LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038946.D
Acq On : 17 Jun 2020 16:07
Operator : SY/MD
Sample : L3040-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L09

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 | 1.404 | 16 | 20 | 30 | rVB3 | 14837 | 14822 | 1.06% | 0.130% |
| 2 | 1.662 | 89 | 100 | 114 | rVB2 | 130850 | 191725 | 13.76% | 1.677% |
| 3 | 1.993 | 194 | 203 | 218 | rBV | 103566 | 143961 | 10.33% | 1.259% |
| 4 | 2.086 | 219 | 232 | 234 | rBV10 | 18389 | 36713 | 2.63% | 0.321% |
| 5 | 2.411 | 328 | 333 | 344 | rVB2 | 29893 | 44863 | 3.22% | 0.392% |
| 6 | 2.645 | 396 | 406 | 425 | rVB | 278946 | 472470 | 33.90% | 4.133% |
| 7 | 2.871 | 472 | 476 | 488 | rBV2 | 13505 | 21975 | 1.58% | 0.192% |
| 8 | 4.562 | 988 | 1002 | 1004 | rBV9 | 9205 | 20024 | 1.44% | 0.175% |
| 9 | 4.838 | 1056 | 1088 | 1124 | rBV2 | 89264 | 496519 | 35.63% | 4.343% |
| 10 | 5.189 | 1181 | 1197 | 1217 | rVB2 | 186877 | 425743 | 30.55% | 3.724% |
| 11 | 5.832 | 1377 | 1397 | 1426 | rBV2 | 413062 | 995605 | 71.44% | 8.709% |
| 12 | 6.340 | 1542 | 1555 | 1573 | rVB | 354466 | 649928 | 46.64% | 5.685% |
| 13 | 6.774 | 1675 | 1690 | 1711 | rBV | 242110 | 463079 | 33.23% | 4.051% |
| 14 | 7.247 | 1811 | 1837 | 1853 | rBV | 101319 | 217806 | 15.63% | 1.905% |
| 15 | 7.626 | 1941 | 1955 | 1968 | rBV2 | 123409 | 216391 | 15.53% | 1.893% |
| 16 | 7.951 | 2044 | 2056 | 2071 | rVB | 432900 | 739207 | 53.04% | 6.466% |
| 17 | 8.227 | 2130 | 2142 | 2156 | rBV | 85824 | 139615 | 10.02% | 1.221% |
| 18 | 8.536 | 2220 | 2238 | 2248 | rBV2 | 21535 | 50787 | 3.64% | 0.444% |
| 19 | 8.597 | 2248 | 2257 | 2267 | rVB7 | 11414 | 20728 | 1.49% | 0.181% |
| 20 | 8.684 | 2267 | 2284 | 2318 | rBV | 692366 | 1393583 | 100.00% | 12.191% |
| 21 | 9.449 | 2510 | 2522 | 2544 | rBV | 510083 | 861833 | 61.84% | 7.539% |
| 22 | 9.639 | 2564 | 2581 | 2587 | rBV4 | 12320 | 26577 | 1.91% | 0.232% |
| 23 | 9.793 | 2617 | 2629 | 2638 | rBV2 | 8885 | 17447 | 1.25% | 0.153% |
| 24 | 9.944 | 2662 | 2676 | 2688 | rBV2 | 13845 | 24432 | 1.75% | 0.214% |
| 25 | 10.703 | 2906 | 2912 | 2923 | rVV2 | 22022 | 33049 | 2.37% | 0.289% |
| 26 | 10.777 | 2923 | 2935 | 2949 | rVB | 209109 | 335251 | 24.06% | 2.933% |
| 27 | 10.909 | 2959 | 2976 | 2986 | rBV6 | 15561 | 27511 | 1.97% | 0.241% |
| 28 | 10.983 | 2988 | 2999 | 3012 | rBV2 | 25559 | 44352 | 3.18% | 0.388% |
| 29 | 11.825 | 3249 | 3261 | 3275 | rBV | 542165 | 859157 | 61.65% | 7.516% |
| 30 | 11.989 | 3307 | 3312 | 3327 | rVB4 | 12423 | 19728 | 1.42% | 0.173% |
| 31 | 12.079 | 3327 | 3340 | 3344 | rBV5 | 9886 | 17140 | 1.23% | 0.150% |
| 32 | 12.208 | 3366 | 3380 | 3393 | rBV | 493677 | 796399 | 57.15% | 6.967% |
| 33 | 12.336 | 3402 | 3420 | 3433 | rBV2 | 24183 | 48417 | 3.47% | 0.424% |
| 34 | 12.529 | 3469 | 3480 | 3484 | rBV6 | 9442 | 16748 | 1.20% | 0.147% |

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038946.D
Acq On : 17 Jun 2020 16:07
Operator : SY/MD
Sample : L3040-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L09

