LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110222\
Data File : VU051711.D
Acq On : 03 Nov 2022 00:09
Operator : JC/MD
Sample : N5301-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
DBWM4

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\SFAMUTR102822WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU051711.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.469 | 30 | 40 | 53 | rBV | 244997 | 438113 | 38.07% | 4.418% |
| 2 | 1.598 | 74 | 80 | 119 | rVB5 | 188692 | 350831 | 30.48% | 3.538% |
| 3 | 1.913 | 170 | 178 | 194 | rVB | 75938 | 102811 | 8.93% | 1.037% |
| 4 | 1.993 | 195 | 203 | 213 | rVB | 104779 | 141463 | 12.29% | 1.426% |
| 5 | 2.565 | 369 | 381 | 394 | rBV2 | 140353 | 241411 | 20.98% | 2.434% |
| 6 | 3.135 | 544 | 558 | 571 | rBV2 | 33922 | 71770 | 6.24% | 0.724% |
| 7 | 3.350 | 610 | 625 | 651 | rBV | 479989 | 958242 | 83.26% | 9.663% |
| 8 | 3.848 | 758 | 780 | 792 | rVB | 7831 | 27254 | 2.37% | 0.275% |
| 9 | 4.527 | 974 | 991 | 1008 | rBV6 | 8834 | 20999 | 1.82% | 0.212% |
| 10 | 4.620 | 1008 | 1020 | 1022 | rBV | 141873 | 195646 | 17.00% | 1.973% |
| 11 | 4.665 | 1024 | 1034 | 1059 | rVB | 468794 | 1109859 | 96.43% | 11.191% |
| 12 | 5.061 | 1142 | 1157 | 1181 | rBV | 140434 | 317637 | 27.60% | 3.203% |
| 13 | 5.382 | 1245 | 1257 | 1272 | rVB4 | 17784 | 41165 | 3.58% | 0.415% |
| 14 | 5.723 | 1343 | 1363 | 1391 | rBV3 | 258722 | 699384 | 60.77% | 7.052% |
| 15 | 6.247 | 1510 | 1526 | 1551 | rBV | 205376 | 400220 | 34.77% | 4.036% |
| 16 | 6.540 | 1603 | 1617 | 1645 | rBV | 606085 | 1150892 | 100.00% | 11.605% |
| 17 | 6.691 | 1650 | 1664 | 1682 | rVV | 171910 | 333051 | 28.94% | 3.358% |
| 18 | 7.565 | 1924 | 1936 | 1954 | rBV | 73948 | 131459 | 11.42% | 1.326% |
| 19 | 7.896 | 2026 | 2039 | 2060 | rBV | 275061 | 486317 | 42.26% | 4.904% |
| 20 | 8.179 | 2117 | 2127 | 2142 | rBV3 | 45731 | 79117 | 6.87% | 0.798% |
| 21 | 8.633 | 2251 | 2268 | 2299 | rBV | 427967 | 815113 | 70.82% | 8.219% |
| 22 | 9.417 | 2498 | 2512 | 2535 | rBV | 315181 | 538730 | 46.81% | 5.432% |
| 23 | 10.755 | 2915 | 2928 | 2949 | rBV | 156035 | 254947 | 22.15% | 2.571% |
| 24 | 11.809 | 3244 | 3256 | 3280 | rBV | 284158 | 477691 | 41.51% | 4.817% |
| 25 | 12.063 | 3325 | 3335 | 3349 | rBV3 | 30969 | 62036 | 5.39% | 0.626% |
| 26 | 12.192 | 3363 | 3375 | 3398 | rBV | 279440 | 470963 | 40.92% | 4.749% |

