# LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX041720\
Data File : VX015749.D
Acq On : 17 Apr 2020 19:25
Operator : JC/SP
Sample : L2305-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** I-OC-1

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\82X032720W.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 | 1.064 | 26 | 29 | 37 | rBV | 4685184 | 5582201 | 3.11% | 0.816% |
| 2 | 1.174 | 44 | 47 | 57 | rVB | 3943381 | 4200978 | 2.34% | 0.614% |
| 3 | 1.564 | 108 | 111 | 167 | rVB2 | 50132944 | 120570250 | 67.13% | 17.624% |
| 4 | 2.253 | 218 | 224 | 245 | rBV | 2349380 | 4637726 | 2.58% | 0.678% |
| 5 | 2.417 | 245 | 251 | 256 | rBV | 3081094 | 4801564 | 2.67% | 0.702% |
| 6 | 2.551 | 266 | 273 | 274 | rBV4 | 65957140 | 101149824 | 56.32% | 14.786% |
| 7 | 2.564 | 274 | 275 | 332 | rVB4 | 82584603 | 179600190 | 100.00% | 26.253% |
| 8 | 5.630 | 766 | 778 | 792 | rVV | 1021089 | 2860441 | 1.59% | 0.418% |
| 9 | 6.118 | 850 | 858 | 877 | rVB | 4836896 | 12654357 | 7.05% | 1.850% |
| 10 | 6.831 | 966 | 975 | 988 | rBV | 1627258 | 3837205 | 2.14% | 0.561% |
| 11 | 8.471 | 1235 | 1244 | 1253 | rBV | 16445908 | 35156745 | 19.58% | 5.139% |
| 12 | 8.697 | 1275 | 1281 | 1287 | rBV | 3322260 | 5212078 | 2.90% | 0.762% |
| 13 | 8.770 | 1287 | 1293 | 1303 | rVV | 4693408 | 7229322 | 4.03% | 1.057% |
| 14 | 8.892 | 1307 | 1313 | 1325 | rVB | 7521928 | 11318678 | 6.30% | 1.655% |
| 15 | 9.977 | 1485 | 1491 | 1500 | rBV | 1843721 | 2814790 | 1.57% | 0.411% |
| 16 | 10.099 | 1505 | 1511 | 1515 | rBV | 3561781 | 4773527 | 2.66% | 0.698% |
| 17 | 10.239 | 1529 | 1534 | 1538 | rBV | 1981361 | 2711732 | 1.51% | 0.396% |
| 18 | 10.343 | 1542 | 1551 | 1563 | rVB2 | 9677769 | 16760705 | 9.33% | 2.450% |
| 19 | 10.684 | 1603 | 1607 | 1616 | rVB | 3643111 | 4757177 | 2.65% | 0.695% |
| 20 | 11.123 | 1674 | 1679 | 1685 | rBV | 3356894 | 4099950 | 2.28% | 0.599% |
| 21 | 11.702 | 1768 | 1774 | 1784 | rVB | 15216428 | 20613442 | 11.48% | 3.013% |
| 22 | 11.794 | 1784 | 1789 | 1794 | rVB | 2111435 | 2585275 | 1.44% | 0.378% |
| 23 | 12.062 | 1827 | 1833 | 1839 | rVB2 | 4520244 | 5910675 | 3.29% | 0.864% |
| 24 | 12.129 | 1839 | 1844 | 1850 | rBV | 1520600 | 2096221 | 1.17% | 0.306% |
| 25 | 13.208 | 2016 | 2021 | 2032 | rBV2 | 1382881 | 2096811 | 1.17% | 0.307% |
| 26 | 13.824 | 2116 | 2122 | 2127 | rBV2 | 70056222 | 97847113 | 54.48% | 14.303% |
| 27 | 13.909 | 2132 | 2136 | 2142 | rVB | 5857345 | 7502494 | 4.18% | 1.097% |
| 28 | 14.092 | 2161 | 2166 | 2170 | rBV | 1758223 | 1989388 | 1.11% | 0.291% |
| 29 | 14.677 | 2258 | 2262 | 2270 | rVB | 4303402 | 5493260 | 3.06% | 0.803% |
| 30 | 14.824 | 2281 | 2286 | 2292 | rBV | 2493358 | 3244526 | 1.81% | 0.474% |

