LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050421\
Data File : VU043517.D
Acq On : 04 May 2021 13:48
Operator : SY/MD
Sample : M2195-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** GB3H9

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\SFAMUTR050321WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU043517.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.362 | 3 | 7 | 22 | rVB | 42016 | 43194 | 3.81% | 0.724% |
| 2 | 1.491 | 40 | 47 | 62 | rVB2 | 34207 | 40712 | 3.59% | 0.683% |
| 3 | 1.604 | 72 | 82 | 92 | rBV2 | 76471 | 91080 | 8.03% | 1.527% |
| 4 | 1.916 | 171 | 179 | 191 | rVB | 39552 | 52158 | 4.60% | 0.875% |
| 5 | 1.999 | 196 | 205 | 215 | rBV | 23108 | 32165 | 2.84% | 0.539% |
| 6 | 2.208 | 262 | 270 | 282 | rVB | 13574 | 20411 | 1.80% | 0.342% |
| 7 | 2.571 | 371 | 383 | 396 | rBV | 84131 | 137579 | 12.13% | 2.307% |
| 8 | 2.645 | 396 | 406 | 416 | rVV | 10997 | 20425 | 1.80% | 0.342% |
| 9 | 2.803 | 440 | 455 | 478 | rBV3 | 7851 | 20844 | 1.84% | 0.350% |
| 10 | 3.054 | 520 | 533 | 554 | rBV2 | 17349 | 40621 | 3.58% | 0.681% |
| 11 | 3.195 | 566 | 577 | 595 | rVB2 | 10063 | 22774 | 2.01% | 0.382% |
| 12 | 4.639 | 1008 | 1026 | 1066 | rBV2 | 94555 | 262246 | 23.13% | 4.397% |
| 13 | 4.816 | 1066 | 1081 | 1107 | rVV | 105034 | 238605 | 21.04% | 4.001% |
| 14 | 5.099 | 1146 | 1169 | 1195 | rBV2 | 463773 | 1133813 | 100.00% | 19.011% |
| 15 | 5.735 | 1345 | 1367 | 1394 | rBV2 | 151480 | 410077 | 36.17% | 6.876% |
| 16 | 6.259 | 1513 | 1530 | 1549 | rBV | 127887 | 238012 | 20.99% | 3.991% |
| 17 | 6.549 | 1611 | 1620 | 1630 | rBV5 | 8318 | 14614 | 1.29% | 0.245% |
| 18 | 6.700 | 1652 | 1667 | 1680 | rBV | 101271 | 193231 | 17.04% | 3.240% |
| 19 | 6.774 | 1680 | 1690 | 1700 | rVB6 | 7277 | 14074 | 1.24% | 0.236% |
| 20 | 7.574 | 1926 | 1939 | 1957 | rVB | 51492 | 90002 | 7.94% | 1.509% |
| 21 | 7.906 | 2021 | 2042 | 2055 | rBV | 172771 | 298565 | 26.33% | 5.006% |
| 22 | 7.976 | 2055 | 2064 | 2076 | rVB | 28124 | 46852 | 4.13% | 0.786% |
| 23 | 8.185 | 2119 | 2129 | 2143 | rBV | 32345 | 54170 | 4.78% | 0.908% |
| 24 | 8.562 | 2233 | 2246 | 2259 | rBV | 563075 | 942244 | 83.10% | 15.799% |
| 25 | 8.642 | 2259 | 2271 | 2300 | rVB | 261107 | 491249 | 43.33% | 8.237% |
| 26 | 8.925 | 2349 | 2359 | 2370 | rBV2 | 8387 | 14134 | 1.25% | 0.237% |
| 27 | 9.423 | 2502 | 2514 | 2536 | rBV | 185467 | 307993 | 27.16% | 5.164% |
| 28 | 9.578 | 2552 | 2562 | 2573 | rVB2 | 9623 | 14570 | 1.29% | 0.244% |
| 29 | 9.700 | 2589 | 2600 | 2611 | rBV | 11461 | 17362 | 1.53% | 0.291% |
| 30 | 10.764 | 2919 | 2931 | 2948 | rVB | 72952 | 116693 | 10.29% | 1.957% |
| 31 | 11.819 | 3247 | 3259 | 3274 | rBV | 176609 | 276647 | 24.40% | 4.639% |
| 32 | 12.201 | 3366 | 3378 | 3392 | rBV | 165789 | 266777 | 23.53% | 4.473% |

