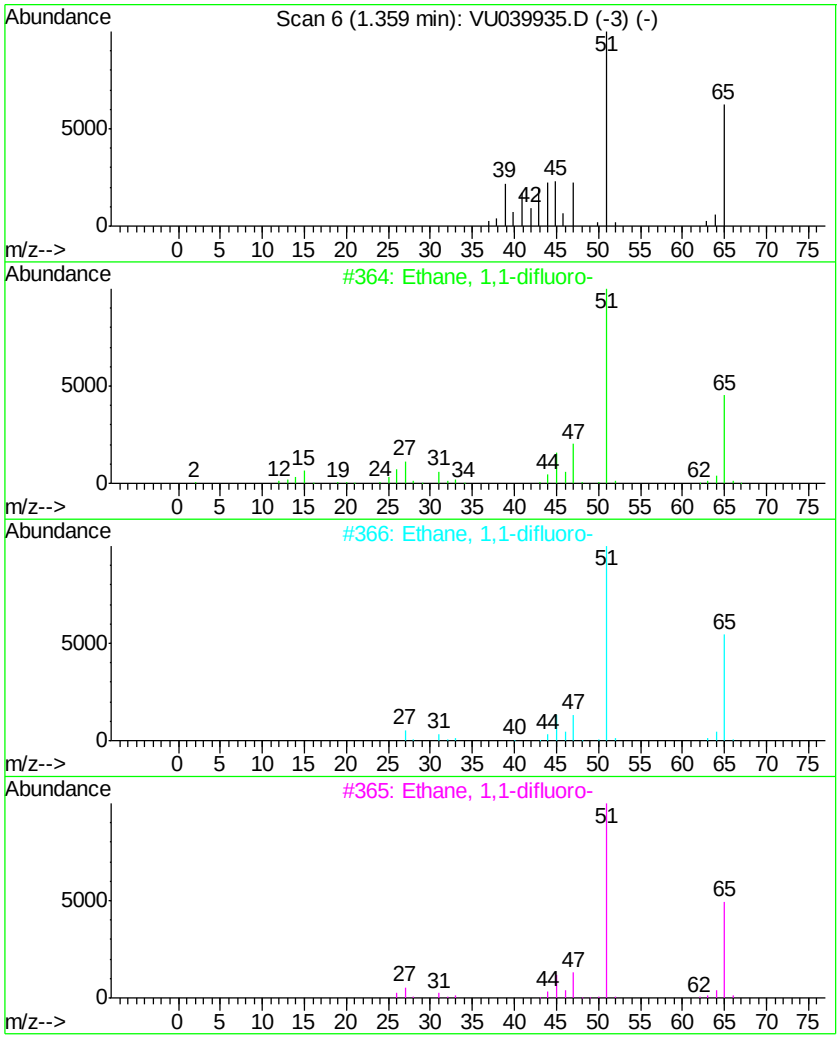
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

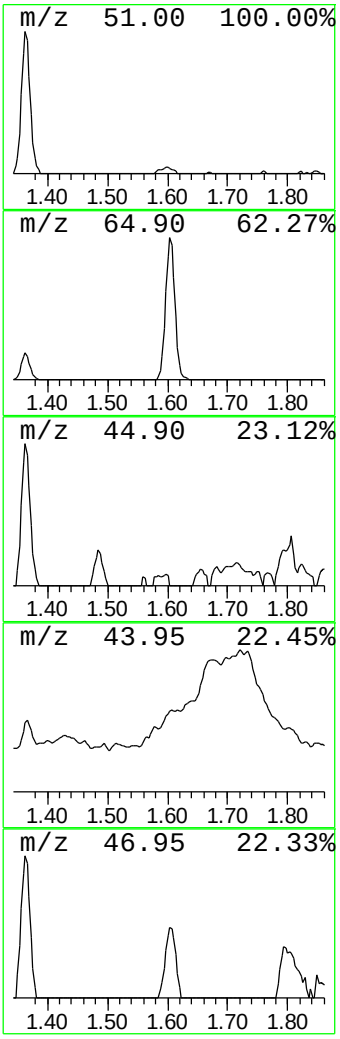
**********

Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.36 | 0.68 ug/L | 24605 | 1,4-Difluorobenzene | 6.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethane, 1,1-difluoro- | 66 | C2H4F2 | 000075-37-6 | 78 |
| 2 | Ethane, 1,1-difluoro- | 66 | C2H4F2 | 000075-37-6 | 64 |
| 3 | Ethane, 1,1-difluoro- | 66 | C2H4F2 | 000075-37-6 | 64 |
| 4 | Propiolonitrile | 51 | C3HN | 001070-71-9 | 4 |
| 5 | Propane, 2,2-difluoro- | 80 | C3H6F2 | 000420-45-1 | 1 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