Sum of corrected areas: 9917121

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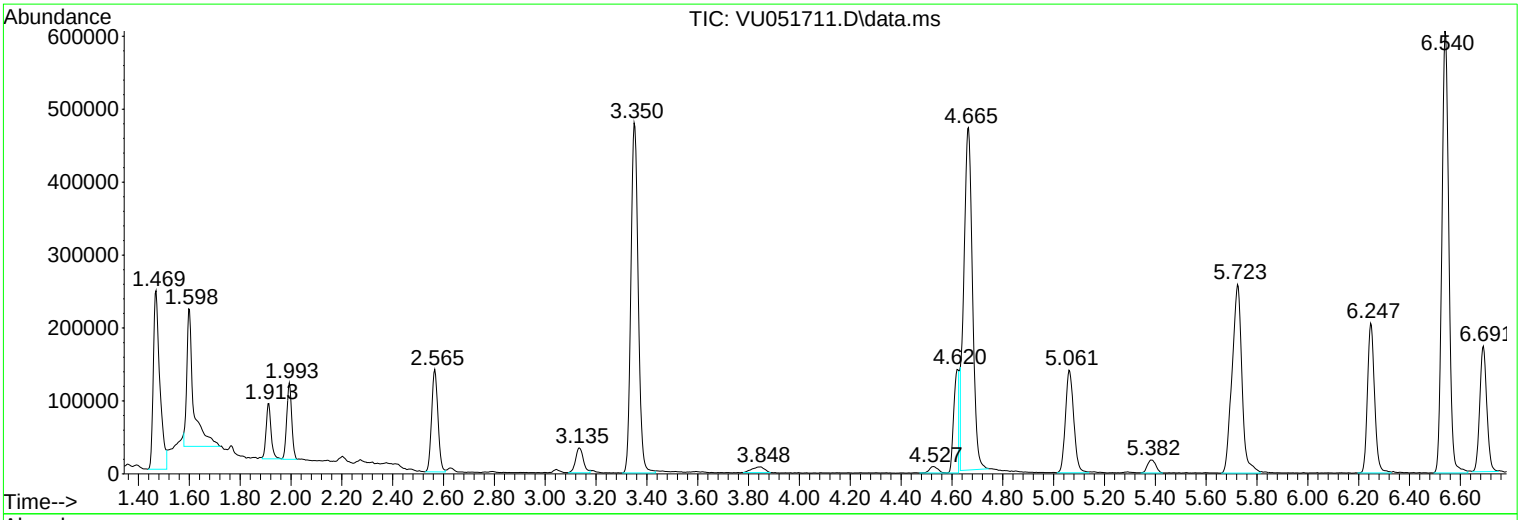
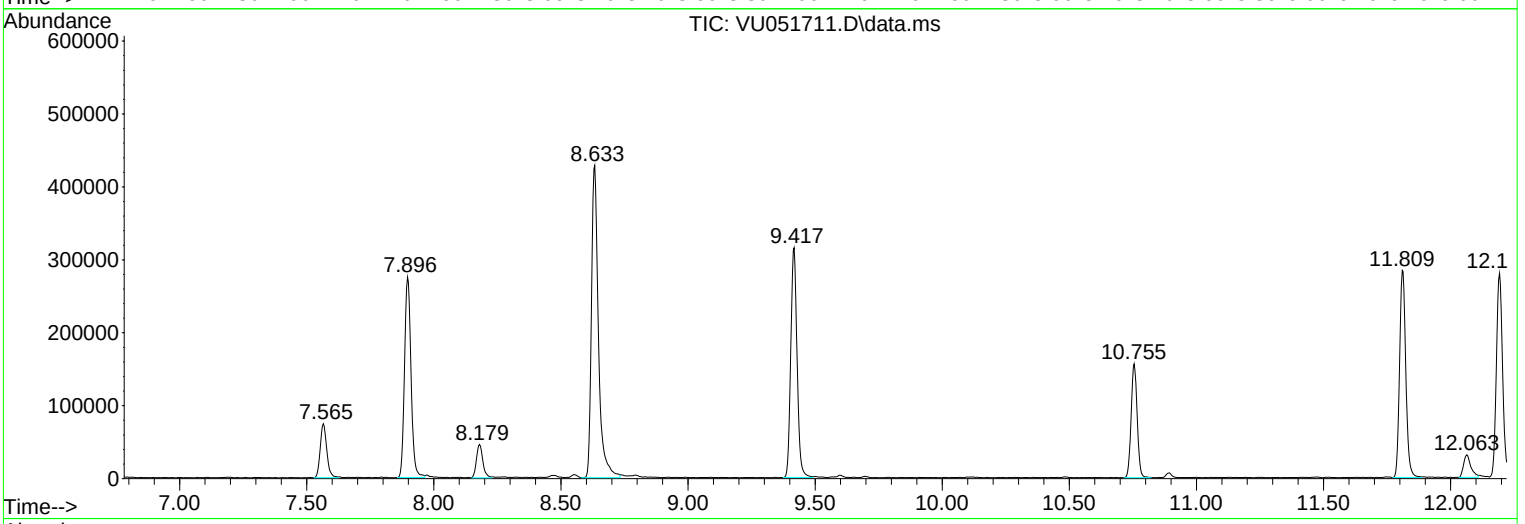
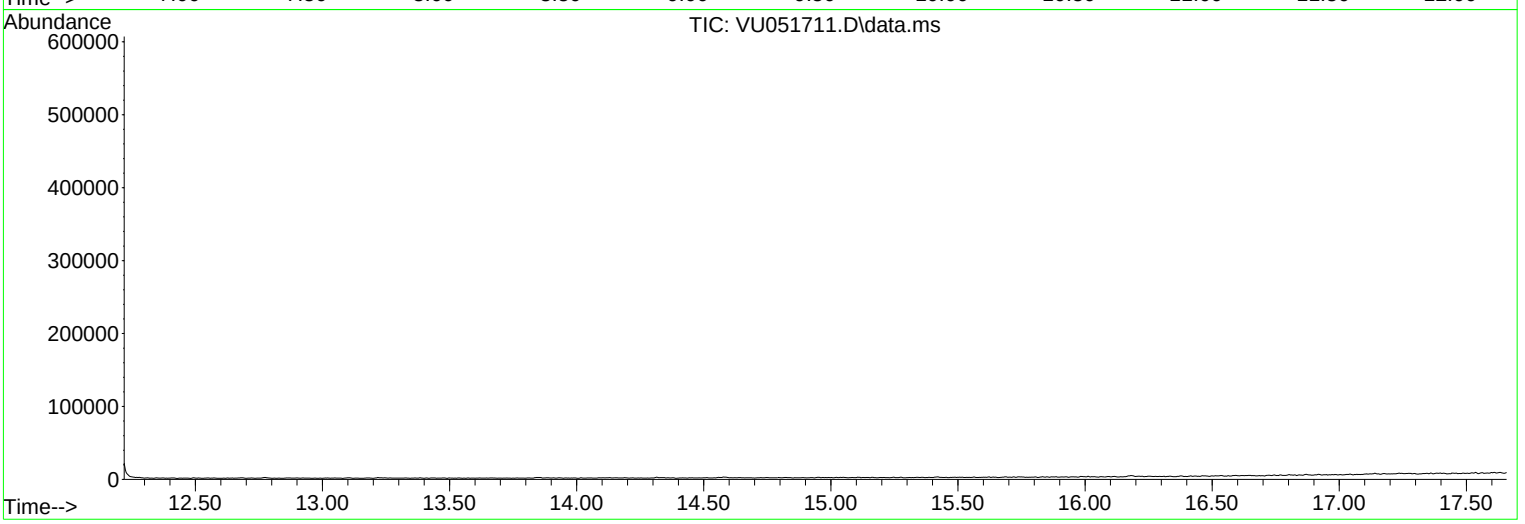
**Instrument :**
MSVOA_U
**ClientSampleId :**
DBWM4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Quant Title : TRACE VOA SFAM1.0

