LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070120\
Data File : VX017101.D
Acq On : 01 Jul 2020 16:23
Operator : JC/SP
Sample : L3129-11 20X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** 1308

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_X\METHOD\82X062920W.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 | 1.624 | 74 | 88 | 91 | rBV | 18589 | 67950 | 5.45% | 0.875% |
| 2 | 1.697 | 98 | 100 | 108 | rVB3 | 23662 | 42065 | 3.37% | 0.541% |
| 3 | 3.050 | 313 | 322 | 330 | rBV | 13885 | 35405 | 2.84% | 0.456% |
| 4 | 4.690 | 580 | 591 | 605 | rBV3 | 7357 | 27733 | 2.22% | 0.357% |
| 5 | 5.465 | 705 | 718 | 732 | rBV2 | 133823 | 380824 | 30.52% | 4.902% |
| 6 | 5.629 | 732 | 745 | 760 | rVB | 214166 | 605849 | 48.56% | 7.798% |
| 7 | 6.031 | 799 | 811 | 824 | rBV | 142778 | 373730 | 29.95% | 4.810% |
| 8 | 6.830 | 932 | 942 | 957 | rBV | 340948 | 806965 | 64.68% | 10.386% |
| 9 | 7.958 | 1120 | 1127 | 1139 | rVB | 80097 | 157150 | 12.59% | 2.023% |
| 10 | 8.696 | 1240 | 1248 | 1256 | rBV | 735179 | 1138670 | 91.26% | 14.656% |
| 11 | 10.098 | 1470 | 1478 | 1491 | rBV | 808891 | 1102835 | 88.39% | 14.194% |
| 12 | 11.122 | 1639 | 1646 | 1654 | rBV | 750211 | 935215 | 74.95% | 12.037% |
| 13 | 12.061 | 1794 | 1800 | 1809 | rBV | 1031218 | 1247720 | 100.00% | 16.059% |
| 14 | 14.262 | 2158 | 2161 | 2166 | rVB7 | 9746 | 16049 | 1.29% | 0.207% |
| 15 | 14.524 | 2202 | 2204 | 2209 | rVB4 | 11976 | 13741 | 1.10% | 0.177% |
| 16 | 14.658 | 2223 | 2226 | 2228 | rBV4 | 15145 | 20172 | 1.62% | 0.260% |
| 17 | 14.713 | 2232 | 2235 | 2237 | rBV4 | 11622 | 14880 | 1.19% | 0.192% |
| 18 | 14.792 | 2246 | 2248 | 2251 | rBV3 | 15194 | 15241 | 1.22% | 0.196% |
| 19 | 14.835 | 2252 | 2255 | 2258 | rVB4 | 16199 | 19256 | 1.54% | 0.248% |
| 20 | 14.884 | 2261 | 2263 | 2269 | rVV6 | 14842 | 27448 | 2.20% | 0.353% |
| 21 | 15.255 | 2321 | 2324 | 2327 | rBV3 | 37905 | 41772 | 3.35% | 0.538% |
| 22 | 15.469 | 2355 | 2359 | 2366 | rVB2 | 87072 | 126605 | 10.15% | 1.630% |
| 23 | 15.798 | 2410 | 2413 | 2417 | rVB3 | 72377 | 96876 | 7.76% | 1.247% |
| 24 | 16.152 | 2466 | 2471 | 2478 | rBV2 | 270576 | 455329 | 36.49% | 5.860% |

