LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090919\
Data File : VU034431.D
Acq On : 09 Sep 2019 14:22
Operator : JC/SP
Sample : K4725-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** S13-0271

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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\82U090619W.M
Title : SW846 8260

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.434 | 403 | 418 | 437 | rBV2 | 12507 | 26312 | 1.51% | 0.256% |
| 2 | 3.971 | 880 | 896 | 914 | rBV5 | 9040 | 24572 | 1.41% | 0.239% |
| 3 | 4.196 | 947 | 966 | 987 | rBV5 | 6854 | 23195 | 1.33% | 0.225% |
| 4 | 4.862 | 1157 | 1173 | 1191 | rBV | 257296 | 595441 | 34.08% | 5.784% |
| 5 | 4.961 | 1191 | 1204 | 1221 | rVV | 313646 | 713237 | 40.82% | 6.929% |
| 6 | 5.061 | 1223 | 1235 | 1257 | rVB | 59365 | 150824 | 8.63% | 1.465% |
| 7 | 5.289 | 1288 | 1306 | 1336 | rBV | 264673 | 583710 | 33.41% | 5.671% |
| 8 | 5.514 | 1349 | 1376 | 1395 | rVB | 85955 | 217024 | 12.42% | 2.108% |
| 9 | 5.868 | 1472 | 1486 | 1506 | rBV | 437138 | 889960 | 50.94% | 8.646% |
| 10 | 6.373 | 1630 | 1643 | 1658 | rVB4 | 32979 | 68420 | 3.92% | 0.665% |
| 11 | 6.569 | 1695 | 1704 | 1719 | rVB2 | 8950 | 18960 | 1.09% | 0.184% |
| 12 | 6.720 | 1735 | 1751 | 1774 | rBV3 | 38456 | 81349 | 4.66% | 0.790% |
| 13 | 6.907 | 1794 | 1809 | 1827 | rBV2 | 76387 | 154815 | 8.86% | 1.504% |
| 14 | 7.029 | 1832 | 1847 | 1866 | rBV | 126951 | 257761 | 14.75% | 2.504% |
| 15 | 7.546 | 1984 | 2008 | 2041 | rVV | 958775 | 1747151 | 100.00% | 16.973% |
| 16 | 7.688 | 2042 | 2052 | 2070 | rVB2 | 49223 | 98979 | 5.67% | 0.962% |
| 17 | 7.897 | 2105 | 2117 | 2135 | rVB2 | 130171 | 237562 | 13.60% | 2.308% |
| 18 | 8.025 | 2147 | 2157 | 2169 | rVB4 | 12540 | 21106 | 1.21% | 0.205% |
| 19 | 8.469 | 2283 | 2295 | 2313 | rVB5 | 25905 | 51959 | 2.97% | 0.505% |
| 20 | 8.826 | 2396 | 2406 | 2419 | rBV3 | 17318 | 31061 | 1.78% | 0.302% |
| 21 | 9.067 | 2465 | 2481 | 2508 | rBV | 645111 | 1125484 | 64.42% | 10.934% |
| 22 | 9.225 | 2521 | 2530 | 2543 | rVB6 | 12751 | 25170 | 1.44% | 0.245% |
| 23 | 9.363 | 2556 | 2573 | 2584 | rVB7 | 29090 | 72960 | 4.18% | 0.709% |
| 24 | 9.710 | 2662 | 2681 | 2695 | rBV8 | 22065 | 71574 | 4.10% | 0.695% |
| 25 | 9.894 | 2725 | 2738 | 2745 | rBV8 | 8664 | 20139 | 1.15% | 0.196% |
| 26 | 10.032 | 2768 | 2781 | 2795 | rBV8 | 9769 | 22448 | 1.28% | 0.218% |
| 27 | 10.286 | 2848 | 2860 | 2876 | rBV | 688143 | 1117611 | 63.97% | 10.857% |
| 28 | 10.469 | 2909 | 2917 | 2928 | rVB6 | 19290 | 32020 | 1.83% | 0.311% |
| 29 | 10.958 | 3054 | 3069 | 3083 | rBV7 | 9609 | 19422 | 1.11% | 0.189% |
| 30 | 11.270 | 3150 | 3166 | 3186 | rBV2 | 21578 | 45313 | 2.59% | 0.440% |
| 31 | 11.459 | 3214 | 3225 | 3248 | rBV | 798165 | 1327230 | 75.97% | 12.894% |
| 32 | 11.845 | 3333 | 3345 | 3364 | rVB10 | 11166 | 29623 | 1.70% | 0.288% |
| 33 | 12.270 | 3468 | 3477 | 3490 | rVB6 | 29567 | 51483 | 2.95% | 0.500% |
| 34 | 12.472 | 3529 | 3540 | 3546 | rBV4 | 13903 | 24066 | 1.38% | 0.234% |