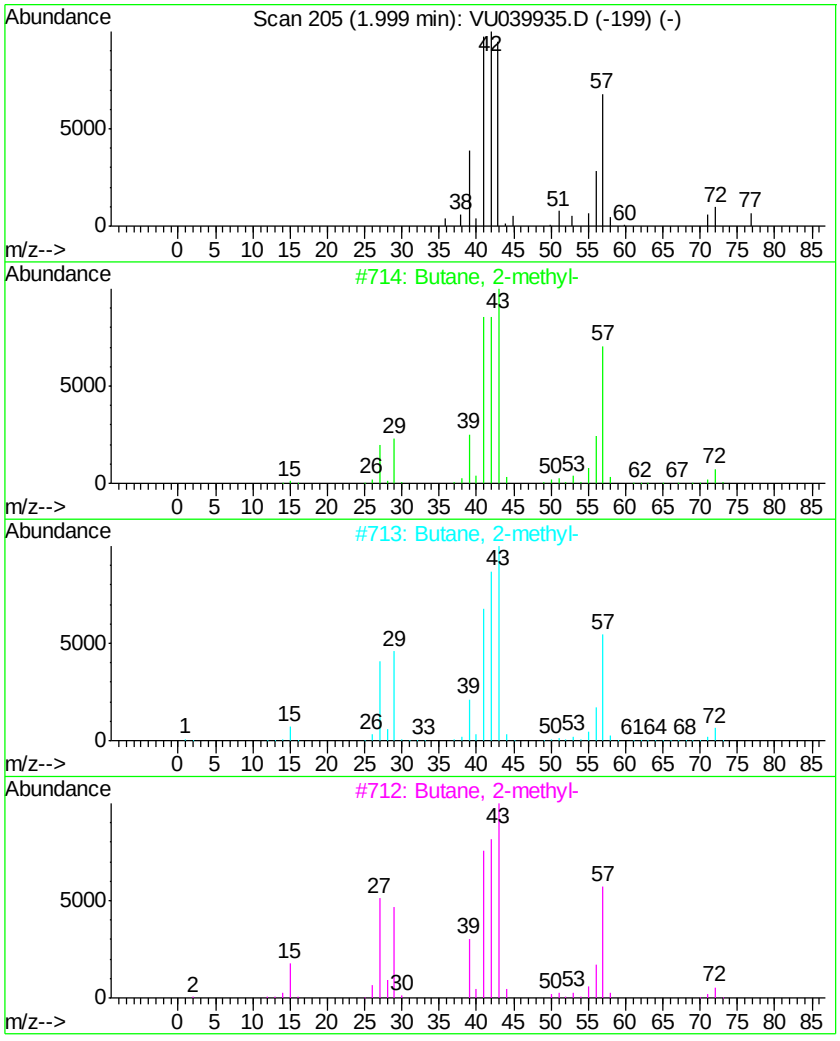
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

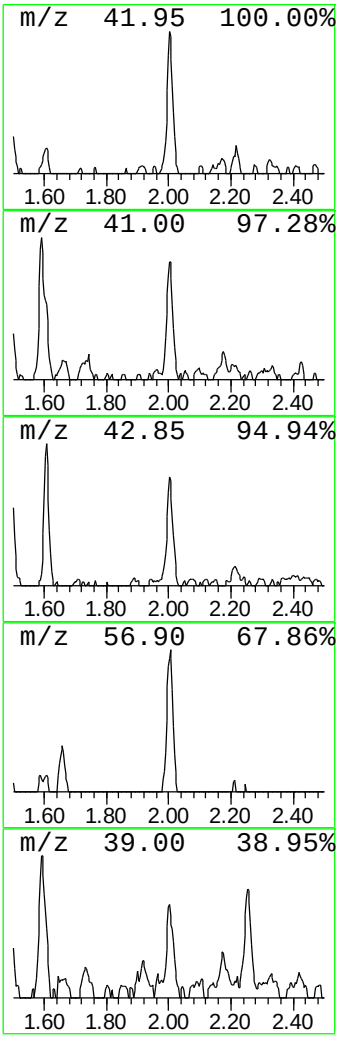
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.00 | 0.54 ug/L | 19430 | 1,4-Difluorobenzene | 6.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methyl- | 72 | C5H12 | 000078-78-4 | 80 |
| 2 | Butane, 2-methyl- | 72 | C5H12 | 000078-78-4 | 59 |
| 3 | Butane, 2-methyl- | 72 | C5H12 | 000078-78-4 | 50 |
| 4 | 1-Butene | 56 | C4H8 | 000106-98-9 | 9 |
| 5 | 3-Buten-1-ol | 72 | C4H8O | 000627-27-0 | 9 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

