LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** 210609018-02-VOA

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\82X061021W.M
Title : SW846 8260

Signal : TIC: VX022679.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.124 | 3 | 6 | 26 | rVB | 193595 | 469723 | 15.68% | 3.538% |
| 2 | 1.258 | 26 | 28 | 41 | rVB | 58632 | 105650 | 3.53% | 0.796% |
| 3 | 1.545 | 71 | 75 | 83 | rBV | 139717 | 141312 | 4.72% | 1.064% |
| 4 | 2.386 | 207 | 213 | 222 | rBV | 206317 | 334628 | 11.17% | 2.520% |
| 5 | 2.550 | 236 | 240 | 248 | rVV | 20503 | 42839 | 1.43% | 0.323% |
| 6 | 2.977 | 297 | 310 | 328 | rBV | 899607 | 1964315 | 65.58% | 14.793% |
| 7 | 4.599 | 561 | 576 | 610 | rBV2 | 826630 | 2995431 | 100.00% | 22.559% |
| 8 | 5.013 | 633 | 644 | 661 | rBV | 250068 | 775203 | 25.88% | 5.838% |
| 9 | 5.397 | 696 | 707 | 719 | rBV | 47717 | 136753 | 4.57% | 1.030% |
| 10 | 5.562 | 722 | 734 | 744 | rBV | 79200 | 219821 | 7.34% | 1.655% |
| 11 | 5.964 | 790 | 800 | 808 | rBV | 60900 | 159372 | 5.32% | 1.200% |
| 12 | 6.080 | 808 | 819 | 833 | rVB6 | 29391 | 117557 | 3.92% | 0.885% |
| 13 | 6.245 | 839 | 846 | 856 | rVB2 | 18332 | 47449 | 1.58% | 0.357% |
| 14 | 6.769 | 921 | 932 | 943 | rBV | 135059 | 321804 | 10.74% | 2.424% |
| 15 | 8.653 | 1234 | 1241 | 1247 | rBV | 293130 | 450307 | 15.03% | 3.391% |
| 16 | 8.720 | 1247 | 1252 | 1261 | rVB2 | 34339 | 57991 | 1.94% | 0.437% |
| 17 | 8.805 | 1261 | 1266 | 1271 | rBV | 25788 | 41481 | 1.38% | 0.312% |
| 18 | 9.378 | 1352 | 1360 | 1366 | rBV | 77027 | 115957 | 3.87% | 0.873% |
| 19 | 10.055 | 1461 | 1471 | 1484 | rBV | 291882 | 446693 | 14.91% | 3.364% |
| 20 | 10.195 | 1490 | 1494 | 1501 | rBV2 | 64191 | 101244 | 3.38% | 0.762% |
| 21 | 10.305 | 1505 | 1512 | 1518 | rVB | 60351 | 89102 | 2.97% | 0.671% |
| 22 | 10.647 | 1563 | 1568 | 1572 | rBV | 39843 | 53950 | 1.80% | 0.406% |
| 23 | 11.085 | 1634 | 1640 | 1645 | rBV | 221447 | 291853 | 9.74% | 2.198% |
| 24 | 11.506 | 1704 | 1709 | 1716 | rVB5 | 25086 | 38909 | 1.30% | 0.293% |
| 25 | 11.756 | 1743 | 1750 | 1754 | rVB | 25137 | 38406 | 1.28% | 0.289% |
| 26 | 11.890 | 1768 | 1772 | 1781 | rVB | 39627 | 51087 | 1.71% | 0.385% |
| 27 | 12.024 | 1788 | 1794 | 1801 | rVB | 292307 | 393680 | 13.14% | 2.965% |
| 28 | 12.104 | 1801 | 1807 | 1811 | rBV3 | 39931 | 67951 | 2.27% | 0.512% |
| 29 | 12.244 | 1828 | 1830 | 1840 | rVB | 29790 | 44419 | 1.48% | 0.335% |
| 30 | 12.415 | 1855 | 1858 | 1867 | rBV3 | 17410 | 33119 | 1.11% | 0.249% |
| 31 | 12.579 | 1882 | 1885 | 1889 | rVB | 25922 | 32057 | 1.07% | 0.241% |
| 32 | 12.768 | 1911 | 1916 | 1920 | rVV2 | 71961 | 100497 | 3.36% | 0.757% |
| 33 | 12.908 | 1928 | 1939 | 1944 | rBV | 515062 | 673475 | 22.48% | 5.072% |
| 34 | 12.963 | 1944 | 1948 | 1953 | rVB5 | 24832 | 44456 | 1.48% | 0.335% |
| 35 | 13.219 | 1985 | 1990 | 1996 | rVV6 | 19299 | 37066 | 1.24% | 0.279% |
| 36 | 13.341 | 2005 | 2010 | 2015 | rBV | 46252 | 70386 | 2.35% | 0.530% |

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** 210609018-02-VOA

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\82X061021W.M
Title : SW846 8260

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 13.427 | 2020 | 2024 | 2028 | rVB3 | 24070 | 33125 | 1.11% | 0.249% |
| 38 | 13.475 | 2028 | 2032 | 2034 | rBV2 | 84121 | 113731 | 3.80% | 0.857% |
| 39 | 13.512 | 2034 | 2038 | 2046 | rVB | 745056 | 975417 | 32.56% | 7.346% |
| 40 | 13.591 | 2046 | 2051 | 2061 | rBV2 | 149094 | 224927 | 7.51% | 1.694% |
| 41 | 13.731 | 2070 | 2074 | 2077 | rBV2 | 42483 | 56485 | 1.89% | 0.425% |
| 42 | 13.780 | 2077 | 2082 | 2088 | rVB | 333158 | 426263 | 14.23% | 3.210% |
| 43 | 13.926 | 2101 | 2106 | 2114 | rBV4 | 21288 | 53985 | 1.80% | 0.407% |
| 44 | 14.103 | 2130 | 2135 | 2147 | rBV | 103741 | 158134 | 5.28% | 1.191% |
| 45 | 14.640 | 2220 | 2223 | 2227 | rVV | 30323 | 37732 | 1.26% | 0.284% |
| 46 | 14.780 | 2240 | 2246 | 2251 | rVB3 | 25853 | 40912 | 1.37% | 0.308% |
| 47 | 16.097 | 2456 | 2462 | 2472 | rVB3 | 25830 | 51607 | 1.72% | 0.389% |

