

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_Y\Data\VY052423\  
 Data File : VY013850.D  
 Acq On : 24 May 2023 16:45  
 Operator : KP/MD  
 Sample : 02848-01  
 Misc : 4.10g/5.0mL/MSVOA\_Y/SOIL  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_Y  
 ClientSampleId :  
 TP4

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\_Y\methods\82Y052323S.M  
 Title : SW846 8260

Signal : TIC: VY013850.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         | 3.948       | 338           | 349         | 368          | rBV      | 191025         | 619080        | 57.63%          | 8.573%        |
| 2         | 4.710       | 463           | 474         | 488          | rBV2     | 28075          | 87400         | 8.14%           | 1.210%        |
| 3         | 5.741       | 634           | 643         | 654          | rBV5     | 5942           | 18880         | 1.76%           | 0.261%        |
| 4         | 6.972       | 834           | 845         | 856          | rBV3     | 22350          | 73614         | 6.85%           | 1.019%        |
| 5         | 7.710       | 954           | 966         | 972          | rBV      | 128557         | 305213        | 28.41%          | 4.226%        |
| 6         | 7.783       | 972           | 978         | 989          | rVB      | 204588         | 458491        | 42.68%          | 6.349%        |
| 7         | 8.136       | 1027          | 1036        | 1047         | rBV      | 129270         | 289069        | 26.91%          | 4.003%        |
| 8         | 8.386       | 1071          | 1077        | 1087         | rVB5     | 5101           | 12410         | 1.16%           | 0.172%        |
| 9         | 8.685       | 1117          | 1126        | 1132         | rBV      | 323135         | 624827        | 58.17%          | 8.652%        |
| 10        | 8.752       | 1132          | 1137        | 1152         | rVB      | 119094         | 244362        | 22.75%          | 3.384%        |
| 11        | 9.502       | 1254          | 1260        | 1272         | rVB5     | 5837           | 12524         | 1.17%           | 0.173%        |
| 12        | 10.173      | 1359          | 1370        | 1379         | rBV      | 502713         | 876461        | 81.59%          | 12.137%       |
| 13        | 10.386      | 1397          | 1405        | 1416         | rBV      | 667106         | 1074224       | 100.00%         | 14.875%       |
| 14        | 10.941      | 1487          | 1496        | 1505         | rBV3     | 9051           | 15563         | 1.45%           | 0.216%        |
| 15        | 11.416      | 1567          | 1574        | 1578         | rBV4     | 12872          | 21988         | 2.05%           | 0.304%        |
| 16        | 11.483      | 1578          | 1585        | 1597         | rVB      | 490763         | 807148        | 75.14%          | 11.177%       |
| 17        | 12.331      | 1717          | 1724        | 1732         | rBV      | 59947          | 101968        | 9.49%           | 1.412%        |
| 18        | 12.477      | 1740          | 1748        | 1759         | rBV      | 393651         | 620066        | 57.72%          | 8.586%        |
| 19        | 12.599      | 1760          | 1768        | 1779         | rVB2     | 26087          | 55819         | 5.20%           | 0.773%        |
| 20        | 12.886      | 1809          | 1815        | 1822         | rBV5     | 6523           | 12119         | 1.13%           | 0.168%        |
| 21        | 13.099      | 1842          | 1850        | 1856         | rBV      | 14539          | 22040         | 2.05%           | 0.305%        |
| 22        | 13.337      | 1884          | 1889        | 1897         | rBV6     | 11165          | 20791         | 1.94%           | 0.288%        |
| 23        | 13.422      | 1897          | 1903        | 1909         | rVV      | 480243         | 725163        | 67.51%          | 10.042%       |
| 24        | 14.026      | 1997          | 2002        | 2007         | rBV3     | 7897           | 12815         | 1.19%           | 0.177%        |
| 25        | 14.172      | 2018          | 2026        | 2031         | rBV2     | 13576          | 24275         | 2.26%           | 0.336%        |
| 26        | 14.940      | 2145          | 2152        | 2158         | rBV2     | 24992          | 42822         | 3.99%           | 0.593%        |
| 27        | 15.178      | 2186          | 2191        | 2199         | rVB      | 16881          | 27348         | 2.55%           | 0.379%        |
| 28        | 15.312      | 2206          | 2213        | 2219         | rVB3     | 7773           | 14988         | 1.40%           | 0.208%        |