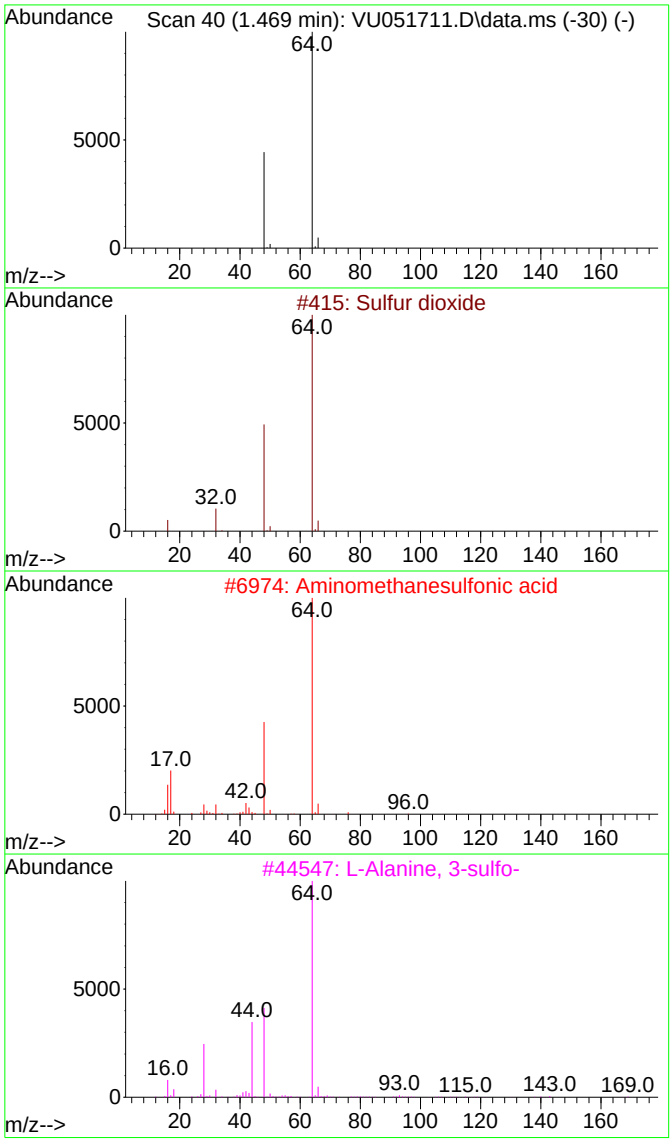
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