Sum of corrected areas: 684108645

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX041720\
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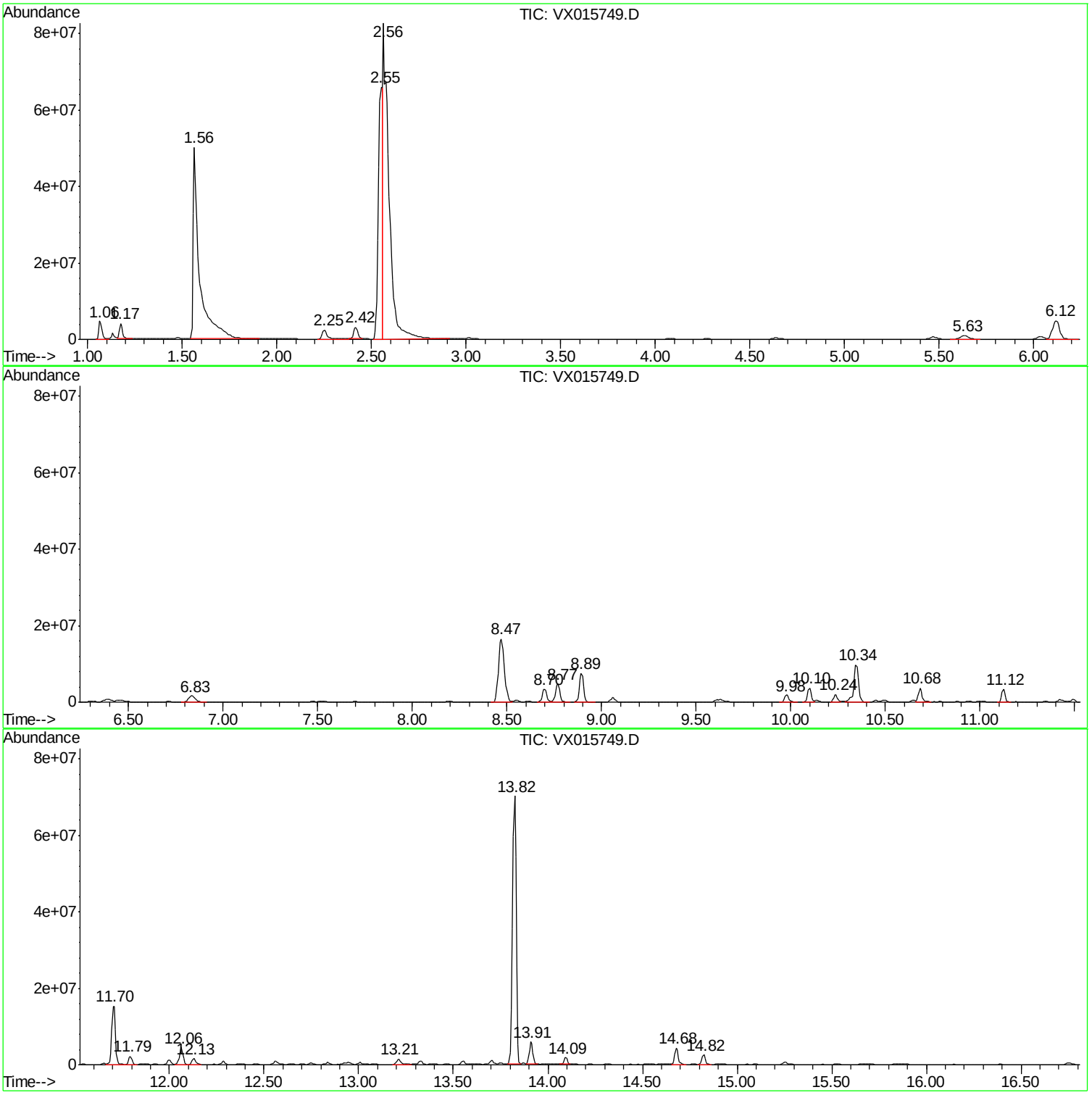
Acq On : 17 Apr 2020 19:25
Operator : JC/SP
Sample : L2305-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
I-OC-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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



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TIC Integration Parameters: LSCINT.P

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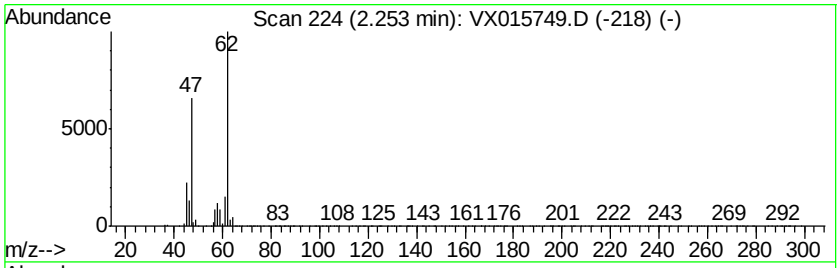
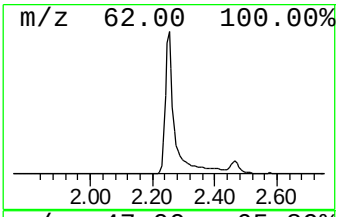
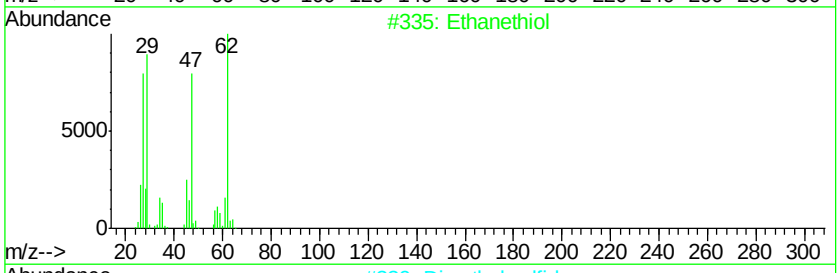
Peak Number 4 Ethanethiol Concentration Rank 6

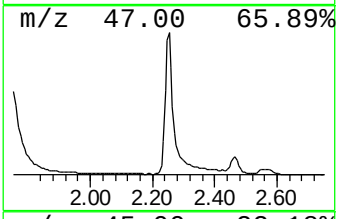
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.25 | 81.07 ug/l | 4637730 | Pentafluorobenzene | 5.63 |