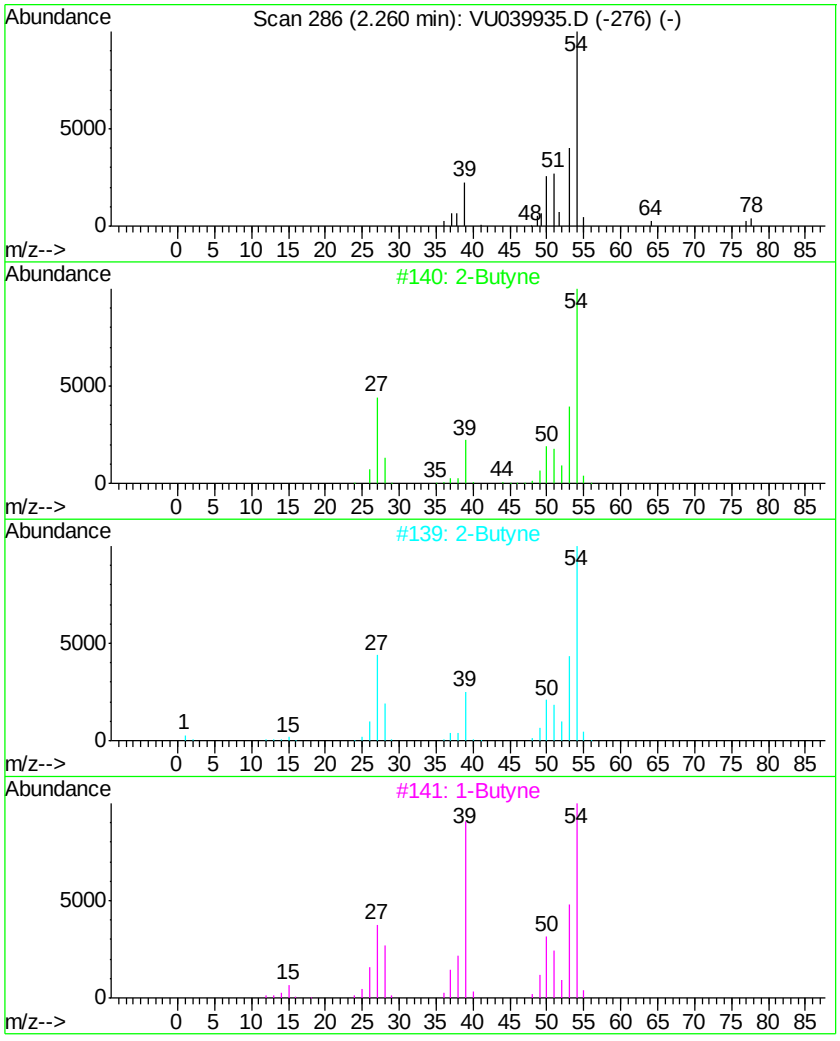
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

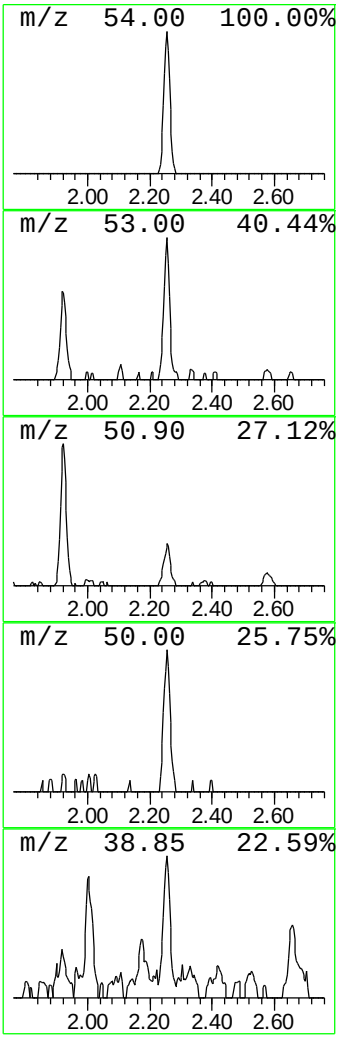
**********

Peak Number 3 2-Butyne Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.26 | 0.53 ug/L | 19221 | 1,4-Difluorobenzene | 6.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Butyne | 54 | C4H6 | 000503-17-3 | 86 |
| 2 | 2-Butyne | 54 | C4H6 | 000503-17-3 | 86 |
| 3 | 1-Butyne | 54 | C4H6 | 000107-00-6 | 78 |
| 4 | 2-Butyne | 54 | C4H6 | 000503-17-3 | 78 |
| 5 | 1,2-Butadiene | 54 | C4H6 | 000590-19-2 | 78 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

