LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050418\
Data File : VU023645.D
Acq On : 04 May 2018 21:53
Operator : MD/SY
Sample : J2630-05
Misc : 25mL/MSVOA U/WATER
ALS Vial : 42 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_U\METHOD\SOMUTR050418WMA.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 | 1.092 | 134 | 156 | 177 | rBV | 1338381 | 1624140 | 45.88% | 10.026% |
| 2 | 1.185 | 177 | 185 | 207 | rBV | 3520808 | 3540335 | 100.00% | 21.854% |
| 3 | 1.304 | 208 | 222 | 244 | rBV | 801960 | 1004827 | 28.38% | 6.203% |
| 4 | 1.404 | 245 | 253 | 263 | rBV2 | 683953 | 734937 | 20.76% | 4.537% |
| 5 | 1.516 | 283 | 288 | 298 | rVB | 55928 | 66983 | 1.89% | 0.413% |
| 6 | 1.680 | 333 | 339 | 353 | rVB | 58175 | 73649 | 2.08% | 0.455% |
| 7 | 1.757 | 355 | 363 | 379 | rVB | 180425 | 233713 | 6.60% | 1.443% |
| 8 | 1.947 | 415 | 422 | 433 | rVB | 35925 | 48632 | 1.37% | 0.300% |
| 9 | 2.272 | 513 | 523 | 534 | rBV | 115480 | 179828 | 5.08% | 1.110% |
| 10 | 2.455 | 571 | 580 | 597 | rVB2 | 27643 | 55481 | 1.57% | 0.342% |
| 11 | 2.789 | 673 | 684 | 696 | rBV | 43560 | 77577 | 2.19% | 0.479% |
| 12 | 2.982 | 732 | 744 | 768 | rVB2 | 72240 | 141697 | 4.00% | 0.875% |
| 13 | 4.085 | 1067 | 1087 | 1107 | rBV3 | 26121 | 70479 | 1.99% | 0.435% |
| 14 | 4.227 | 1107 | 1131 | 1167 | rBV2 | 931607 | 2468717 | 69.73% | 15.239% |
| 15 | 4.651 | 1247 | 1263 | 1289 | rBV | 97138 | 226320 | 6.39% | 1.397% |
| 16 | 4.992 | 1354 | 1369 | 1386 | rBV3 | 46838 | 110557 | 3.12% | 0.682% |
| 17 | 5.342 | 1457 | 1478 | 1509 | rVB2 | 191356 | 534291 | 15.09% | 3.298% |
| 18 | 5.892 | 1634 | 1649 | 1671 | rBV | 175370 | 351103 | 9.92% | 2.167% |
| 19 | 6.188 | 1727 | 1741 | 1774 | rBV | 273480 | 541063 | 15.28% | 3.340% |
| 20 | 6.336 | 1774 | 1787 | 1801 | rVV | 130670 | 263496 | 7.44% | 1.627% |
| 21 | 6.416 | 1801 | 1812 | 1828 | rVB3 | 18671 | 45024 | 1.27% | 0.278% |
| 22 | 7.233 | 2054 | 2066 | 2084 | rBV | 57010 | 103013 | 2.91% | 0.636% |
| 23 | 7.571 | 2151 | 2171 | 2188 | rBV | 231930 | 407638 | 11.51% | 2.516% |
| 24 | 7.857 | 2246 | 2260 | 2274 | rBV2 | 34534 | 59352 | 1.68% | 0.366% |
| 25 | 8.230 | 2363 | 2376 | 2393 | rBV | 700639 | 1192529 | 33.68% | 7.361% |
| 26 | 8.320 | 2393 | 2404 | 2432 | rVB | 388377 | 660808 | 18.67% | 4.079% |
| 27 | 9.095 | 2632 | 2645 | 2668 | rBV | 266267 | 440974 | 12.46% | 2.722% |
| 28 | 10.439 | 3051 | 3063 | 3077 | rBV | 103560 | 164726 | 4.65% | 1.017% |
| 29 | 11.490 | 3378 | 3390 | 3412 | rBV | 242652 | 396924 | 11.21% | 2.450% |
| 30 | 11.866 | 3495 | 3507 | 3527 | rBV | 234446 | 380759 | 10.75% | 2.350% |