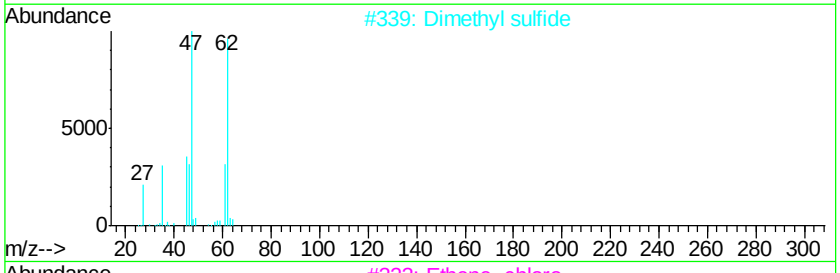
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanethiol | 62 | C2H6S | 000075-08-1 | 91 |
| 2 | Dimethyl sulfide | 62 | C2H6S | 000075-18-3 | 64 |
| 3 | Ethene, chloro- | 62 | C2H3Cl | 000075-01-4 | 50 |
| 4 | Borane-methyl sulfide complex | 76 | C2H9BS | 013292-87-0 | 25 |
| 5 | Phosphine, ethyl- | 62 | C2H7P | 000593-68-0 | 9 |

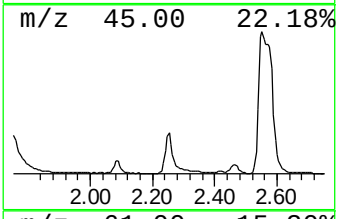


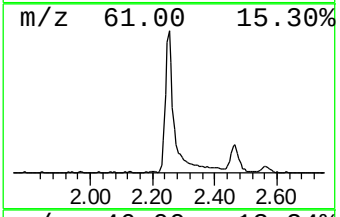



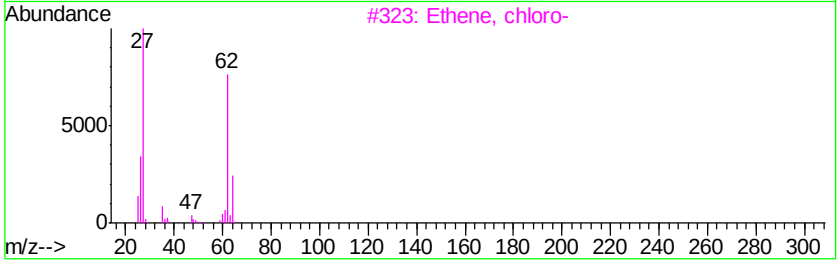



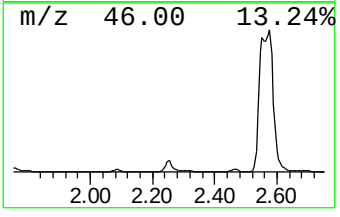



# Library Search Compound Report

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Data File : VX015749.D
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Operator : JC/SP
Sample : L2305-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** I-OC-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

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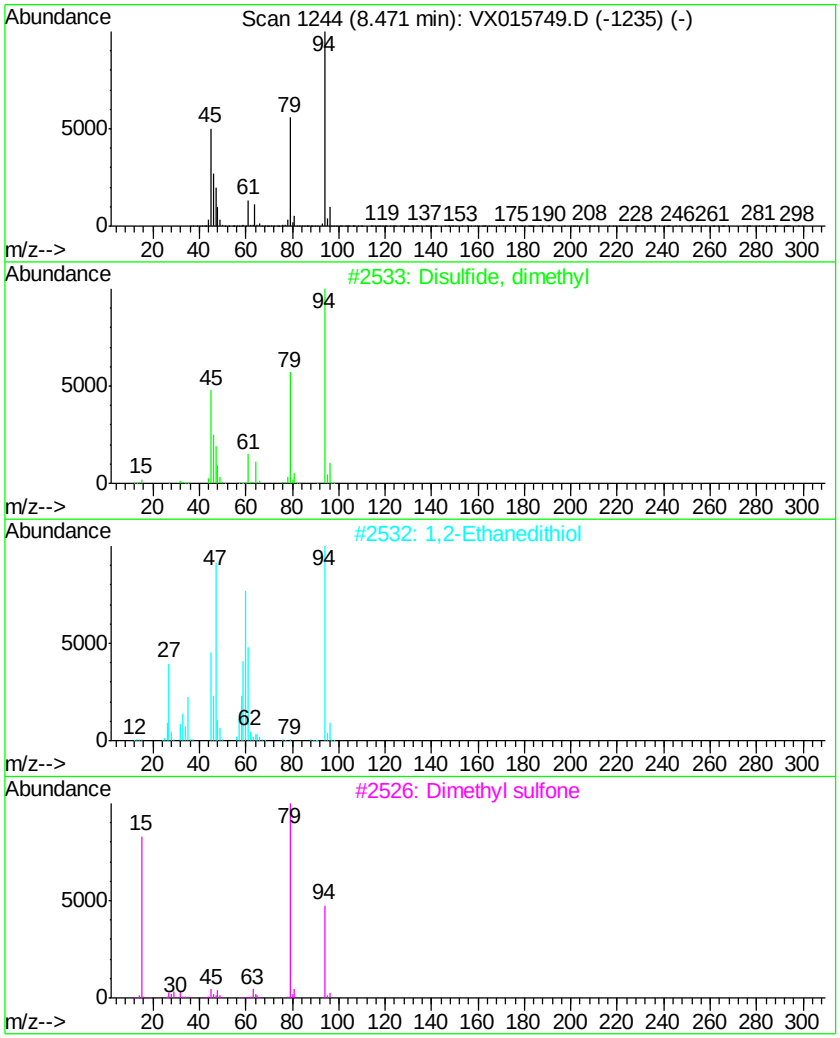
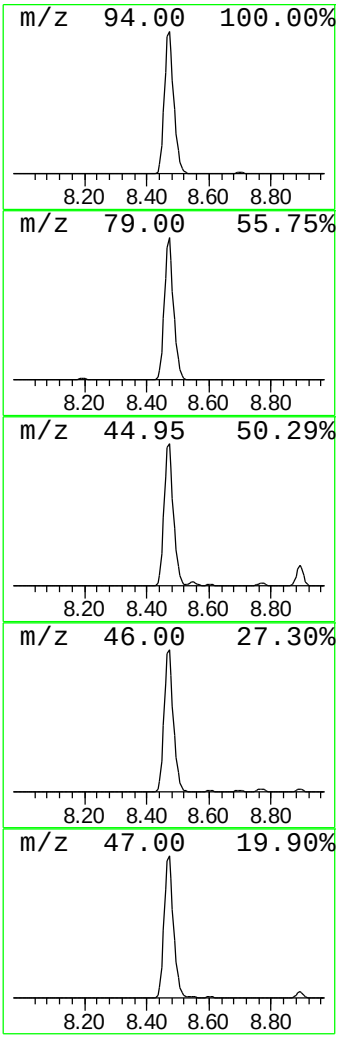
Peak Number 5 Disulfide, dimethyl Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.47 | 368.25 ug/l | 35156700 | Chlorobenzene-d5 | 10.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Disulfide, dimethyl | 94 | C2H6S2 | 000624-92-0 | 97 |
| 2 | 1,2-Ethanedithiol | 94 | C2H6S2 | 000540-63-6 | 52 |
| 3 | Dimethyl sulfone | 94 | C2H6O2S | 000067-71-0 | 46 |
| 4 | Methanesulfonylacetic acid | 138 | C3H6O4S | 002516-97-4 | 9 |
| 5 | Methanesulfonyl chloride | 114 | CH3ClO2S | 000124-63-0 | 7 |