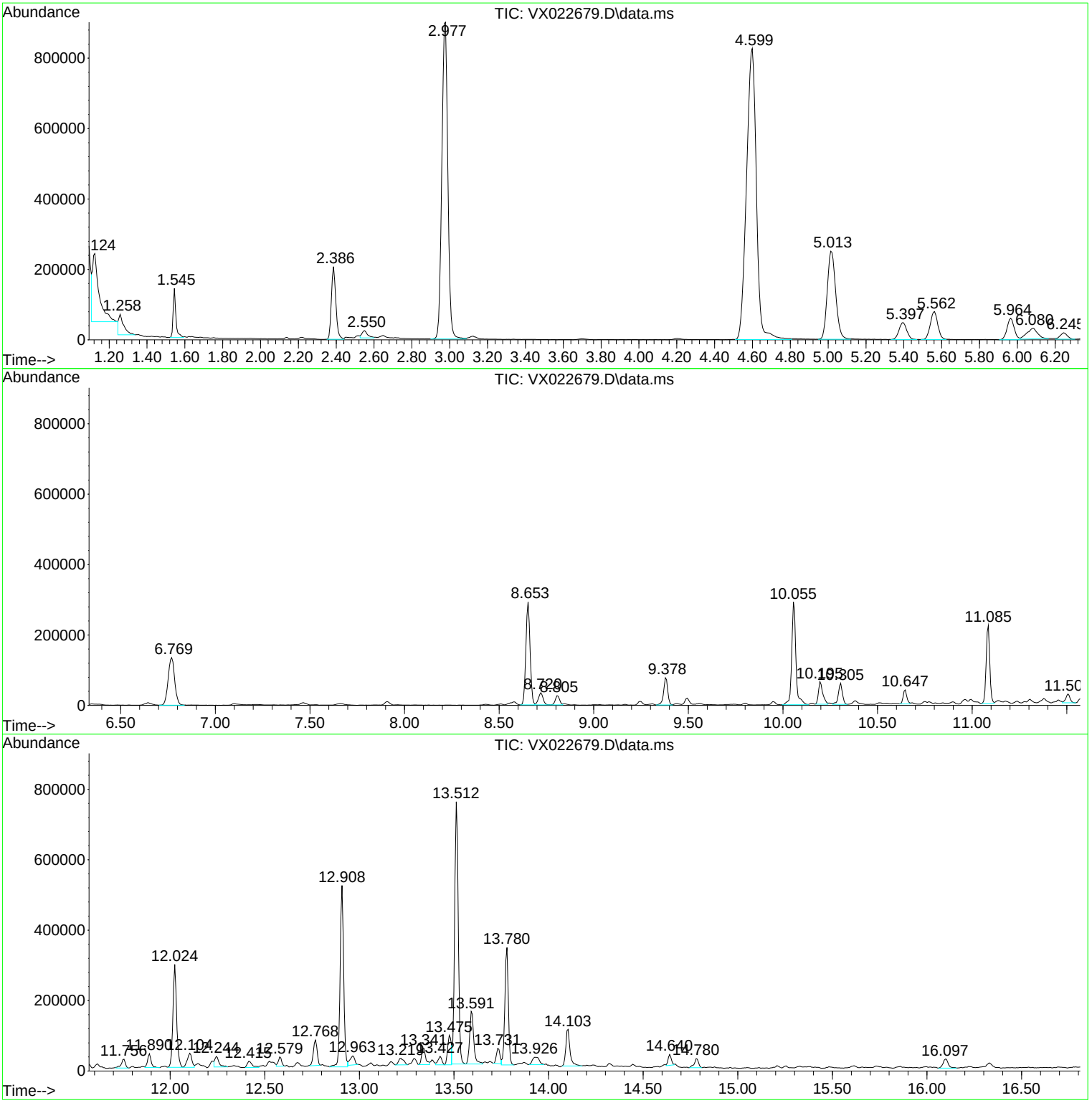
Sum of corrected areas: 13278261

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
210609018-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
210609018-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