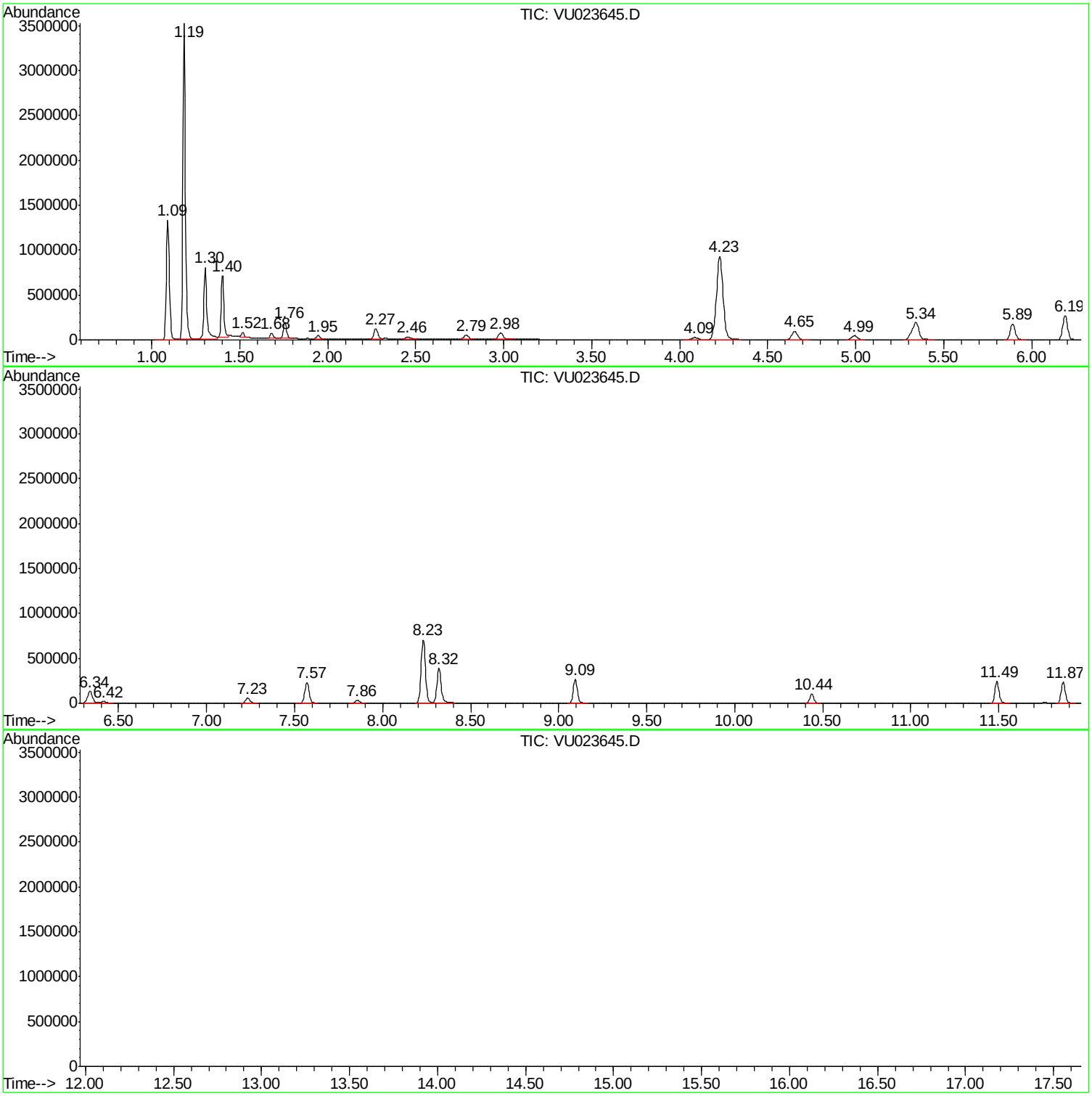
Sum of corrected areas: 16199572

LSC Report - Integrated Chromatogram

Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050418\
Data File : VU023645.D
Acq On : 04 May 2018 21:53
Operator : MD/SY
Sample : J2630-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMUTR050418WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050418\
Data File : VU023645.D
Acq On : 04 May 2018 21:53
Operator : MD/SY
Sample : J2630-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMUTR050418WMA.M
Quant Title : TRACE VOA SOM01.0

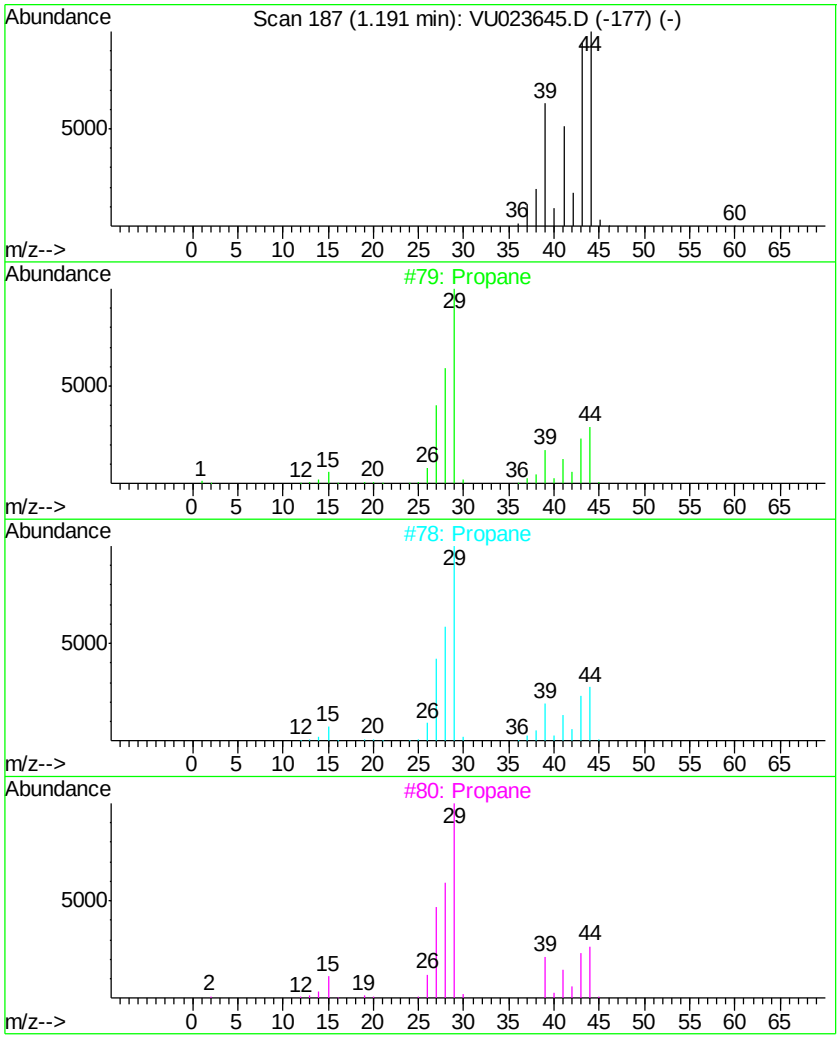
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

