

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX031621\  
 Data File : VX021257.D  
 Acq On : 16 Mar 2021 20:17  
 Operator : JC/MD  
 Sample : M1694-01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 23 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 JG-W

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\82X031621W.M  
 Title : SW846 8260

Signal : TIC: VX021257.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 4.635       | 592           | 603         | 620          | rVB2     | 23659          | 69785         | 1.47%           | 0.292%        |
| 2         | 5.176       | 683           | 695         | 709          | rVB      | 96282          | 287679        | 6.06%           | 1.205%        |
| 3         | 5.464       | 731           | 744         | 756          | rBV2     | 54269          | 156752        | 3.30%           | 0.657%        |
| 4         | 5.629       | 760           | 772         | 786          | rVB      | 100580         | 276725        | 5.83%           | 1.159%        |
| 5         | 6.029       | 828           | 840         | 852          | rBV      | 64000          | 169594        | 3.57%           | 0.711%        |
| 6         | 6.829       | 965           | 976         | 987          | rBV      | 148009         | 346730        | 7.30%           | 1.453%        |
| 7         | 8.694       | 1286          | 1293        | 1300         | rBV      | 301904         | 474971        | 10.00%          | 1.990%        |
| 8         | 8.765       | 1300          | 1305        | 1312         | rVB      | 42310          | 66218         | 1.39%           | 0.277%        |
| 9         | 10.094      | 1525          | 1531        | 1544         | rBV      | 299551         | 398410        | 8.39%           | 1.669%        |
| 10        | 10.235      | 1550          | 1555        | 1564         | rVB      | 120642         | 155419        | 3.27%           | 0.651%        |
| 11        | 10.341      | 1564          | 1573        | 1584         | rBV      | 458980         | 637020        | 13.41%          | 2.669%        |
| 12        | 10.682      | 1624          | 1631        | 1638         | rBV      | 250738         | 324246        | 6.83%           | 1.359%        |
| 13        | 10.983      | 1676          | 1682        | 1692         | rBV      | 296731         | 393800        | 8.29%           | 1.650%        |
| 14        | 11.118      | 1700          | 1705        | 1711         | rBV      | 238419         | 312630        | 6.58%           | 1.310%        |
| 15        | 11.177      | 1711          | 1715        | 1717         | rVV      | 86599          | 111115        | 2.34%           | 0.466%        |
| 16        | 11.212      | 1717          | 1721        | 1727         | rVB      | 318088         | 425561        | 8.96%           | 1.783%        |
| 17        | 11.606      | 1783          | 1788        | 1794         | rBV      | 60012          | 71343         | 1.50%           | 0.299%        |
| 18        | 11.906      | 1834          | 1839        | 1841         | rBV      | 46895          | 65031         | 1.37%           | 0.272%        |
| 19        | 12.012      | 1848          | 1857        | 1859         | rBV      | 766955         | 891019        | 18.76%          | 3.733%        |
| 20        | 12.047      | 1859          | 1863        | 1874         | rVV      | 3717670        | 4748622       | 100.00%         | 19.896%       |
| 21        | 12.141      | 1874          | 1879        | 1887         | rVB      | 93146          | 119577        | 2.52%           | 0.501%        |
| 22        | 12.277      | 1894          | 1902        | 1909         | rBV2     | 30703          | 51597         | 1.09%           | 0.216%        |
| 23        | 12.565      | 1945          | 1951        | 1959         | rBV      | 531525         | 659286        | 13.88%          | 2.762%        |
| 24        | 12.947      | 2010          | 2016        | 2025         | rBV      | 602822         | 798897        | 16.82%          | 3.347%        |
| 25        | 13.206      | 2052          | 2060        | 2068         | rBV      | 2136014        | 2876452       | 60.57%          | 12.052%       |
| 26        | 13.289      | 2068          | 2074        | 2083         | rVV3     | 144254         | 273059        | 5.75%           | 1.144%        |
| 27        | 13.377      | 2084          | 2089        | 2090         | rVV      | 92575          | 108656        | 2.29%           | 0.455%        |
| 28        | 13.400      | 2090          | 2093        | 2100         | rVB      | 206200         | 265167        | 5.58%           | 1.111%        |
| 29        | 13.512      | 2107          | 2112        | 2115         | rBV      | 175229         | 237527        | 5.00%           | 0.995%        |
| 30        | 13.553      | 2115          | 2119        | 2124         | rVV      | 951535         | 1260704       | 26.55%          | 5.282%        |
| 31        | 13.618      | 2124          | 2130        | 2138         | rVV2     | 329706         | 577260        | 12.16%          | 2.419%        |
| 32        | 13.706      | 2138          | 2145        | 2150         | rVV2     | 1970190        | 2779169       | 58.53%          | 11.644%       |
| 33        | 13.771      | 2150          | 2156        | 2161         | rVV      | 2786734        | 3385163       | 71.29%          | 14.183%       |
| 34        | 13.812      | 2161          | 2163        | 2169         | rVV      | 67471          | 92574         | 1.95%           | 0.388%        |