Sum of corrected areas: 5963893

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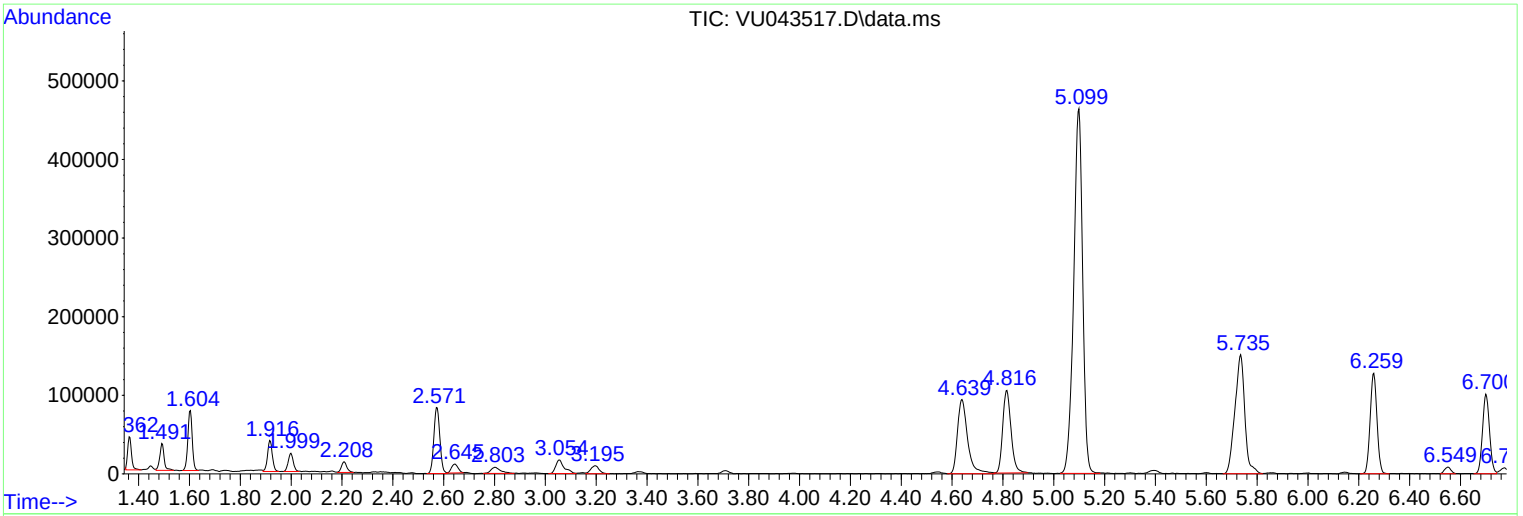
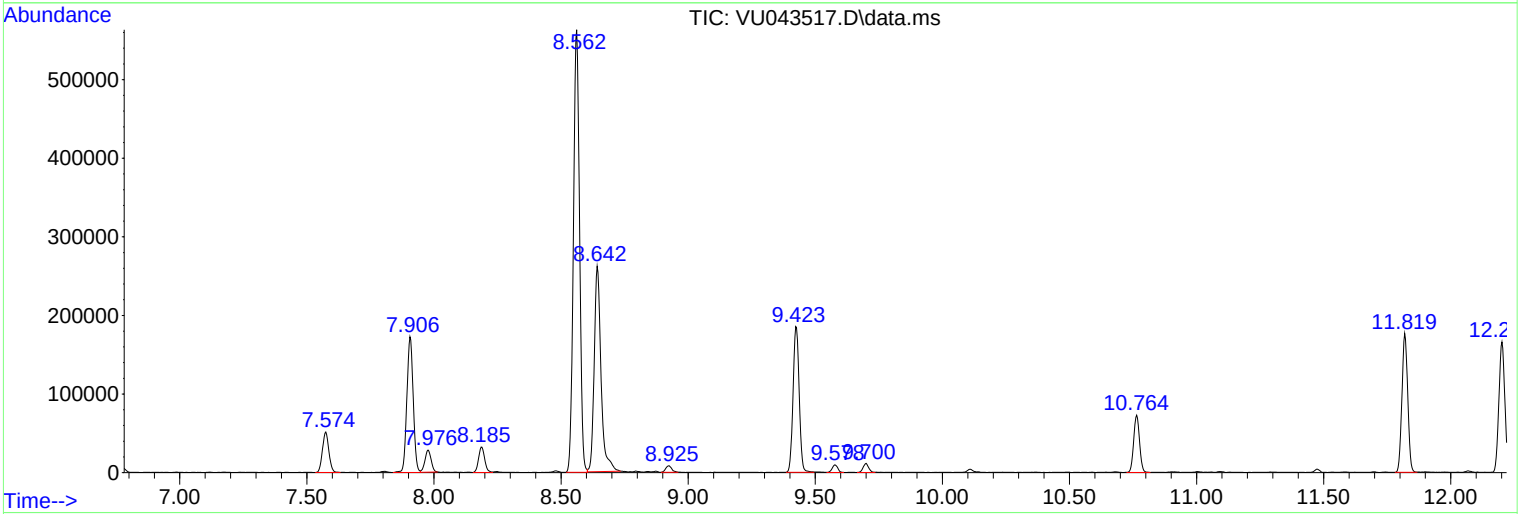
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