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090919\
Data File : VU034431.D
Acq On : 09 Sep 2019 14:22
Operator : JC/SP
Sample : K4725-13
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** S13-0271

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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\82U090619W.M
Title : SW846 8260

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 12.517 | 3547 | 3554 | 3568 | rVB3 | 18462 | 32200 | 1.84% | 0.313% |
| 36 | 12.771 | 3622 | 3633 | 3648 | rBV3 | 15550 | 25550 | 1.46% | 0.248% |
| 37 | 12.903 | 3664 | 3674 | 3684 | rBV3 | 14751 | 25580 | 1.46% | 0.249% |
| 38 | 12.977 | 3690 | 3697 | 3709 | rVB2 | 14391 | 22677 | 1.30% | 0.220% |
| 39 | 13.540 | 3863 | 3872 | 3874 | rBV3 | 13786 | 20761 | 1.19% | 0.202% |
| 40 | 13.736 | 3919 | 3933 | 3938 | rBV2 | 14365 | 31171 | 1.78% | 0.303% |
| 41 | 14.003 | 4005 | 4016 | 4024 | rBV5 | 14662 | 25828 | 1.48% | 0.251% |
| 42 | 14.527 | 4168 | 4179 | 4191 | rVB6 | 14375 | 29280 | 1.68% | 0.284% |
| 43 | 14.675 | 4212 | 4225 | 4235 | rBV5 | 12207 | 29057 | 1.66% | 0.282% |
| 44 | 14.913 | 4290 | 4299 | 4317 | rVB5 | 14060 | 35066 | 2.01% | 0.341% |
| 45 | 15.057 | 4334 | 4344 | 4356 | rVB6 | 19148 | 38633 | 2.21% | 0.375% |

Sum of corrected areas: 10293744

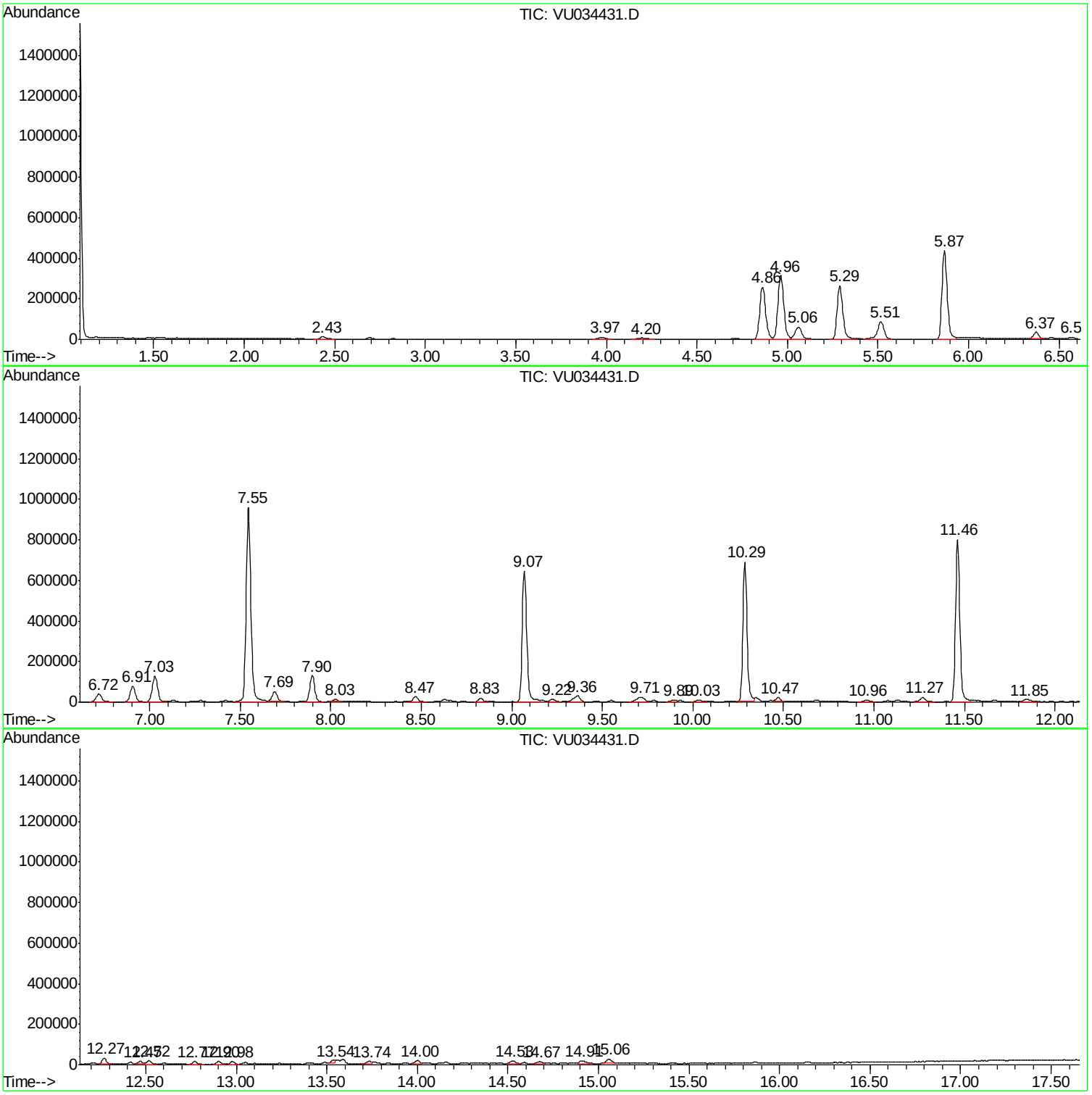
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090919\
Data File : VU034431.D
Acq On : 09 Sep 2019 14:22
Operator : JC/SP
Sample : K4725-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** S13-0271