Sum of corrected areas: 23867758

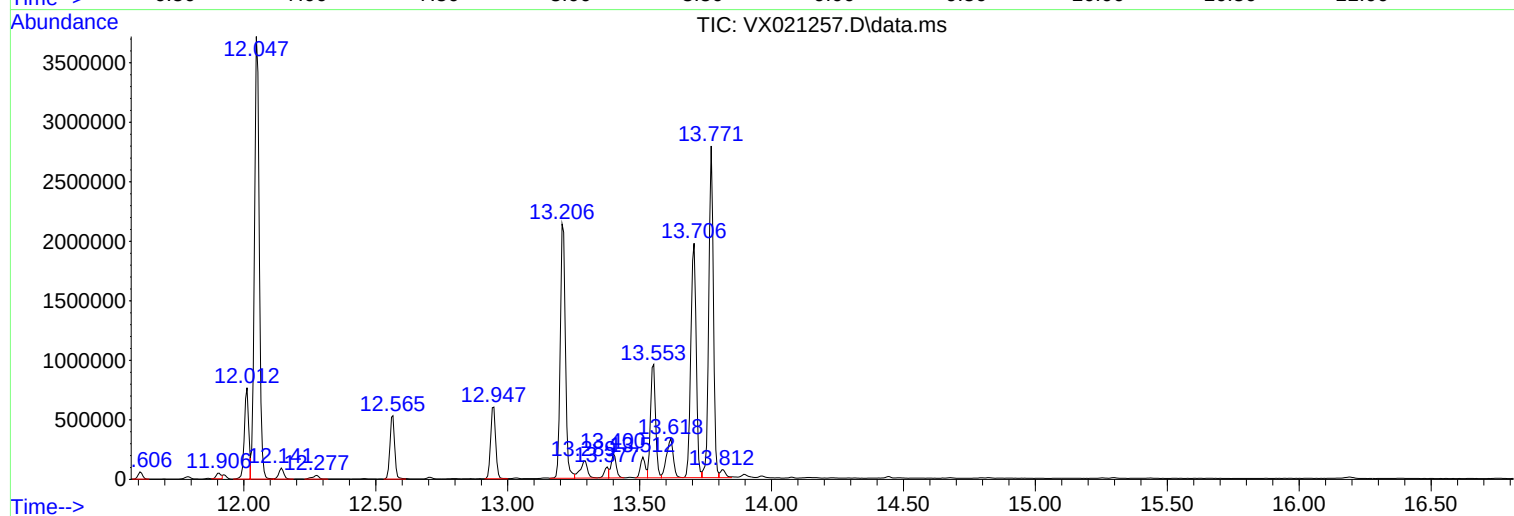
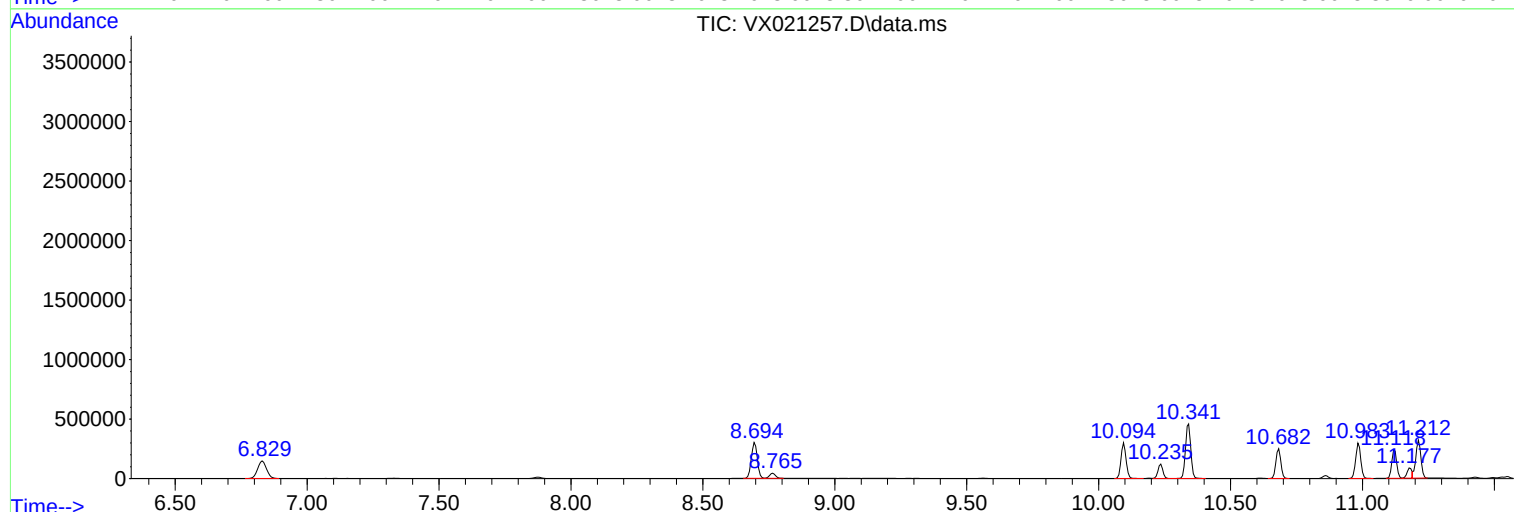
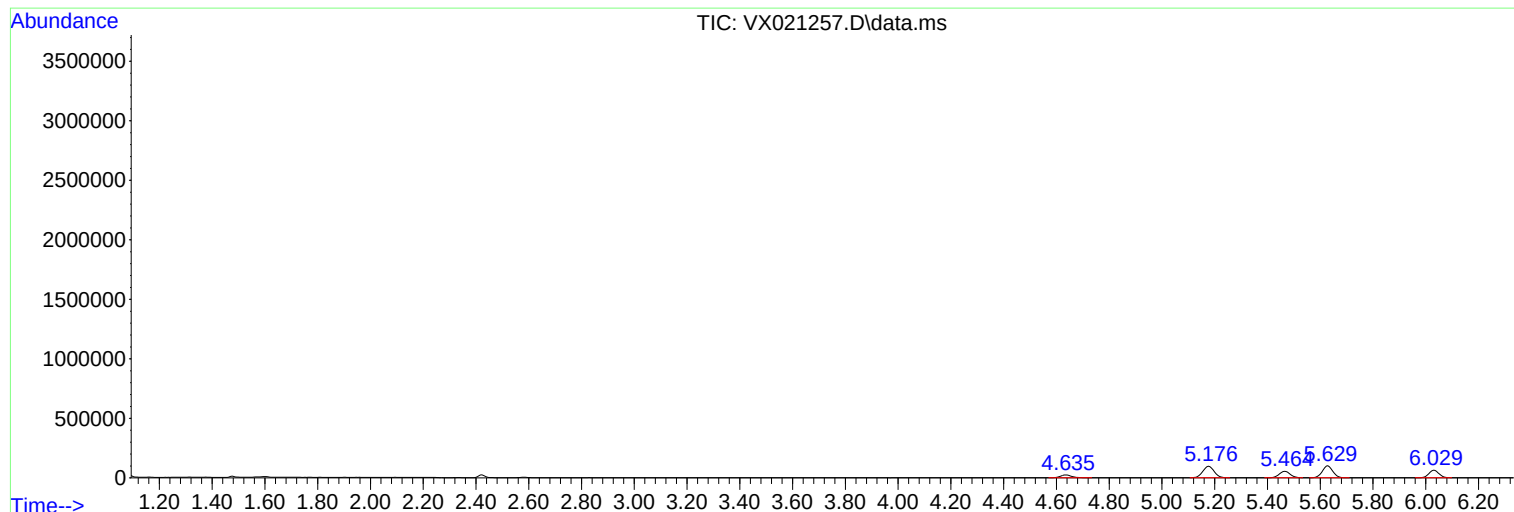
**Instrument :**  
MSVOA\_X  
**ClientSampleId :**  
JG-W