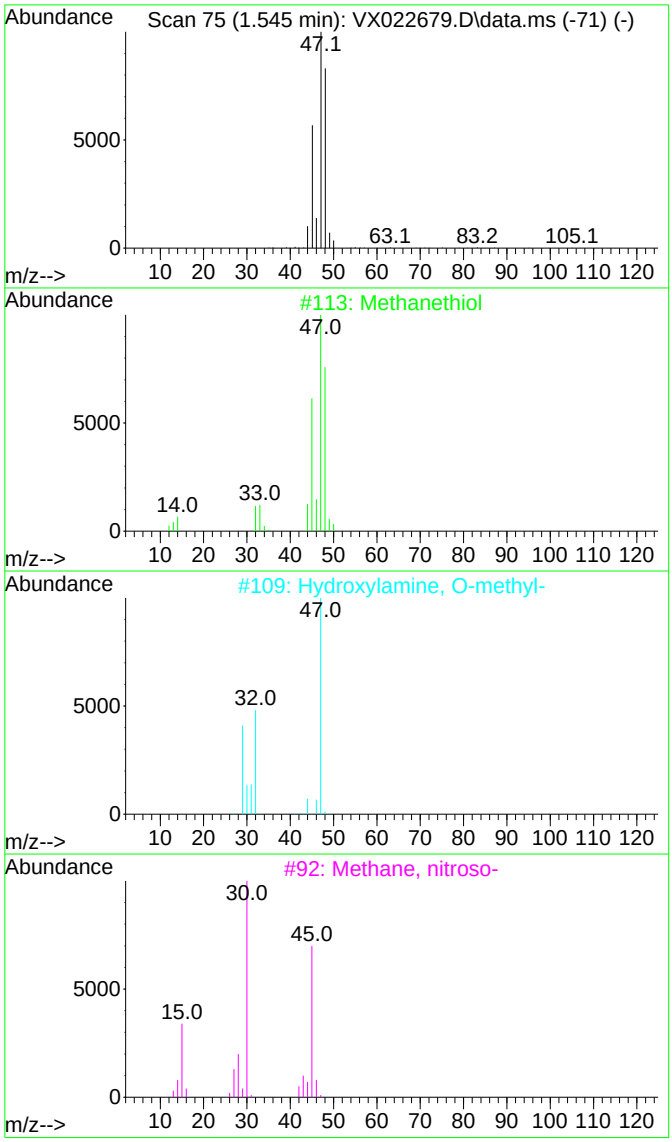
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

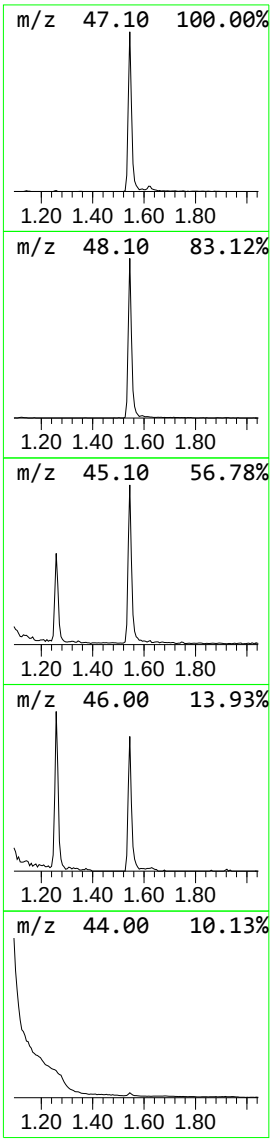
**********

Peak Number 3 Methanethiol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 1.545 | 32.14 ug/l | 141312 | Pentafluorobenzene | 5.556 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methanethiol | 48 | CH4S | 000074-93-1 | 91 |
| 2 | Hydroxylamine, O-methyl- | 47 | CH5NO | 000067-62-9 | 9 |
| 3 | Methane, nitroso- | 45 | CH3NO | 000865-40-7 | 5 |
| 4 | Ethane, fluoro- | 48 | C2H5F | 000353-36-6 | 4 |
| 5 | Formamide | 45 | CH3NO | 000075-12-7 | 4 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
210609018-02-VOA

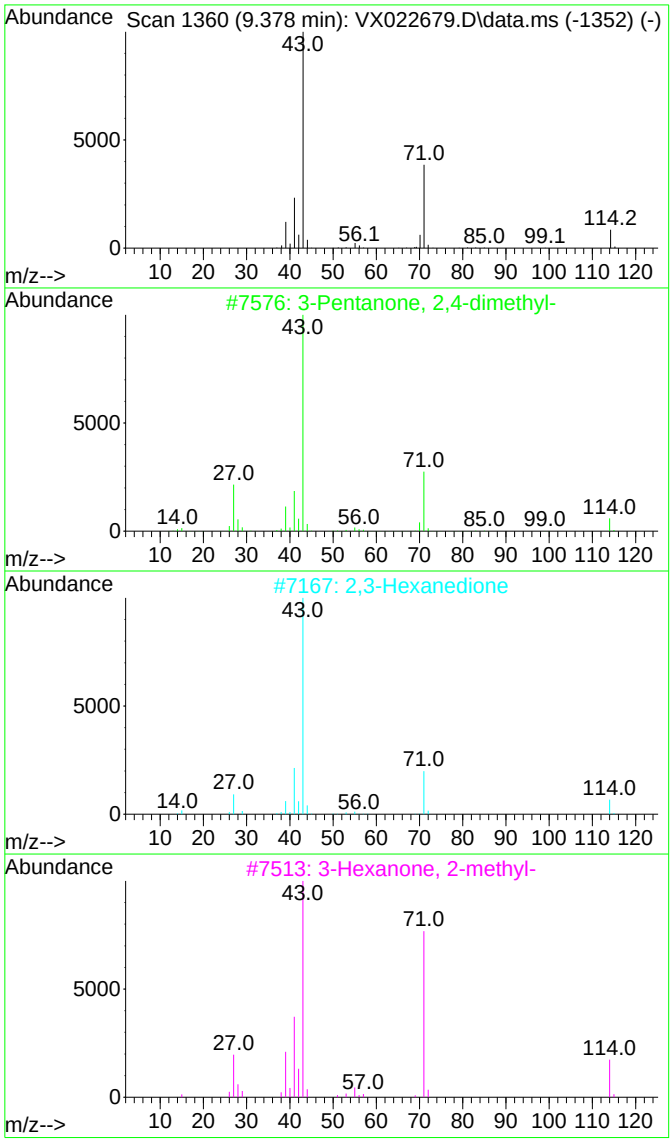
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