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Operator : JC/SP
Sample : L2305-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** I-OC-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

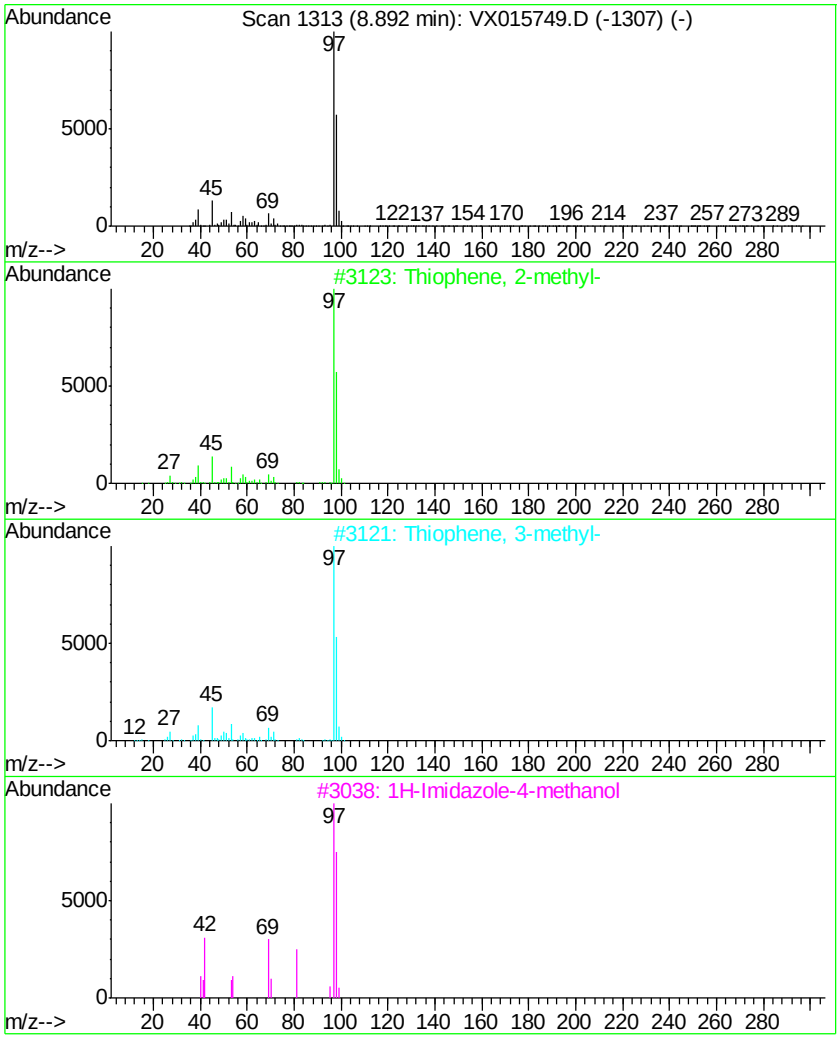
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