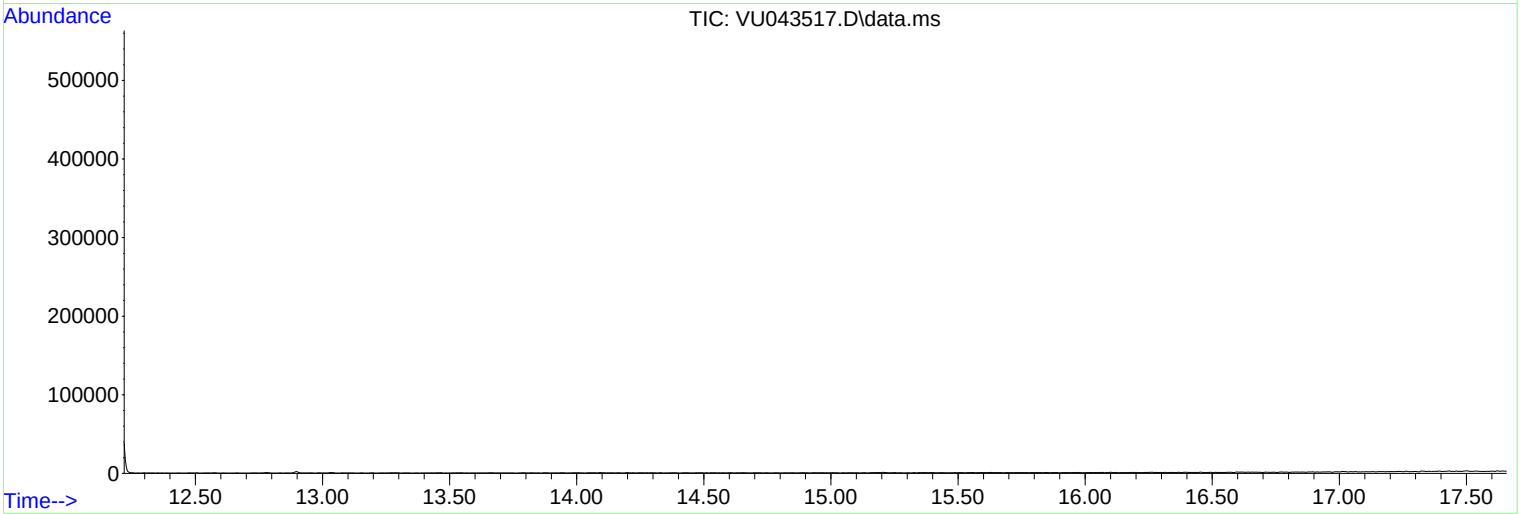
**Instrument :**
MSVOA_U
**ClientSampleId :**
GB3H9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR050321WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Data File : VU043517.D
Acq On : 04 May 2021 13:48
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** GB3H9