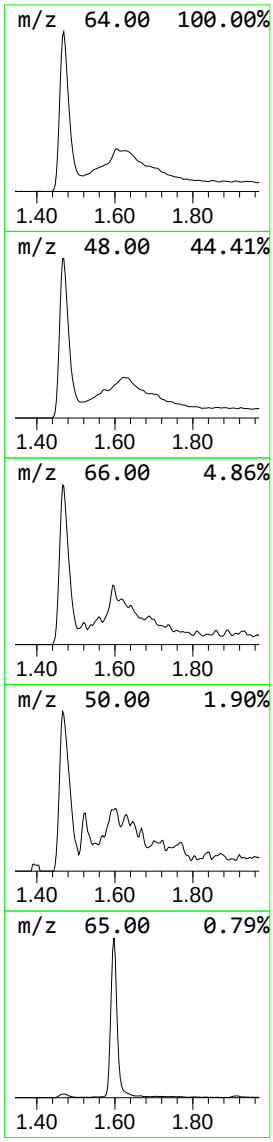
**********

Peak Number 1 Sulfur dioxide Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.469 | 5.47 ug/L | 438113 | 1,4-Difluorobenzene | 6.247 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 83 |
| 2 | Aminomethanesulfonic acid | 111 | CH5NO3S | 013881-91-9 | 74 |
| 3 | L-Alanine, 3-sulfo- | 169 | C3H7NO5S | 000498-40-8 | 9 |
| 4 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 4 |
| 5 | Ethene, 1,1-difluoro- | 64 | C2H2F2 | 000075-38-7 | 4 |



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Acq On : 03 Nov 2022 00:09
Operator : JC/MD
Sample : N5301-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
DBWM4