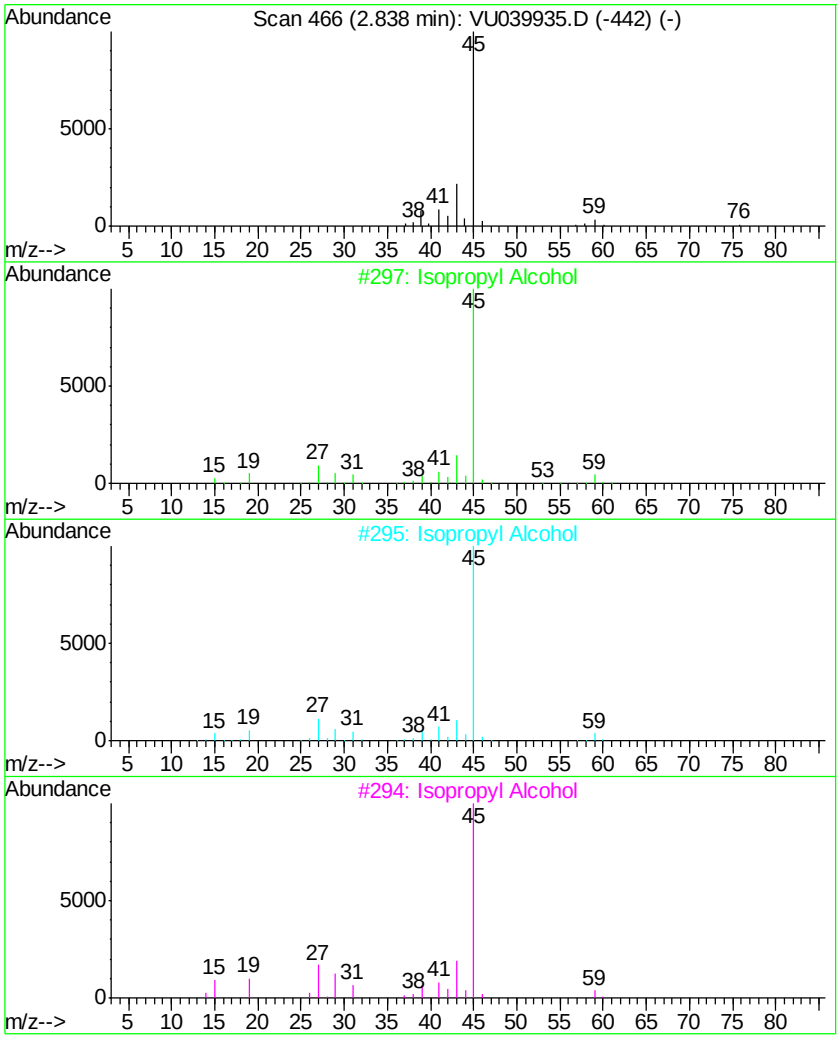
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

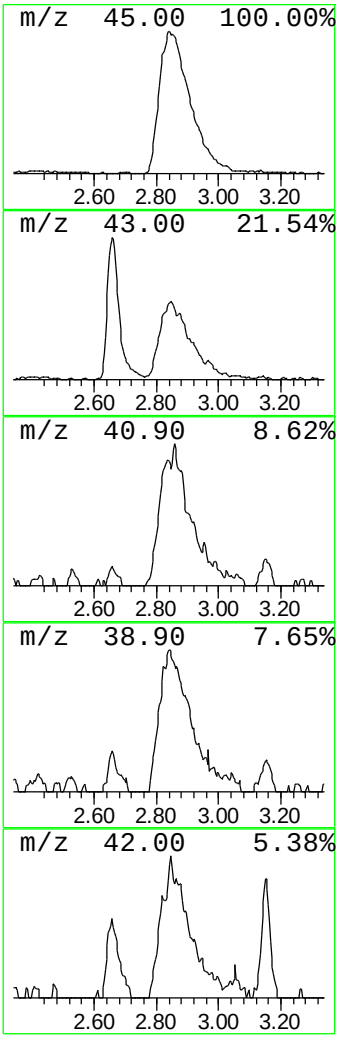
**********

Peak Number 4 Isopropyl Alcohol Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.84 | 10.05 ug/L | 363577 | 1,4-Difluorobenzene | 6.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Isopropyl Alcohol | 60 | C3H8O | 000067-63-0 | 86 |
| 2 | Isopropyl Alcohol | 60 | C3H8O | 000067-63-0 | 86 |
| 3 | Isopropyl Alcohol | 60 | C3H8O | 000067-63-0 | 78 |
| 4 | Isopropyl Alcohol | 60 | C3H8O | 000067-63-0 | 72 |
| 5 | Propane, 2-ethoxy- | 88 | C5H12O | 000625-54-7 | 40 |