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX031621\  
Data File : VX021257.D  
Acq On : 16 Mar 2021 20:17  
Operator : JC/MD  
Sample : M1694-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
JG-W

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X031621W.M  
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX031621\  
Data File : VX021257.D  
Acq On : 16 Mar 2021 20:17  
Operator : JC/MD  
Sample : M1694-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
JG-W

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X031621W.M  
Quant Title : SW846 8260

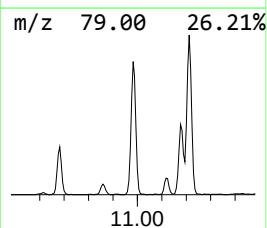
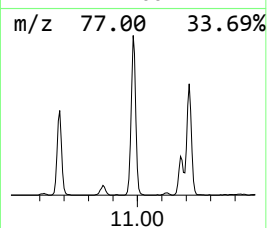
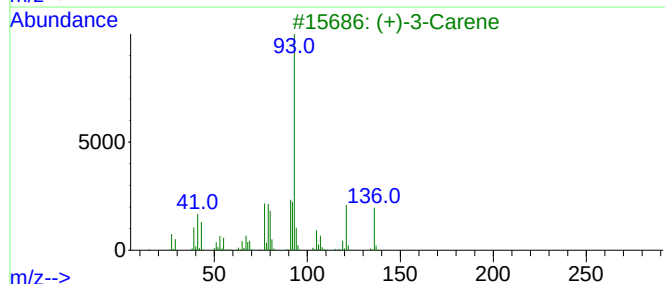
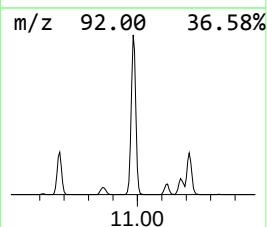
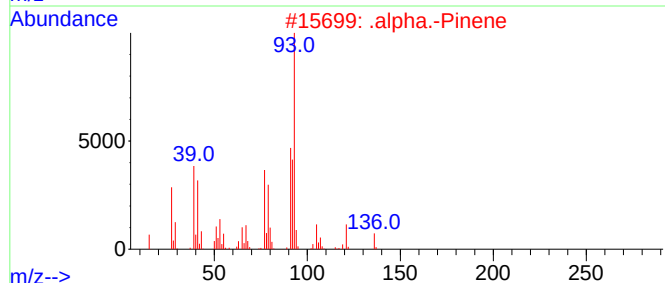
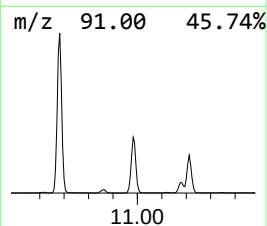
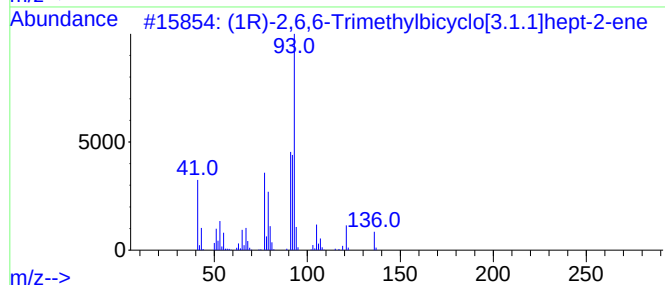
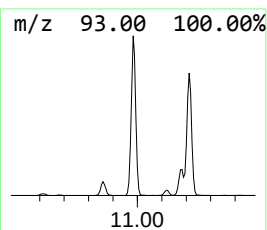
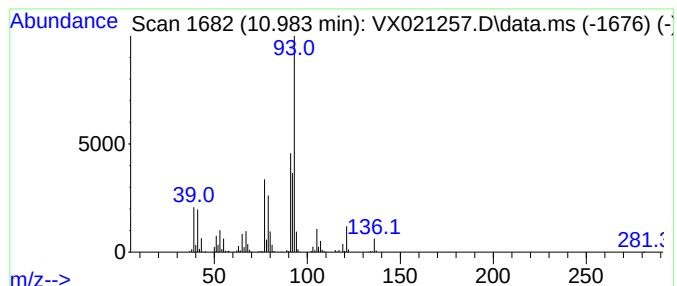
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 1 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 1

| R.T.   | EstConc    | Area   | Relative to ISTD | R.T.   |
|--------|------------|--------|------------------|--------|
| 10.983 | 49.42 ug/l | 393800 | Chlorobenzene-d5 | 10.094 |

| Hit# | of | 5 | Tentative ID                                    | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------------------|-----|---------|-------------|------|
| 1    |    |   | (1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene    | 136 | C10H16  | 007785-70-8 | 97   |
| 2    |    |   | .alpha.-Pinene                                  | 136 | C10H16  | 000080-56-8 | 95   |
| 3    |    |   | (+)-3-Carene                                    | 136 | C10H16  | 000498-15-7 | 91   |
| 4    |    |   | Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-      | 136 | C10H16  | 004889-83-2 | 91   |
| 5    |    |   | Tricyclo[2.2.1.0(2,6)]heptane, 1,1,2-trimethyl- | 136 | C10H16  | 000508-32-7 | 91   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX031621\  
Data File : VX021257.D  
Acq On : 16 Mar 2021 20:17  
Operator : JC/MD  
Sample : M1694-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
JG-W