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

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



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090919\
Data File : VU034431.D
Acq On : 09 Sep 2019 14:22
Operator : JC/SP
Sample : K4725-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** S13-0271

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

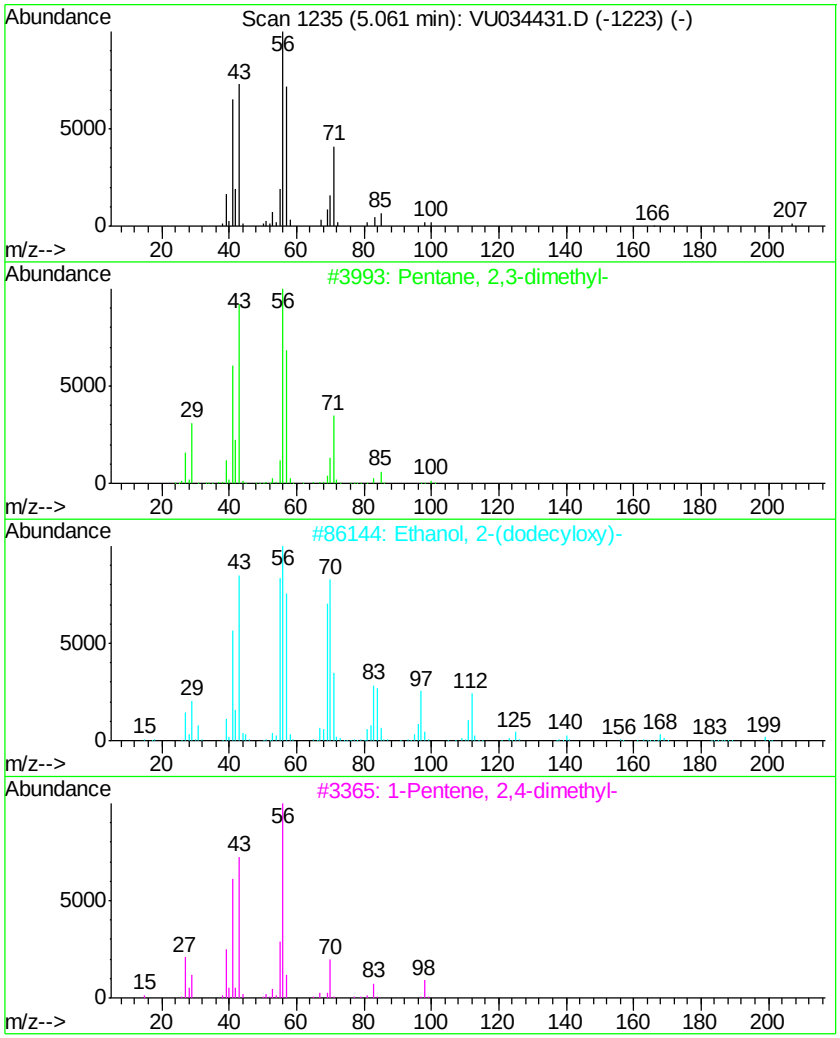
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