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

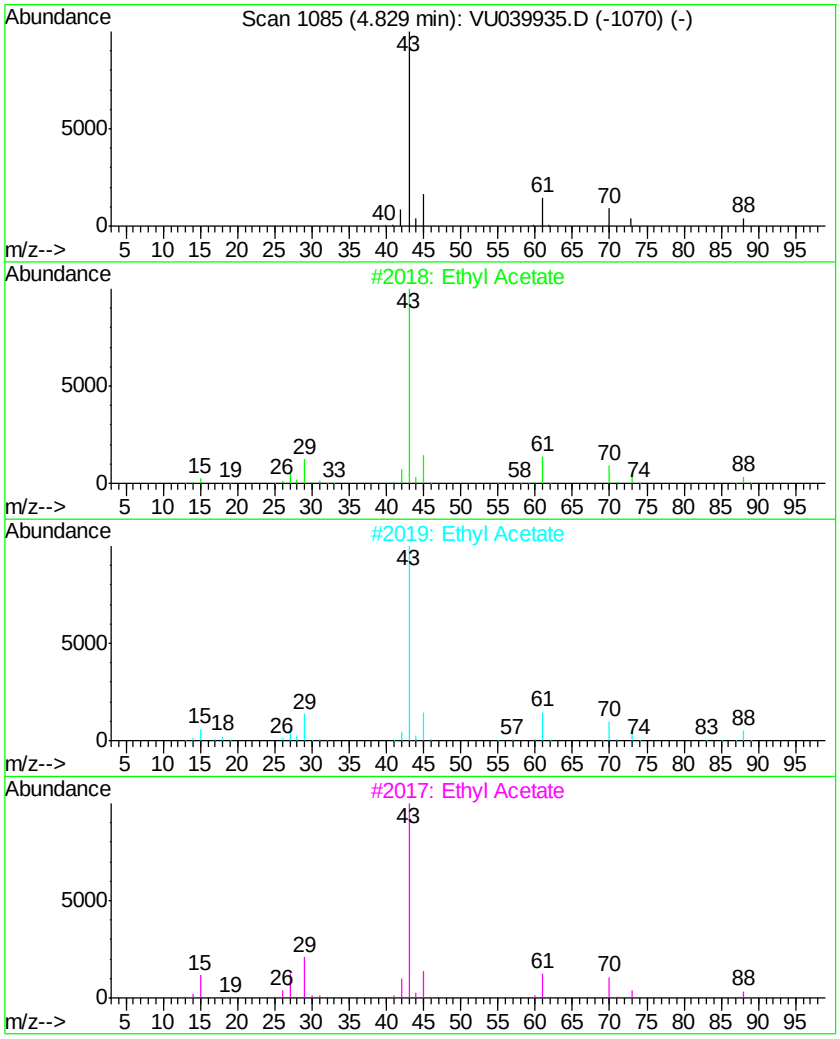
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

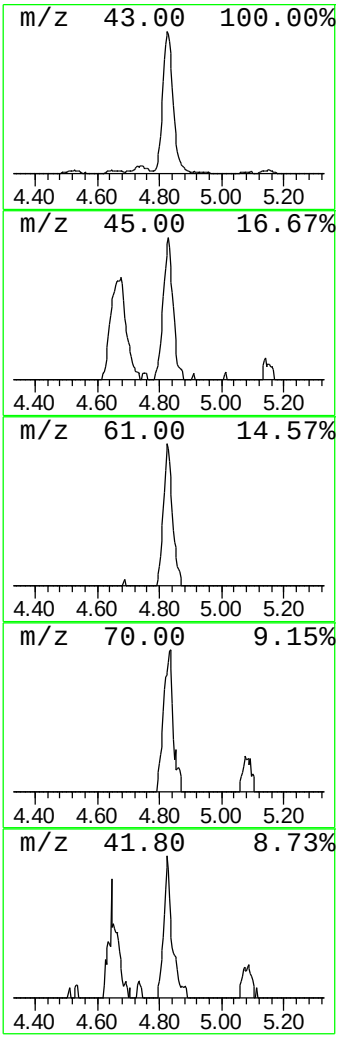
**********

Peak Number 5 Ethyl Acetate Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.83 | 1.51 ug/L | 54528 | 1,4-Difluorobenzene | 6.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethyl Acetate | 88 | C4H8O2 | 000141-78-6 | 90 |
| 2 | Ethyl Acetate | 88 | C4H8O2 | 000141-78-6 | 78 |
| 3 | Ethyl Acetate | 88 | C4H8O2 | 000141-78-6 | 64 |
| 4 | Ethyl Acetate | 88 | C4H8O2 | 000141-78-6 | 42 |
| 5 | CH3C(O)CH2CH2OH | 88 | C4H8O2 | 000590-90-9 | 38 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