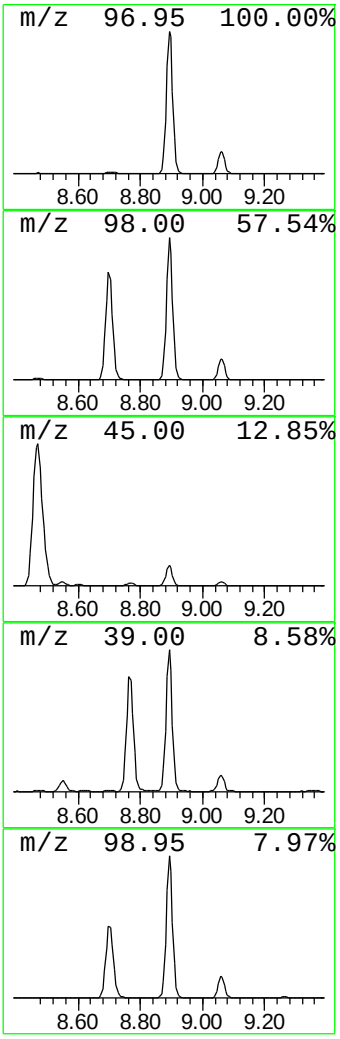
**********

Peak Number 6 Thiophene, 2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.89 | 118.56 ug/l | 11318700 | Chlorobenzene-d5 | 10.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Thiophene, 2-methyl- | 98 | C5H6S | 000554-14-3 | 95 |
| 2 | Thiophene, 3-methyl- | 98 | C5H6S | 000616-44-4 | 91 |
| 3 | 1H-Imidazole-4-methanol | 98 | C4H6N2O | 000822-55-9 | 72 |
| 4 | Propennitrile, 3-ethoxy-2-(2-thi... | 257 | C10H11NO3S2 | 1000267-97-5 | 50 |
| 5 | 2-Fluoropyridine | 97 | C5H4FN | 000372-48-5 | 28 |



# Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX041720\
Data File : VX015749.D
Acq On : 17 Apr 2020 19:25
Operator : JC/SP
Sample : L2305-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** I-OC-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

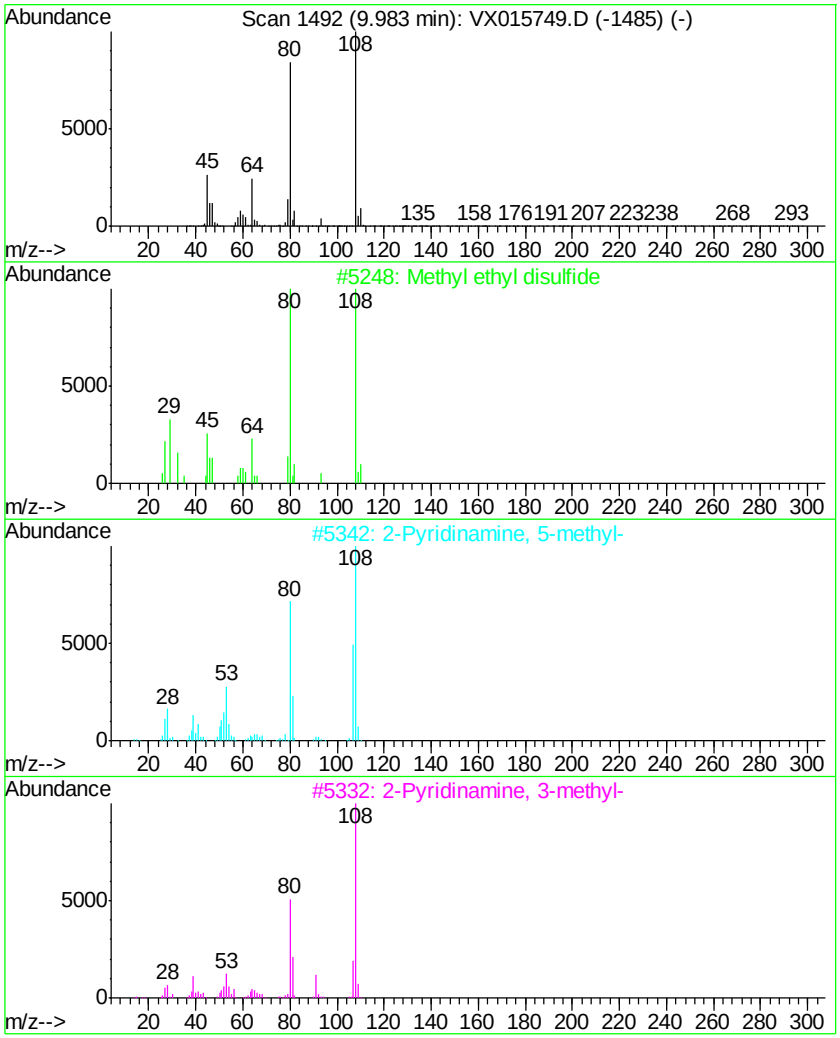
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

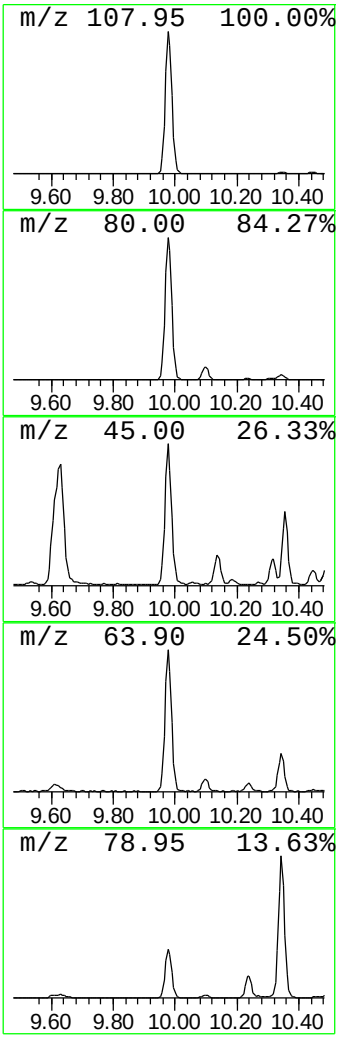
**********

Peak Number 7 Methyl ethyl disulfide Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.98 | 29.48 ug/l | 2814790 | Chlorobenzene-d5 | 10.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl ethyl disulfide | 108 | C3H8S2 | 020333-39-5 | 91 |
| 2 | 2-Pyridinamine, 5-methyl- | 108 | C6H8N2 | 001603-41-4 | 80 |
| 3 | 2-Pyridinamine, 3-methyl- | 108 | C6H8N2 | 001603-40-3 | 72 |
| 4 | Nicotinyl alcohol | 109 | C6H7NO | 000100-55-0 | 64 |
| 5 | Dimethyl phosphite | 110 | C2H7O3P | 000868-85-9 | 53 |