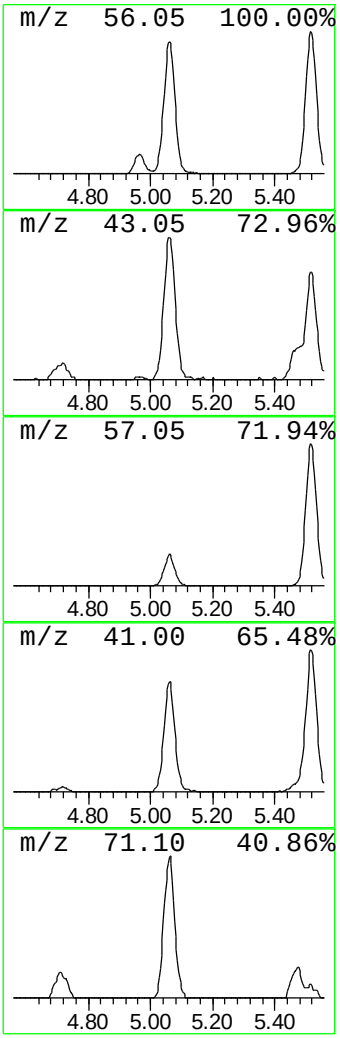
**********

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.06 | 10.57 ug/l | 150824 | Pentafluorobenzene | 4.96 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentane, 2,3-dimethyl- | 100 | C7H16 | 000565-59-3 | 91 |
| 2 | Ethanol, 2-(dodecyloxy)- | 230 | C14H30O2 | 004536-30-5 | 56 |
| 3 | 1-Pentene, 2,4-dimethyl- | 98 | C7H14 | 002213-32-3 | 50 |
| 4 | Nonane, 5-methylene- | 140 | C10H20 | 006795-79-5 | 50 |
| 5 | 1-Hexene, 5-methyl- | 98 | C7H14 | 003524-73-0 | 47 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090919\
Data File : VU034431.D
Acq On : 09 Sep 2019 14:22
Operator : JC/SP
Sample : K4725-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** S13-0271

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

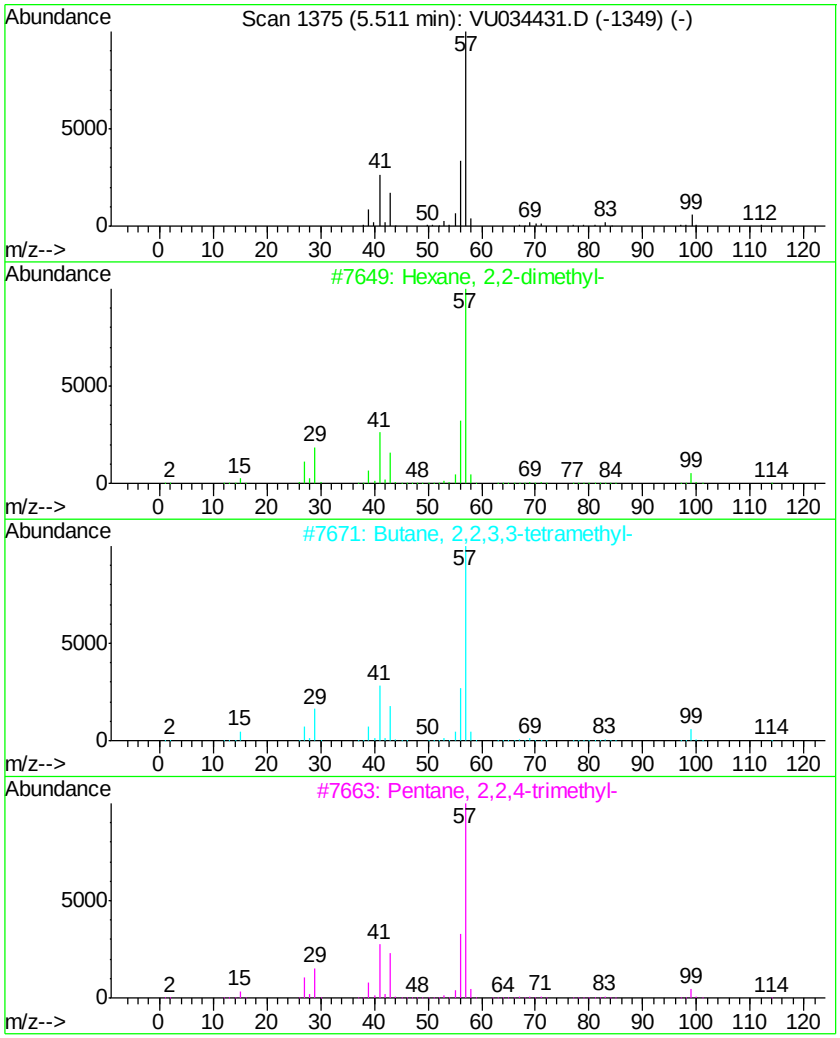
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