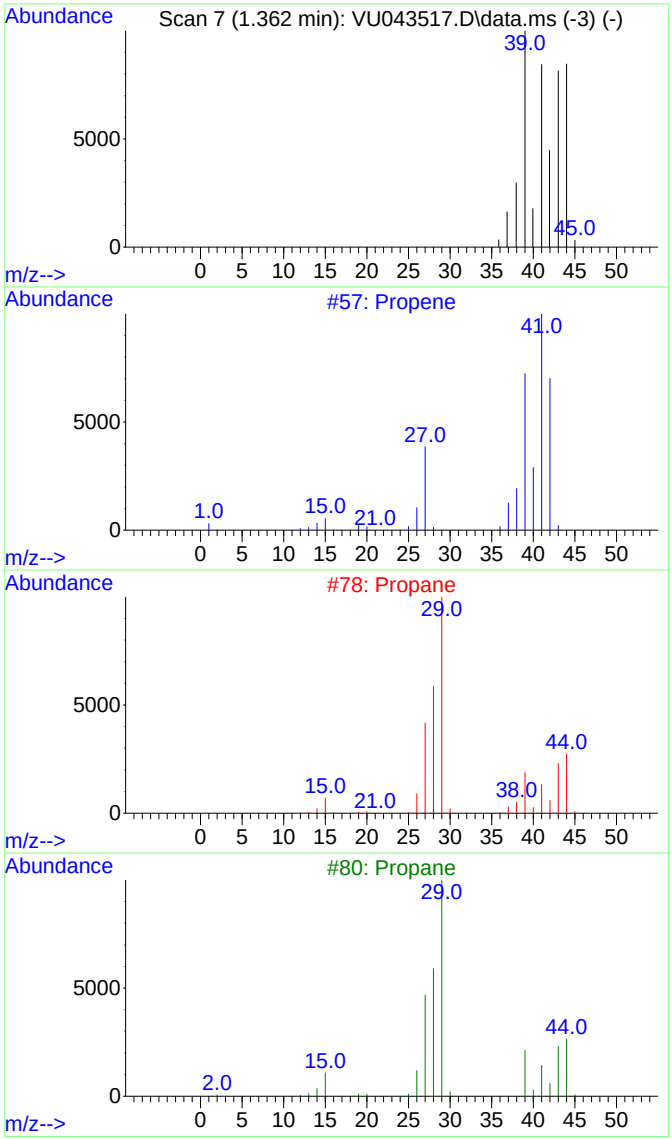
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR050321WMA.M
Quant Title : TRACE VOA SFAM1.0

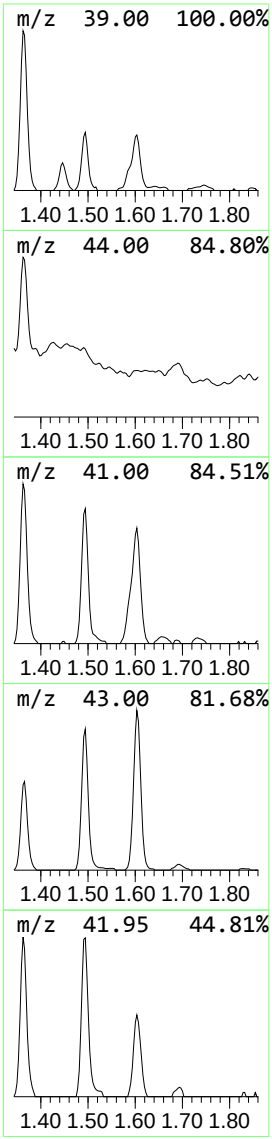
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.362 | 0.91 ug/L | 43194 | 1,4-Difluorobenzene | 6.259 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propene | 42 | C3H6 | 000115-07-1 | 9 |
| 2 | Propane | 44 | C3H8 | 000074-98-6 | 4 |
| 3 | Propane | 44 | C3H8 | 000074-98-6 | 4 |
| 4 | Propane | 44 | C3H8 | 000074-98-6 | 4 |
| 5 | Cyclopropene | 40 | C3H4 | 002781-85-3 | 4 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050421\
Data File : VU043517.D
Acq On : 04 May 2021 13:48
Operator : SY/MD
Sample : M2195-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** GB3H9