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 | 12.793 | 3555 | 3562 | 3574 | rBV2 | 10528 | 17482 | 1.25% | 0.153% |
| 36 | 12.909 | 3585 | 3598 | 3605 | rBV8 | 9751 | 15362 | 1.10% | 0.134% |
| 37 | 12.970 | 3608 | 3617 | 3627 | rBV4 | 13167 | 20010 | 1.44% | 0.175% |
| 38 | 13.166 | 3668 | 3678 | 3691 | rVB4 | 8594 | 18179 | 1.30% | 0.159% |
| 39 | 14.230 | 3993 | 4009 | 4022 | rBV | 139340 | 226720 | 16.27% | 1.983% |
| 40 | 14.352 | 4037 | 4047 | 4061 | rVB2 | 61971 | 101577 | 7.29% | 0.889% |
| 41 | 15.044 | 4251 | 4262 | 4273 | rBV6 | 17283 | 33955 | 2.44% | 0.297% |
| 42 | 15.147 | 4284 | 4294 | 4312 | rBV3 | 15088 | 27023 | 1.94% | 0.236% |
| 43 | 15.507 | 4395 | 4406 | 4414 | rBV5 | 11031 | 18104 | 1.30% | 0.158% |
| 44 | 15.642 | 4441 | 4448 | 4456 | rVB5 | 12711 | 18137 | 1.30% | 0.159% |
| 45 | 15.748 | 4470 | 4481 | 4494 | rVB2 | 38789 | 71641 | 5.14% | 0.627% |
| 46 | 16.195 | 4608 | 4620 | 4630 | rBV3 | 55916 | 91692 | 6.58% | 0.802% |
| 47 | 16.417 | 4682 | 4689 | 4701 | rVB3 | 9930 | 18484 | 1.33% | 0.162% |
| 48 | 16.838 | 4811 | 4820 | 4830 | rBV3 | 100870 | 161468 | 11.59% | 1.412% |
| 49 | 16.963 | 4847 | 4859 | 4877 | rBV | 415949 | 708082 | 50.81% | 6.194% |

Sum of corrected areas: 11431501

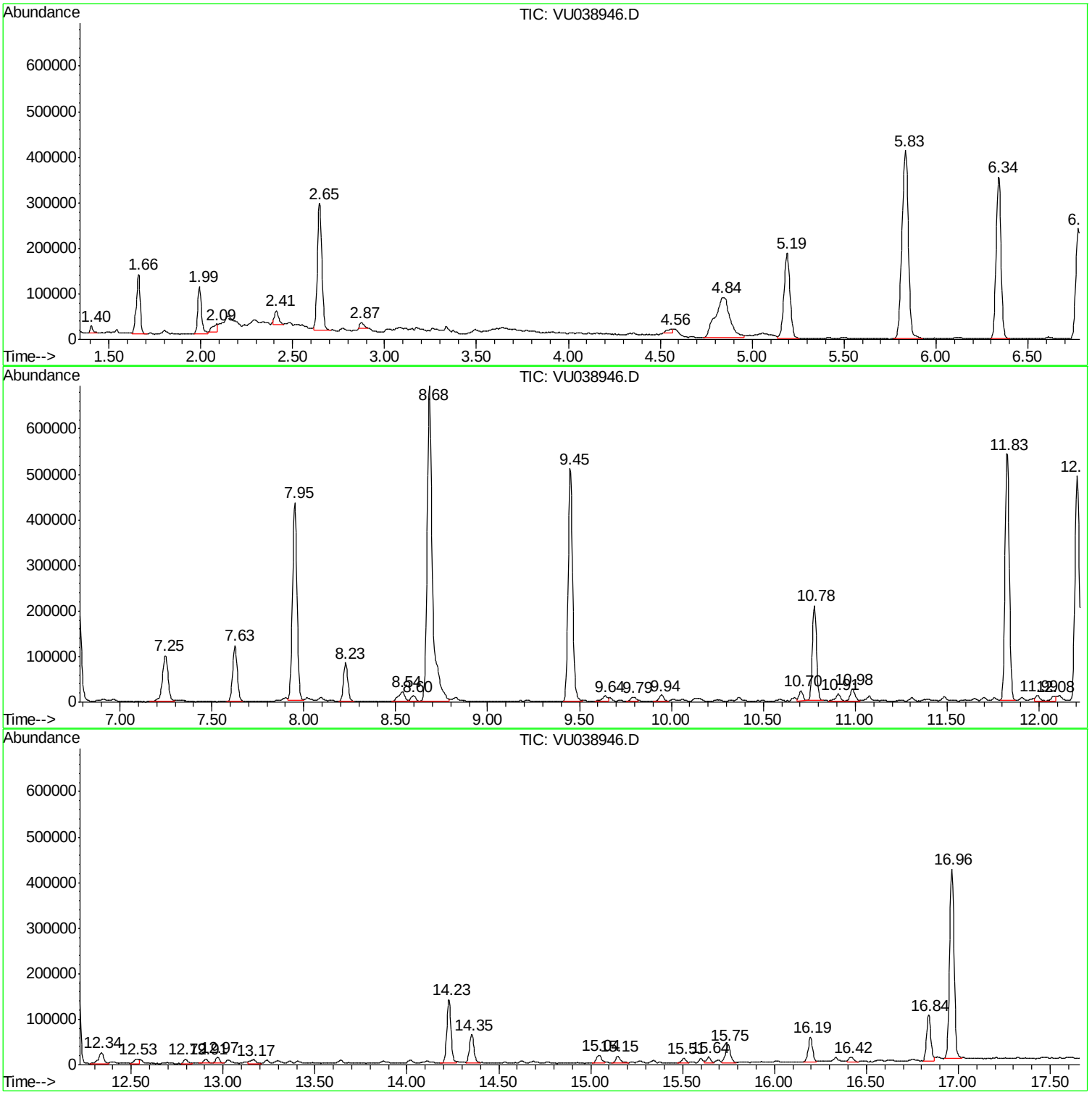
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038946.D
Acq On : 17 Jun 2020 16:07
Operator : SY/MD
Sample : L3040-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L09

