LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

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\SOMUTR061720WMA.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 | 1.629 | 79 | 90 | 103 | rBV2 | 122602 | 184672 | 16.02% | 1.492% |
| 2 | 1.765 | 127 | 132 | 142 | rVB3 | 12882 | 19091 | 1.66% | 0.154% |
| 3 | 1.951 | 182 | 190 | 203 | rBV | 103783 | 127440 | 11.06% | 1.030% |
| 4 | 2.067 | 211 | 226 | 231 | rBV3 | 28984 | 66597 | 5.78% | 0.538% |
| 5 | 2.617 | 385 | 397 | 411 | rBV | 299549 | 509633 | 44.21% | 4.117% |
| 6 | 2.893 | 479 | 483 | 491 | rBV2 | 12424 | 16585 | 1.44% | 0.134% |
| 7 | 4.565 | 978 | 1003 | 1020 | rBV5 | 26527 | 91175 | 7.91% | 0.737% |
| 8 | 4.809 | 1048 | 1079 | 1121 | rBV2 | 82653 | 419422 | 36.39% | 3.388% |
| 9 | 5.015 | 1129 | 1143 | 1145 | rBV3 | 11804 | 22444 | 1.95% | 0.181% |
| 10 | 5.163 | 1174 | 1189 | 1207 | rVB | 199229 | 429003 | 37.22% | 3.466% |
| 11 | 5.803 | 1366 | 1388 | 1410 | rBV2 | 408374 | 995574 | 86.37% | 8.043% |
| 12 | 6.317 | 1534 | 1548 | 1563 | rVB | 340652 | 620727 | 53.85% | 5.015% |
| 13 | 6.694 | 1658 | 1665 | 1671 | rBV2 | 8272 | 12031 | 1.04% | 0.097% |
| 14 | 6.755 | 1671 | 1684 | 1704 | rVV | 245678 | 479102 | 41.57% | 3.870% |
| 15 | 6.864 | 1709 | 1718 | 1733 | rVV6 | 10345 | 26960 | 2.34% | 0.218% |
| 16 | 6.944 | 1735 | 1743 | 1753 | rVV5 | 8251 | 16496 | 1.43% | 0.133% |
| 17 | 7.005 | 1753 | 1762 | 1772 | rVB2 | 6810 | 14153 | 1.23% | 0.114% |
| 18 | 7.231 | 1806 | 1832 | 1848 | rBV | 150059 | 315096 | 27.34% | 2.546% |
| 19 | 7.317 | 1848 | 1859 | 1873 | rVB3 | 10224 | 22811 | 1.98% | 0.184% |
| 20 | 7.613 | 1937 | 1951 | 1966 | rVB2 | 126347 | 219386 | 19.03% | 1.772% |
| 21 | 7.848 | 2009 | 2024 | 2027 | rBV3 | 14239 | 23351 | 2.03% | 0.189% |
| 22 | 7.890 | 2030 | 2037 | 2041 | rVV3 | 22687 | 40775 | 3.54% | 0.329% |
| 23 | 7.941 | 2041 | 2053 | 2069 | rVB | 452395 | 788491 | 68.41% | 6.370% |
| 24 | 8.083 | 2086 | 2097 | 2107 | rVV | 15844 | 27196 | 2.36% | 0.220% |
| 25 | 8.218 | 2127 | 2139 | 2150 | rBV2 | 85164 | 139810 | 12.13% | 1.129% |
| 26 | 8.530 | 2220 | 2236 | 2244 | rBV3 | 17620 | 40258 | 3.49% | 0.325% |
| 27 | 8.587 | 2245 | 2254 | 2264 | rBV4 | 11274 | 18541 | 1.61% | 0.150% |
| 28 | 8.674 | 2264 | 2281 | 2290 | rBV | 644758 | 1152654 | 100.00% | 9.312% |
| 29 | 8.822 | 2319 | 2327 | 2349 | rVB5 | 20322 | 39149 | 3.40% | 0.316% |
| 30 | 8.948 | 2356 | 2366 | 2376 | rBV3 | 7481 | 16631 | 1.44% | 0.134% |
| 31 | 9.443 | 2507 | 2520 | 2540 | rBV | 491357 | 822466 | 71.35% | 6.644% |
| 32 | 9.661 | 2563 | 2588 | 2599 | rBV | 91903 | 161658 | 14.02% | 1.306% |
| 33 | 9.793 | 2613 | 2629 | 2645 | rBV6 | 26519 | 68367 | 5.93% | 0.552% |
| 34 | 9.941 | 2662 | 2675 | 2689 | rBV5 | 14834 | 28042 | 2.43% | 0.227% |

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

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\SOMUTR061720WMA.M
Title : TRACE VOA SOM01.0

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 10.153 | 2734 | 2741 | 2749 | rVB4 | 7984 | 11818 | 1.03% | 0.095% |
| 36 | 10.256 | 2760 | 2773 | 2787 | rBV | 56193 | 98358 | 8.53% | 0.795% |
| 37 | 10.365 | 2799 | 2807 | 2826 | rVB9 | 11662 | 26535 | 2.30% | 0.214% |
| 38 | 10.665 | 2890 | 2900 | 2905 | rBV6 | 9410 | 15976 | 1.39% | 0.129% |
| 39 | 10.700 | 2906 | 2911 | 2922 | rVB5 | 9817 | 16275 | 1.41% | 0.131% |
| 40 | 10.774 | 2922 | 2934 | 2950 | rBV | 207182 | 341245 | 29.61% | 2.757% |
| 41 | 10.906 | 2959 | 2975 | 2983 | rVB | 9651 | 22149 | 1.92% | 0.179% |
| 42 | 10.986 | 2990 | 3000 | 3012 | rVV3 | 13429 | 23042 | 2.00% | 0.186% |
| 43 | 11.066 | 3012 | 3025 | 3036 | rVV7 | 8801 | 20691 | 1.80% | 0.167% |
| 44 | 11.131 | 3036 | 3045 | 3061 | rVB2 | 13444 | 24456 | 2.12% | 0.198% |
| 45 | 11.288 | 3085 | 3094 | 3108 | rBV3 | 12003 | 22006 | 1.91% | 0.178% |
| 46 | 11.484 | 3146 | 3155 | 3163 | rBV3 | 27082 | 40479 | 3.51% | 0.327% |
| 47 | 11.587 | 3176 | 3187 | 3197 | rBV2 | 24638 | 40346 | 3.50% | 0.326% |
| 48 | 11.700 | 3214 | 3222 | 3233 | rVB4 | 29752 | 44432 | 3.85% | 0.359% |
| 49 | 11.825 | 3248 | 3261 | 3277 | rVB | 524341 | 829708 | 71.98% | 6.703% |
| 50 | 12.076 | 3326 | 3339 | 3361 | rBV | 129345 | 294593 | 25.56% | 2.380% |
| 51 | 12.205 | 3368 | 3379 | 3394 | rVB | 513617 | 822663 | 71.37% | 6.646% |
| 52 | 12.336 | 3413 | 3420 | 3425 | rBV3 | 13729 | 18908 | 1.64% | 0.153% |
| 53 | 12.372 | 3426 | 3431 | 3439 | rVB4 | 18038 | 24697 | 2.14% | 0.200% |
| 54 | 12.549 | 3482 | 3486 | 3500 | rVB6 | 9683 | 17323 | 1.50% | 0.140% |
| 55 | 12.793 | 3552 | 3562 | 3572 | rBV3 | 51033 | 79700 | 6.91% | 0.644% |
| 56 | 12.906 | 3588 | 3597 | 3608 | rVB4 | 20581 | 33355 | 2.89% | 0.269% |
| 57 | 13.163 | 3666 | 3677 | 3684 | rBV5 | 6632 | 11602 | 1.01% | 0.094% |
| 58 | 14.015 | 3934 | 3942 | 3953 | rBV5 | 15245 | 22404 | 1.94% | 0.181% |
| 59 | 14.227 | 3996 | 4008 | 4032 | rBV | 258603 | 406224 | 35.24% | 3.282% |
| 60 | 14.352 | 4039 | 4047 | 4058 | rVB7 | 15200 | 25748 | 2.23% | 0.208% |
| 61 | 14.873 | 4201 | 4209 | 4215 | rBV5 | 7237 | 13256 | 1.15% | 0.107% |
| 62 | 14.922 | 4218 | 4224 | 4236 | rVB6 | 19002 | 31866 | 2.76% | 0.257% |
| 63 | 15.047 | 4252 | 4263 | 4271 | rBV4 | 18851 | 35462 | 3.08% | 0.286% |
| 64 | 15.147 | 4287 | 4294 | 4303 | rBV3 | 14962 | 21902 | 1.90% | 0.177% |
| 65 | 15.504 | 4396 | 4405 | 4413 | rBV4 | 13987 | 21689 | 1.88% | 0.175% |
| 66 | 15.600 | 4427 | 4435 | 4441 | rBV5 | 12942 | 19530 | 1.69% | 0.158% |
| 67 | 15.645 | 4442 | 4449 | 4457 | rVV4 | 14265 | 24120 | 2.09% | 0.195% |
| 68 | 15.693 | 4457 | 4464 | 4469 | rVV8 | 8277 | 12993 | 1.13% | 0.105% |
| 69 | 15.748 | 4471 | 4481 | 4492 | rVB5 | 35698 | 66548 | 5.77% | 0.538% |
| 70 | 16.195 | 4607 | 4620 | 4631 | rBV2 | 63423 | 106991 | 9.28% | 0.864% |
| 71 | 16.413 | 4677 | 4688 | 4699 | rBV6 | 22162 | 38644 | 3.35% | 0.312% |