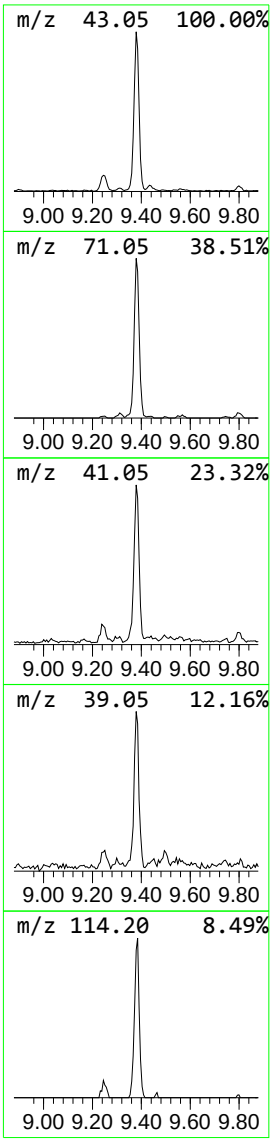
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.378 | 12.98 ug/l | 115957 | Chlorobenzene-d5 | 10.055 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Pentanone, 2,4-dimethyl- | 114 | C7H14O | 000565-80-0 | 90 |
| 2 | 2,3-Hexanedione | 114 | C6H10O2 | 003848-24-6 | 72 |
| 3 | 3-Hexanone, 2-methyl- | 114 | C7H14O | 007379-12-6 | 59 |
| 4 | 4-Heptanone | 114 | C7H14O | 000123-19-3 | 45 |
| 5 | Propanoic acid, 2-methyl-, 2-pro... | 128 | C7H12O2 | 015727-77-2 | 40 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
210609018-02-VOA

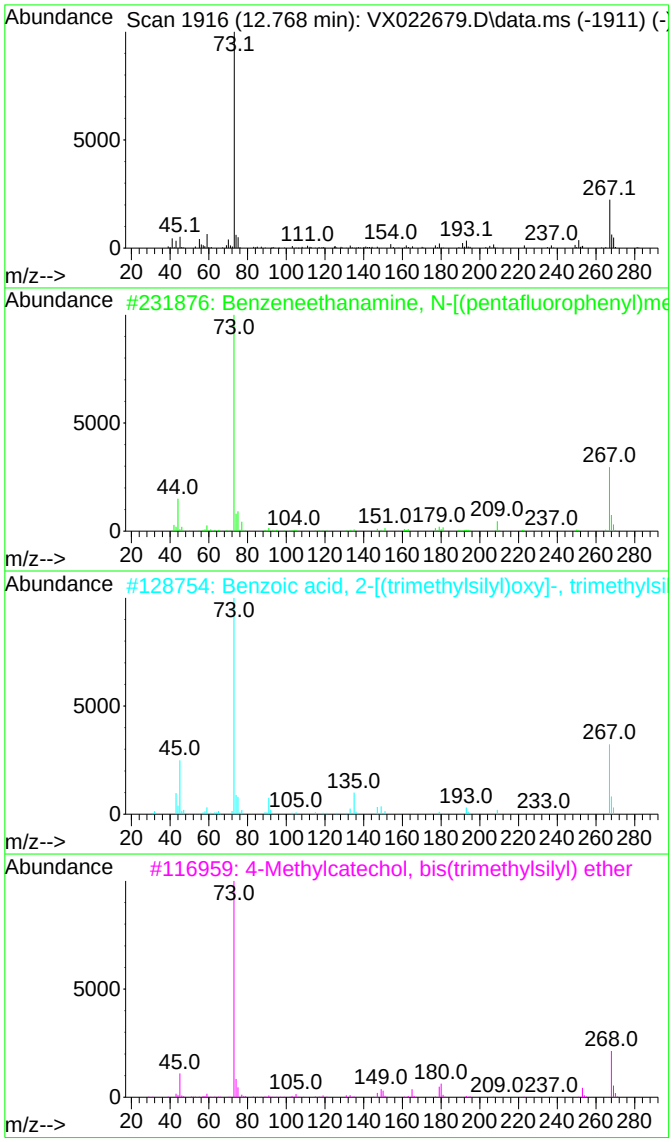
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

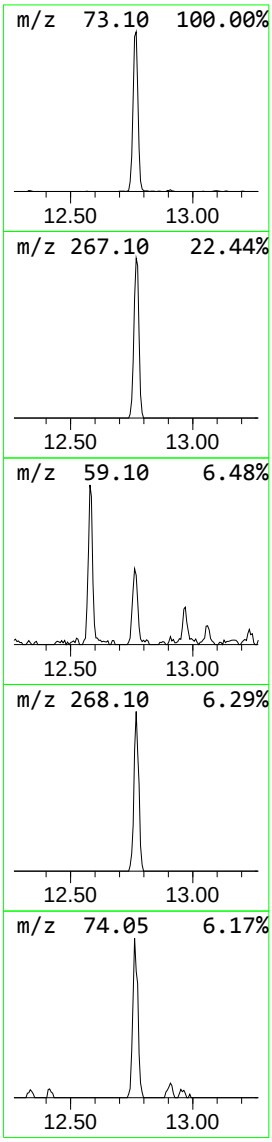
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 unknown12.768 Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.768 | 12.76 ug/l | 100497 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzeneethanamine, N-[(pentafluo... | 475 | C21H26F5NO2Si2 | 055429-85-1 | 37 |
| 2 | Benzoic acid, 2-[(trimethylsilyl... | 282 | C13H22O3Si2 | 003789-85-3 | 25 |
| 3 | 4-Methylcatechol, bis(trimethyls... | 268 | C13H24O2Si2 | 1000332-79-9 | 16 |
| 4 | 1-(3-Chlorophenyl)piperazine, 4-... | 268 | C13H21ClN2Si | 1000373-99-3 | 12 |
| 5 | 11H-Dibenzo[b,e][1,4]diazepin-11... | 267 | C16H17N3O | 013450-73-2 | 9 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
210609018-02-VOA