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



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038946.D
Acq On : 17 Jun 2020 16:07
Operator : SY/MD
Sample : L3040-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L09

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

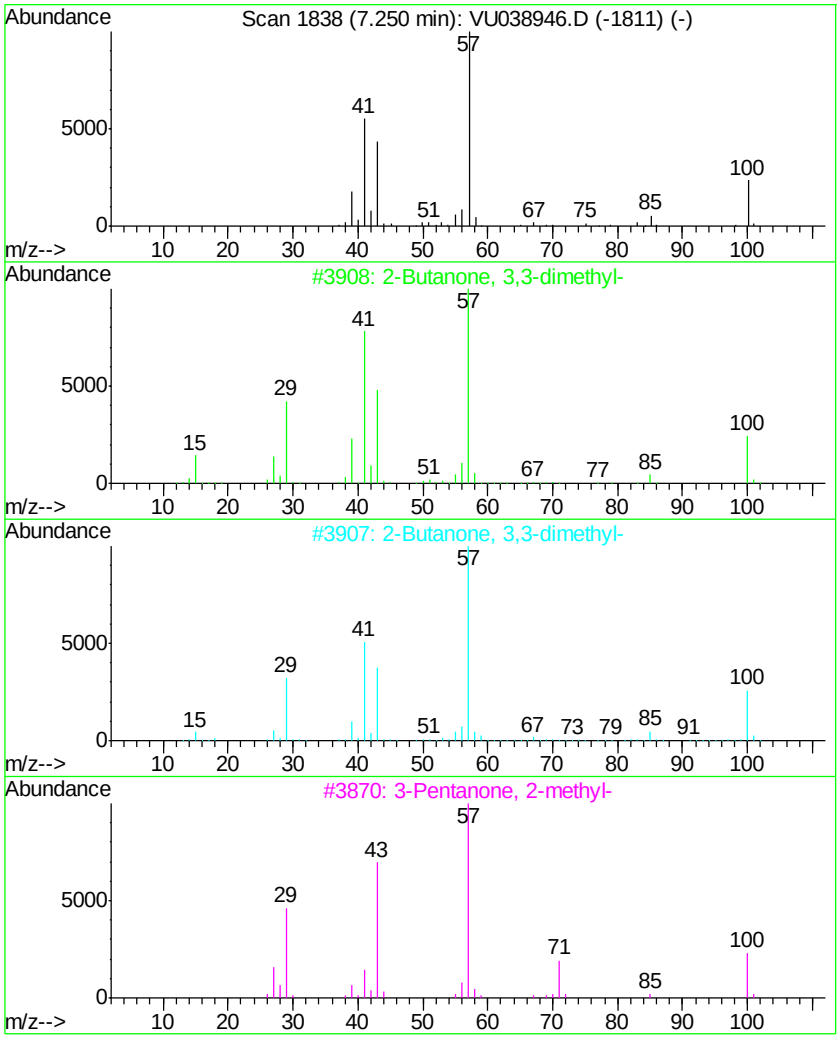
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

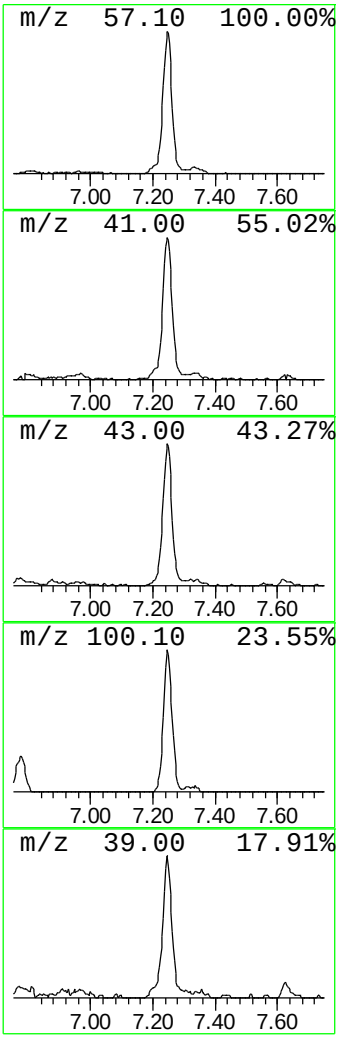
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.25 | 1.68 ug/L | 217806 | 1,4-Difluorobenzene | 6.34 |

| 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 | 87 |
| 3 | 3-Pentanone, 2-methyl- | 100 | C6H12O | 000565-69-5 | 80 |
| 4 | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O | 000075-97-8 | 72 |
| 5 | 3-Pentanone, 2-methyl- | 100 | C6H12O | 000565-69-5 | 53 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038946.D
Acq On : 17 Jun 2020 16:07
Operator : SY/MD
Sample : L3040-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L09