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

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\SOMUTR061720WMA.M
Title : TRACE VOA SOM01.0

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 16.838 | 4809 | 4820 | 4831 | rBV2 | 176966 | 292979 | 25.42% | 2.367% |
| 73 | 16.963 | 4848 | 4859 | 4871 | rBV2 | 221455 | 381864 | 33.13% | 3.085% |

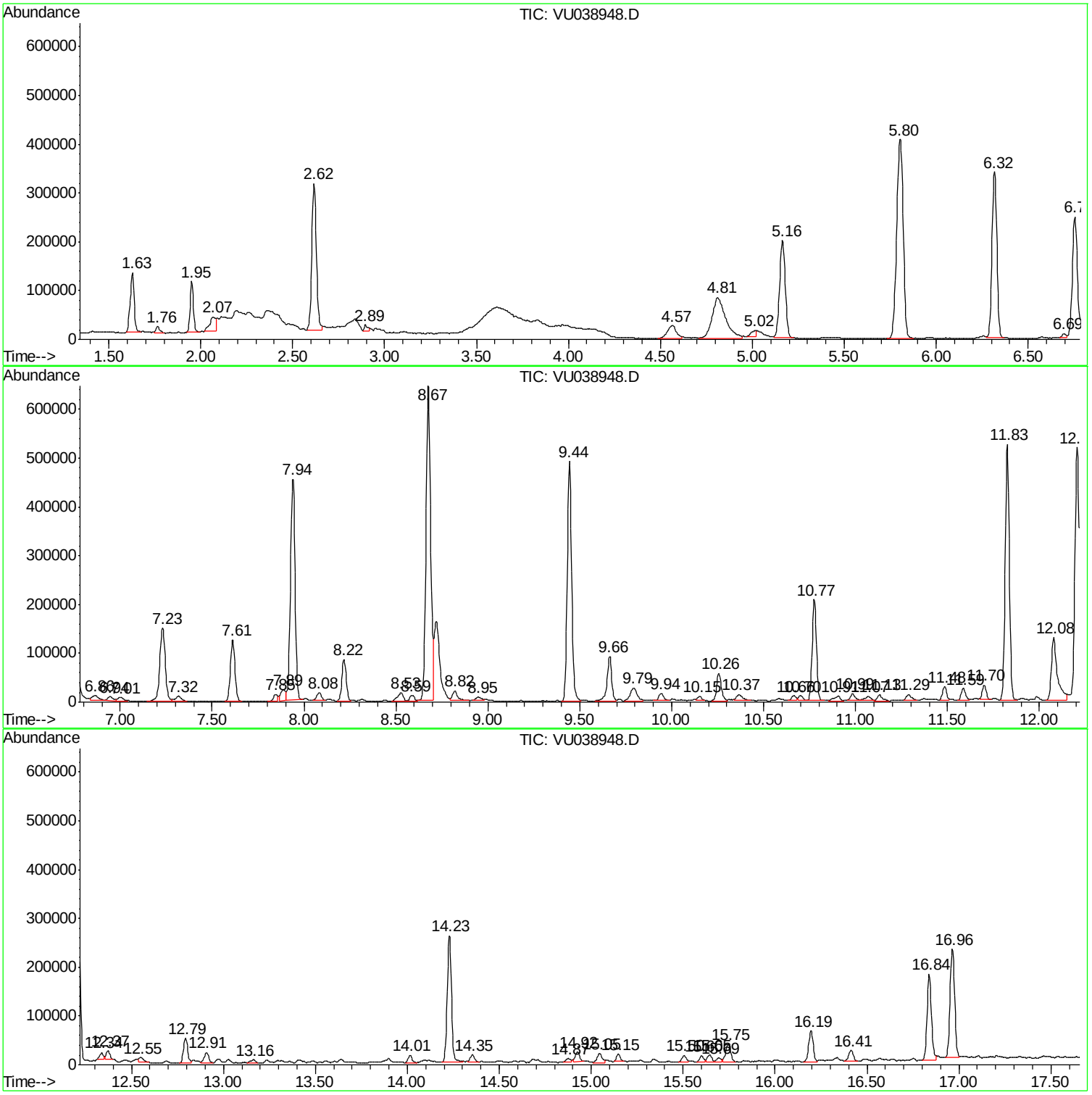
Sum of corrected areas: 12378364

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

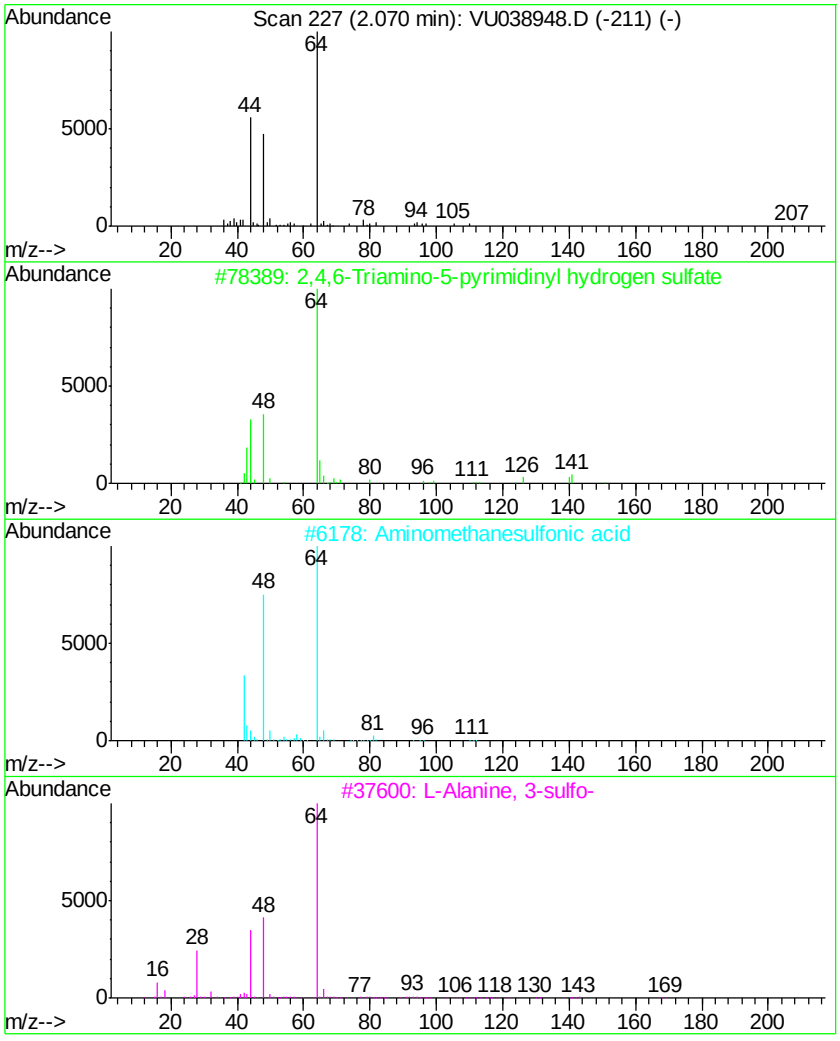
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