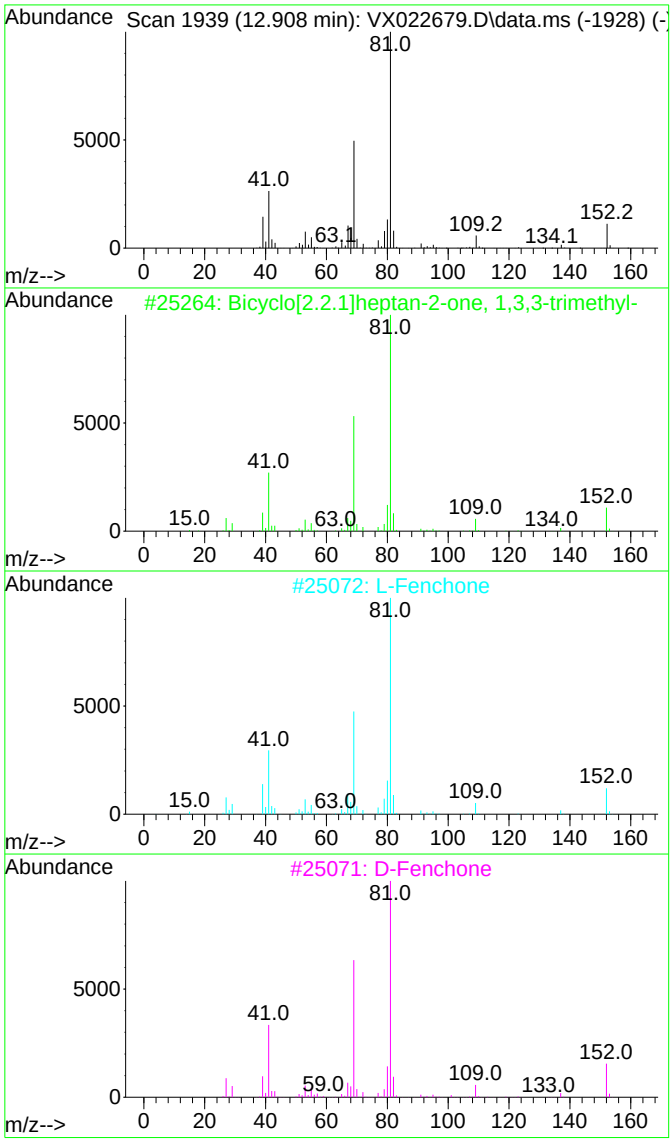
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

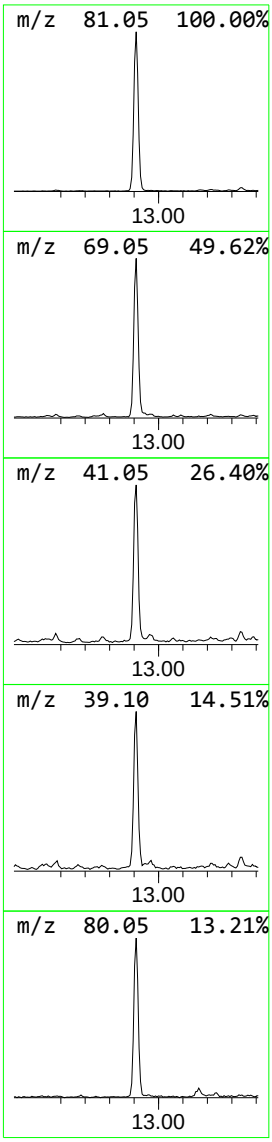
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.908 | 85.54 ug/l | 673475 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bicyclo[2.2.1]heptan-2-one, 1,3,... | 152 | C10H16O | 001195-79-5 | 95 |
| 2 | L-Fenchone | 152 | C10H16O | 007787-20-4 | 94 |
| 3 | D-Fenchone | 152 | C10H16O | 004695-62-9 | 94 |
| 4 | 2,4-Decadienal, (E,E)- | 152 | C10H16O | 025152-84-5 | 59 |
| 5 | 2-Cyclopentene-1-carboxylic acid... | 140 | C8H12O2 | 068317-73-7 | 42 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
210609018-02-VOA

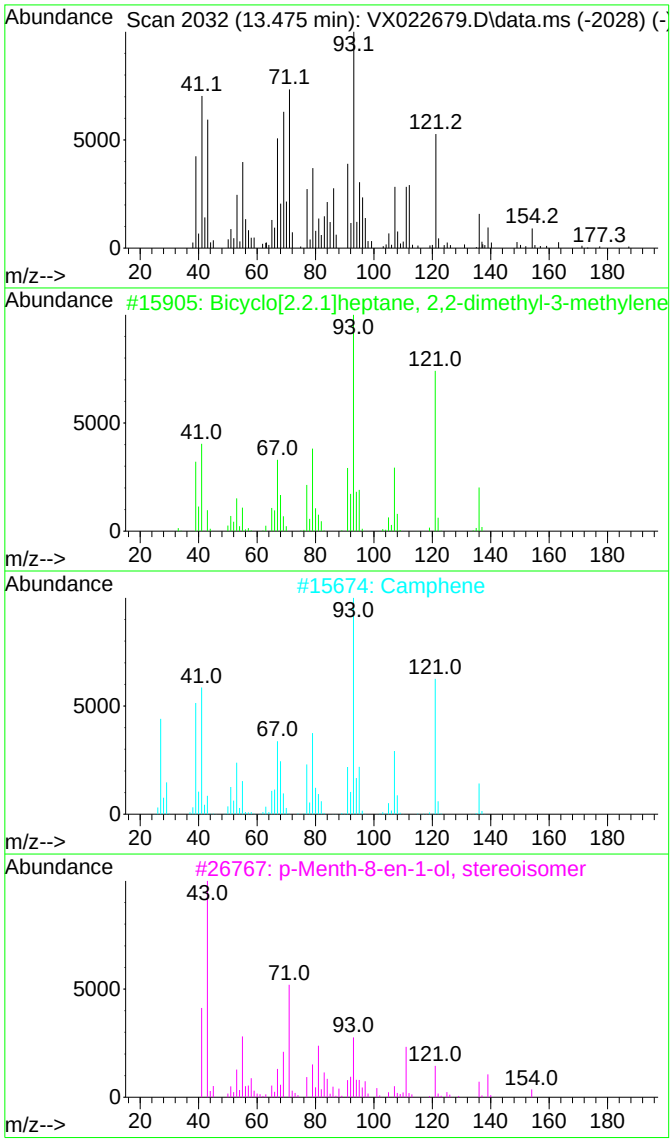
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