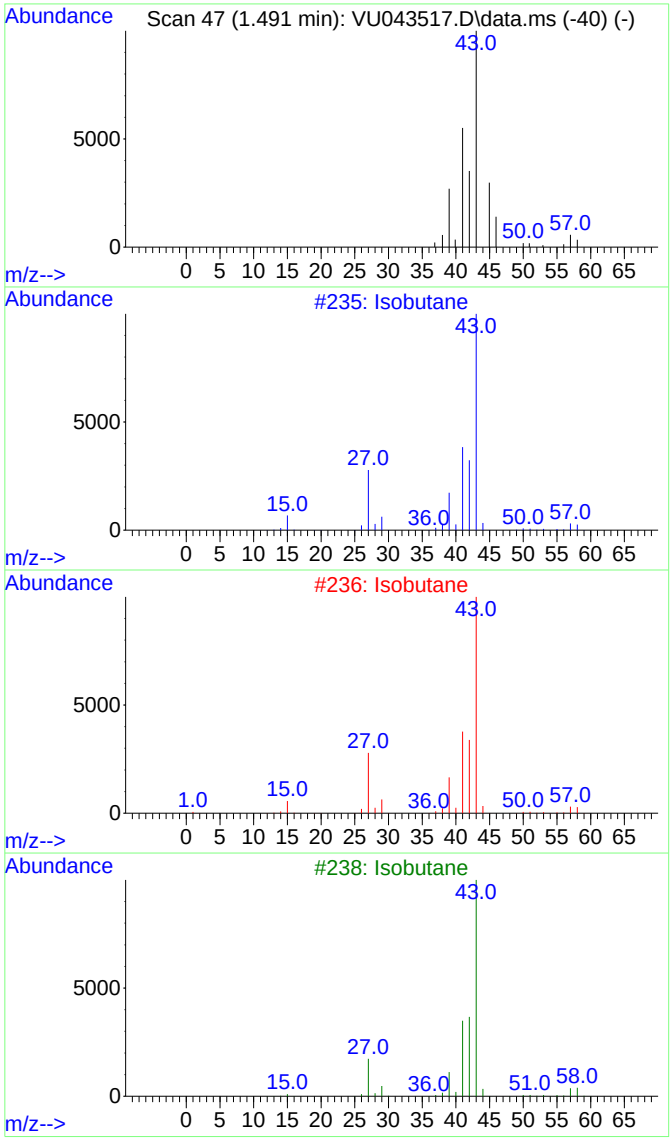
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR050321WMA.M
Quant Title : TRACE VOA SFAM1.0

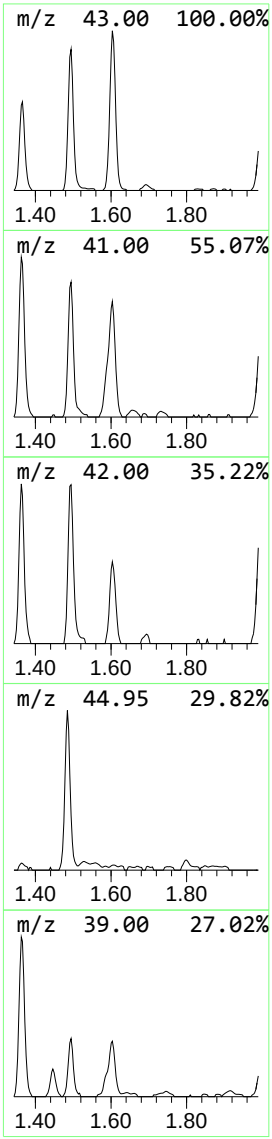
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.491 | 0.86 ug/L | 40712 | 1,4-Difluorobenzene | 6.259 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Isobutane | 58 | C4H10 | 000075-28-5 | 37 |
| 2 | Isobutane | 58 | C4H10 | 000075-28-5 | 37 |
| 3 | Isobutane | 58 | C4H10 | 000075-28-5 | 32 |
| 4 | Isobutane | 58 | C4H10 | 000075-28-5 | 32 |
| 5 | Propane, 1-chloro-2-methyl- | 92 | C4H9Cl | 000513-36-0 | 9 |



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Data File : VU043517.D
Acq On : 04 May 2021 13:48
Operator : SY/MD
Sample : M2195-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** GB3H9