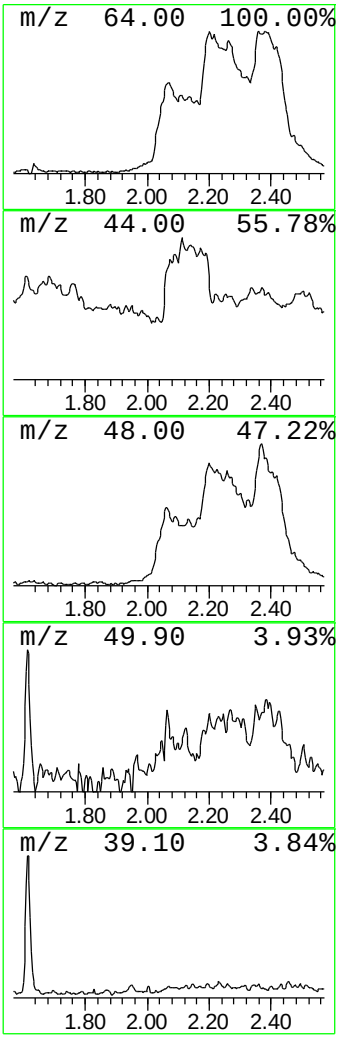
**********

Peak Number 1 2,4,6-Triamino-5-pyrimidiny... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.07 | 0.54 ug/L | 66597 | 1,4-Difluorobenzene | 6.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,6-Triamino-5-pyrimidinyl hyd... | 221 | C4H7N5O4S | 071552-23-3 | 74 |
| 2 | Aminomethanesulfonic acid | 111 | CH5NO3S | 013881-91-9 | 72 |
| 3 | L-Alanine, 3-sulfo- | 169 | C3H7NO5S | 000498-40-8 | 64 |
| 4 | Sulfur dioxide | 64 | O2S | 007446-09-5 | 56 |
| 5 | 4,6-Diamino-5-pyrimidinyl hydrog... | 206 | C4H6N4O4S | 071525-41-2 | 43 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

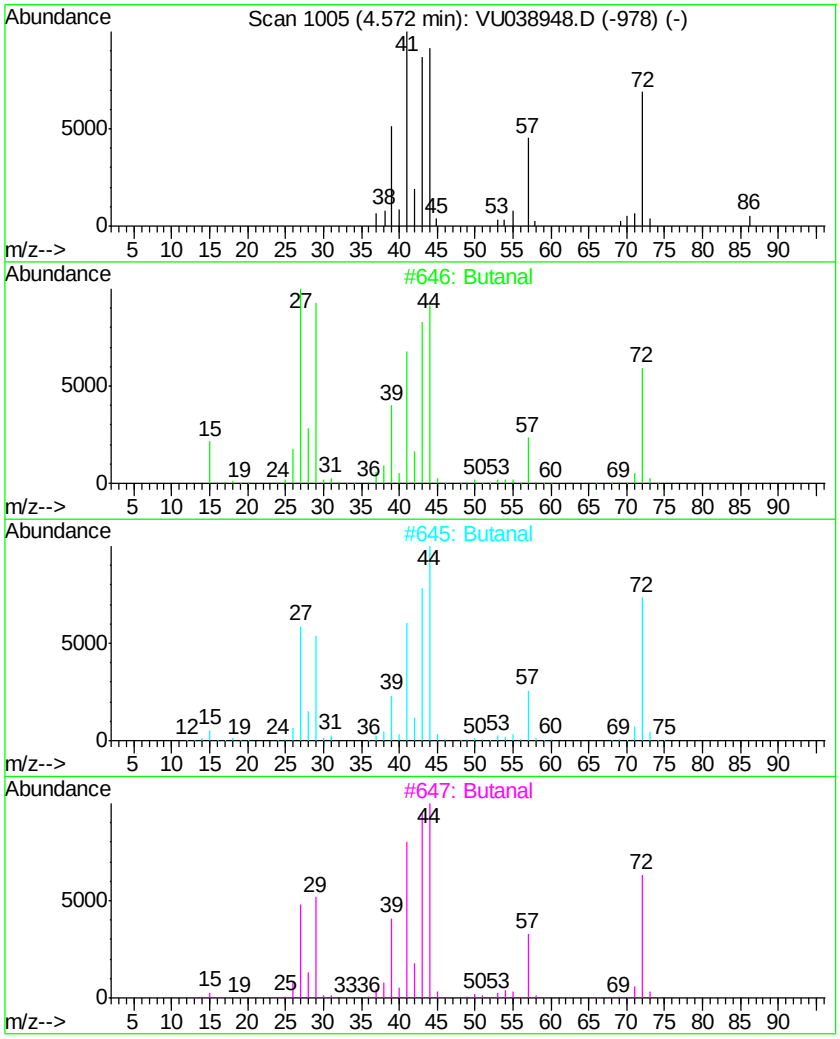
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

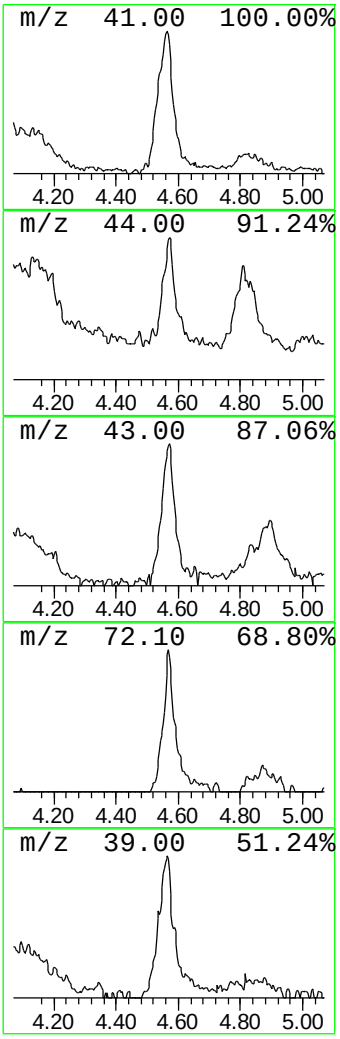
**********

Peak Number 2 Butanal Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.57 | 0.73 ug/L | 91175 | 1,4-Difluorobenzene | 6.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butanal | 72 | C4H8O | 000123-72-8 | 64 |
| 2 | Butanal | 72 | C4H8O | 000123-72-8 | 50 |
| 3 | Butanal | 72 | C4H8O | 000123-72-8 | 43 |
| 4 | Butanal | 72 | C4H8O | 000123-72-8 | 38 |
| 5 | Propanal, 2-methyl- | 72 | C4H8O | 000078-84-2 | 38 |