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X031621W.M  
Quant Title : SW846 8260

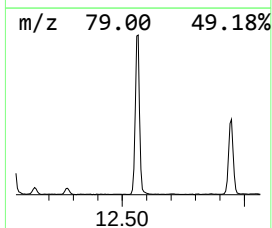
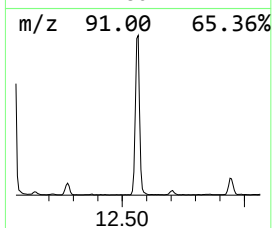
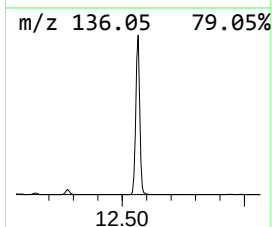
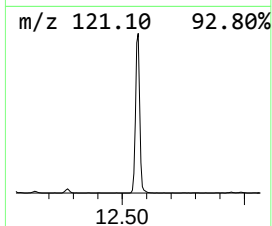
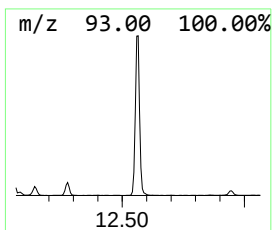
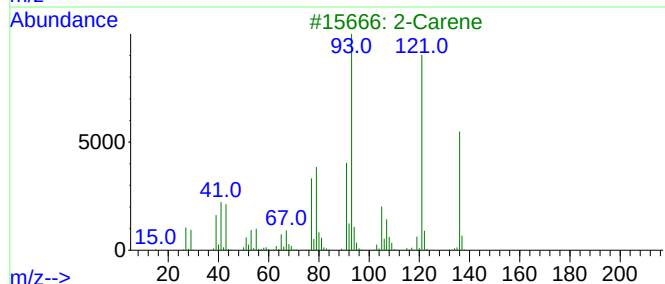
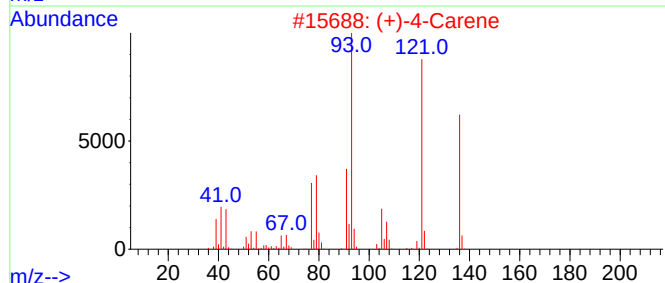
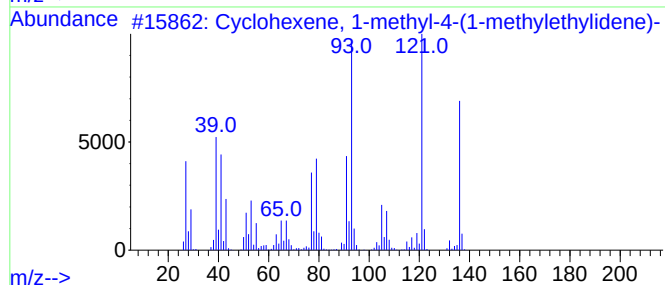
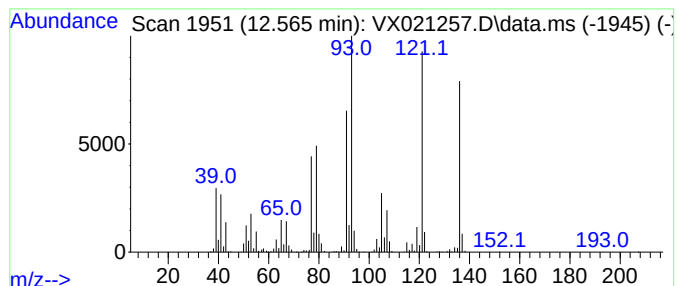
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 2 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 6

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 12.565 | 6.94 ug/l | 659286 | 1,4-Dichlorobenzene-d4 | 12.059 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexene, 1-methyl-4-(1-methy... | 136 | C10H16  | 000586-62-9 | 97   |
| 2    |    |   | (+)-4-Carene                        | 136 | C10H16  | 029050-33-7 | 96   |
| 3    |    |   | 2-Carene                            | 136 | C10H16  | 000554-61-0 | 94   |
| 4    |    |   | 1,3-Cyclohexadiene, 1-methyl-4-(... | 136 | C10H16  | 000099-86-5 | 93   |
| 5    |    |   | 3-Octen-5-yne, 2,7-dimethyl-, (Z)-  | 136 | C10H16  | 028935-76-4 | 90   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX031621\  
Data File : VX021257.D  
Acq On : 16 Mar 2021 20:17  
Operator : JC/MD  
Sample : M1694-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
JG-W

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X031621W.M  
Quant Title : SW846 8260