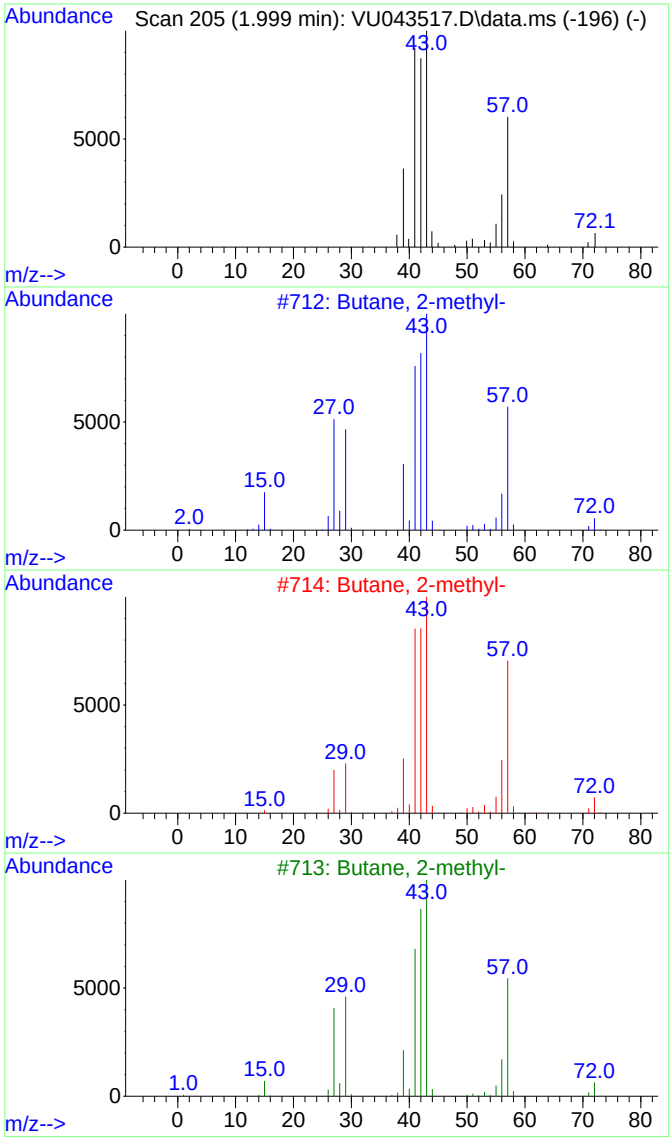
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR050321WMA.M
Quant Title : TRACE VOA SFAM1.0

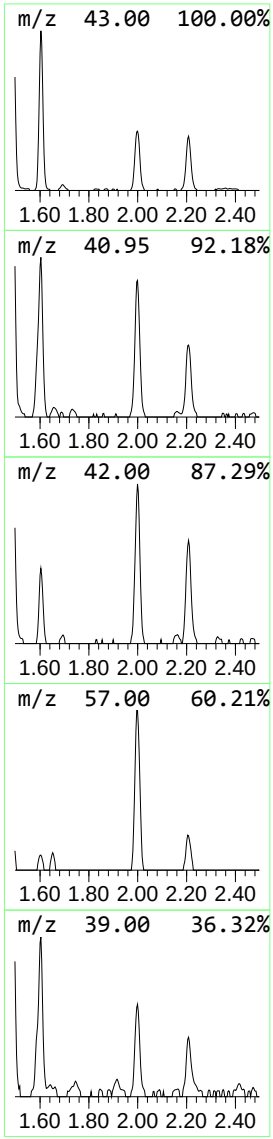
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.999 | 0.68 ug/L | 32165 | 1,4-Difluorobenzene | 6.259 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methyl- | 72 | C5H12 | 000078-78-4 | 91 |
| 2 | Butane, 2-methyl- | 72 | C5H12 | 000078-78-4 | 87 |
| 3 | Butane, 2-methyl- | 72 | C5H12 | 000078-78-4 | 86 |
| 4 | 3-Buten-1-ol | 72 | C4H8O | 000627-27-0 | 43 |
| 5 | 3-Buten-1-ol | 72 | C4H8O | 000627-27-0 | 37 |



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Acq On : 04 May 2021 13:48
Operator : SY/MD
Sample : M2195-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** GB3H9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR050321WMA.M
Quant Title : TRACE VOA SFAM1.0