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

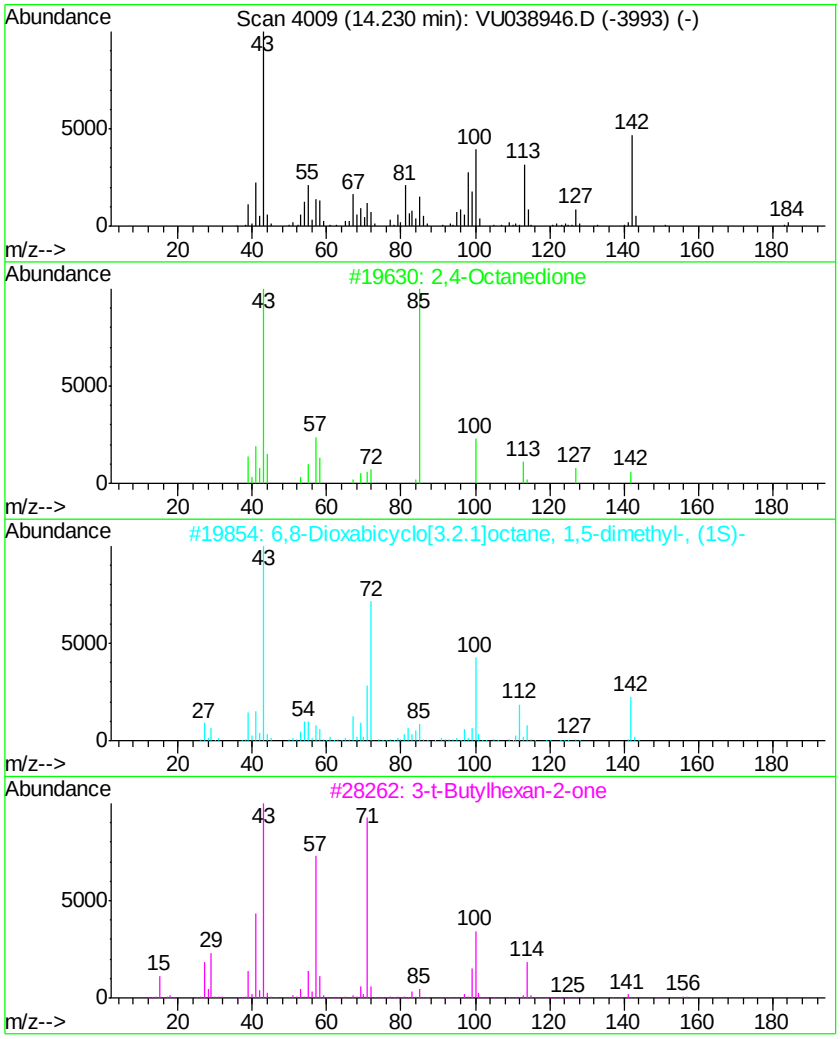
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

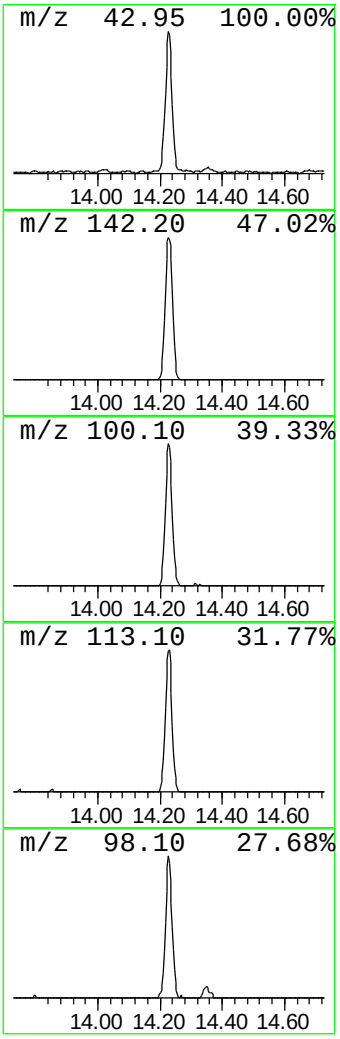
**********

Peak Number 3 2,4-Octanedione Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.23 | 1.32 ug/L | 226720 | 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 | 16 |
| 3 | 3-t-Butylhexan-2-one | 156 | C10H20O | 1000202-22-9 | 12 |
| 4 | Acetylacetone | 100 | C5H8O2 | 000123-54-6 | 10 |
| 5 | 5-Undecanone, 2-methyl- | 184 | C12H24O | 050639-02-6 | 10 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038946.D
Acq On : 17 Jun 2020 16:07
Operator : SY/MD
Sample : L3040-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L09