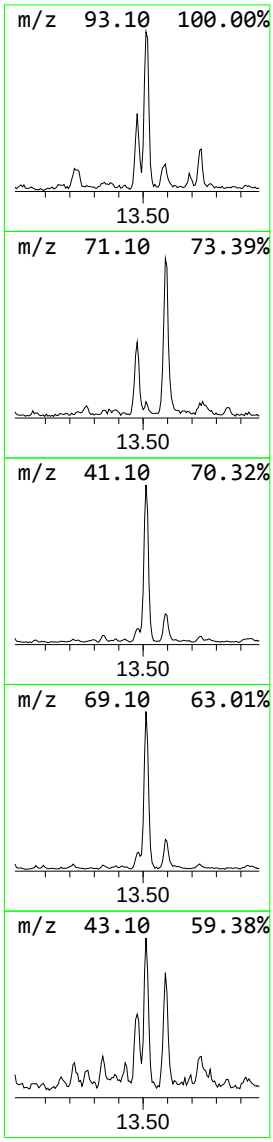
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 Bicyclo[2.2.1]heptane, 2,2-... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.475 | 14.44 ug/l | 113731 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bicyclo[2.2.1]heptane, 2,2-dimet... | 136 | C10H16 | 005794-04-7 | 74 |
| 2 | Camphene | 136 | C10H16 | 000079-92-5 | 51 |
| 3 | p-Menth-8-en-1-ol, stereoisomer | 154 | C10H18O | 007299-40-3 | 30 |
| 4 | 5-Caranol, (1S,3R,5S,6R)-(-)- | 154 | C10H18O | 006909-21-3 | 25 |
| 5 | Bicyclo[2.2.1]hept-2-ene, 1,7,7-... | 136 | C10H16 | 000464-17-5 | 25 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
210609018-02-VOA

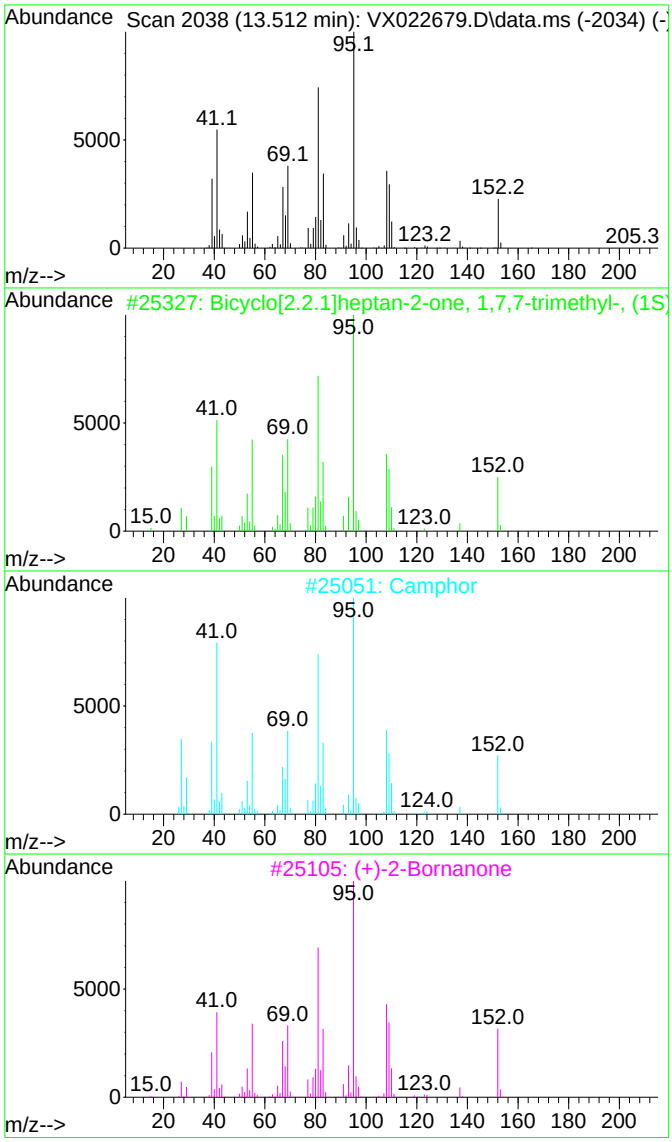
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