Sum of corrected areas: 7769480

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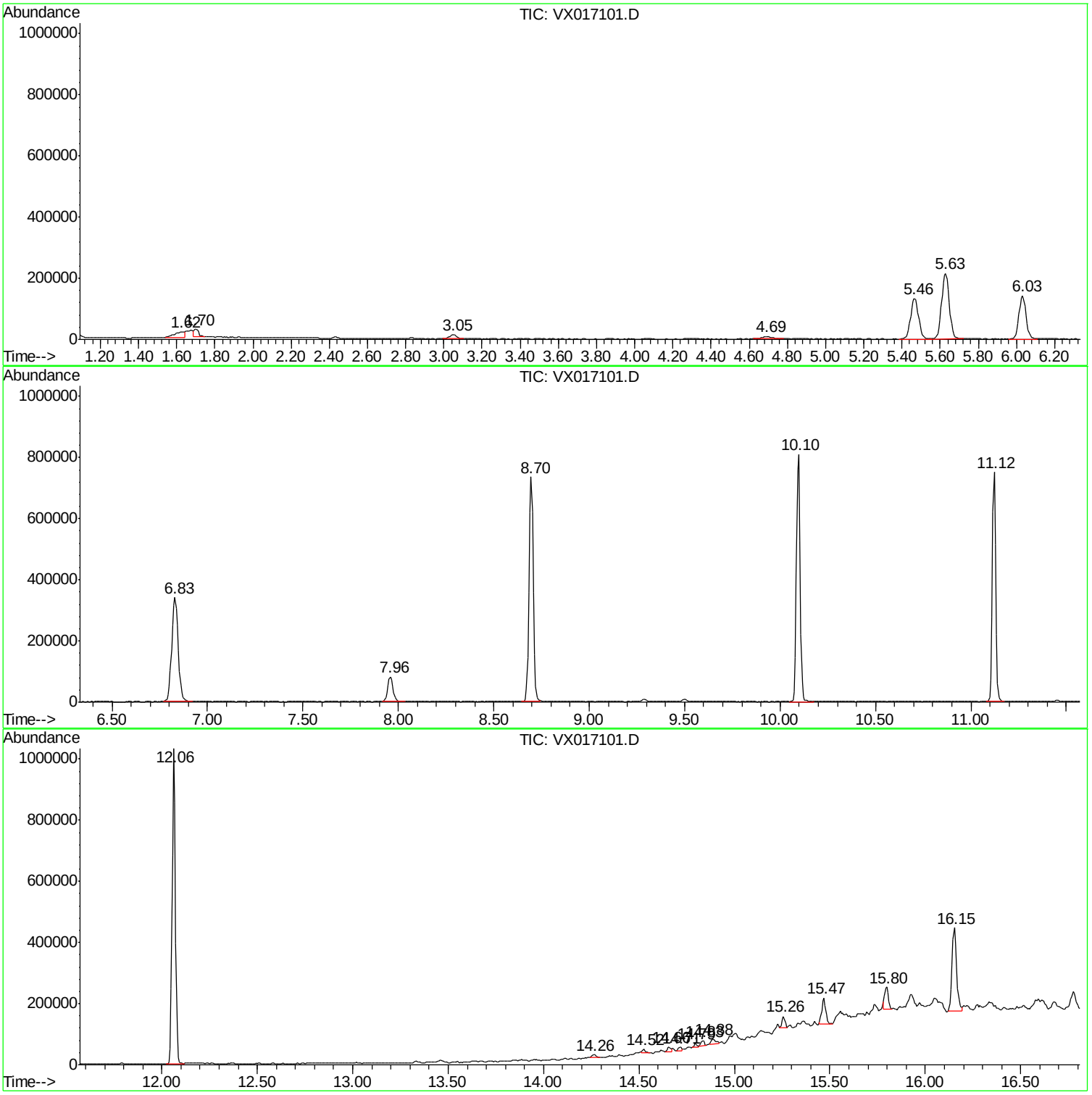
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
1308

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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Data File : VX017101.D
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Operator : JC/SP
Sample : L3129-11 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** 1308