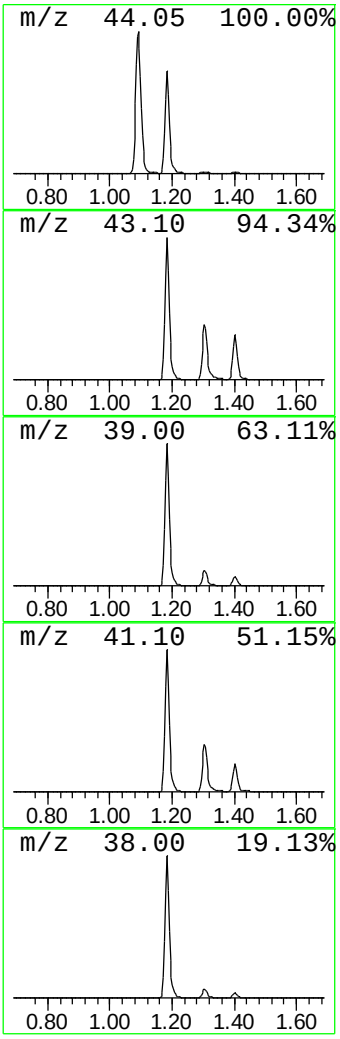
**********

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.19 | 50.42 ug/L | 3540340 | 1,4-Difluorobenzene | 5.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane | 44 | C3H8 | 000074-98-6 | 83 |
| 2 | Propane | 44 | C3H8 | 000074-98-6 | 83 |
| 3 | Propane | 44 | C3H8 | 000074-98-6 | 9 |
| 4 | Propene | 42 | C3H6 | 000115-07-1 | 9 |
| 5 | Acetaldehyde | 44 | C2H4O | 000075-07-0 | 5 |



Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050418\
Data File : VU023645.D
Acq On : 04 May 2018 21:53
Operator : MD/SY
Sample : J2630-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMUTR050418WMA.M
Quant Title : TRACE VOA SOM01.0

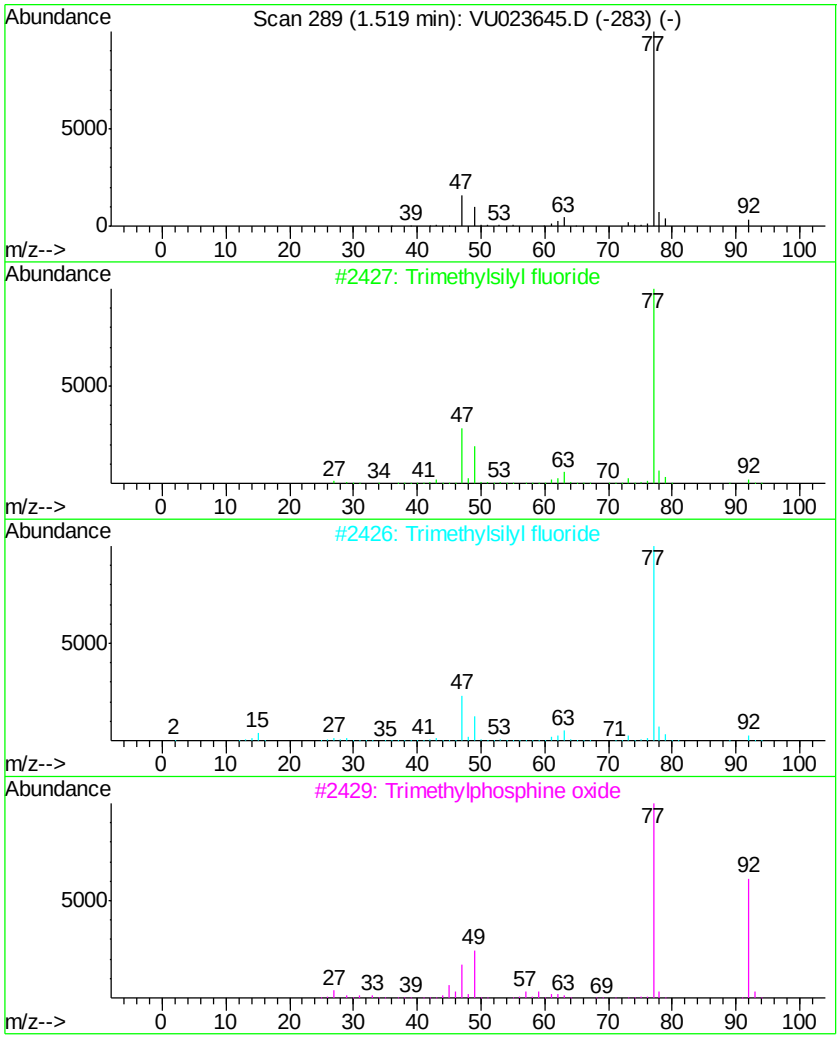
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