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

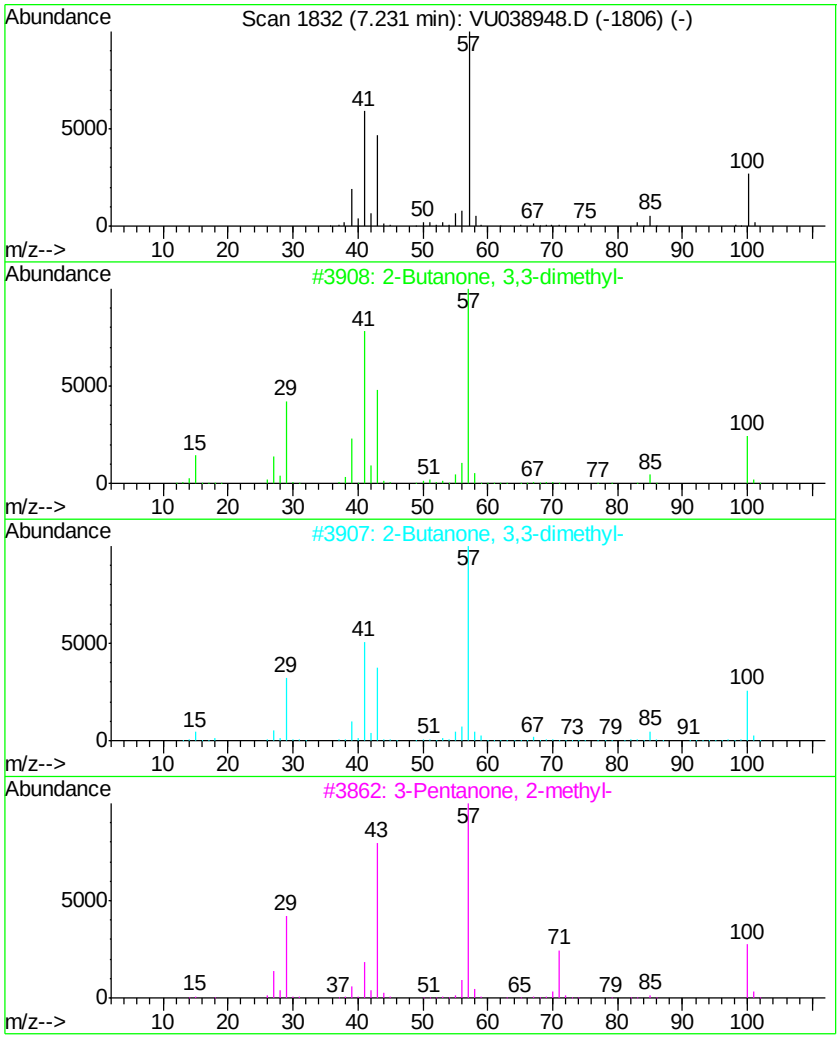
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

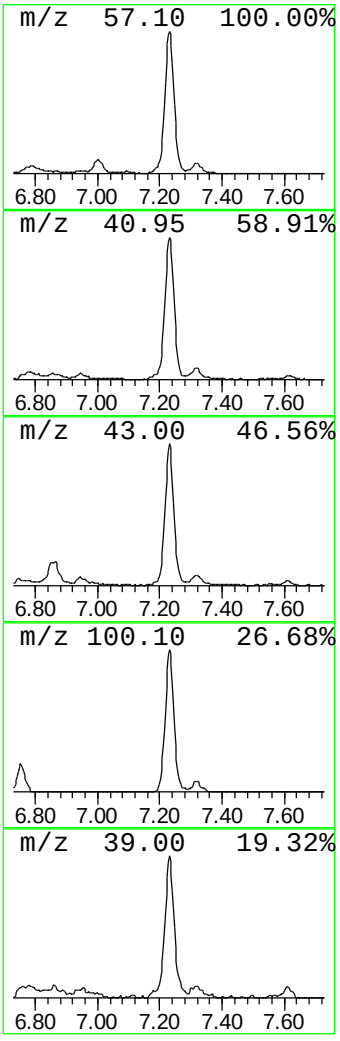
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.23 | 2.54 ug/L | 315096 | 1,4-Difluorobenzene | 6.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O | 000075-97-8 | 91 |
| 2 | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O | 000075-97-8 | 86 |
| 3 | 3-Pentanone, 2-methyl- | 100 | C6H12O | 000565-69-5 | 80 |
| 4 | 3-Pentanone, 2-methyl- | 100 | C6H12O | 000565-69-5 | 59 |
| 5 | 3-Hexanone | 100 | C6H12O | 000589-38-8 | 59 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

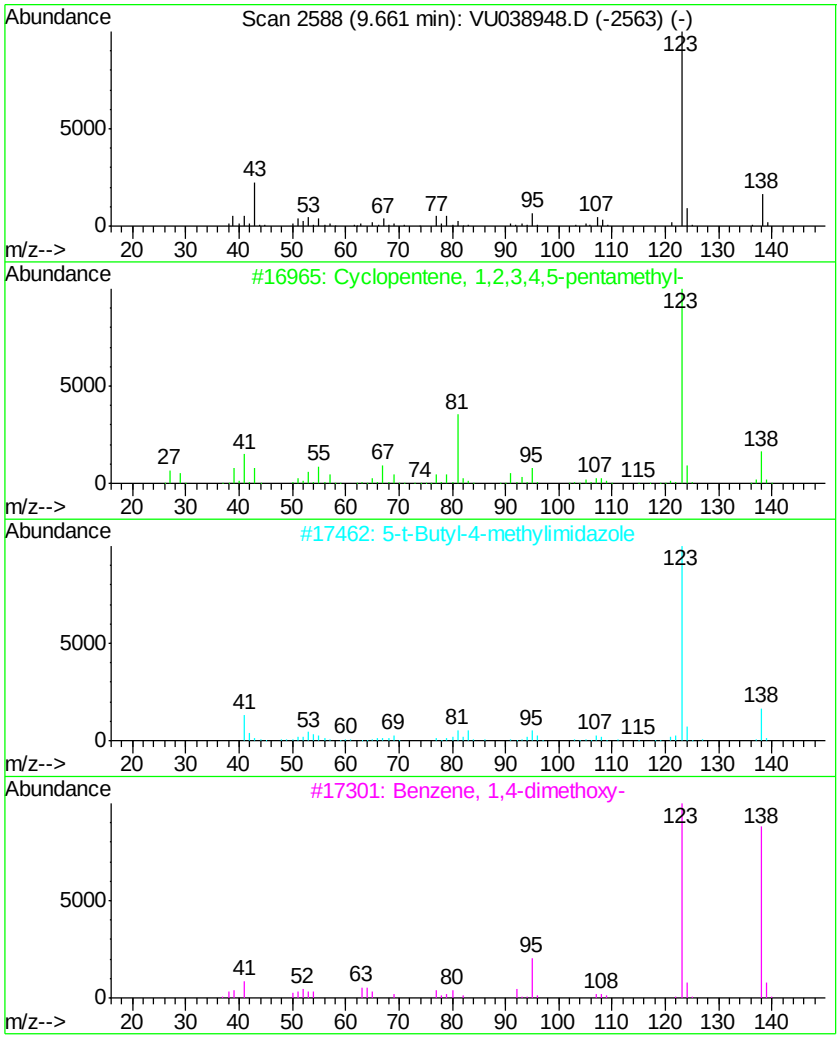
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