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

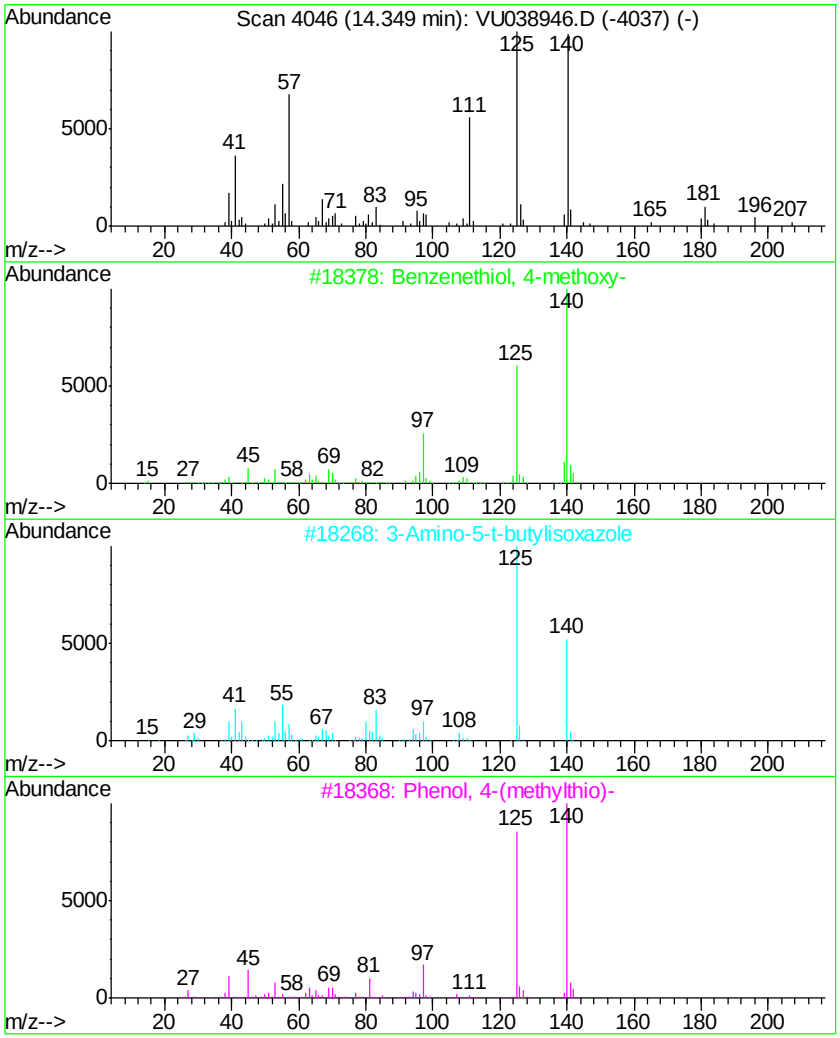
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

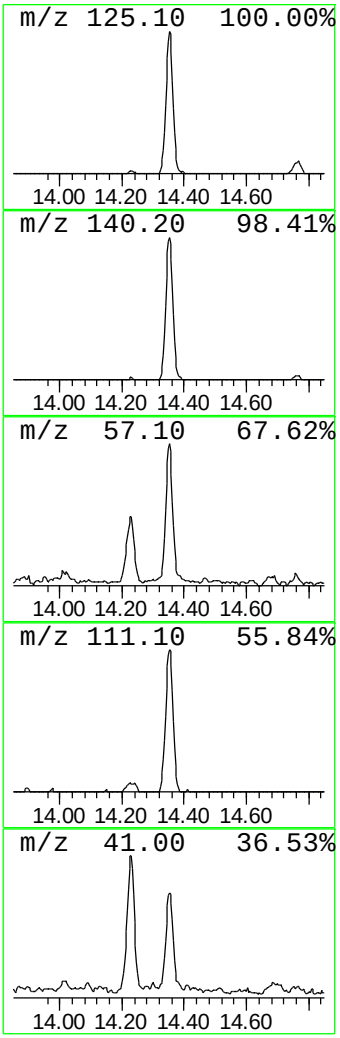
**********

Peak Number 4 Benzenethiol, 4-methoxy- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.35 | 0.59 ug/L | 101577 | 1,4-Dichlorobenzene-d4 | 11.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenethiol, 4-methoxy- | 140 | C7H8OS | 000696-63-9 | 53 |
| 2 | 3-Amino-5-t-butylisoxazole | 140 | C7H12N2O | 055809-36-4 | 53 |
| 3 | Phenol, 4-(methylthio)- | 140 | C7H8OS | 001073-72-9 | 53 |
| 4 | 1,4-Benzenediol, 2-methoxy- | 140 | C7H8O3 | 000824-46-4 | 53 |
| 5 | 1,2-Benzenediol, 3-methoxy- | 140 | C7H8O3 | 000934-00-9 | 53 |



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038946.D
Acq On : 17 Jun 2020 16:07
Operator : SY/MD
Sample : L3040-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L09