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

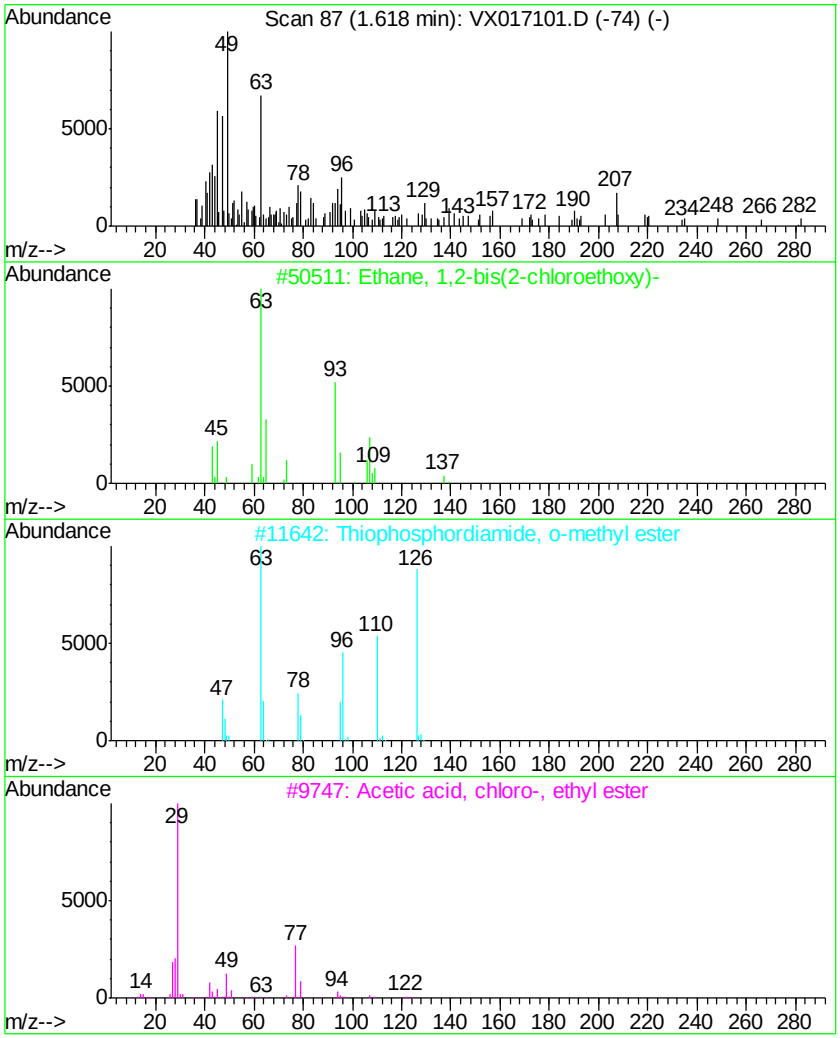
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

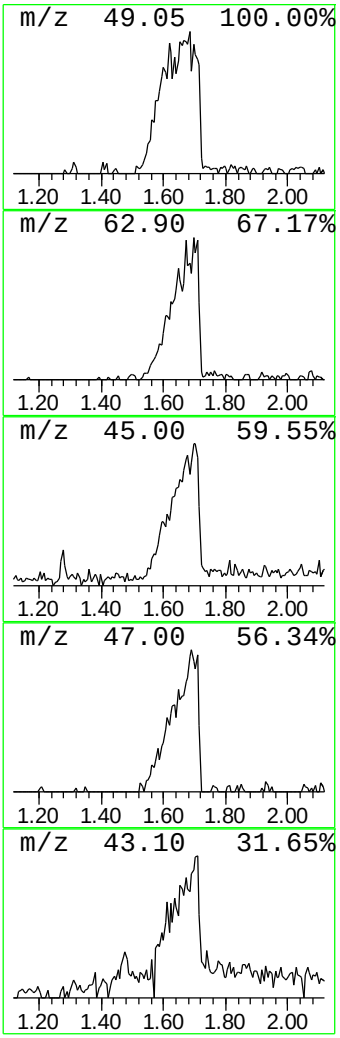
**********

Peak Number 1 unknown1.62 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.62 | 5.61 ug/l | 67950 | Pentafluorobenzene | 5.63 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethane, 1,2-bis(2-chloroethoxy)- | 186 | C6H12Cl2O2 | 000112-26-5 | 35 |
| 2 | Thiophosphordiamide, o-methyl ester | 126 | CH7N2OPS | 1000306-03-3 | 17 |
| 3 | Acetic acid, chloro-, ethyl ester | 122 | C4H7ClO2 | 000105-39-5 | 17 |
| 4 | 2-[2-(2-Chloro-ethoxy)-ethoxy]-p... | 216 | C10H13ClO3 | 1000317-46-1 | 17 |
| 5 | Methane, chloromethoxy- | 80 | C2H5ClO | 000107-30-2 | 12 |