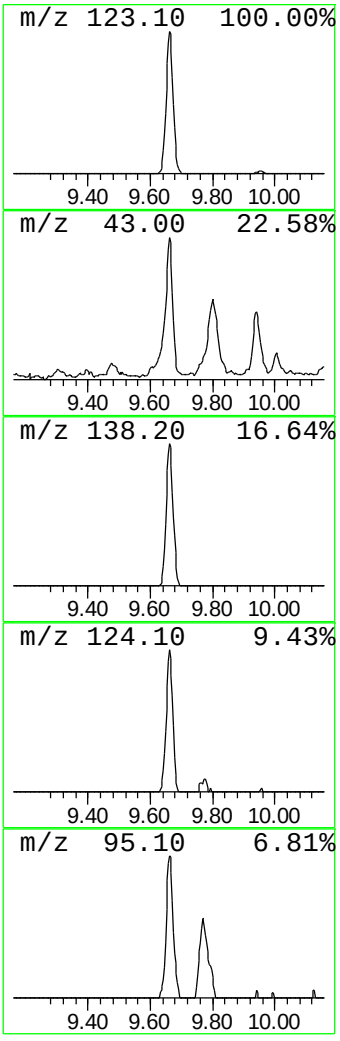
**********

Peak Number 5 Cyclopentene, 1,2,3,4,5-pen... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.66 | 0.98 ug/L | 161658 | Chlorobenzene-d5 | 9.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopentene, 1,2,3,4,5-pentamet... | 138 | C10H18 | 1000154-28-6 | 90 |
| 2 | 5-t-Butyl-4-methylimidazole | 138 | C8H14N2 | 146979-50-2 | 86 |
| 3 | Benzene, 1,4-dimethoxy- | 138 | C8H10O2 | 000150-78-7 | 80 |
| 4 | 1,6,6-Trimethyl-7-(3-oxobut-1-en... | 236 | C13H16O4 | 1000192-00-9 | 78 |
| 5 | Cyclopentene, 1,2,3,3,4-pentamet... | 138 | C10H18 | 197390-29-7 | 78 |



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

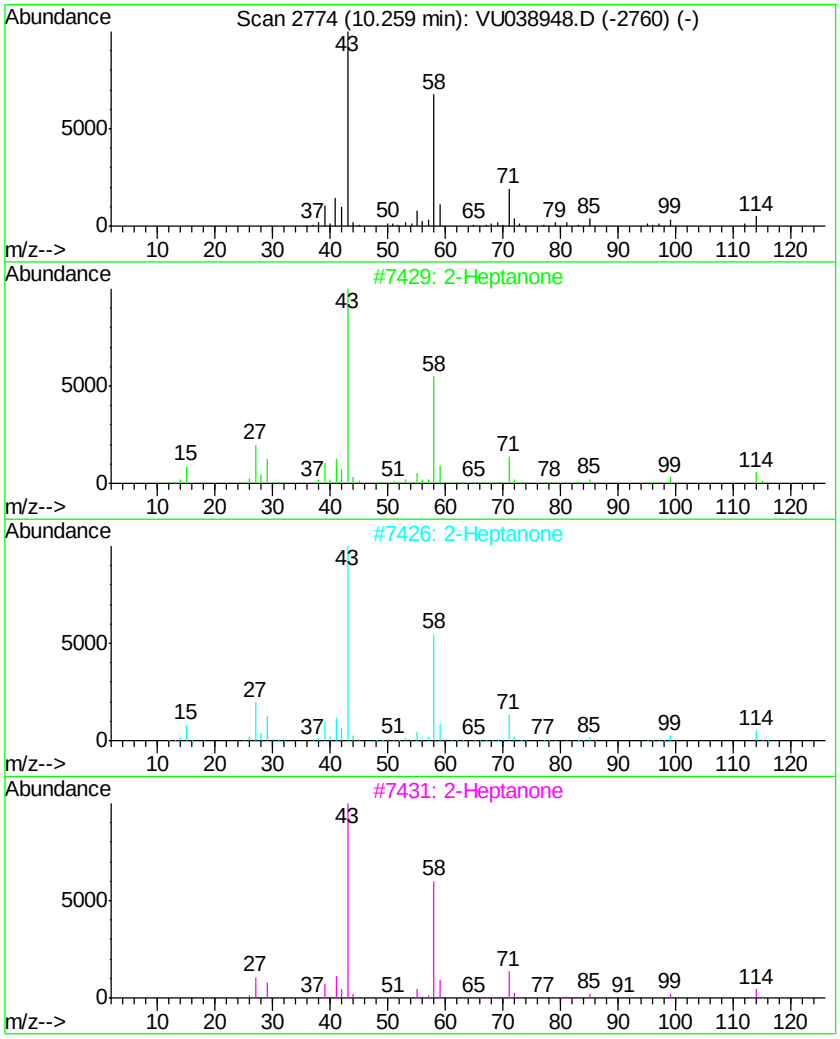
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

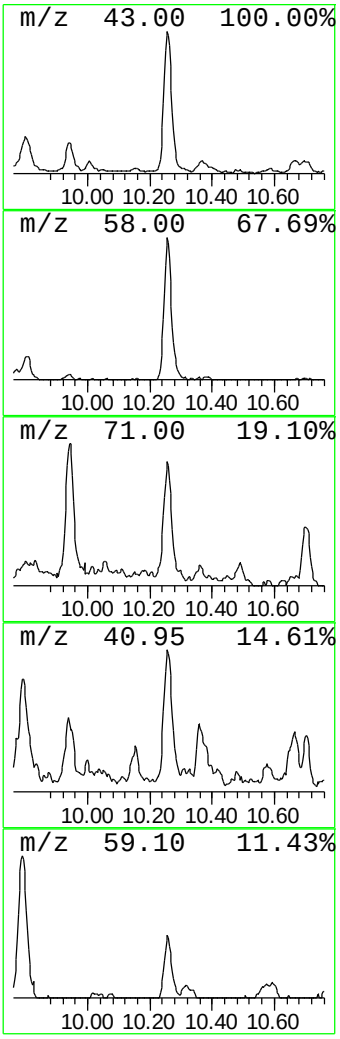
**********

Peak Number 6 2-Heptanone Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.26 | 0.60 ug/L | 98358 | Chlorobenzene-d5 | 9.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Heptanone | 114 | C7H14O | 000110-43-0 | 91 |
| 2 | 2-Heptanone | 114 | C7H14O | 000110-43-0 | 91 |
| 3 | 2-Heptanone | 114 | C7H14O | 000110-43-0 | 90 |
| 4 | 2-Hexanone, 5-methyl- | 114 | C7H14O | 000110-12-3 | 78 |
| 5 | 2-Hexanone, 5-methyl- | 114 | C7H14O | 000110-12-3 | 59 |