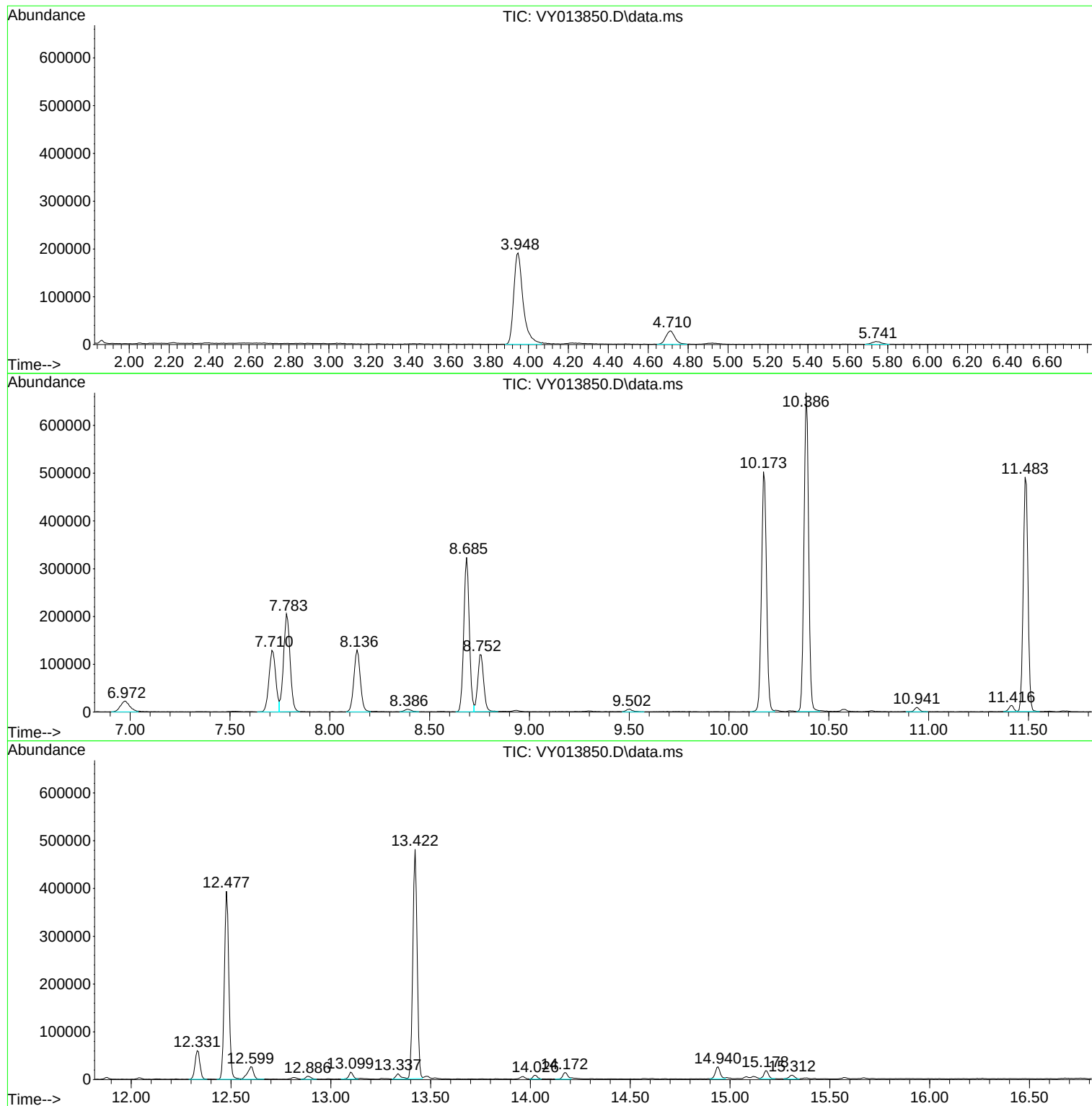
Sum of corrected areas: 7221468

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_Y\Data\VY052423\  
Data File : VY013850.D  
Acq On : 24 May 2023 16:45  
Operator : KP/MD  
Sample : 02848-01  
Misc : 4.10g/5.0mL/MSVOA\_Y/SOIL  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_Y  
ClientSampleId :  
TP4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y052323S.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_Y\Data\VY052423\  