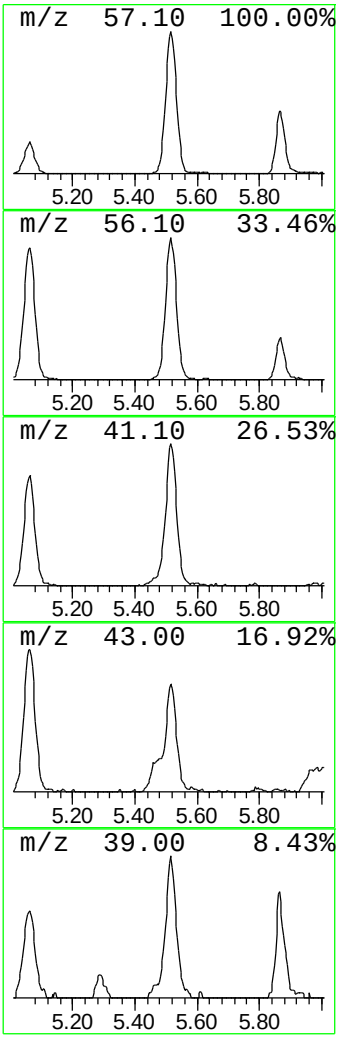
**********

Peak Number 2 Hexane, 2,2-dimethyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.51 | 12.19 ug/l | 217024 | 1,4-Difluorobenzene | 5.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexane, 2,2-dimethyl- | 114 | C8H18 | 000590-73-8 | 72 |
| 2 | Butane, 2,2,3,3-tetramethyl- | 114 | C8H18 | 000594-82-1 | 72 |
| 3 | Pentane, 2,2,4-trimethyl- | 114 | C8H18 | 000540-84-1 | 72 |
| 4 | Heptane, 2,2,4,6,6-pentamethyl- | 170 | C12H26 | 013475-82-6 | 64 |
| 5 | Hexane, 2,2,4-trimethyl- | 128 | C9H20 | 016747-26-5 | 59 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090919\
Data File : VU034431.D
Acq On : 09 Sep 2019 14:22
Operator : JC/SP
Sample : K4725-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** S13-0271

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

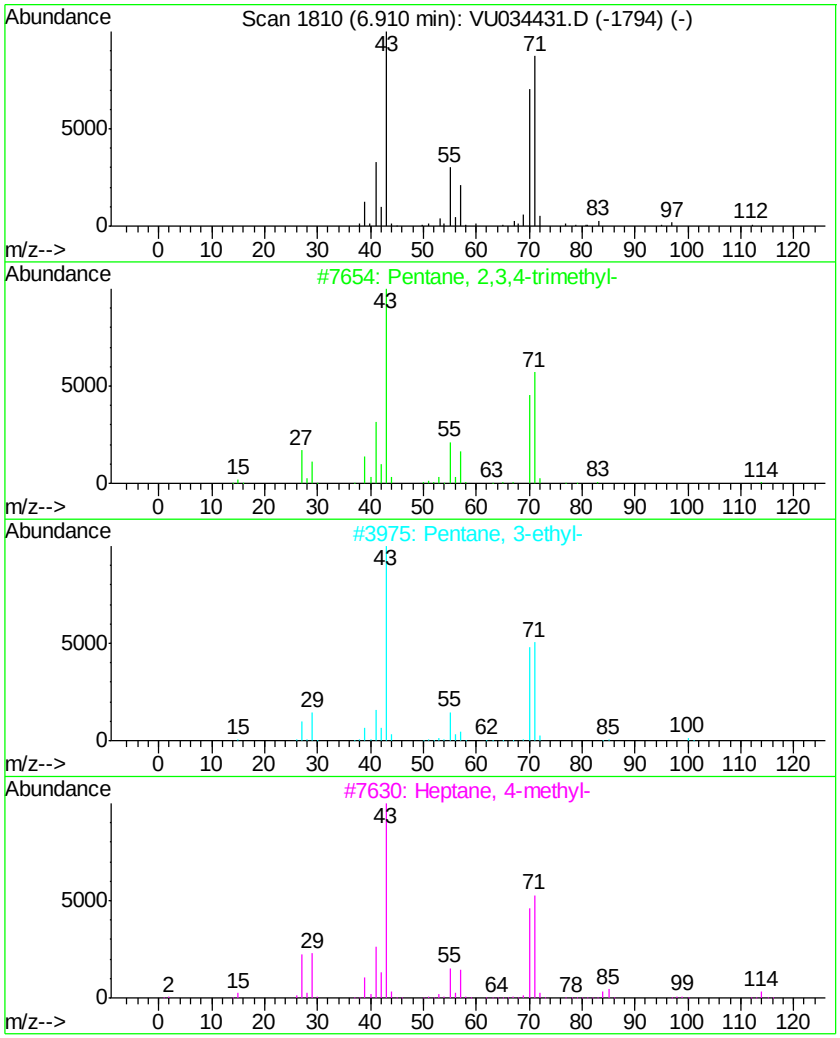
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