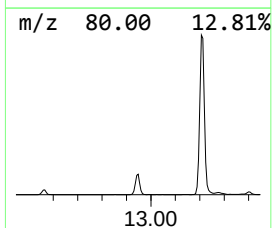
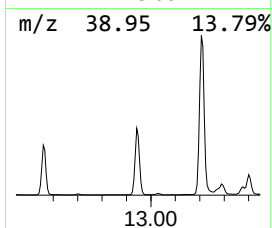
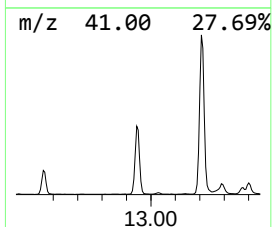
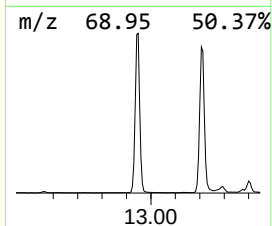
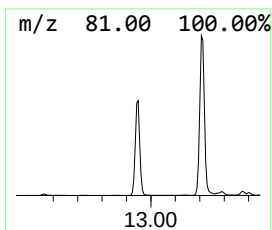
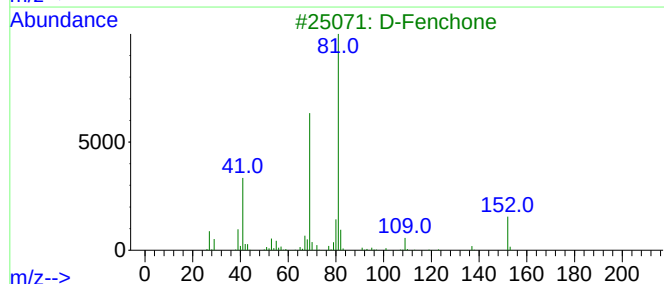
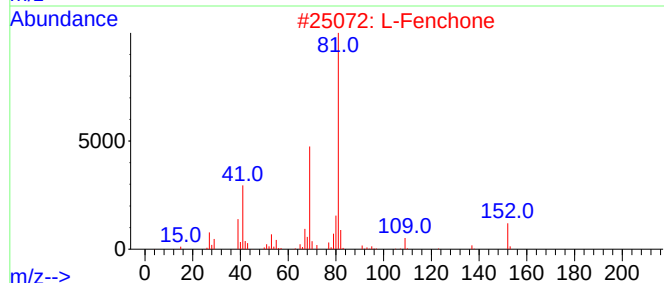
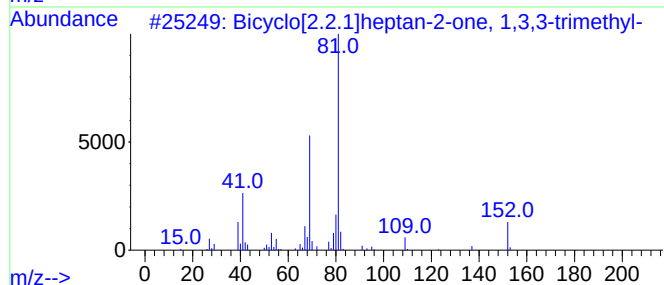
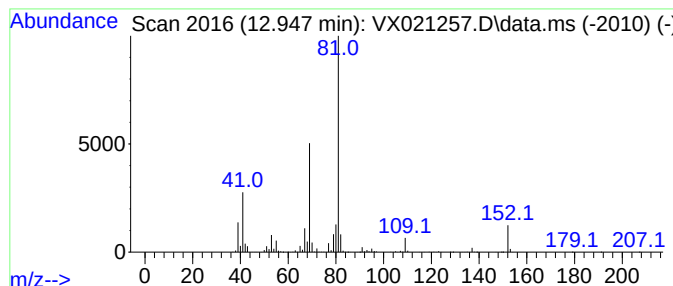
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 3 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 5

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 12.948 | 8.41 ug/l | 798897 | 1,4-Dichlorobenzene-d4 | 12.059 |

| 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 | 95   |
| 3    |    |   | D-Fenchone                          | 152 | C10H16O | 004695-62-9 | 91   |
| 4    |    |   | 2,4-Decadienal, (E,E)-              | 152 | C10H16O | 025152-84-5 | 59   |
| 5    |    |   | 2,4-Nonadienal, (E,E)-              | 138 | C9H14O  | 005910-87-2 | 53   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX031621\  
Data File : VX021257.D  
Acq On : 16 Mar 2021 20:17  
Operator : JC/MD  
Sample : M1694-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
JG-W

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X031621W.M  
Quant Title : SW846 8260

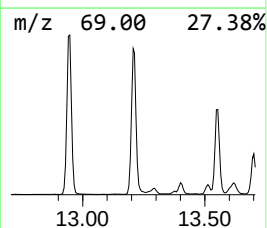
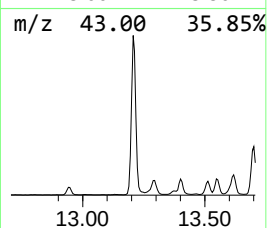
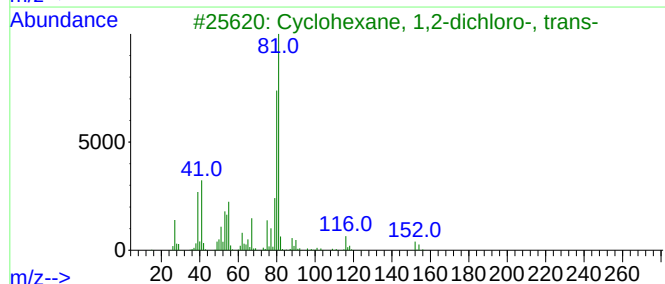
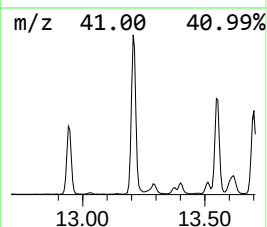
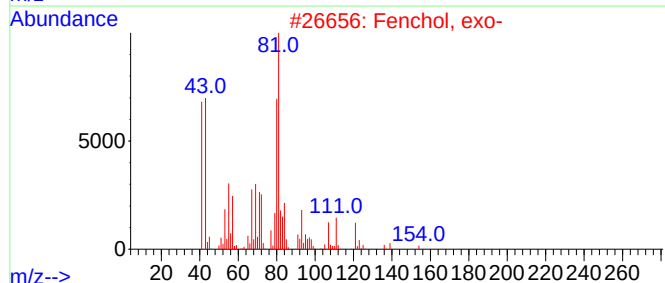
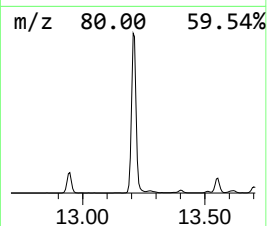
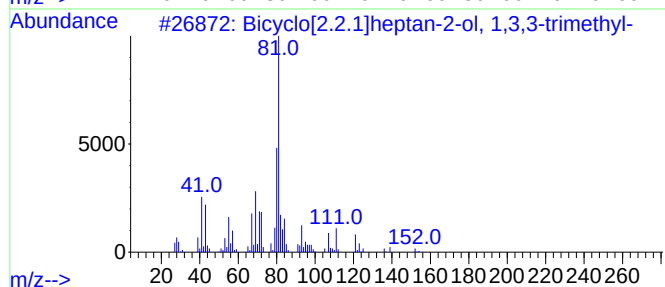
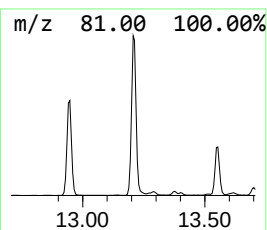
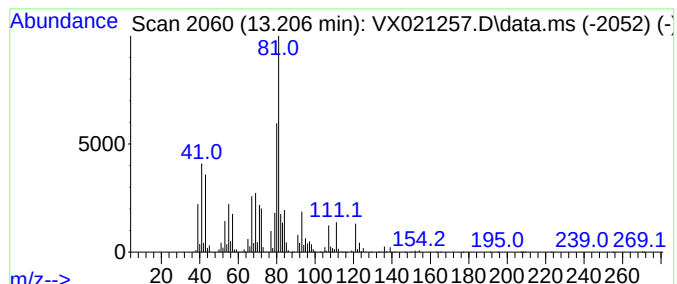
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 4 Bicyclo[2.2.1]heptan-2-ol, ... Concentration Rank 2