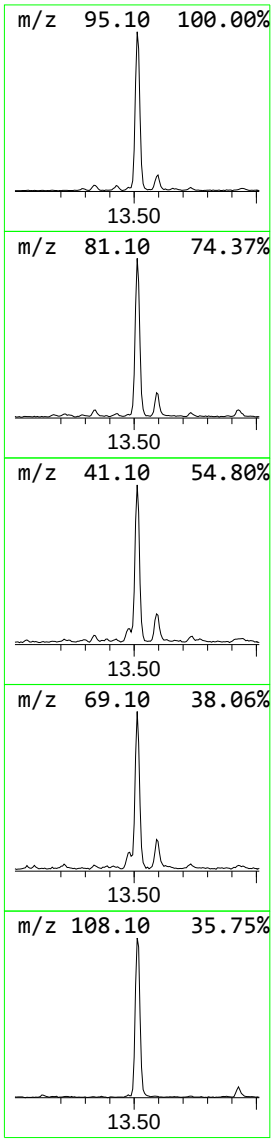
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 8 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.512 | 123.89 ug/l | 975417 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bicyclo[2.2.1]heptan-2-one, 1,7,... | 152 | C10H16O | 000464-48-2 | 98 |
| 2 | Camphor | 152 | C10H16O | 000076-22-2 | 96 |
| 3 | (+)-2-Bornanone | 152 | C10H16O | 000464-49-3 | 96 |
| 4 | Cyclohexanone, 5-methyl-2-(1-met... | 152 | C10H16O | 000529-00-0 | 45 |
| 5 | 5,7-Octadien-4-one, 2,6-dimethyl... | 152 | C10H16O | 006752-80-3 | 43 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
210609018-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

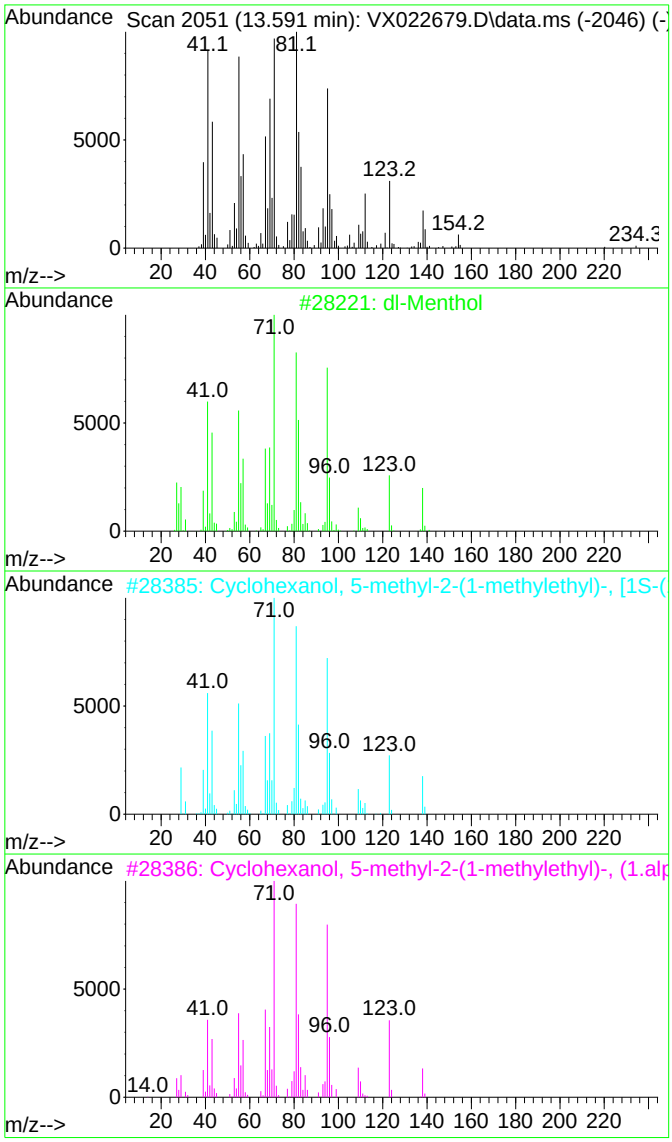
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

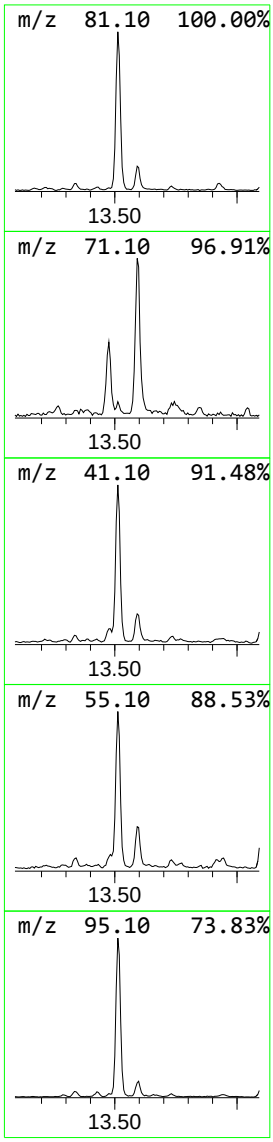
**********

Peak Number 9 dl-Menthol Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.591 | 28.57 ug/l | 224927 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | dl-Menthol | 156 | C10H20O | 000089-78-1 | 86 |
| 2 | Cyclohexanol, 5-methyl-2-(1-meth... | 156 | C10H20O | 002216-52-6 | 86 |
| 3 | Cyclohexanol, 5-methyl-2-(1-meth... | 156 | C10H20O | 015356-70-4 | 80 |
| 4 | Bicyclo[3.1.0]hexan-2-one, 5-(1-... | 138 | C9H14O | 000513-20-2 | 60 |
| 5 | Cyclohexane, 1-methyl-4-(1-methy... | 138 | C10H18 | 001879-07-8 | 58 |