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

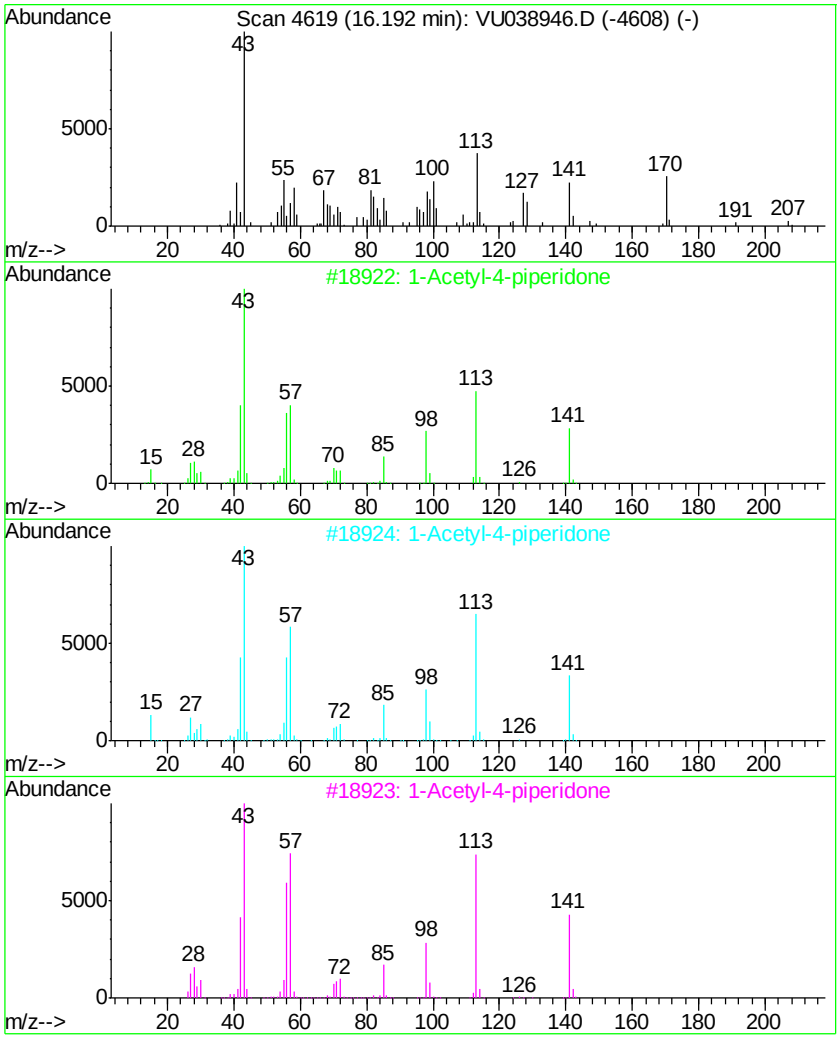
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

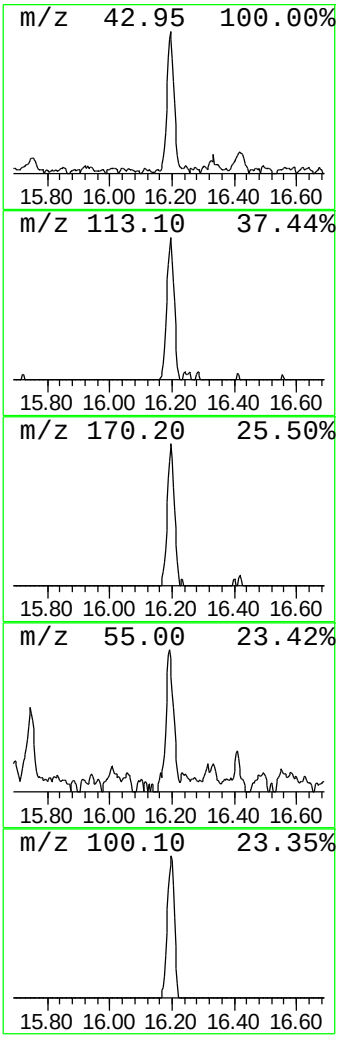
**********

Peak Number 5 unknown-01 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.19 | 0.53 ug/L | 91692 | 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 | 1-Acetyl-4-piperidone | 141 | C7H11NO2 | 032161-06-1 | 32 |
| 3 | 1-Acetyl-4-piperidone | 141 | C7H11NO2 | 032161-06-1 | 32 |
| 4 | Pyrrolidine, 1-(1-oxobutyl)- | 141 | C8H15NO | 033527-93-4 | 32 |
| 5 | 3,4-Diethoxy-3-cyclobutene-1,2-d... | 170 | C8H10O4 | 005231-87-8 | 27 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038946.D
Acq On : 17 Jun 2020 16:07
Operator : SY/MD
Sample : L3040-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L09