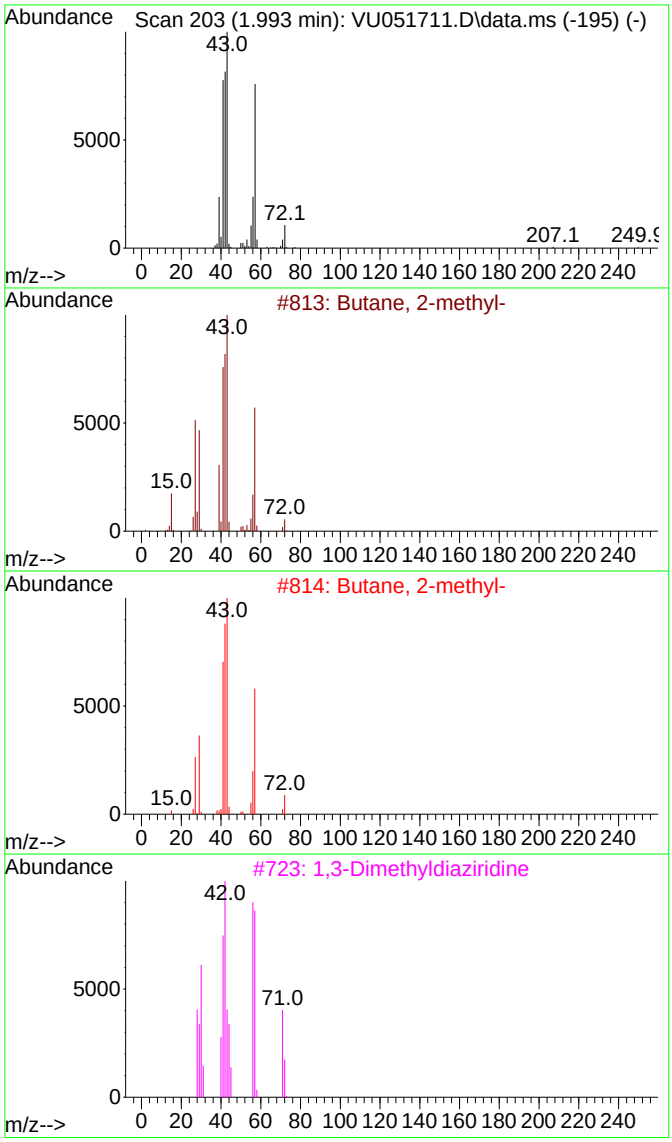
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

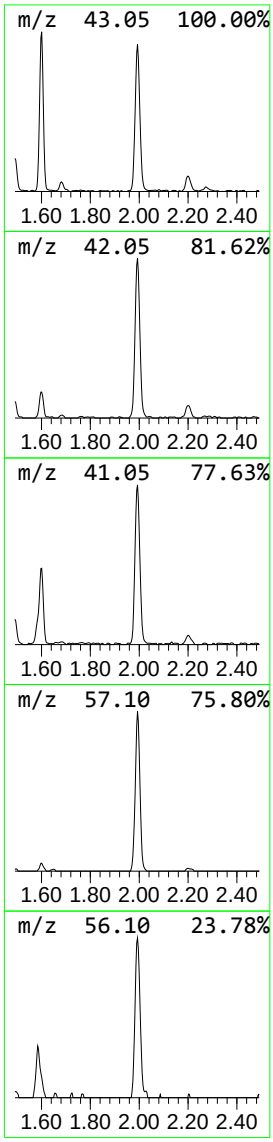
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.993 | 1.77 ug/L | 141463 | 1,4-Difluorobenzene | 6.247 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methyl- | 72 | C5H12 | 000078-78-4 | 90 |
| 2 | Butane, 2-methyl- | 72 | C5H12 | 000078-78-4 | 86 |
| 3 | 1,3-Dimethyldiaziridine | 72 | C3H8N2 | 026177-36-6 | 36 |
| 4 | Pentane | 72 | C5H12 | 000109-66-0 | 36 |
| 5 | 1,1-Diisobutoxy-butane | 202 | C12H26O2 | 013002-16-9 | 16 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110222\
Data File : VU051711.D
Acq On : 03 Nov 2022 00:09
Operator : JC/MD
Sample : N5301-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
DBWM4