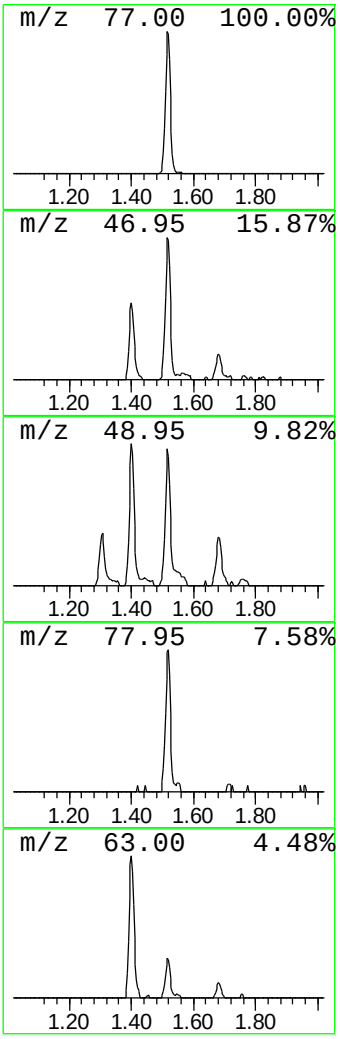
**********

Peak Number 3 Trimethylsilyl fluoride Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.52 | 0.95 ug/L | 66983 | 1,4-Difluorobenzene | 5.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trimethylsilyl fluoride | 92 | C3H9FSi | 000420-56-4 | 91 |
| 2 | Trimethylsilyl fluoride | 92 | C3H9FSi | 000420-56-4 | 91 |
| 3 | Trimethylphosphine oxide | 92 | C3H9OP | 000676-96-0 | 4 |
| 4 | Propane, 2-chloro-2-nitro- | 123 | C3H6ClNO2 | 000594-71-8 | 4 |
| 5 | Mercaptamine | 77 | C2H7NS | 000060-23-1 | 3 |



Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050418\
Data File : VU023645.D
Acq On : 04 May 2018 21:53
Operator : MD/SY
Sample : J2630-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMUTR050418WMA.M
Quant Title : TRACE VOA SOM01.0

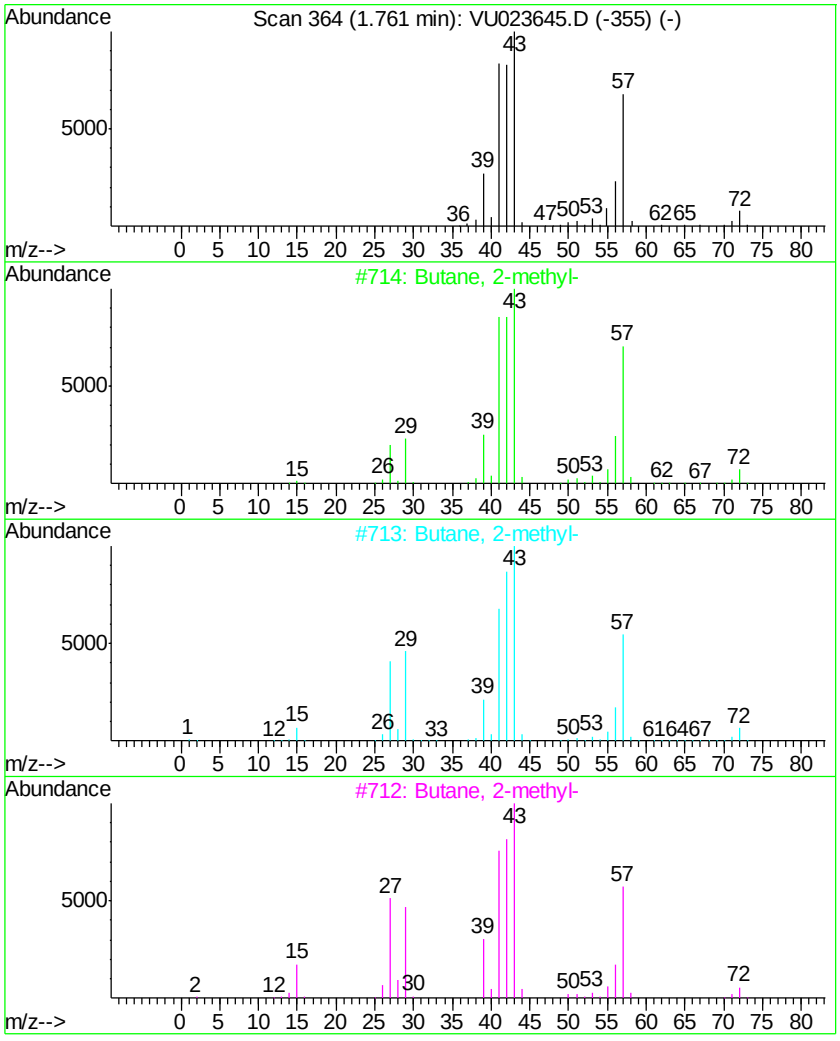
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