Library Search Compound Report

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Data File : VX017101.D
Acq On : 01 Jul 2020 16:23
Operator : JC/SP
Sample : L3129-11 20X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** 1308

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

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

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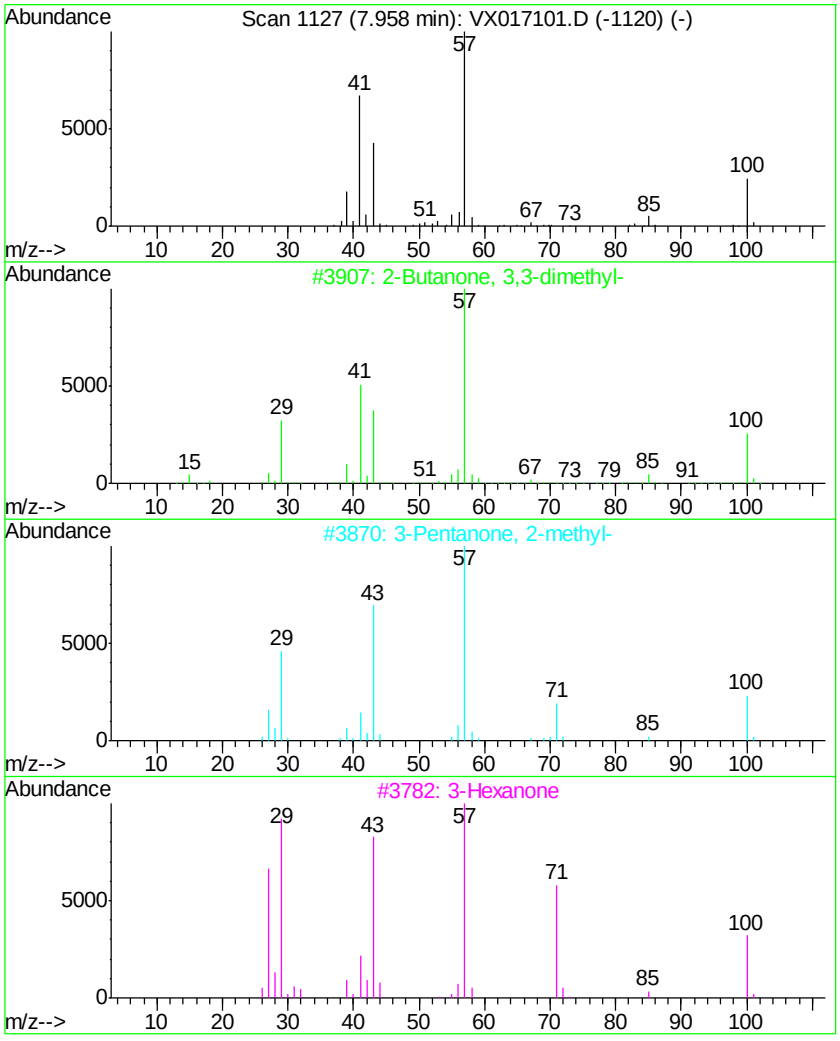
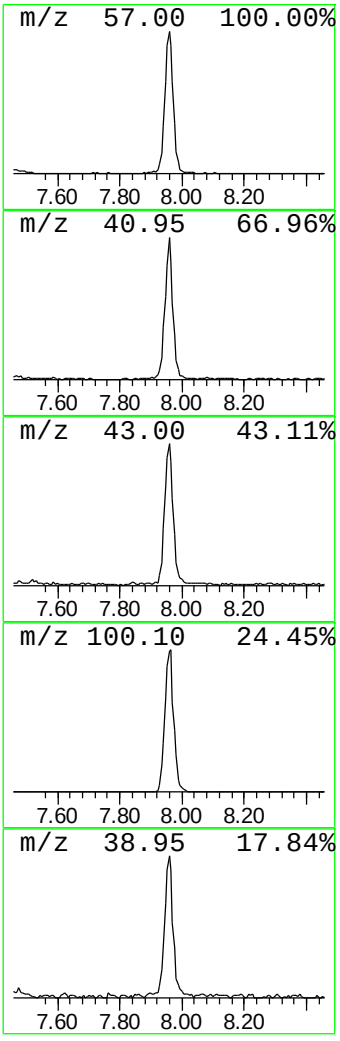
Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.96 | 9.74 ug/l | 157150 | 1,4-Difluorobenzene | 6.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Butanone, 3,3-dimethyl- | 100 | C6H12O | 000075-97-8 | 87 |
| 2 | 3-Pentanone, 2-methyl- | 100 | C6H12O | 000565-69-5 | 80 |
| 3 | 3-Hexanone | 100 | C6H12O | 000589-38-8 | 59 |
| 4 | Propane, 1-(ethenyloxy)-2-methyl- | 100 | C6H12O | 000109-53-5 | 50 |
| 5 | trans-1-Ethoxy-1-butene | 100 | C6H12O | 1000139-43-9 | 50 |