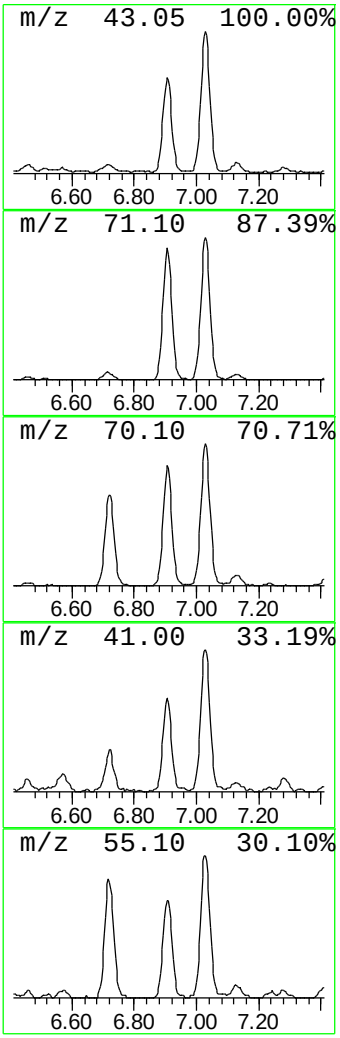
**********

Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.91 | 8.70 ug/l | 154815 | 1,4-Difluorobenzene | 5.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentane, 2,3,4-trimethyl- | 114 | C8H18 | 000565-75-3 | 90 |
| 2 | Pentane, 3-ethyl- | 100 | C7H16 | 000617-78-7 | 83 |
| 3 | Heptane, 4-methyl- | 114 | C8H18 | 000589-53-7 | 83 |
| 4 | 3,3-Dimethyl-2-pentanol | 116 | C7H16O | 019781-24-9 | 74 |
| 5 | Hexane, 3,3,4-trimethyl- | 128 | C9H20 | 016747-31-2 | 64 |



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090919\
Data File : VU034431.D
Acq On : 09 Sep 2019 14:22
Operator : JC/SP
Sample : K4725-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** S13-0271

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

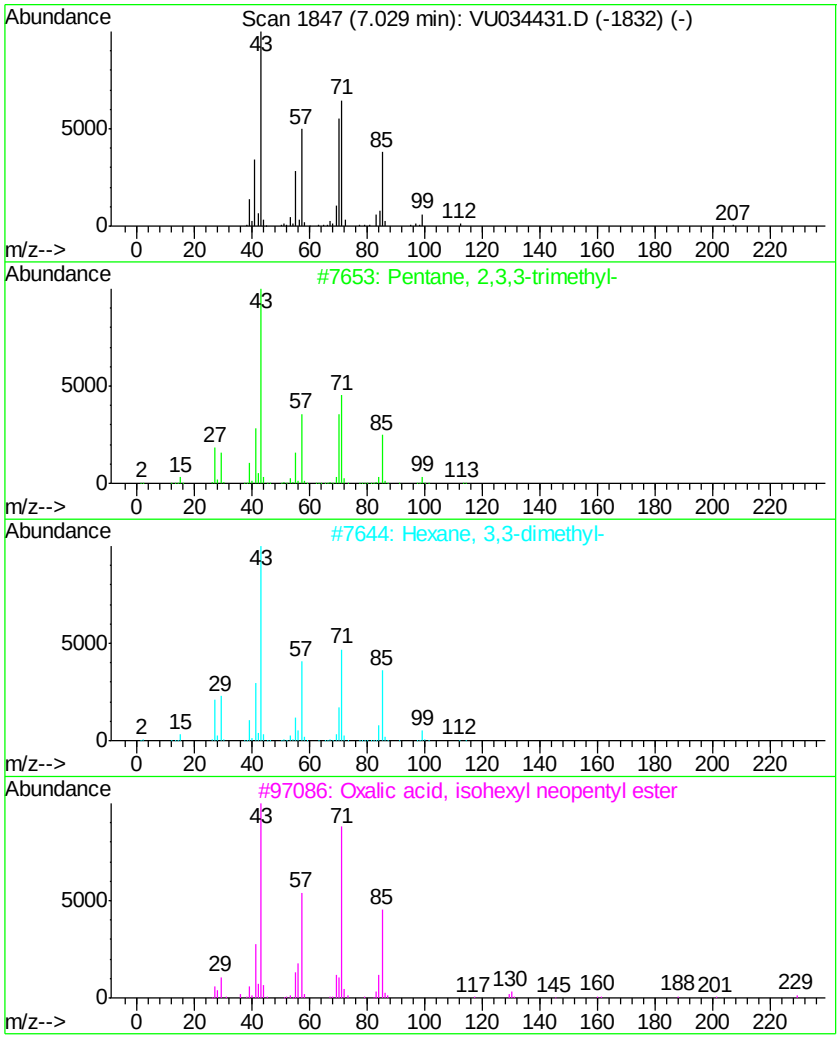
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