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 13.206 | 30.29 ug/l | 2876450 | 1,4-Dichlorobenzene-d4 | 12.059 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Bicyclo[2.2.1]heptan-2-ol, 1,3,3... | 154 | C10H18O  | 001632-73-1 | 96   |
| 2    |    |   | Fenchol, exo-                       | 154 | C10H18O  | 022627-95-8 | 83   |
| 3    |    |   | Cyclohexane, 1,2-dichloro-, trans-  | 152 | C6H10Cl2 | 000822-86-6 | 43   |
| 4    |    |   | Bi-2-cyclohexen-1-yl                | 162 | C12H18   | 001541-20-4 | 38   |
| 5    |    |   | Cyclohexene, 3-ethyl-               | 110 | C8H14    | 002808-71-1 | 35   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX031621\  
Data File : VX021257.D  
Acq On : 16 Mar 2021 20:17  
Operator : JC/MD  
Sample : M1694-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
JG-W

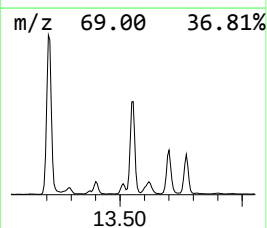
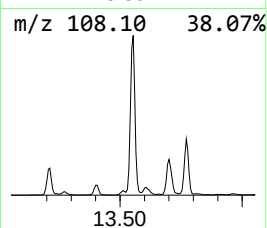
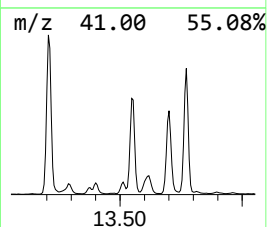
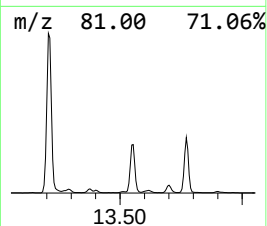
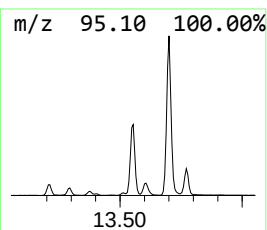
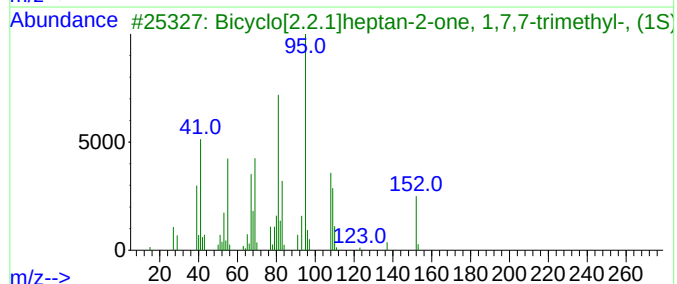
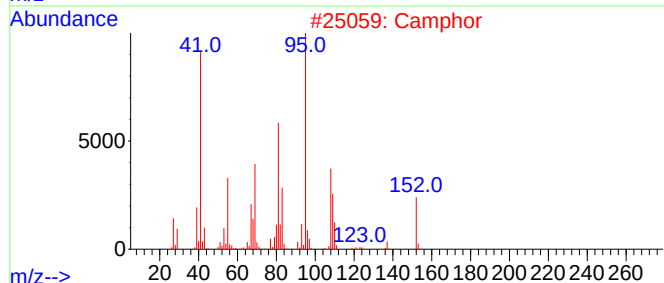
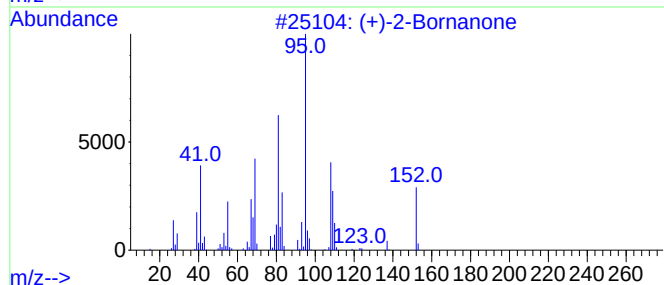
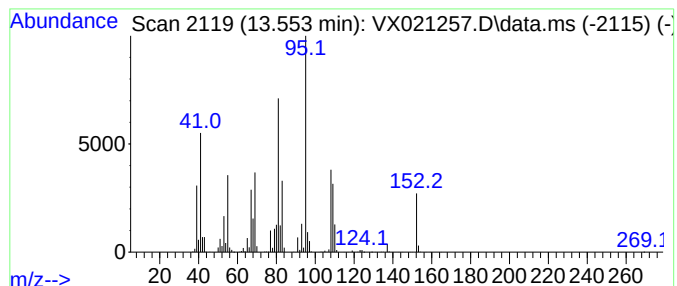
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X031621W.M  
Quant Title : SW846 8260