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

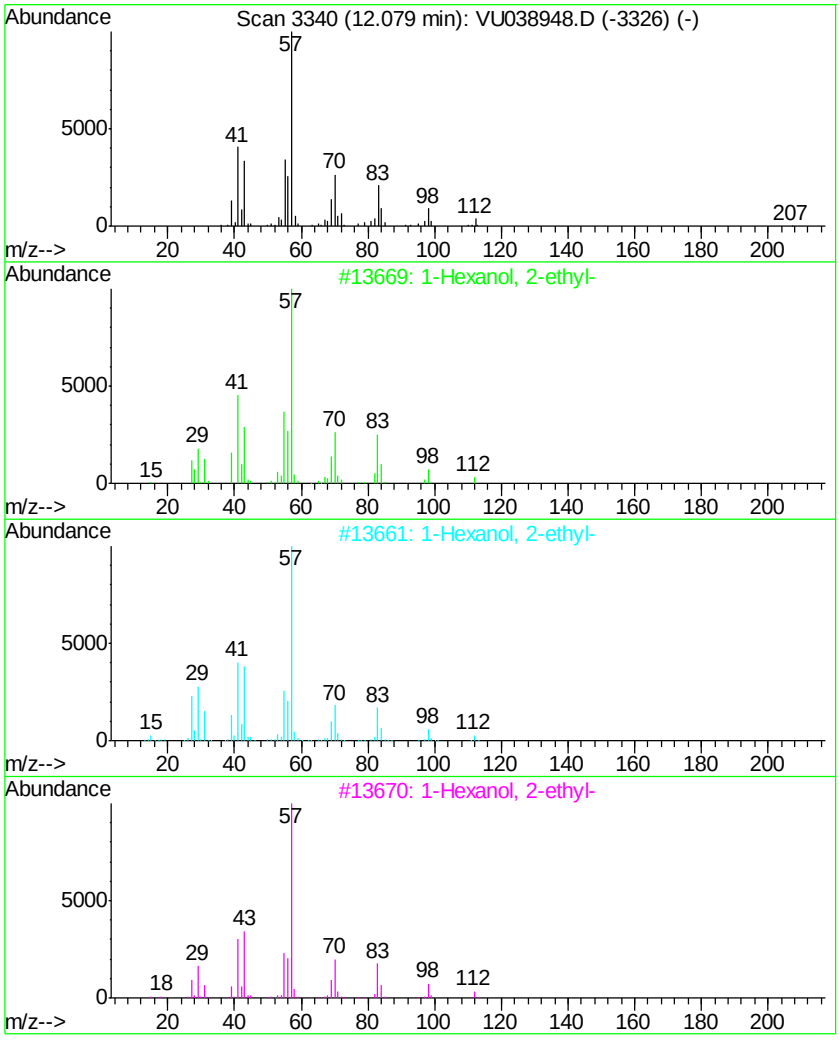
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

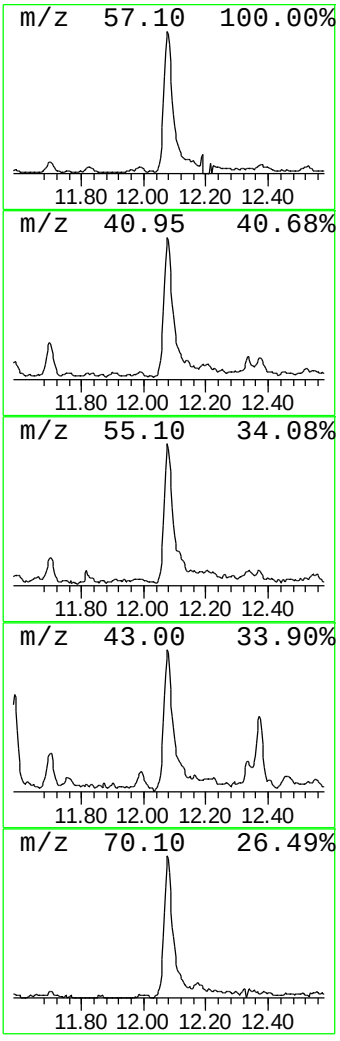
**********

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.08 | 1.78 ug/L | 294593 | 1,4-Dichlorobenzene-d4 | 11.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 90 |
| 2 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 90 |
| 3 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 83 |
| 4 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 78 |
| 5 | 2-Ethyl-1-hexanol, pentafluoropr... | 276 | C11H17F5O2 | 1000365-51-1 | 59 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

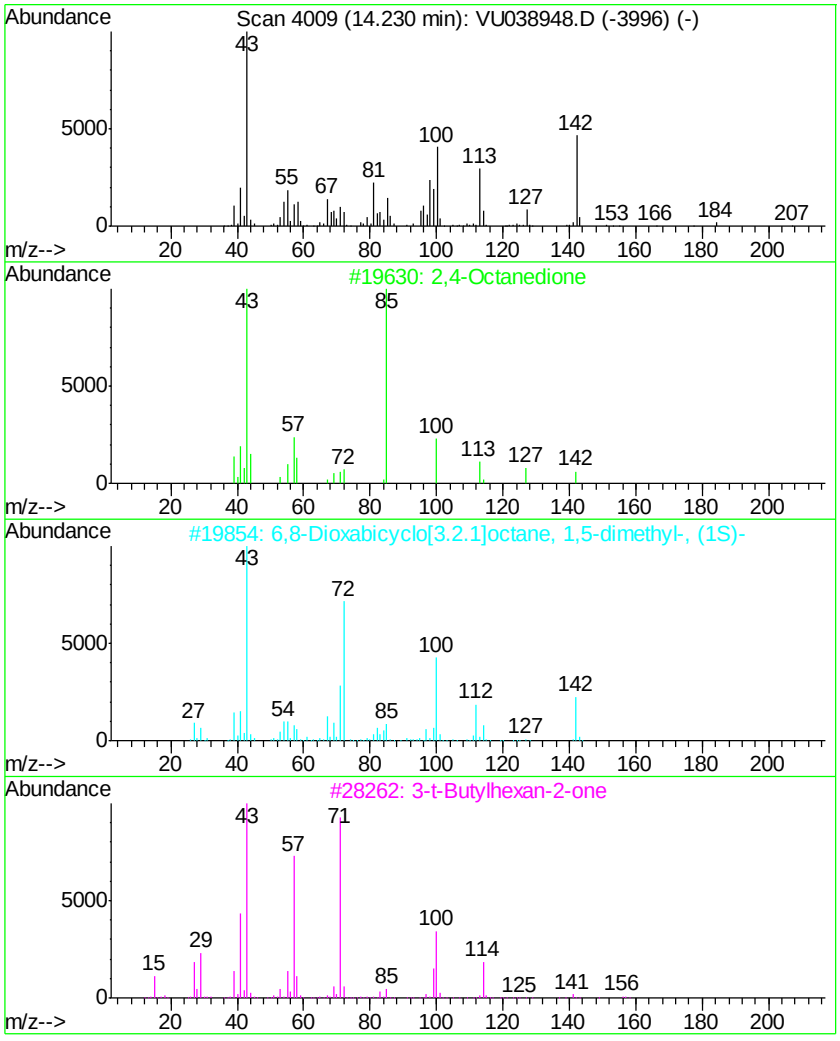
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

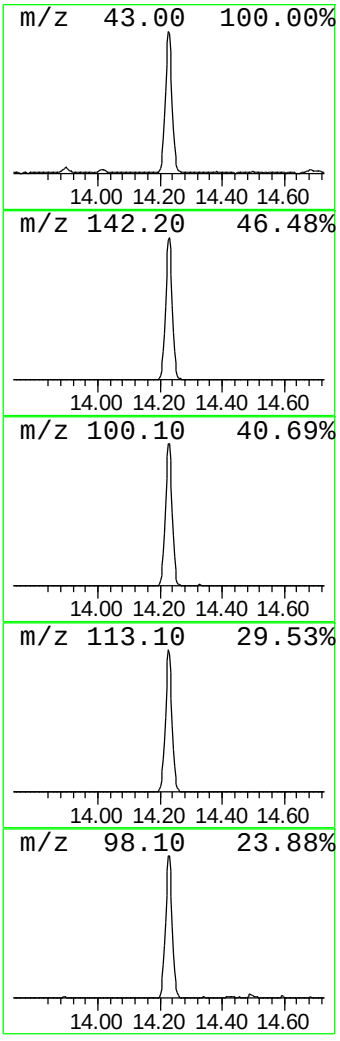
**********

Peak Number 8 2,4-Octanedione Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.23 | 2.45 ug/L | 406224 | 1,4-Dichlorobenzene-d4 | 11.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4-Octanedione | 142 | C8H14O2 | 014090-87-0 | 50 |
| 2 | 6,8-Dioxabicyclo[3.2.1]octane, 1... | 142 | C8H14O2 | 028401-39-0 | 38 |
| 3 | 3-t-Butylhexan-2-one | 156 | C10H20O | 1000202-22-9 | 12 |
| 4 | Cyclohexanemethylamine | 113 | C7H15N | 003218-02-8 | 11 |
| 5 | 6-Dodecanone | 184 | C12H24O | 006064-27-3 | 10 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