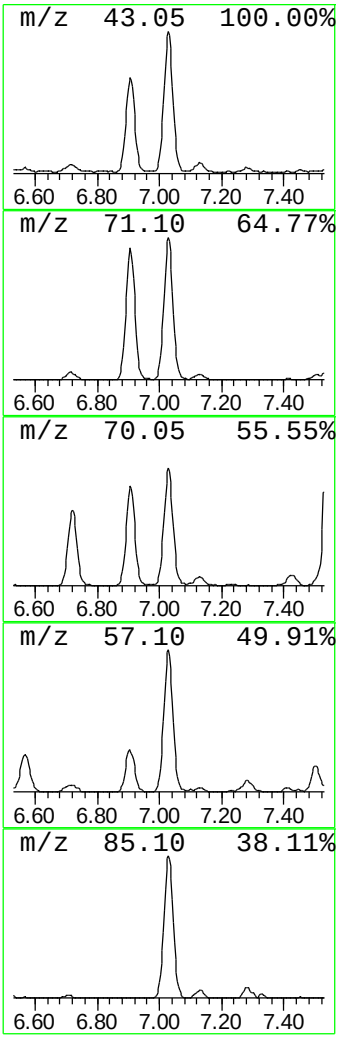
**********

Peak Number 4 Pentane, 2,3,3-trimethyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.03 | 14.48 ug/l | 257761 | 1,4-Difluorobenzene | 5.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentane, 2,3,3-trimethyl- | 114 | C8H18 | 000560-21-4 | 90 |
| 2 | Hexane, 3,3-dimethyl- | 114 | C8H18 | 000563-16-6 | 59 |
| 3 | Oxalic acid, isohexyl neopentyl ... | 244 | C13H24O4 | 1000309-73-0 | 59 |
| 4 | Hexane, 3-methyl- | 100 | C7H16 | 000589-34-4 | 53 |
| 5 | 2-Bromononane | 206 | C9H19Br | 002216-35-5 | 53 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090919\
Data File : VU034431.D
Acq On : 09 Sep 2019 14:22
Operator : JC/SP
Sample : K4725-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** S13-0271