Library Search Compound Report

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Data File : VX015749.D
Acq On : 17 Apr 2020 19:25
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Sample : L2305-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** I-OC-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

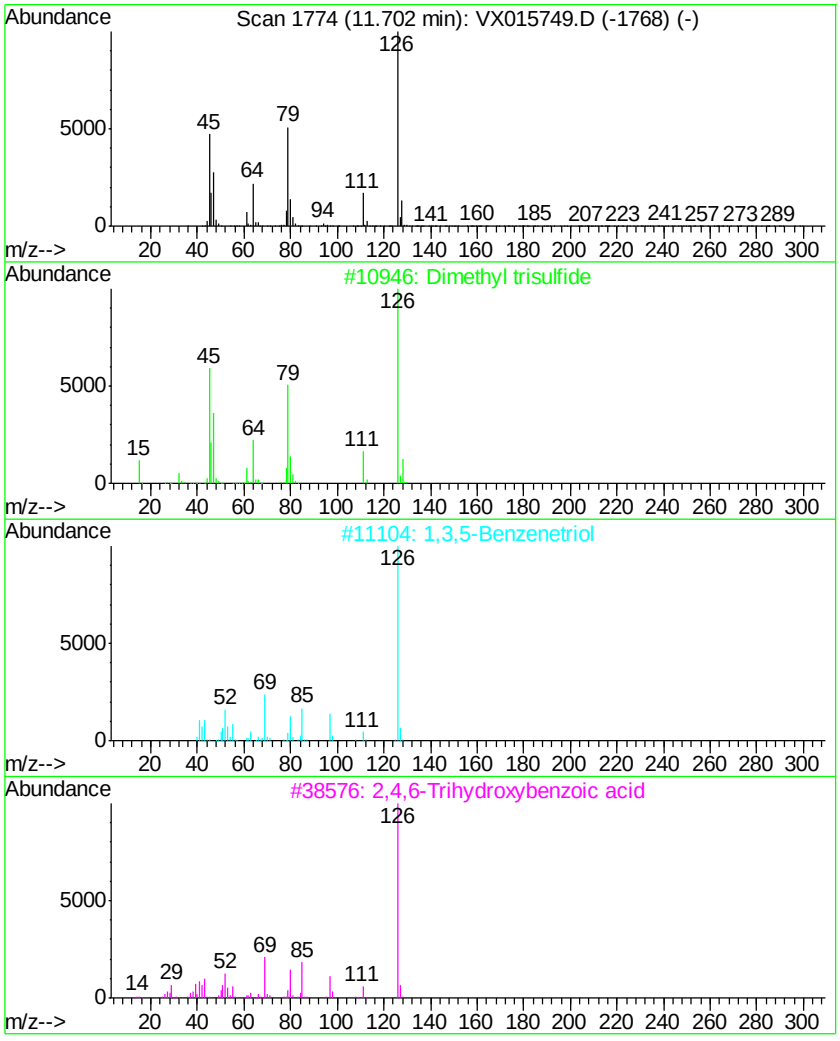
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

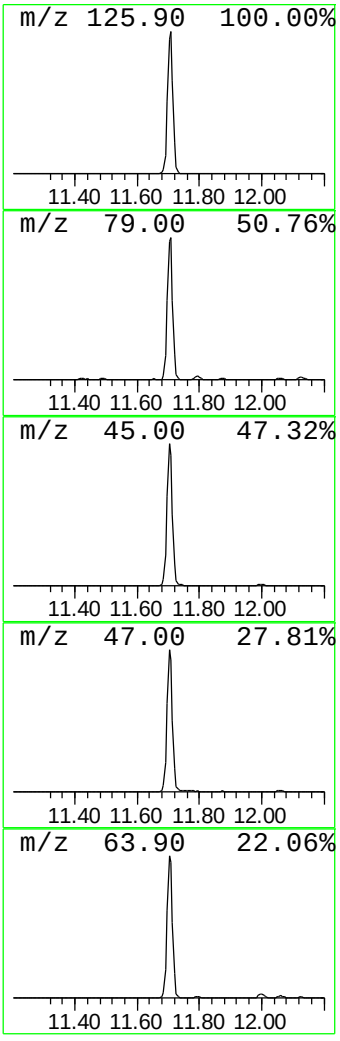
**********

Peak Number 8 Dimethyl trisulfide Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.70 | 174.38 ug/l | 20613400 | 1,4-Dichlorobenzene-d4 | 12.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dimethyl trisulfide | 126 | C2H6S3 | 003658-80-8 | 97 |
| 2 | 1,3,5-Benzenetriol | 126 | C6H6O3 | 000108-73-6 | 16 |
| 3 | 2,4,6-Trihydroxybenzoic acid | 170 | C7H6O5 | 000083-30-7 | 16 |
| 4 | Dimethyldithiophosphinic acid | 126 | C2H7PS2 | 016367-68-3 | 16 |
| 5 | (2,2,2-Trifluoroethoxy)ethene | 126 | C4H5F3O | 1000306-54-7 | 9 |