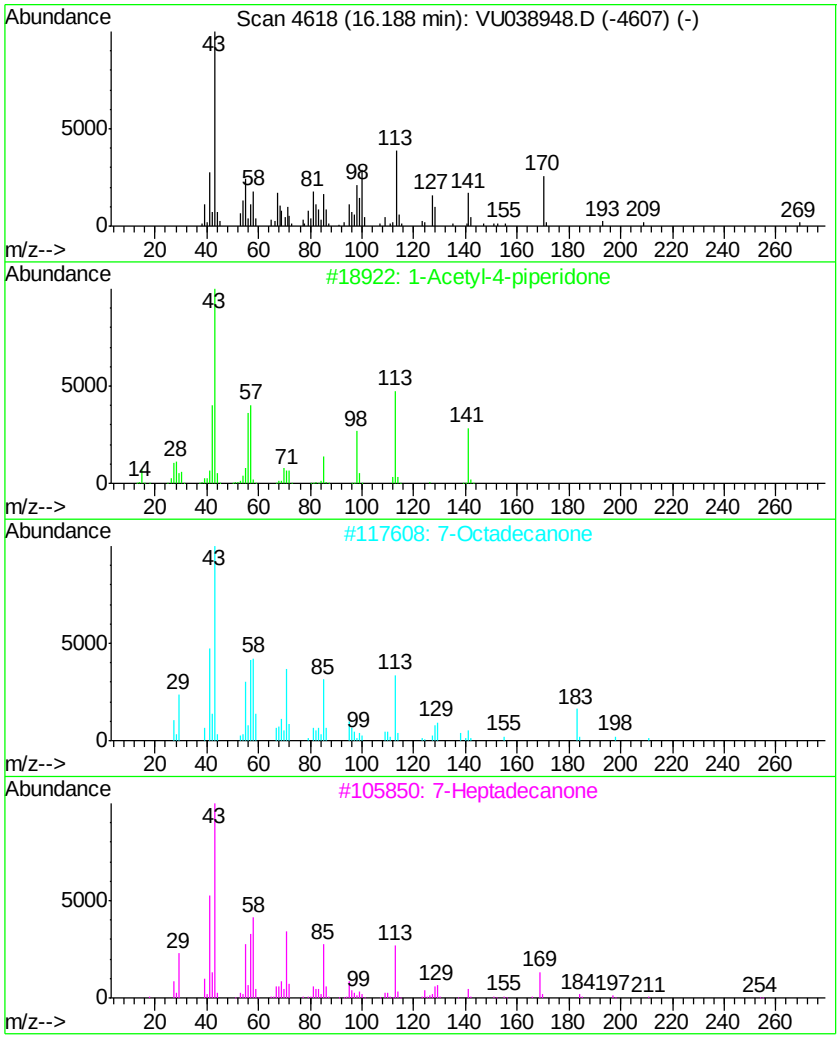
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