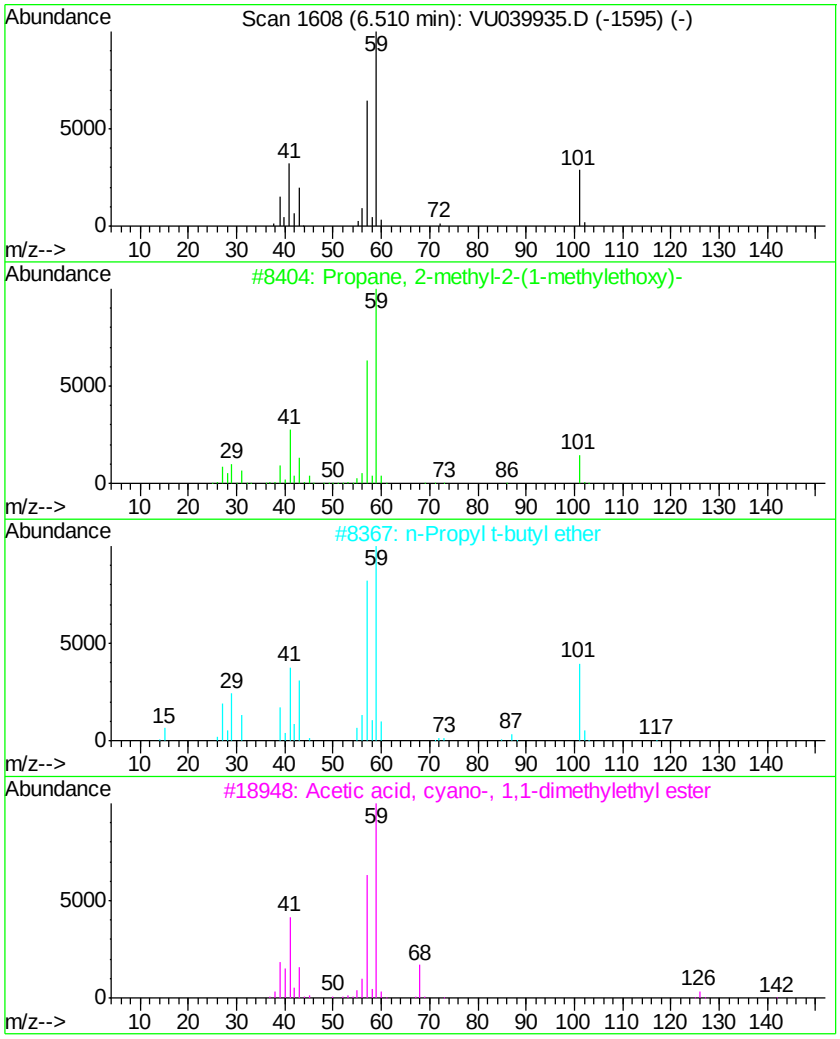
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

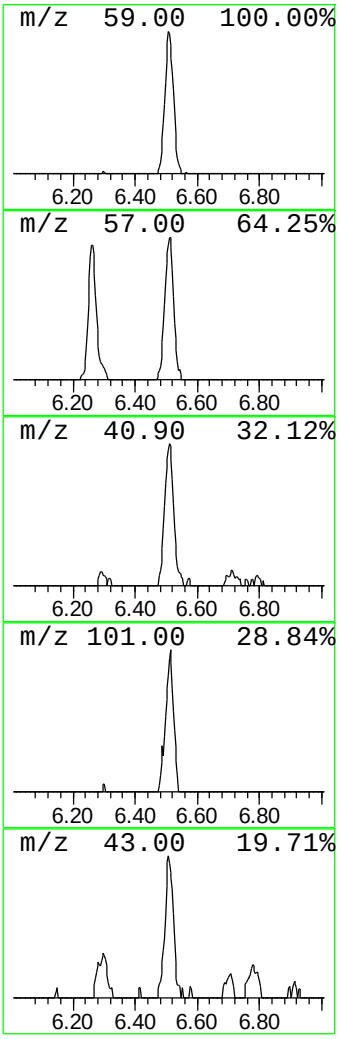
**********

Peak Number 6 Propane, 2-methyl-2-(1-meth... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.51 | 1.31 ug/L | 47292 | 1,4-Difluorobenzene | 6.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 83 |
| 2 | n-Propyl t-butyl ether | 116 | C7H16O | 1000334-81-9 | 64 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 50 |
| 4 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 36 |
| 5 | 1-Methyl-3-pyrrolidinol | 101 | C5H11NO | 013220-33-2 | 9 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