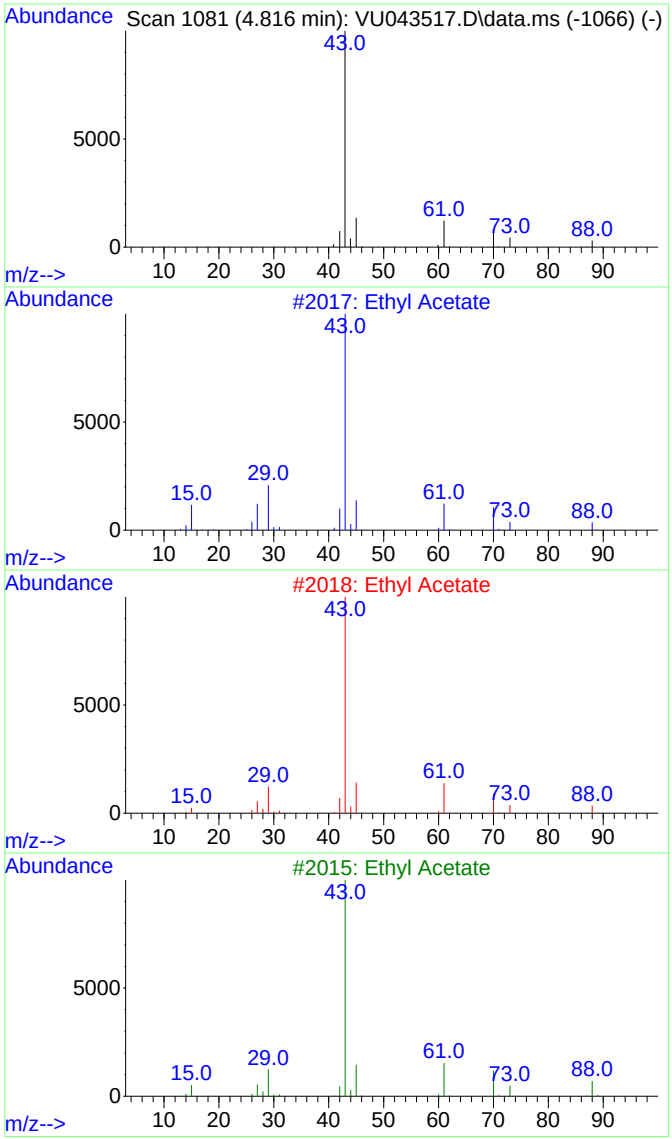
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

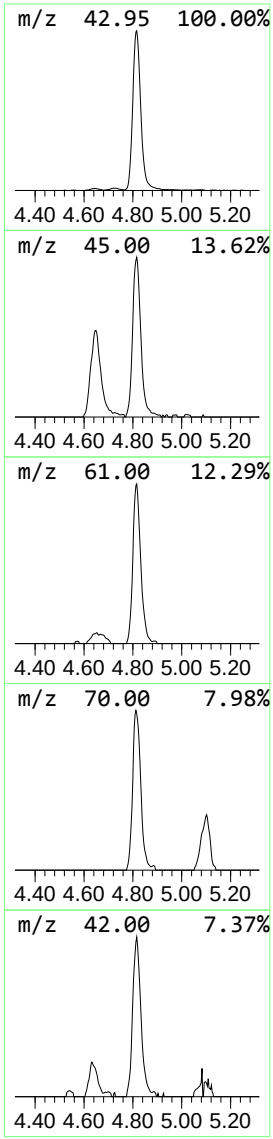
**********

Peak Number 4 Ethyl Acetate Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.816 | 5.01 ug/L | 238605 | 1,4-Difluorobenzene | 6.259 |

| 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 | 90 |
| 3 | Ethyl Acetate | 88 | C4H8O2 | 000141-78-6 | 64 |
| 4 | Ethyl Acetate | 88 | C4H8O2 | 000141-78-6 | 64 |
| 5 | (3-Methyl-oxiran-2-yl)-methanol | 88 | C4H8O2 | 1000194-22-9 | 9 |



Tentatively Identified Compound (LSC) summary

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ALS Vial : 13 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** GB3H9

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Quant Title : TRACE VOA SFAM1.0

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| (DEL) Alkane: S... | 1.362 | 0.9 | ug/L | 43194 | 1 | 6.259 | 238012 | 5.0 |
| (DEL) Alkane: S... | 1.491 | 0.9 | ug/L | 40712 | 1 | 6.259 | 238012 | 5.0 |
| (DEL) Alkane: S... | 1.999 | 0.7 | ug/L | 32165 | 1 | 6.259 | 238012 | 5.0 |
| Ethyl Acetate | 4.816 | 5.0 | ug/L | 238605 | 1 | 6.259 | 238012 | 5.0 |