Library Search Compound Report

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

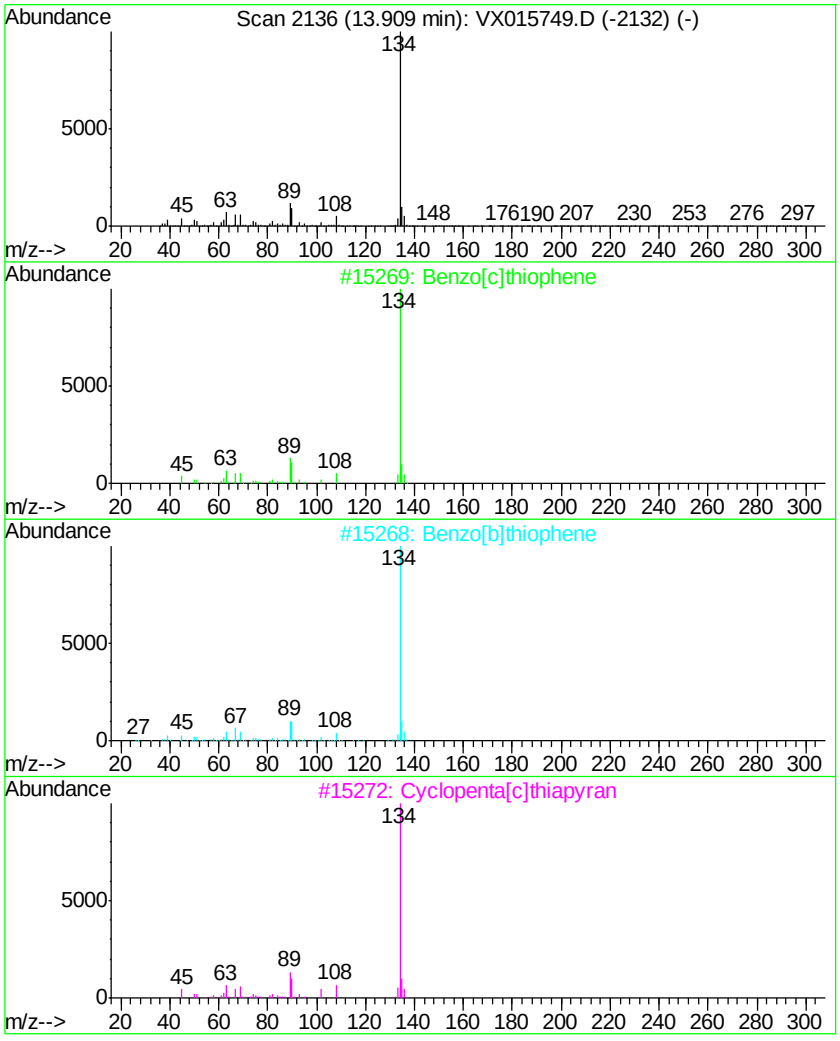
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

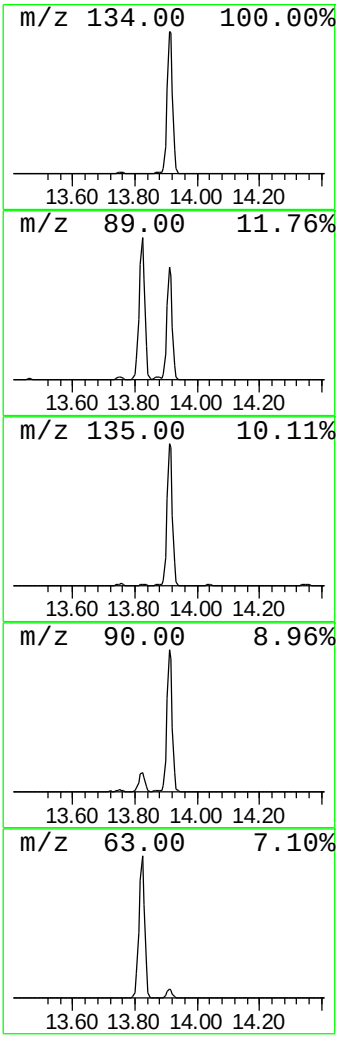
**********

Peak Number 9 Benzo[c]thiophene Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.91 | 63.47 ug/l | 7502490 | 1,4-Dichlorobenzene-d4 | 12.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[c]thiophene | 134 | C8H6S | 000270-82-6 | 97 |
| 2 | Benzo[b]thiophene | 134 | C8H6S | 000095-15-8 | 95 |
| 3 | Cyclopenta[c]thiapyran | 134 | C8H6S | 000270-63-3 | 94 |
| 4 | 2H-Benzimidazol-2-one, 1,3-dihydro- | 134 | C7H6N2O | 000615-16-7 | 45 |
| 5 | [1]Benzothieno[2',3':3,4]cyclobu... | 246 | C13H10O3S | 034002-19-2 | 40 |



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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