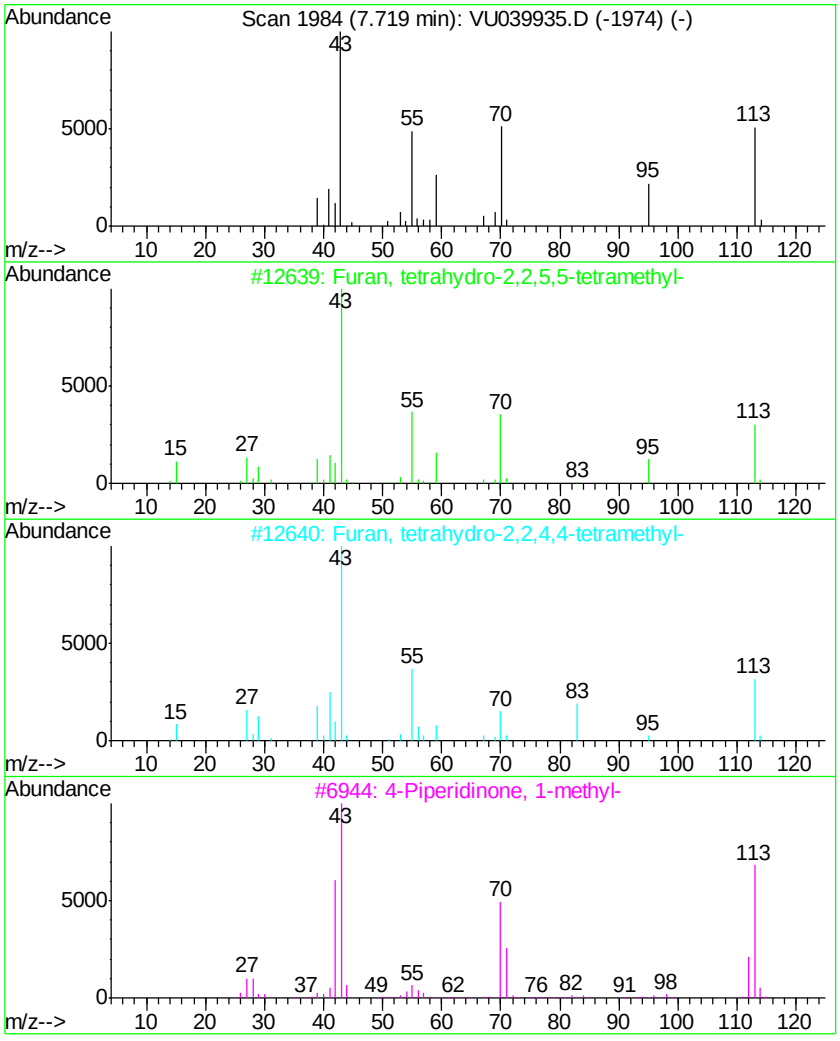
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

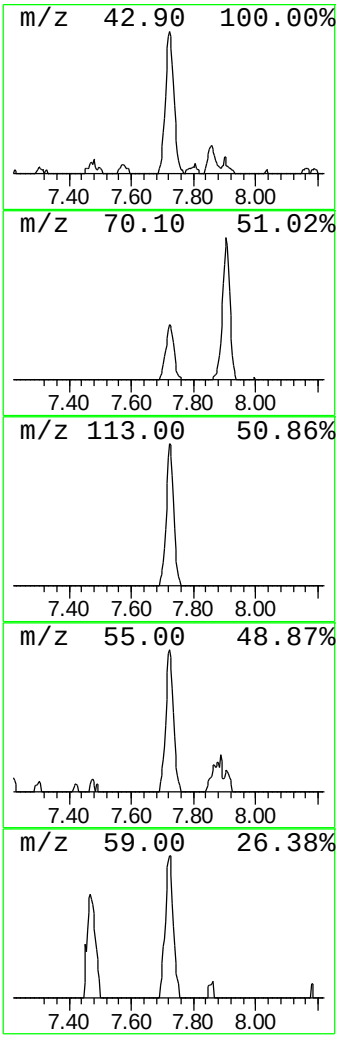
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 8 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.72 | 0.95 ug/L | 34245 | 1,4-Difluorobenzene | 6.26 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Furan, tetrahydro-2,2,5,5-tetram... | 128 | C8H16O | 015045-43-9 | 53 |
| 2 | Furan, tetrahydro-2,2,4,4-tetram... | 128 | C8H16O | 003358-28-9 | 53 |
| 3 | 4-Piperidinone, 1-methyl- | 113 | C6H11NO | 001445-73-4 | 50 |
| 4 | 1,3,5-Triazine-2,4(1H,3H)-dione | 113 | C3H3N3O2 | 000071-33-0 | 47 |
| 5 | Piperazine, 1-[(2,4-dichlorobenz... | 286 | C13H16Cl2N2O | 1000137-95-1 | 43 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