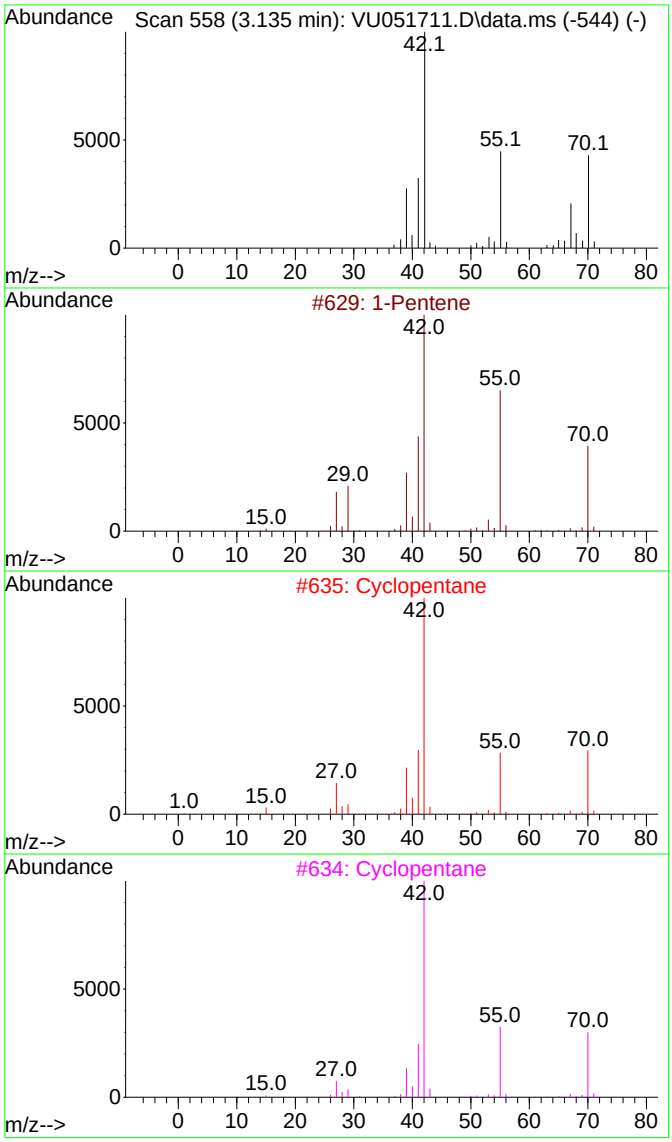
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

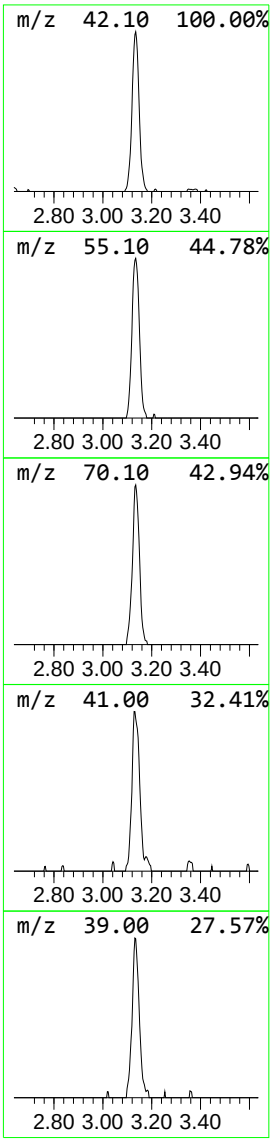
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.135 | 0.90 ug/L | 71770 | 1,4-Difluorobenzene | 6.247 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Pentene | 70 | C5H10 | 000109-67-1 | 64 |
| 2 | Cyclopentane | 70 | C5H10 | 000287-92-3 | 64 |
| 3 | Cyclopentane | 70 | C5H10 | 000287-92-3 | 59 |
| 4 | Cyclopentane | 70 | C5H10 | 000287-92-3 | 45 |
| 5 | 1-Pentene | 70 | C5H10 | 000109-67-1 | 42 |



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Operator : JC/MD
Sample : N5301-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