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
MSVOA_X
**ClientSampleId :**
210609018-02-VOA

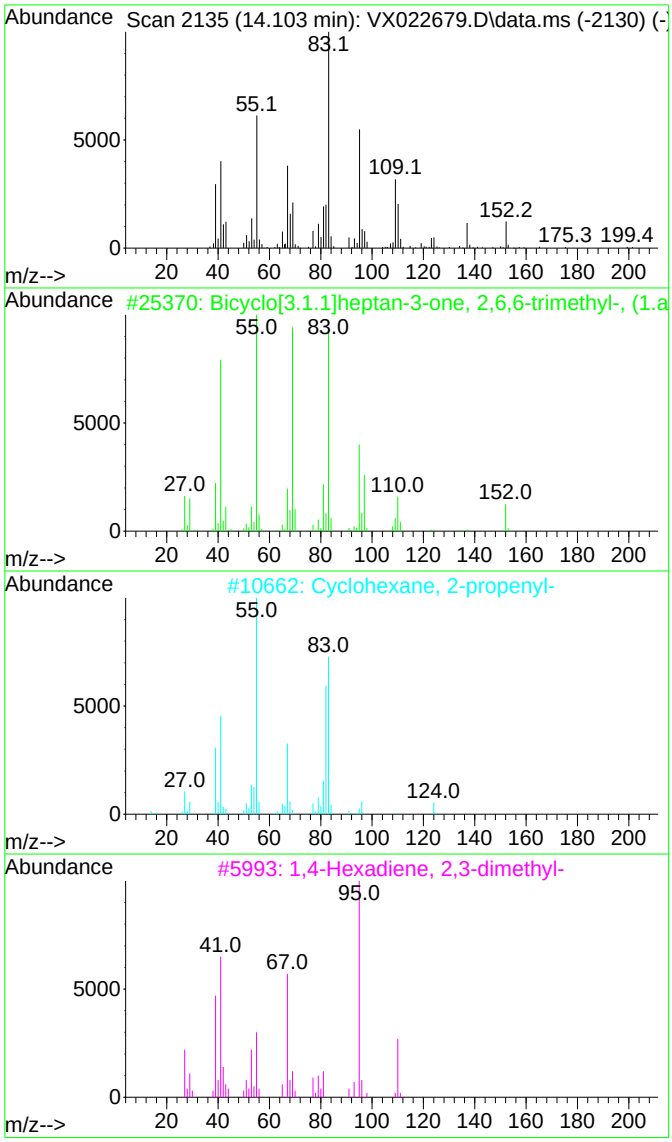
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.M
Quant Title : SW846 8260

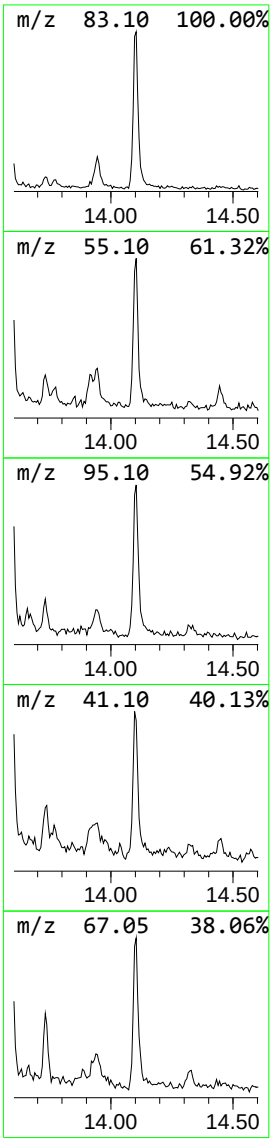
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 Bicyclo[3.1.1]heptan-3-one,... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.103 | 20.08 ug/l | 158134 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bicyclo[3.1.1]heptan-3-one, 2,6,... | 152 | C10H16O | 000547-60-4 | 58 |
| 2 | Cyclohexane, 2-propenyl- | 124 | C9H16 | 002114-42-3 | 50 |
| 3 | 1,4-Hexadiene, 2,3-dimethyl- | 110 | C8H14 | 018669-52-8 | 42 |
| 4 | 5,5-Dimethyl-1,3-hexadiene | 110 | C8H14 | 001515-79-3 | 38 |
| 5 | 1-Methyl-2-methylenecyclohexane | 110 | C8H14 | 002808-75-5 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061121\
Data File : VX022679.D
Acq On : 11 Jun 2021 19:52
Operator : JC/MD
Sample : M2703-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** MSVOA_X
**ClientSampleId :** 210609018-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061021W.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 |
| Methanethiol | 1.545 | 32.1 | ug/l | 141312 | 1 | 5.556 | 219821 | 50.0 |
| 3-Pentanone, 2,... | 9.378 | 13.0 | ug/l | 115957 | 3 | 10.055 | 446693 | 50.0 |
| unknown12.768 | 12.768 | 12.8 | ug/l | 100497 | 4 | 12.024 | 393680 | 50.0 |
| Bicyclo[2.2.1]h... | 12.908 | 85.5 | ug/l | 673475 | 4 | 12.024 | 393680 | 50.0 |
| Bicyclo[2.2.1]h... | 13.475 | 14.4 | ug/l | 113731 | 4 | 12.024 | 393680 | 50.0 |
| Bicyclo[2.2.1]h... | 13.512 | 123.9 | ug/l | 975417 | 4 | 12.024 | 393680 | 50.0 |
| dl-Menthol | 13.591 | 28.6 | ug/l | 224927 | 4 | 12.024 | 393680 | 50.0 |
| Bicyclo[3.1.1]h... | 14.103 | 20.1 | ug/l | 158134 | 4 | 12.024 | 393680 | 50.0 |