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

\*\*\*\*\*  
Peak Number 5 (+)-2-Bornanone Concentration Rank 4

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 13.553 | 13.27 ug/l | 1260700 | 1,4-Dichlorobenzene-d4 | 12.059 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | (+)-2-Bornanone                     | 152 | C10H16O | 000464-49-3 | 98   |
| 2    |    |   | Camphor                             | 152 | C10H16O | 000076-22-2 | 98   |
| 3    |    |   | Bicyclo[2.2.1]heptan-2-one, 1,7,... | 152 | C10H16O | 000464-48-2 | 98   |
| 4    |    |   | 5,7-Octadien-4-one, 2,6-dimethyl... | 152 | C10H16O | 006752-80-3 | 52   |
| 5    |    |   | 2-Butanone, 4-(5-methyl-2-furanyl)- | 152 | C9H12O2 | 013679-56-6 | 46   |





Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX031621\  
Data File : VX021257.D  
Acq On : 16 Mar 2021 20:17  
Operator : JC/MD  
Sample : M1694-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
JG-W

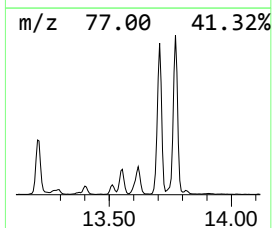
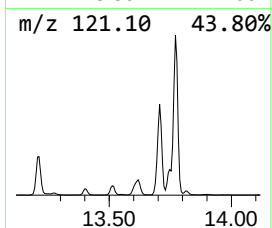
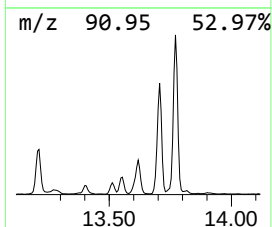
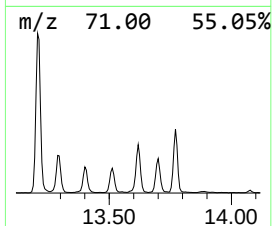
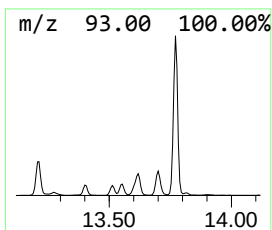
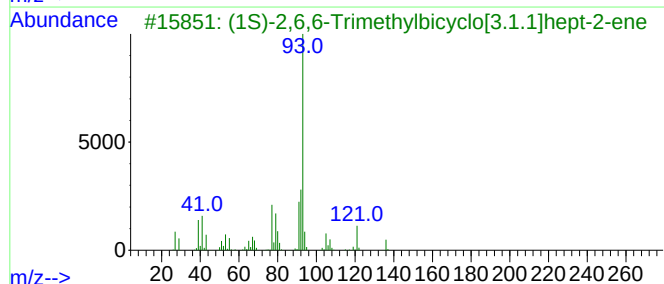
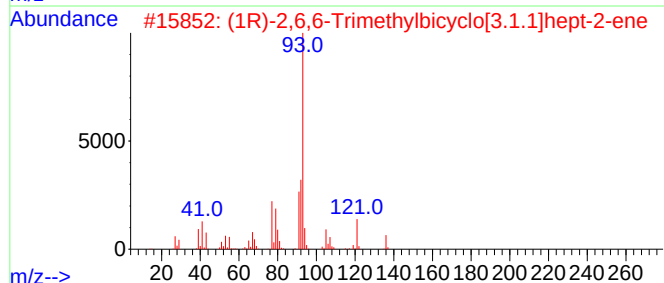
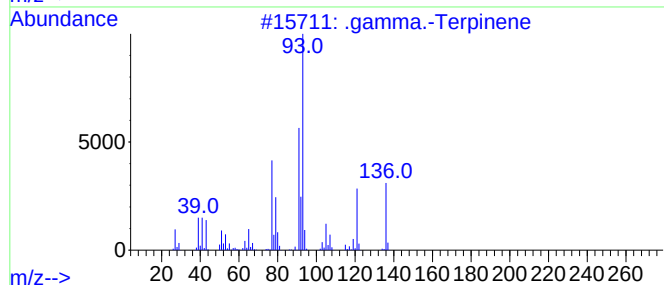
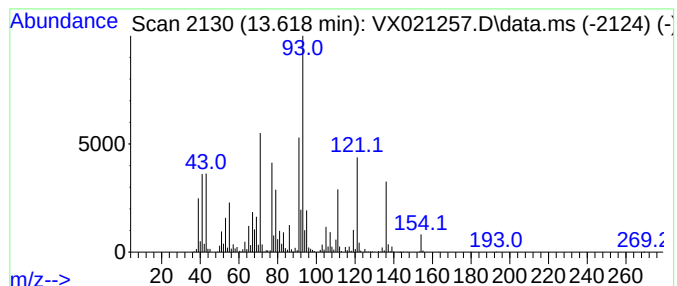
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X031621W.M  
Quant Title : SW846 8260

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

\*\*\*\*\*  
Peak Number 6 .gamma.-Terpinene Concentration Rank 7

| R.T.   | EstConc   | Area   | Relative to ISTD       | R.T.   |
|--------|-----------|--------|------------------------|--------|
| 13.618 | 6.08 ug/l | 577260 | 1,4-Dichlorobenzene-d4 | 12.059 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|------|-------------------------------------|-----|---------|-------------|------|
| 1    |      | .gamma.-Terpinene                   | 136 | C10H16  | 000099-85-4 | 92   |
| 2    |      | (1R)-2,6,6-Trimethylbicyclo[3.1.... | 136 | C10H16  | 007785-70-8 | 78   |
| 3    |      | (1S)-2,6,6-Trimethylbicyclo[3.1.... | 136 | C10H16  | 007785-26-4 | 60   |
| 4    |      | .alpha.-Phellandrene                | 136 | C10H16  | 000099-83-2 | 60   |
| 5    |      | (+)-3-Carene                        | 136 | C10H16  | 000498-15-7 | 60   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX031621\  
Data File : VX021257.D  
Acq On : 16 Mar 2021 20:17  
Operator : JC/MD  
Sample : M1694-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
JG-W