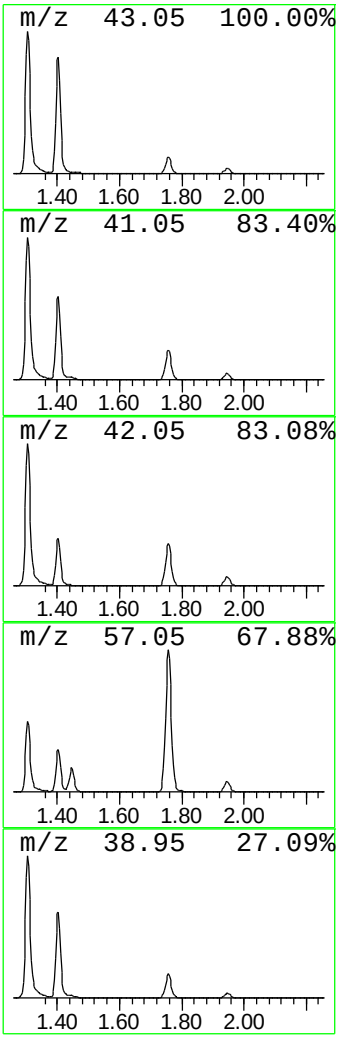
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.76 | 3.33 ug/L | 233713 | 1,4-Difluorobenzene | 5.89 |

| 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 | 91 |
| 3 | Butane, 2-methyl- | 72 | C5H12 | 000078-78-4 | 86 |
| 4 | Pentane | 72 | C5H12 | 000109-66-0 | 50 |
| 5 | 3-Buten-1-ol | 72 | C4H8O | 000627-27-0 | 28 |



Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050418\
Data File : VU023645.D
Acq On : 04 May 2018 21:53
Operator : MD/SY
Sample : J2630-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMUTR050418WMA.M
Quant Title : TRACE VOA SOM01.0

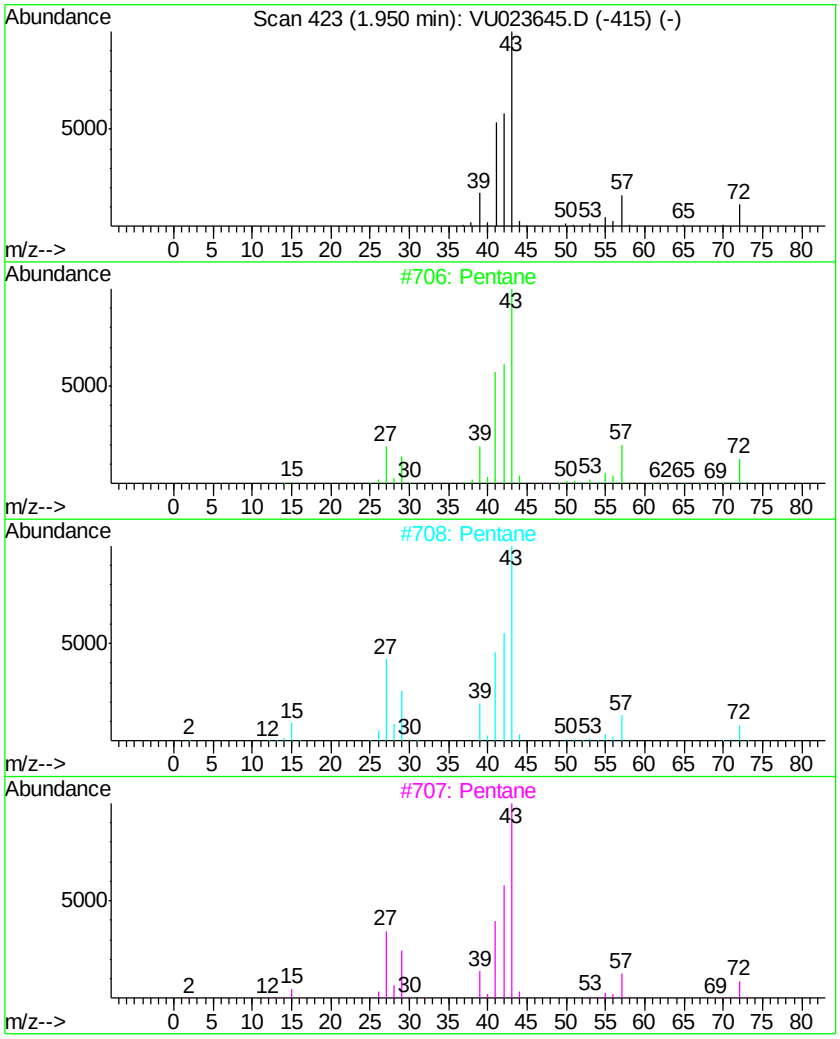
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

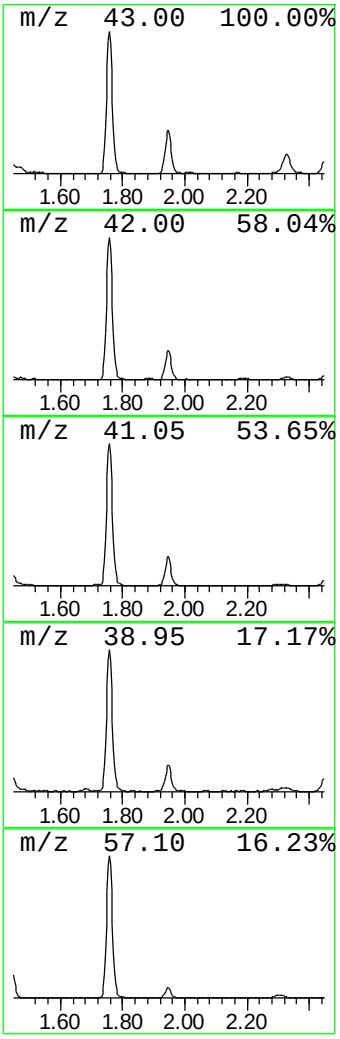
**********

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.95 | 0.69 ug/L | 48632 | 1,4-Difluorobenzene | 5.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentane | 72 | C5H12 | 000109-66-0 | 90 |
| 2 | Pentane | 72 | C5H12 | 000109-66-0 | 86 |
| 3 | Pentane | 72 | C5H12 | 000109-66-0 | 80 |
| 4 | Pentane | 72 | C5H12 | 000109-66-0 | 72 |
| 5 | Oxirane, ethyl- | 72 | C4H8O | 000106-88-7 | 40 |



Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050418\
Data File : VU023645.D
Acq On : 04 May 2018 21:53
Operator : MD/SY
Sample : J2630-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMUTR050418WMA.M
Quant Title : TRACE VOA SOM01.0

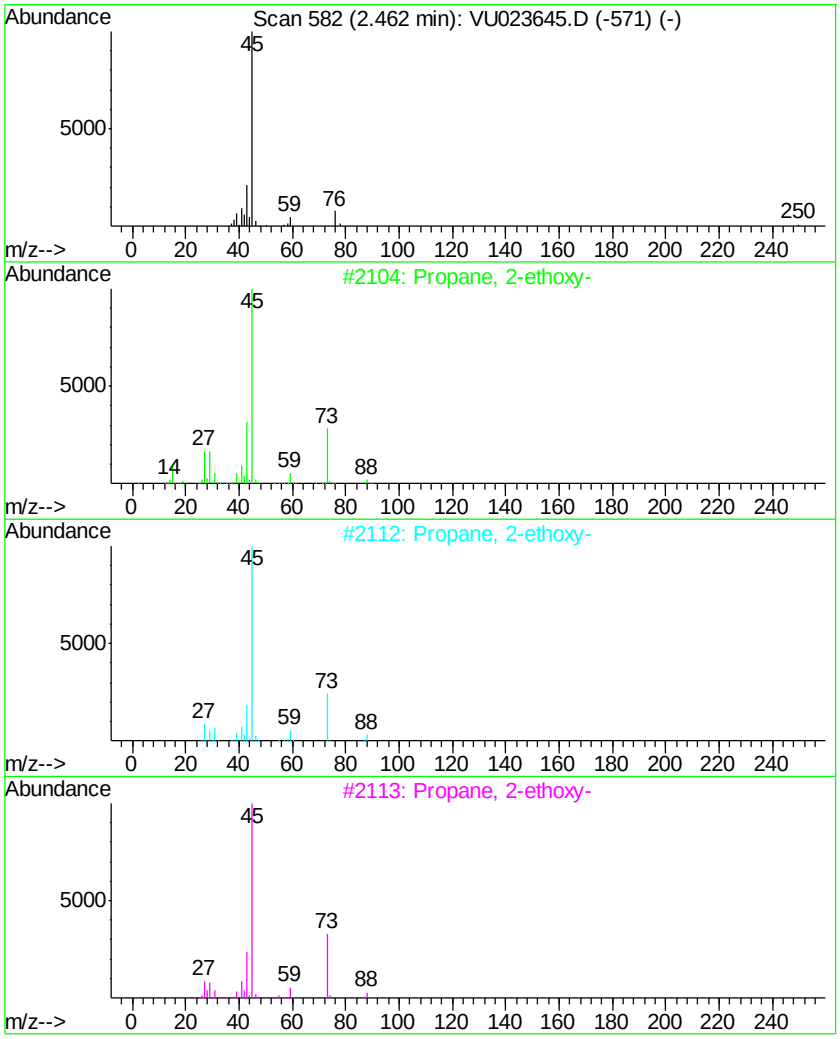
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

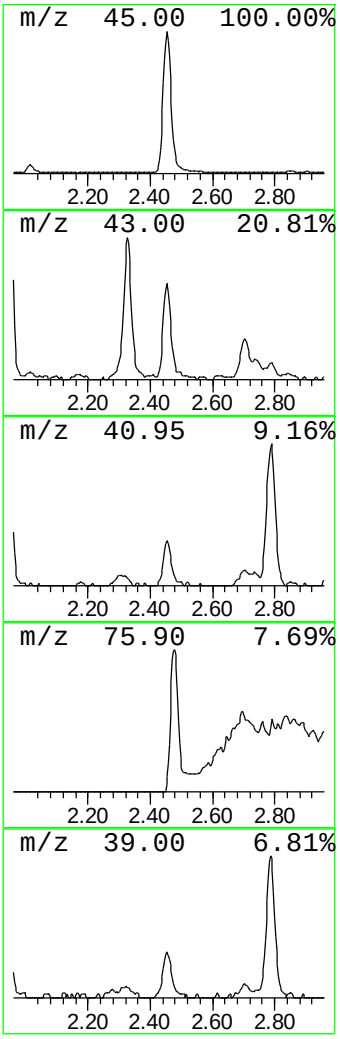
**********

Peak Number 6 Propane, 2-ethoxy- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.46 | 0.79 ug/L | 55481 | 1,4-Difluorobenzene | 5.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2-ethoxy- | 88 | C5H12O | 000625-54-7 | 64 |
| 2 | Propane, 2-ethoxy- | 88 | C5H12O | 000625-54-7 | 56 |
| 3 | Propane, 2-ethoxy- | 88 | C5H12O | 000625-54-7 | 43 |
| 4 | Isopropyl Alcohol | 60 | C3H8O | 000067-63-0 | 40 |
| 5 | Formic acid, 1-methylethyl ester | 88 | C4H8O2 | 000625-55-8 | 40 |



Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050418\
Data File : VU023645.D
Acq On : 04 May 2018 21:53
Operator : MD/SY
Sample : J2630-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMUTR050418WMA.M
Quant Title : TRACE VOA SOM01.0