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

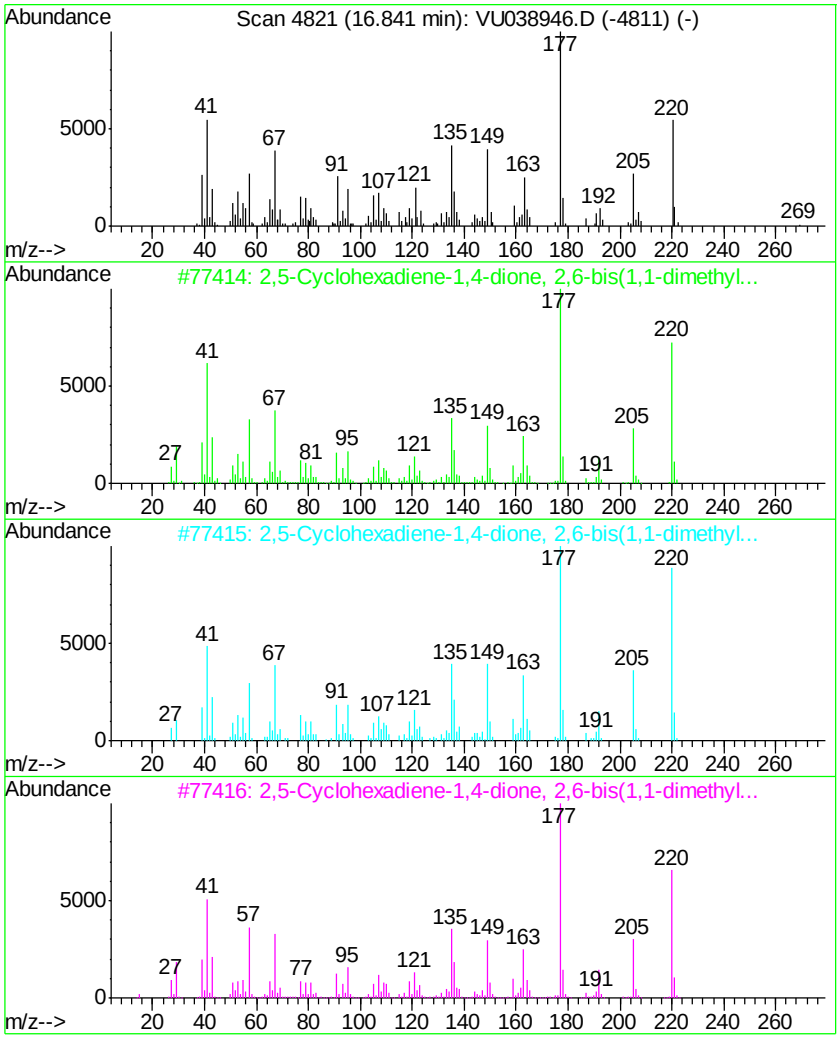
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

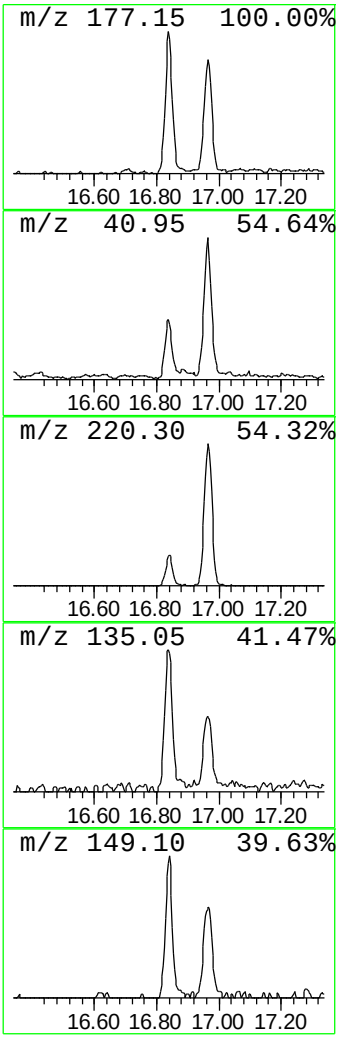
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.84 | 0.94 ug/L | 161468 | 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 | 96 |
| 2 | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 96 |
| 3 | 2,5-Cyclohexadiene-1,4-dione, 2,... | 220 | C14H20O2 | 000719-22-2 | 55 |
| 4 | Thiocoumarine, 4,4,6,7-tetramethyl- | 220 | C13H16OS | 1000128-90-2 | 46 |
| 5 | Thiocoumarin, 4,4,6,8-tetramethyl- | 220 | C13H16OS | 1000128-90-3 | 43 |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038946.D
Acq On : 17 Jun 2020 16:07
Operator : SY/MD
Sample : L3040-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L09