**Instrument :**
MSVOA_U
**ClientSampleId :**
DBWM4

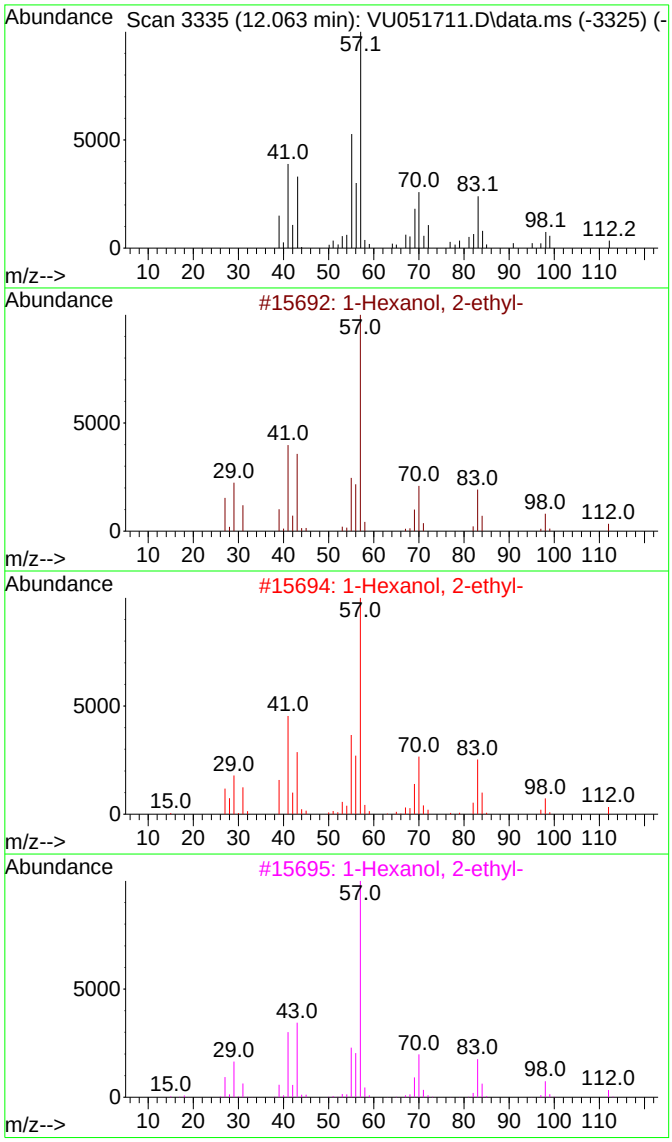
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

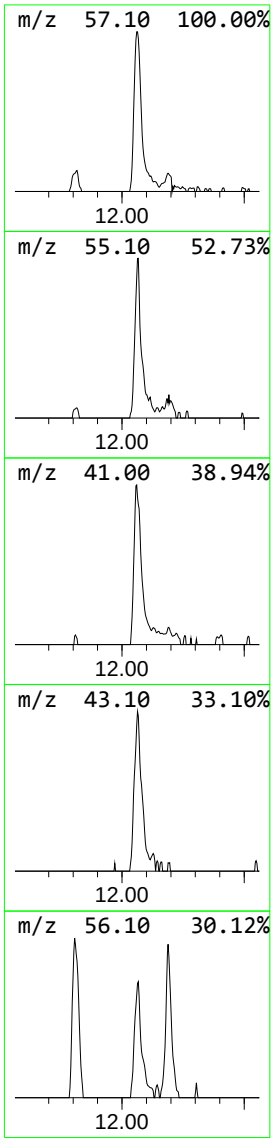
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.063 | 0.65 ug/L | 62036 | 1,4-Dichlorobenzene-d4 | 11.813 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 78 |
| 2 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 78 |
| 3 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 64 |
| 4 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 64 |
| 5 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 59 |



Tentatively Identified Compound (LSC) summary

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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 |
| Sulfur dioxide | 1.469 | 5.5 | ug/L | 438113 | 1 | 6.247 | 400220 | 5.0 |
| (DEL) Alkane: S... | 1.993 | 1.8 | ug/L | 141463 | 1 | 6.247 | 400220 | 5.0 |
| (DEL) Alkane: S... | 3.135 | 0.9 | ug/L | 71770 | 1 | 6.247 | 400220 | 5.0 |
| 1-Hexanol, 2-et... | 12.063 | 0.7 | ug/L | 62036 | 3 | 11.813 | 477691 | 5.0 |