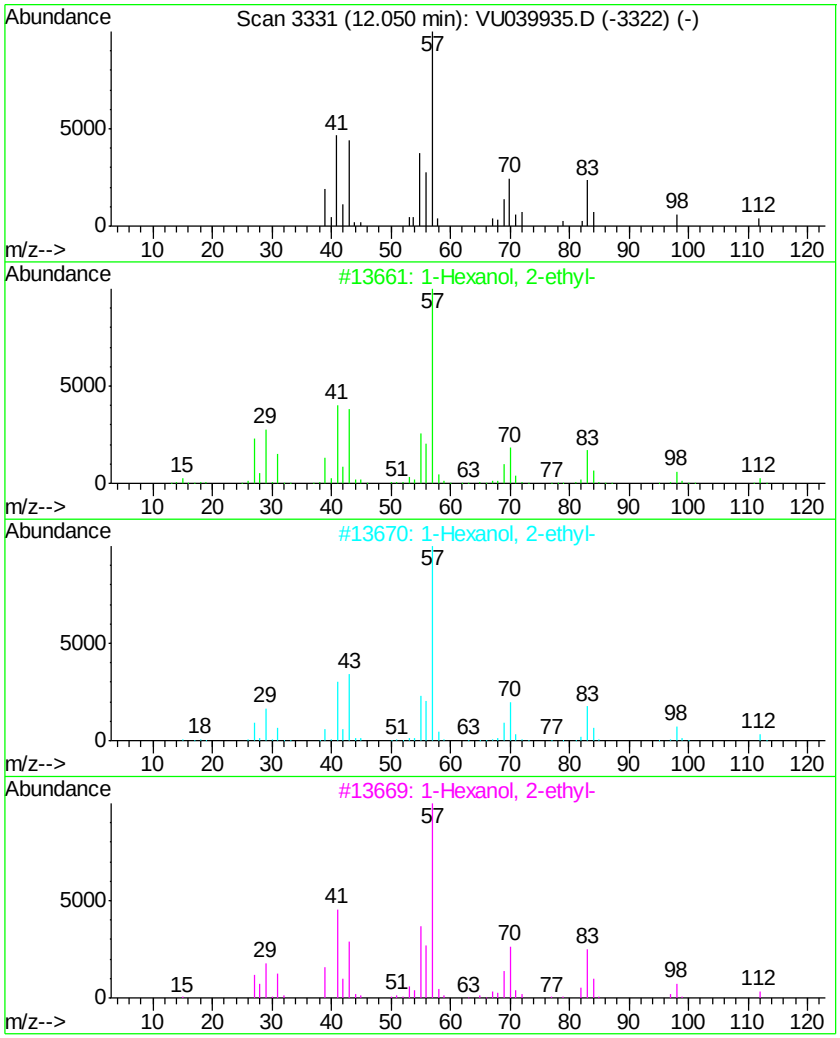
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

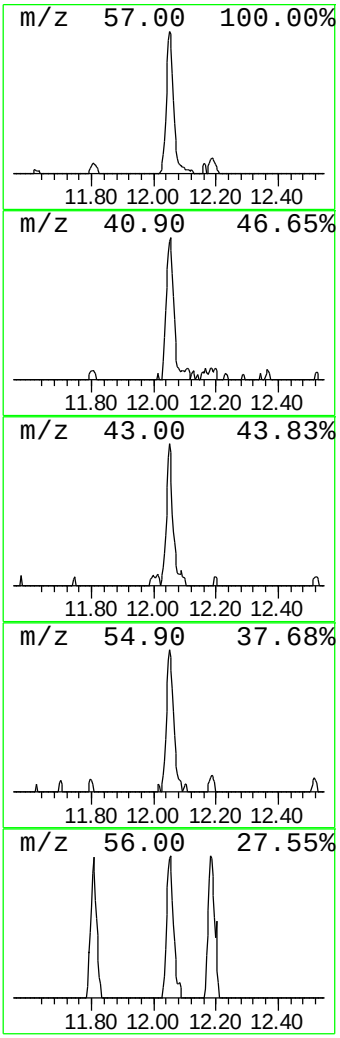
**********

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.05 | 0.79 ug/L | 35666 | 1,4-Dichlorobenzene-d4 | 11.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 64 |
| 2 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 64 |
| 3 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 64 |
| 4 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 59 |
| 5 | 2-Propyl-1-pentanol | 130 | C8H18O | 058175-57-8 | 59 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082120\
Data File : VU039935.D
Acq On : 21 Aug 2020 18:02
Operator : SY/MD
Sample : L3776-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F4Y11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Ethane, 1,1-diflu... | 1.36 | 0.7 | ug/L | 24605 | 1 | 6.26 | 180833 | 5.0 |
| (DEL) Alkane: Str... | 2.00 | 0.5 | ug/L | 19430 | 1 | 6.26 | 180833 | 5.0 |
| 2-Butyne | 2.26 | 0.5 | ug/L | 19221 | 1 | 6.26 | 180833 | 5.0 |
| Isopropyl Alcohol | 2.84 | 10.1 | ug/L | 363577 | 1 | 6.26 | 180833 | 5.0 |
| Ethyl Acetate | 4.83 | 1.5 | ug/L | 54528 | 1 | 6.26 | 180833 | 5.0 |
| Propane, 2-methyl... | 6.51 | 1.3 | ug/L | 47292 | 1 | 6.26 | 180833 | 5.0 |
| Furan, tetrahydro... | 7.72 | 0.9 | ug/L | 34245 | 1 | 6.26 | 180833 | 5.0 |
| 1-Hexanol, 2-ethyl- | 12.05 | 0.8 | ug/L | 35666 | 3 | 11.81 | 226515 | 5.0 |