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

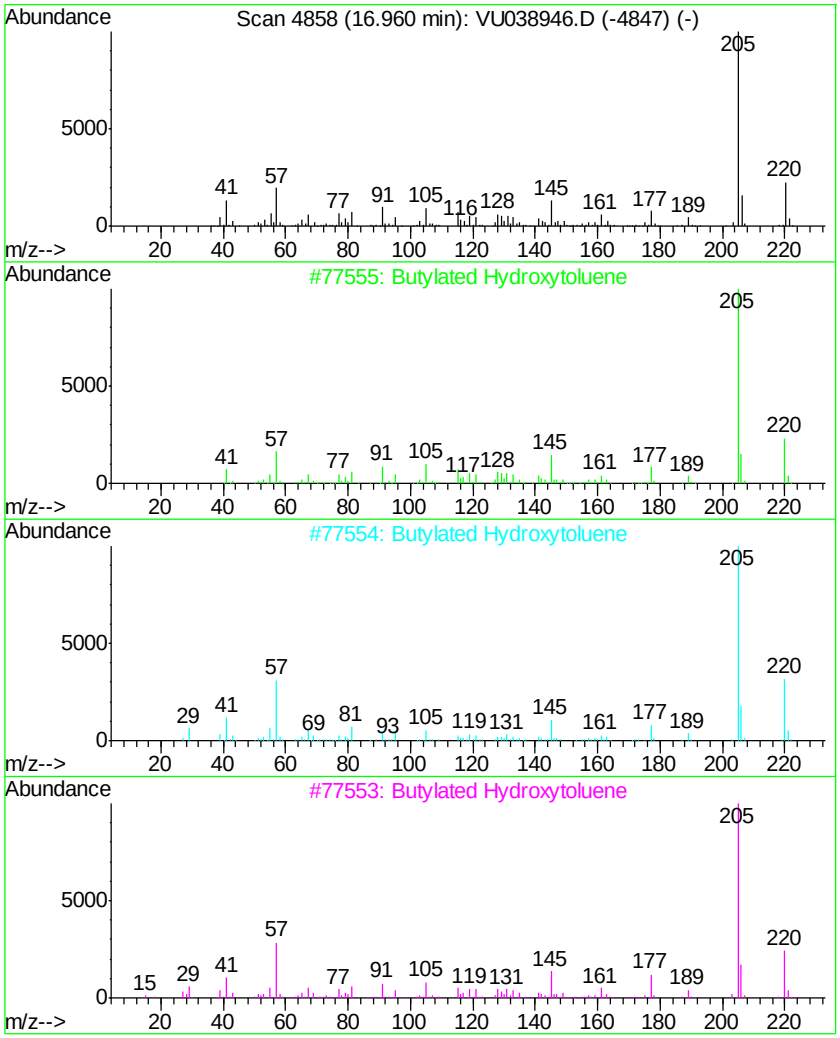
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

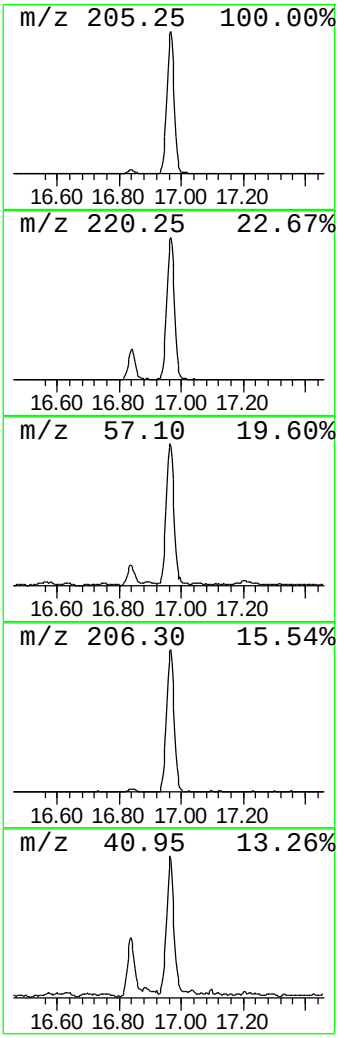
**********

Peak Number 7 Butylated Hydroxytoluene Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.96 | 4.12 ug/L | 708082 | 1,4-Dichlorobenzene-d4 | 11.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 99 |
| 2 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 97 |
| 3 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 96 |
| 4 | Phenol, 4,6-di(1,1-dimethylethyl... | 220 | C15H24O | 000616-55-7 | 94 |
| 5 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 94 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038946.D
Acq On : 17 Jun 2020 16:07
Operator : SY/MD
Sample : L3040-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

**Instrument :** MSVOA_U
**ClientSampleId :** F9L09

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-Butanone, 3,3-d... | 7.25 | 1.7 | ug/L | 217806 | 1 | 6.34 | 649928 | 5.0 |
| 2,4-Octanedione | 14.23 | 1.3 | ug/L | 226720 | 3 | 11.83 | 859157 | 5.0 |
| Benzenethiol, 4-m... | 14.35 | 0.6 | ug/L | 101577 | 3 | 11.83 | 859157 | 5.0 |
| unknown-01 | 16.19 | 0.5 | ug/L | 91692 | 3 | 11.83 | 859157 | 5.0 |
| 2,5-Cyclohexadien... | 16.84 | 0.9 | ug/L | 161468 | 3 | 11.83 | 859157 | 5.0 |
| Butylated Hydroxy... | 16.96 | 4.1 | ug/L | 708082 | 3 | 11.83 | 859157 | 5.0 |