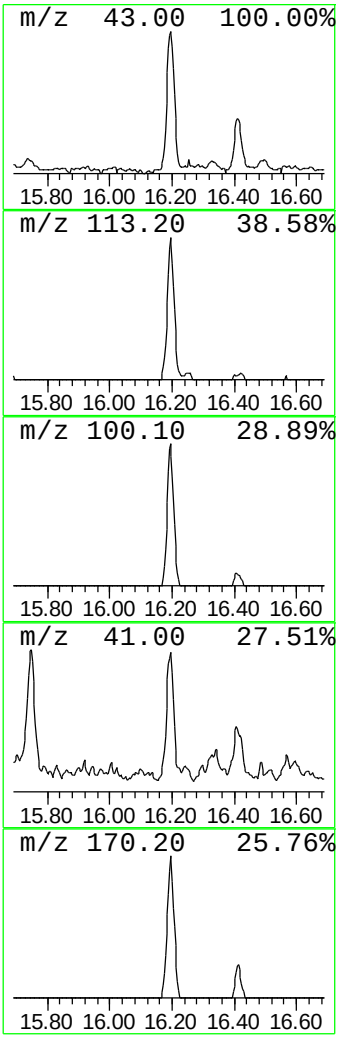
**********

Peak Number 9 unknown-01 Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.19 | 0.64 ug/L | 106991 | 1,4-Dichlorobenzene-d4 | 11.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Acetyl-4-piperidone | 141 | C7H11NO2 | 032161-06-1 | 38 |
| 2 | 7-Octadecanone | 268 | C18H36O | 018277-00-4 | 25 |
| 3 | 7-Heptadecanone | 254 | C17H34O | 006064-42-2 | 25 |
| 4 | Allyl heptanoate | 170 | C10H18O2 | 000142-19-8 | 22 |
| 5 | 1-Acetyl-5,5-dimethyl-2,4-dioxoi... | 170 | C7H10N2O3 | 006341-67-9 | 22 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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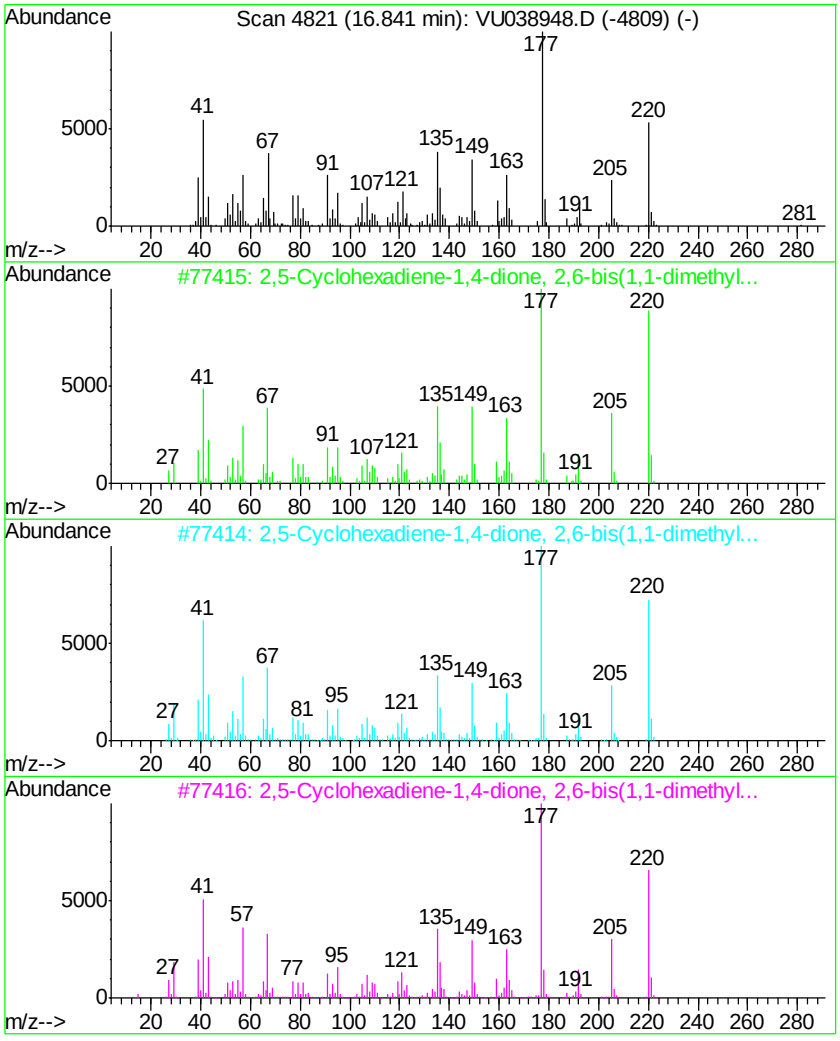
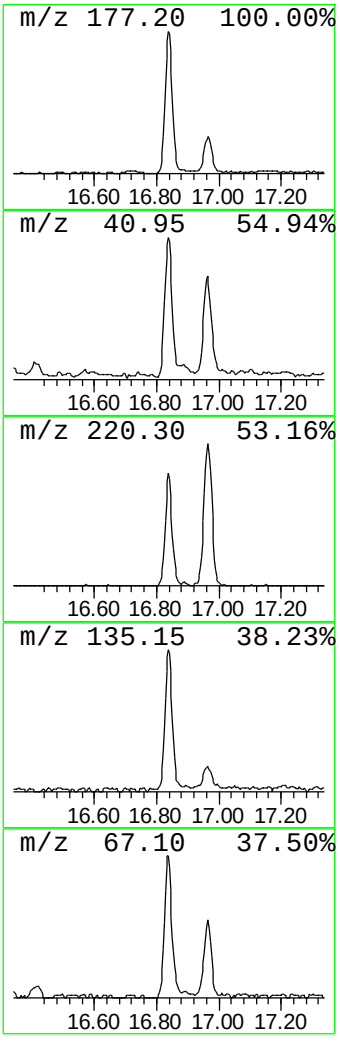
Peak Number 10 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.84 | 1.77 ug/L | 292979 | 1,4-Dichlorobenzene-d4 | 11.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 99 |
| 2 | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 97 |
| 3 | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 87 |
| 4 | Thiocoumarine, 4,4,6,7-tetramethyl- | 220 | C13H16OS | 1000128-90-2 | 53 |
| 5 | N-[4-(Ethyl-methyl-amino)-phenyl... | 192 | C11H16N2O | 099981-45-0 | 46 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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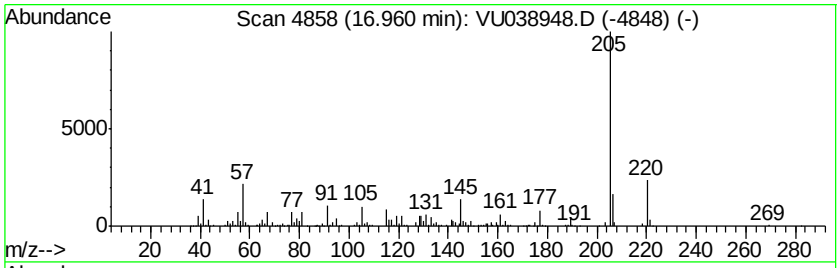
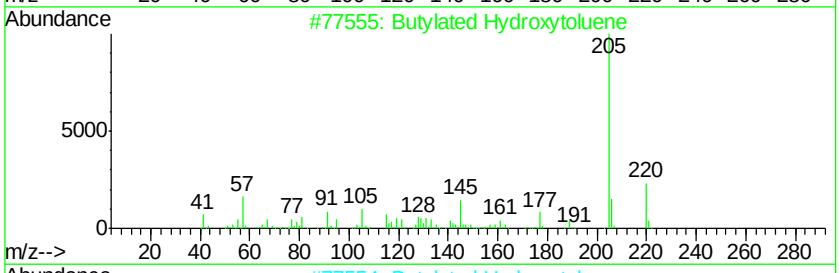
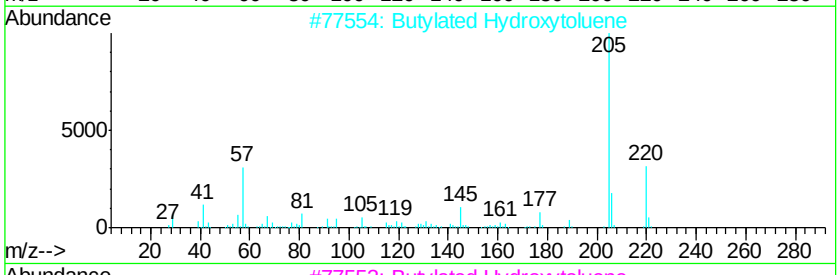
Peak Number 11 Butylated Hydroxytoluene Concentration Rank 3

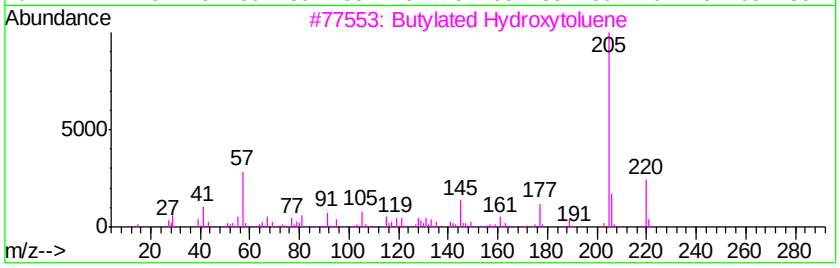
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.96 | 2.30 ug/L | 381864 | 1,4-Dichlorobenzene-d4 | 11.83 |

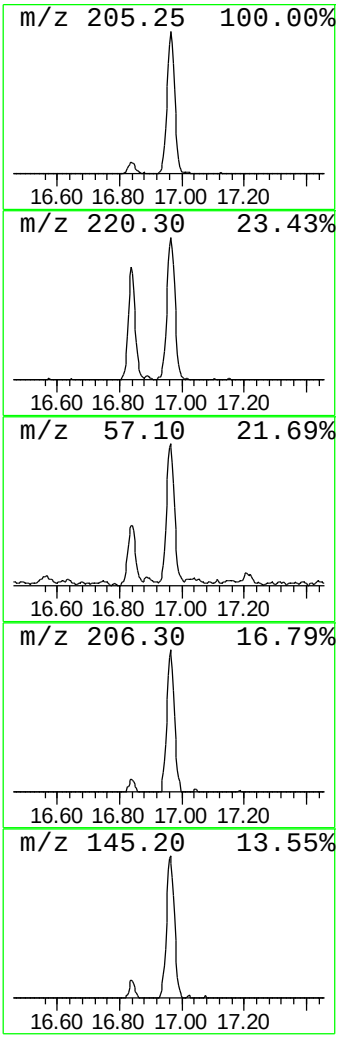
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 98 |
| 2 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 97 |
| 3 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 96 |
| 4 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 94 |
| 5 | Phenol, 4,6-di(1,1-dimethylethyl... | 220 | C15H24O | 000616-55-7 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038948.D
Acq On : 17 Jun 2020 16:53
Operator : SY/MD
Sample : L3040-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L11

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.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 |
| 2,4,6-Triamino-5-... | 2.07 | 0.5 | ug/L | 66597 | 1 | 6.32 | 620727 | 5.0 |
| Butanal | 4.57 | 0.7 | ug/L | 91175 | 1 | 6.32 | 620727 | 5.0 |
| 2-Butanone, 3,3-d... | 7.23 | 2.5 | ug/L | 315096 | 1 | 6.32 | 620727 | 5.0 |
| Cyclopentene, 1,2... | 9.66 | 1.0 | ug/L | 161658 | 2 | 9.44 | 822466 | 5.0 |
| 2-Heptanone | 10.26 | 0.6 | ug/L | 98358 | 2 | 9.44 | 822466 | 5.0 |
| 1-Hexanol, 2-ethyl- | 12.08 | 1.8 | ug/L | 294593 | 3 | 11.83 | 829708 | 5.0 |
| 2,4-Octanedione | 14.23 | 2.5 | ug/L | 406224 | 3 | 11.83 | 829708 | 5.0 |
| unknown-01 | 16.19 | 0.6 | ug/L | 106991 | 3 | 11.83 | 829708 | 5.0 |
| 2,5-Cyclohexadien... | 16.84 | 1.8 | ug/L | 292979 | 3 | 11.83 | 829708 | 5.0 |
| Butylated Hydroxy... | 16.96 | 2.3 | ug/L | 381864 | 3 | 11.83 | 829708 | 5.0 |