Library Search Compound Report

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Acq On : 01 Jul 2020 16:23
Operator : JC/SP
Sample : L3129-11 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** 1308

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

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

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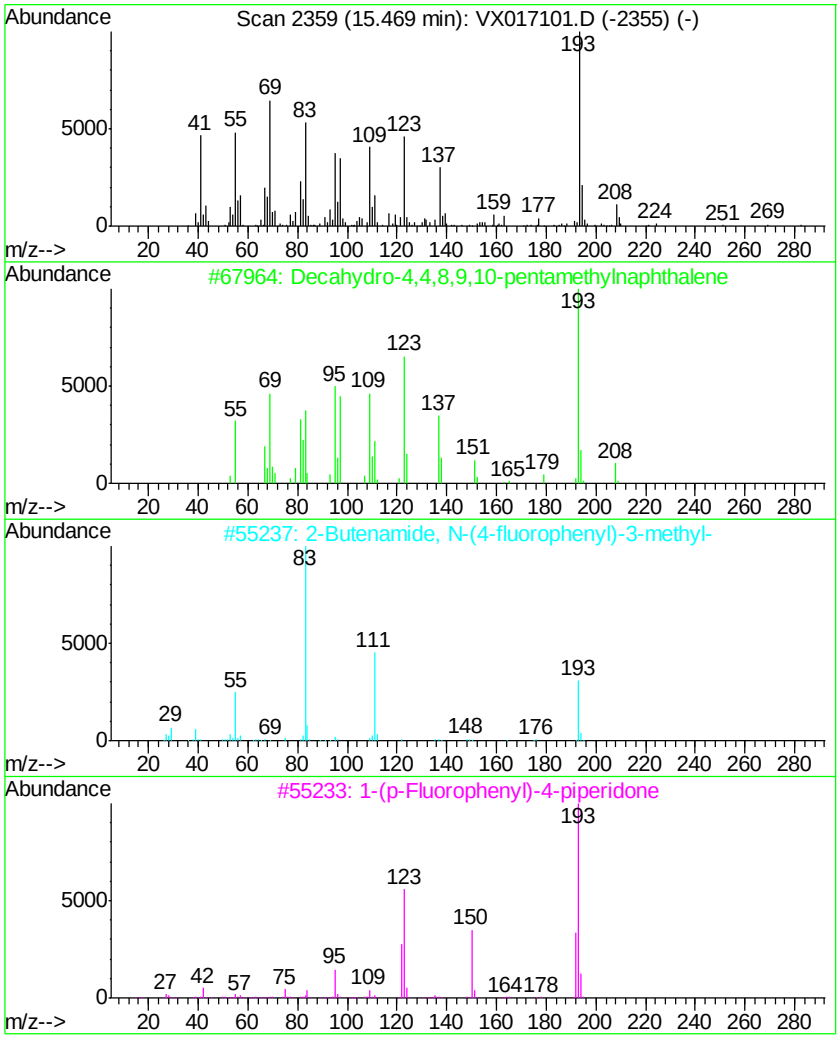
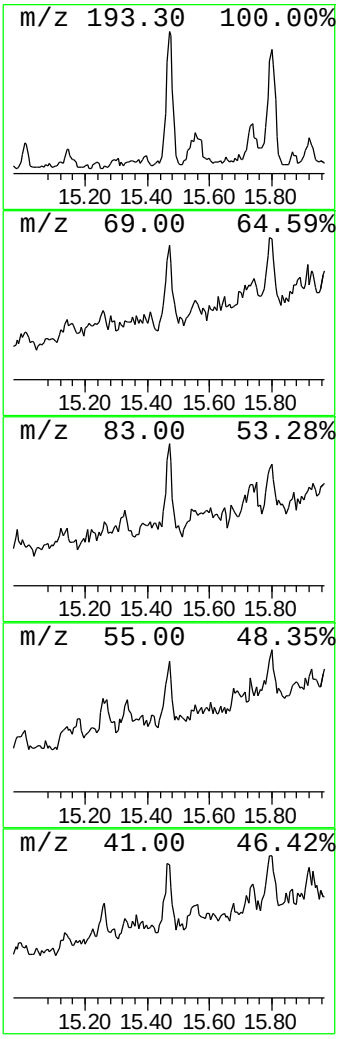
Peak Number 3 Decahydro-4,4,8,9,10-pentam... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.47 | 5.07 ug/l | 126605 | 1,4-Dichlorobenzene-d4 | 12.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Decahydro-4,4,8,9,10-pentamethyl... | 208 | C15H28 | 080655-44-3 | 76 |
| 2 | 2-Butenamide, N-(4-fluorophenyl)... | 193 | C11H12FNO | 1000307-26-7 | 38 |
| 3 | 1-(p-Fluorophenyl)-4-piperidone | 193 | C11H12FNO | 1000238-56-7 | 38 |
| 4 | 1,2-Dicyclohexylbutane | 222 | C16H30 | 054890-01-6 | 37 |
| 5 | 2-Phenylindolizine | 193 | C14H11N | 025379-20-8 | 27 |