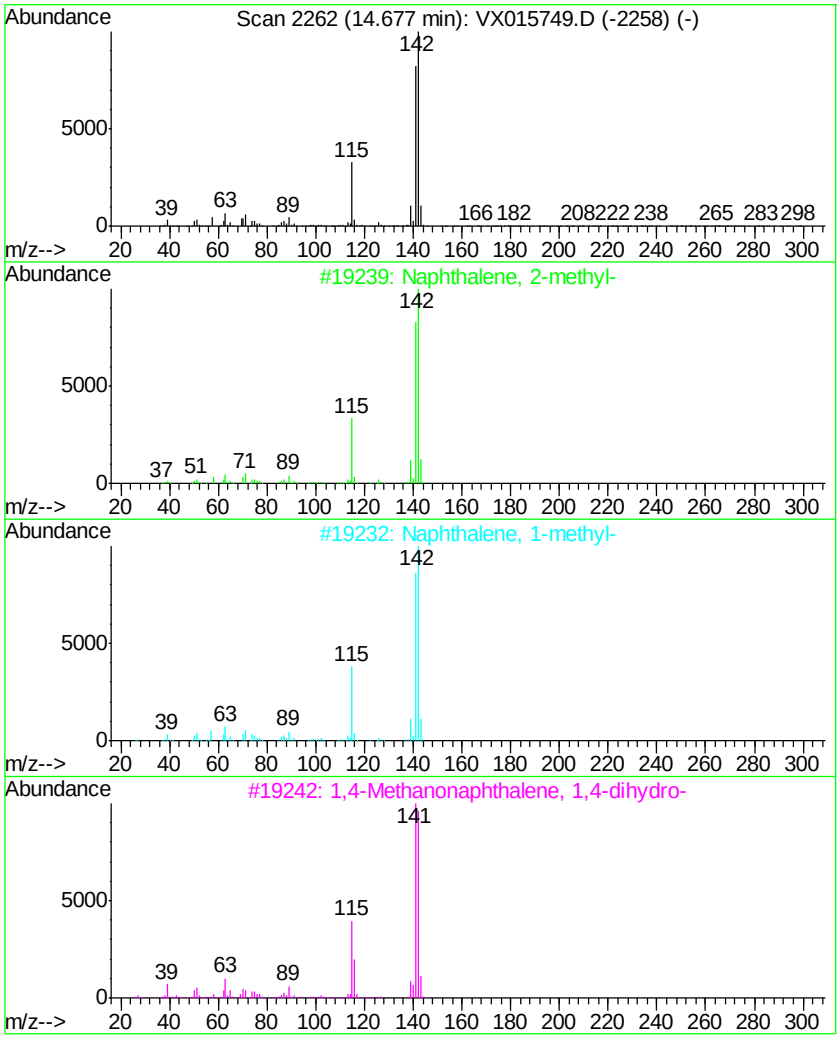
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

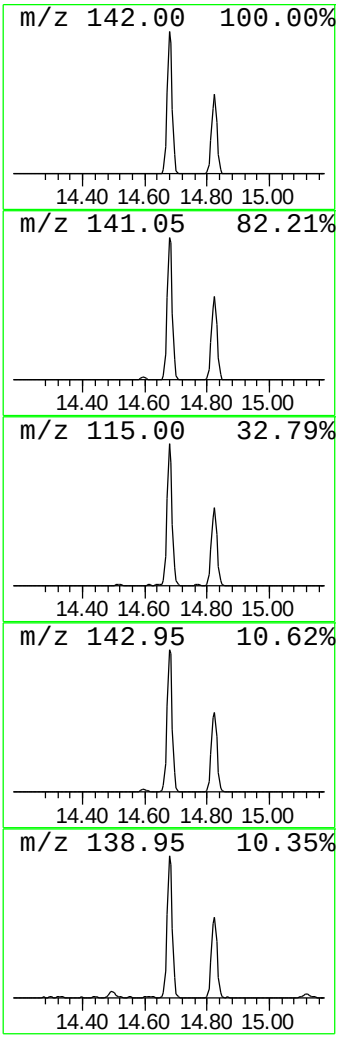
**********

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.68 | 46.47 ug/l | 5493260 | 1,4-Dichlorobenzene-d4 | 12.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Naphthalene, 2-methyl- | 142 | C11H10 | 000091-57-6 | 96 |
| 2 | Naphthalene, 1-methyl- | 142 | C11H10 | 000090-12-0 | 96 |
| 3 | 1,4-Methanonaphthalene, 1,4-dihy... | 142 | C11H10 | 004453-90-1 | 91 |
| 4 | Benzocycloheptatriene | 142 | C11H10 | 000264-09-5 | 91 |
| 5 | 1H-Indene, 1-ethylidene- | 142 | C11H10 | 002471-83-2 | 72 |



Tentatively Identified Compound (LSC) summary

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ALS Vial : 21 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 |
| Ethanethiol | 2.25 | 81.1 | ug/l | 4637730 | 1 | 5.63 | 2860440 | 50.0 |
| Disulfide, dimethyl | 8.47 | 368.3 | ug/l | 35156700 | 3 | 10.10 | 4773530 | 50.0 |
| Thiophene, 2-methyl- | 8.89 | 118.6 | ug/l | 11318700 | 3 | 10.10 | 4773530 | 50.0 |
| Methyl ethyl disu... | 9.98 | 29.5 | ug/l | 2814790 | 3 | 10.10 | 4773530 | 50.0 |
| Dimethyl trisulfide | 11.70 | 174.4 | ug/l | 20613400 | 4 | 12.06 | 5910680 | 50.0 |
| Benzo[c]thiophene | 13.91 | 63.5 | ug/l | 7502490 | 4 | 12.06 | 5910680 | 50.0 |
| Naphthalene, 1-me... | 14.68 | 46.5 | ug/l | 5493260 | 4 | 12.06 | 5910680 | 50.0 |