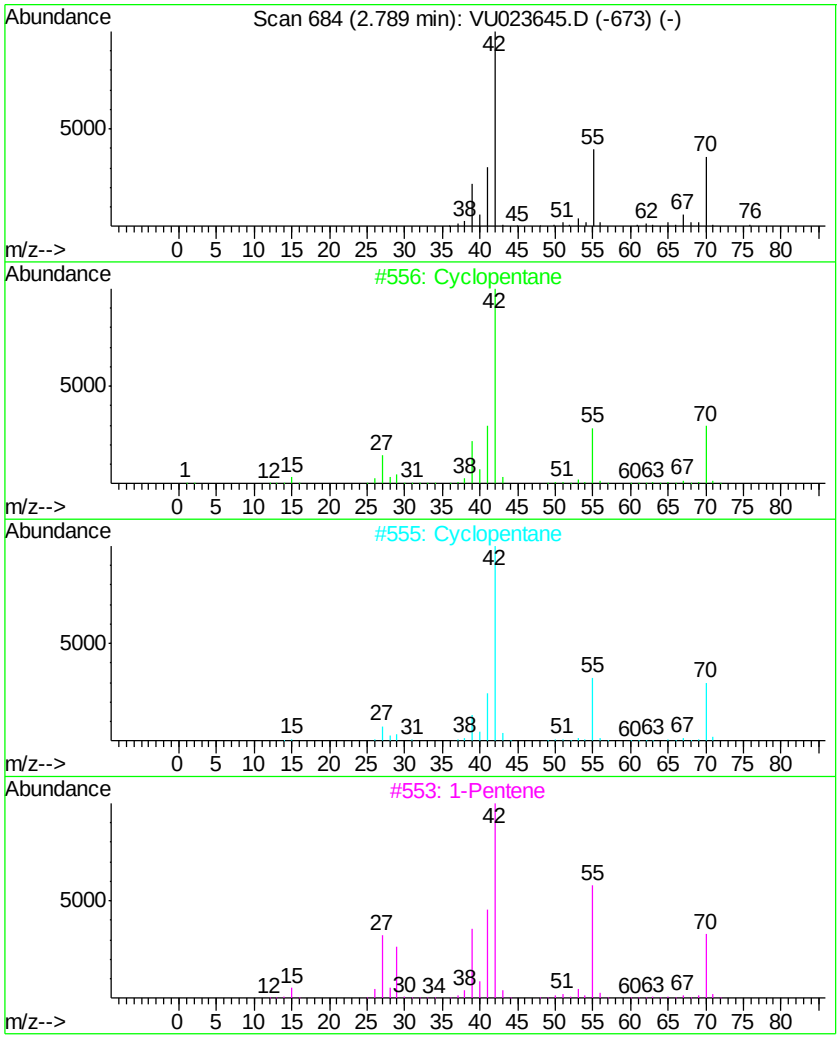
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

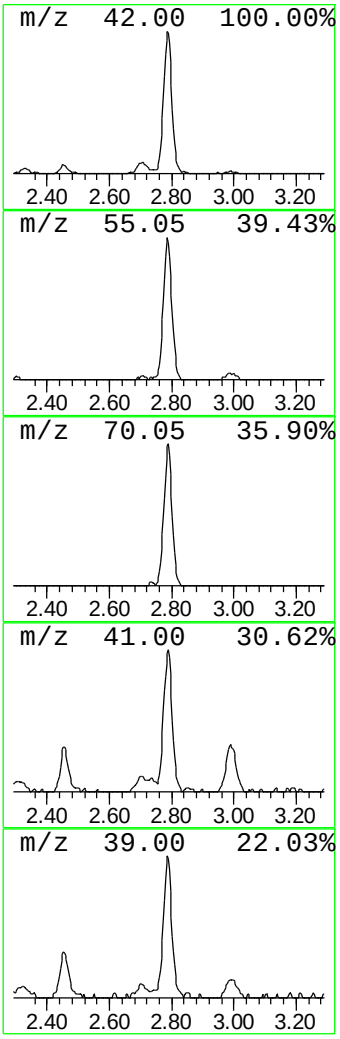
**********

Peak Number 7 (DEL) Alkane: Cyclic2.79 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.79 | 1.10 ug/L | 77577 | 1,4-Difluorobenzene | 5.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopentane | 70 | C5H10 | 000287-92-3 | 86 |
| 2 | Cyclopentane | 70 | C5H10 | 000287-92-3 | 72 |
| 3 | 1-Pentene | 70 | C5H10 | 000109-67-1 | 64 |
| 4 | 1-Pentene | 70 | C5H10 | 000109-67-1 | 37 |
| 5 | Aziridine, 2-ethyl- | 71 | C4H9N | 002549-67-9 | 9 |



Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050418\
Data File : VU023645.D
Acq On : 04 May 2018 21:53
Operator : MD/SY
Sample : J2630-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMUTR050418WMA.M
Quant Title : TRACE VOA SOM01.0