Library Search Compound Report

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Sample : L3129-11 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** 1308

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X062920W.M
Quant Title : SW846 8260

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

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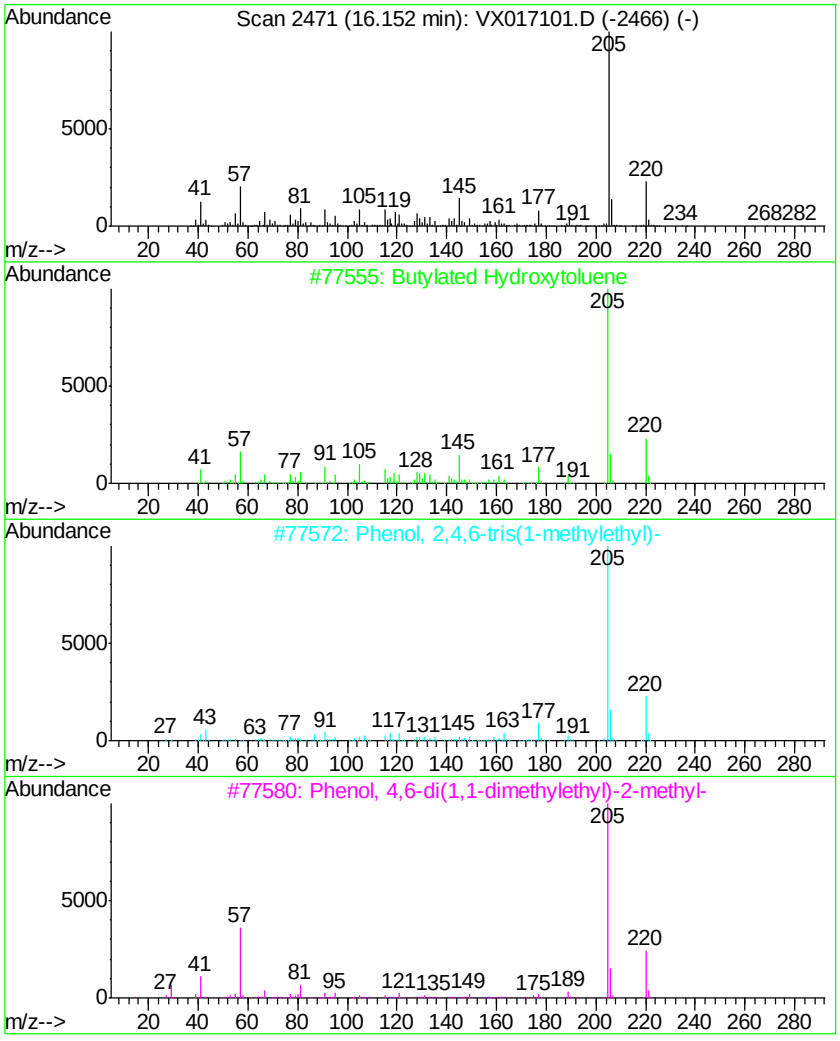
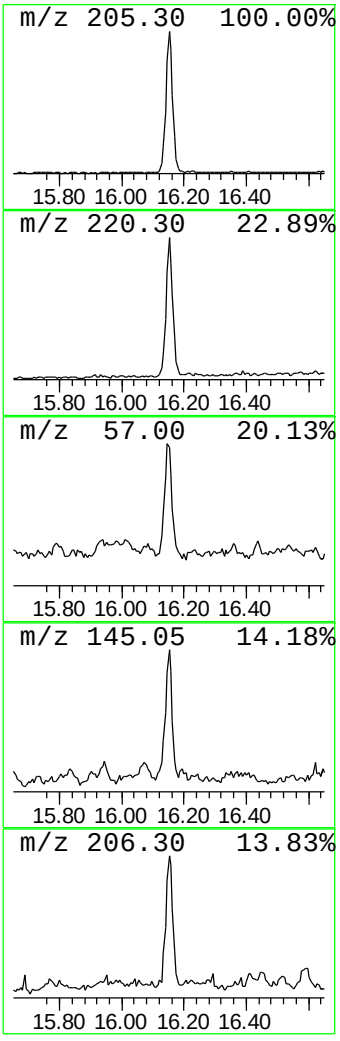
Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.15 | 18.25 ug/l | 455329 | 1,4-Dichlorobenzene-d4 | 12.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butylated Hydroxytoluene | 220 | C15H24O | 000128-37-0 | 98 |
| 2 | Phenol, 2,4,6-tris(1-methylethyl)- | 220 | C15H24O | 002934-07-8 | 87 |
| 3 | Phenol, 4,6-di(1,1-dimethylethyl... | 220 | C15H24O | 000616-55-7 | 87 |
| 4 | 2,4,6-Tris(1,1-dimethylethyl)-4-... | 276 | C19H32O | 019687-22-0 | 78 |
| 5 | Phenol, 2,6-bis(1,1-dimethylethy... | 277 | C17H27NO2 | 001918-11-2 | 78 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX070120\
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ALS Vial : 17 Sample Multiplier: 1

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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 |
| unknown1.62 | 1.62 | 5.6 | ug/l | 67950 | 1 | 5.63 | 605849 | 50.0 |
| 2-Butanone, 3,3-d... | 7.96 | 9.7 | ug/l | 157150 | 2 | 6.83 | 806965 | 50.0 |
| Decahydro-4,4,8,9... | 15.47 | 5.1 | ug/l | 126605 | 4 | 12.06 | 1247720 | 50.0 |
| Butylated Hydroxy... | 16.15 | 18.3 | ug/l | 455329 | 4 | 12.06 | 1247720 | 50.0 |