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

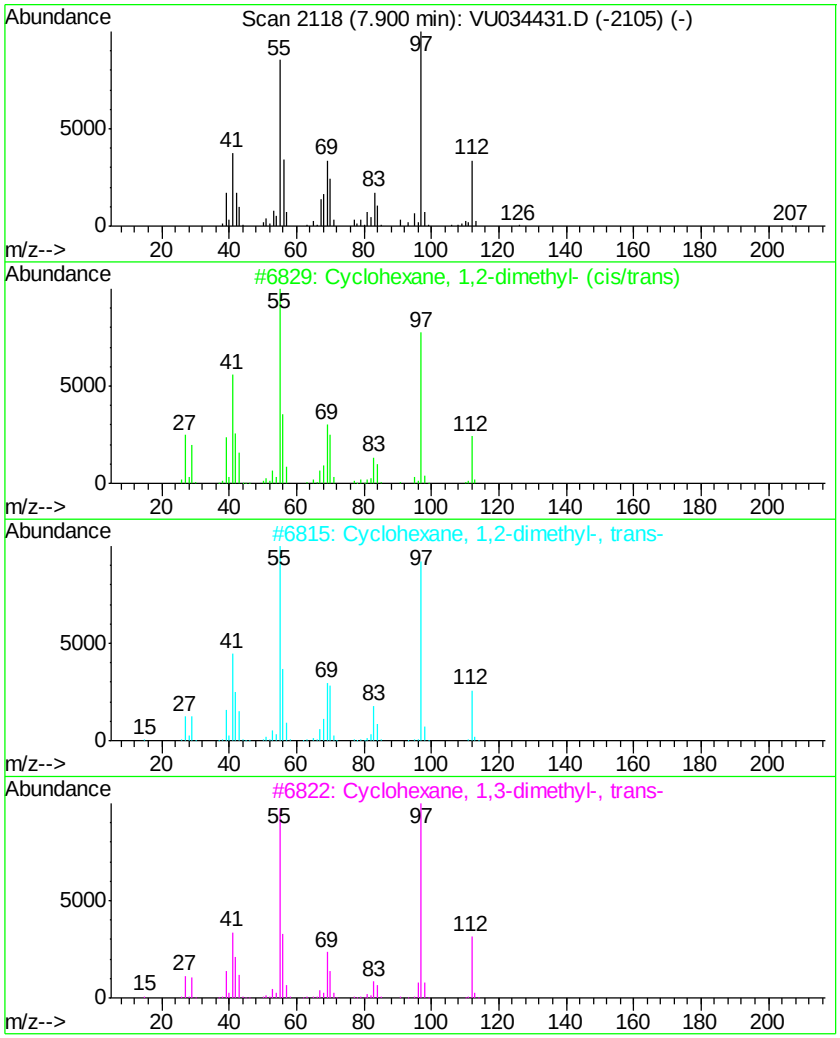
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

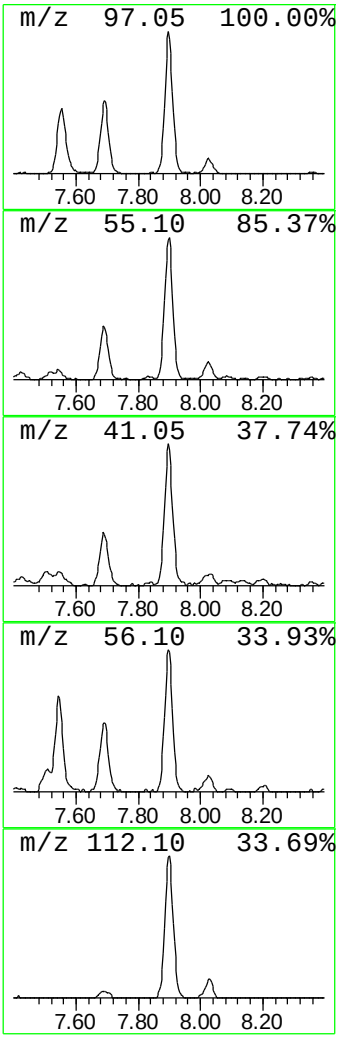
**********

Peak Number 5 Cyclohexane, 1,2-dimethyl- ... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.90 | 10.55 ug/l | 237562 | Chlorobenzene-d5 | 9.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexane, 1,2-dimethyl- (cis/... | 112 | C8H16 | 000583-57-3 | 94 |
| 2 | Cyclohexane, 1,2-dimethyl-, trans- | 112 | C8H16 | 006876-23-9 | 94 |
| 3 | Cyclohexane, 1,3-dimethyl-, trans- | 112 | C8H16 | 002207-03-6 | 87 |
| 4 | Cyclohexane, 1,4-dimethyl-, trans- | 112 | C8H16 | 002207-04-7 | 83 |
| 5 | Cyclohexane, 1,4-dimethyl-, cis- | 112 | C8H16 | 000624-29-3 | 83 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU090919\
Data File : VU034431.D
Acq On : 09 Sep 2019 14:22
Operator : JC/SP
Sample : K4725-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** S13-0271

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U090619W.M
Quant Title : SW846 8260

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Pentane, 2,3-dime... | 5.06 | 10.6 | ug/l | 150824 | 1 | 4.96 | 713237 | 50.0 |
| Hexane, 2,2-dimet... | 5.51 | 12.2 | ug/l | 217024 | 2 | 5.87 | 889960 | 50.0 |
| Pentane, 2,3,4-tr... | 6.91 | 8.7 | ug/l | 154815 | 2 | 5.87 | 889960 | 50.0 |
| Pentane, 2,3,3-tr... | 7.03 | 14.5 | ug/l | 257761 | 2 | 5.87 | 889960 | 50.0 |
| Cyclohexane, 1,2-... | 7.90 | 10.6 | ug/l | 237562 | 3 | 9.07 | 1125480 | 50.0 |