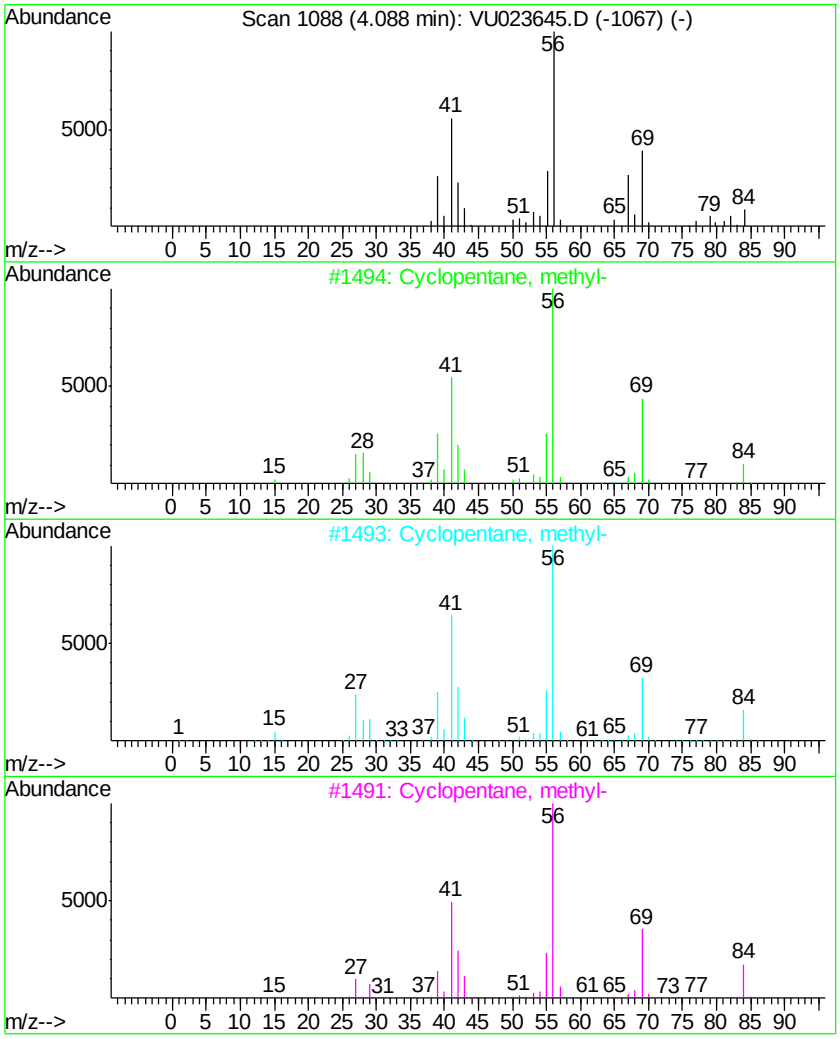
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

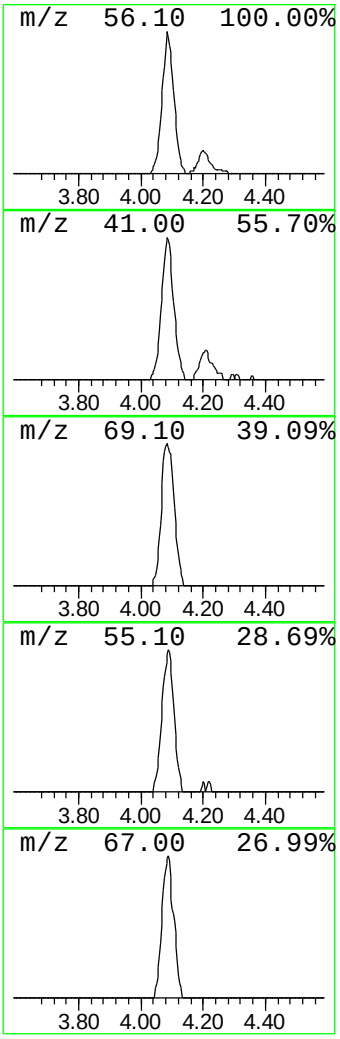
**********

Peak Number 8 (DEL) Alkane: Cyclic4.09 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.09 | 1.00 ug/L | 70479 | 1,4-Difluorobenzene | 5.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopentane, methyl- | 84 | C6H12 | 000096-37-7 | 76 |
| 2 | Cyclopentane, methyl- | 84 | C6H12 | 000096-37-7 | 58 |
| 3 | Cyclopentane, methyl- | 84 | C6H12 | 000096-37-7 | 53 |
| 4 | Cyclobutane, ethyl- | 84 | C6H12 | 004806-61-5 | 50 |
| 5 | Cyclobutane, ethyl- | 84 | C6H12 | 004806-61-5 | 40 |



Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050418\
Data File : VU023645.D
Acq On : 04 May 2018 21:53
Operator : MD/SY
Sample : J2630-05
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMUTR050418WMA.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 |
| (DEL) Alkane: Str... | 1.19 | 50.4 | ug/L | 3540340 | 1 | 5.89 | 351103 | 5.0 |
| Trimethylsilyl fl... | 1.52 | 0.9 | ug/L | 66983 | 1 | 5.89 | 351103 | 5.0 |
| (DEL) Alkane: Str... | 1.76 | 3.3 | ug/L | 233713 | 1 | 5.89 | 351103 | 5.0 |
| (DEL) Alkane: Str... | 1.95 | 0.7 | ug/L | 48632 | 1 | 5.89 | 351103 | 5.0 |
| Propane, 2-ethoxy- | 2.46 | 0.8 | ug/L | 55481 | 1 | 5.89 | 351103 | 5.0 |
| (DEL) Alkane: Cyc... | 2.79 | 1.1 | ug/L | 77577 | 1 | 5.89 | 351103 | 5.0 |
| (DEL) Alkane: Cyc... | 4.09 | 1.0 | ug/L | 70479 | 1 | 5.89 | 351103 | 5.0 |