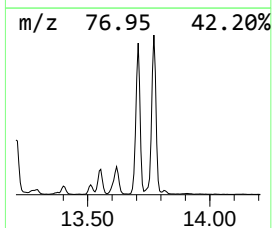
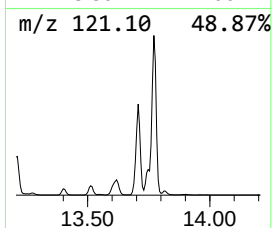
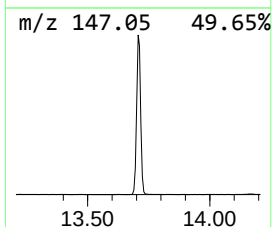
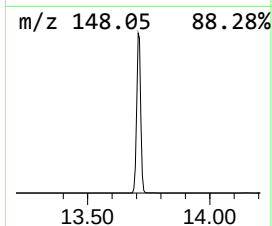
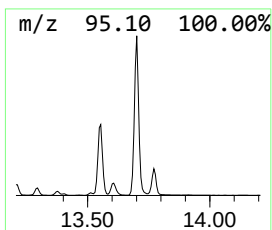
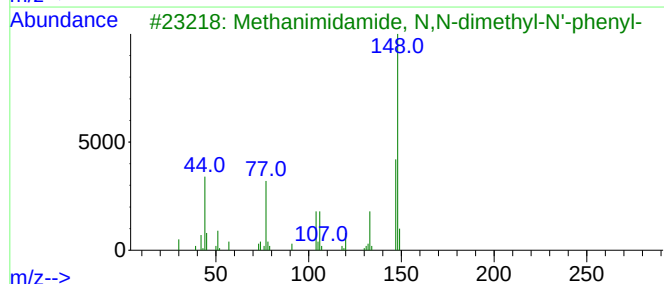
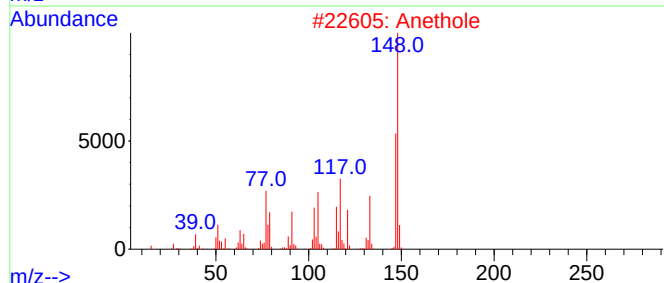
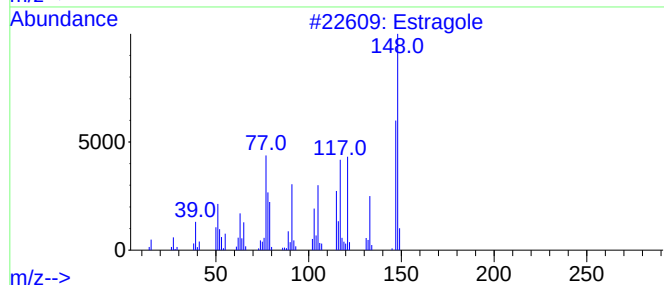
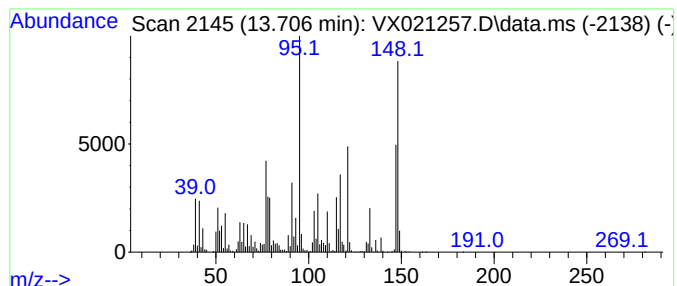
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X031621W.M  
Quant Title : SW846 8260

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

\*\*\*\*\*  
Peak Number 7 Estragole Concentration Rank 3

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 13.706 | 29.26 ug/l | 2779170 | 1,4-Dichlorobenzene-d4 | 12.059 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Estragole                           | 148 | C10H12O | 000140-67-0 | 99   |
| 2    |    |   | Anethole                            | 148 | C10H12O | 000104-46-1 | 96   |
| 3    |    |   | Methanimidamide, N,N-dimethyl-N'... | 148 | C9H12N2 | 001783-25-1 | 46   |
| 4    |    |   | 2-Hydroxymethylbenzimidazole        | 148 | C8H8N2O | 022128-99-0 | 38   |
| 5    |    |   | endo-Borneol                        | 154 | C10H18O | 000507-70-0 | 25   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX031621\  
Data File : VX021257.D  
Acq On : 16 Mar 2021 20:17  
Operator : JC/MD  
Sample : M1694-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
JG-W

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X031621W.M  
Quant Title : SW846 8260

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| (1R)-2,6,6-Trim... | 10.983 | 49.4    | ug/l  | 393800   | 3                     | 10.094 | 398410  | 50.0 |
| Cyclohexene, 1-... | 12.565 | 6.9     | ug/l  | 659286   | 4                     | 12.059 | 4748620 | 50.0 |
| Bicyclo[2.2.1]h... | 12.948 | 8.4     | ug/l  | 798897   | 4                     | 12.059 | 4748620 | 50.0 |
| Bicyclo[2.2.1]h... | 13.206 | 30.3    | ug/l  | 2876450  | 4                     | 12.059 | 4748620 | 50.0 |
| (+)-2-Bornanone    | 13.553 | 13.3    | ug/l  | 1260700  | 4                     | 12.059 | 4748620 | 50.0 |
| .gamma.-Terpinene  | 13.618 | 6.1     | ug/l  | 577260   | 4                     | 12.059 | 4748620 | 50.0 |
| Estragole          | 13.706 | 29.3    | ug/l  | 2779170  | 4                     | 12.059 | 4748620 | 50.0 |