Data File : VY013850.D  
Acq On : 24 May 2023 16:45  
Operator : KP/MD  
Sample : 02848-01  
Misc : 4.10g/5.0mL/MSVOA\_Y/SOIL  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_Y  
ClientSampleId :  
TP4

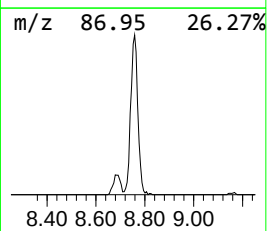
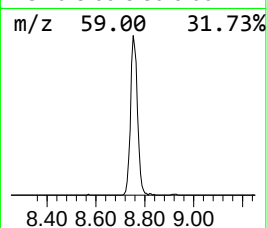
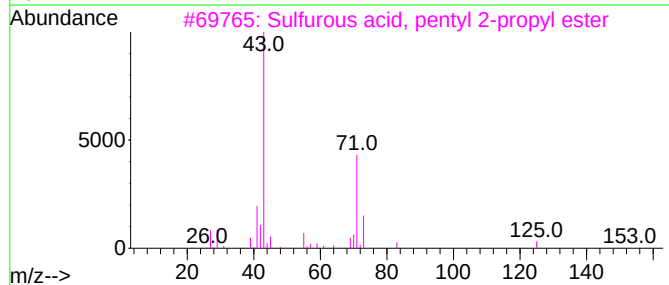
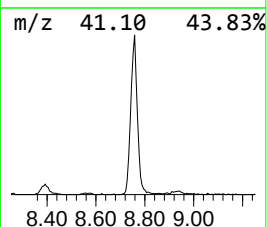
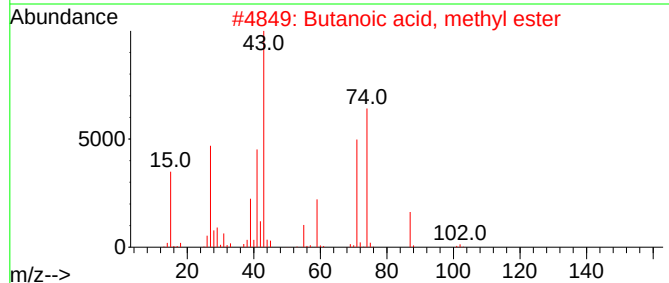
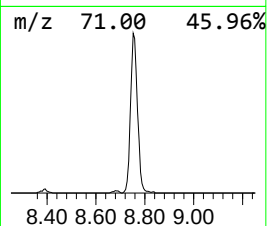
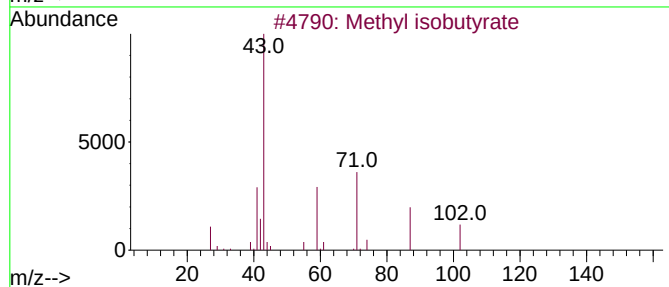
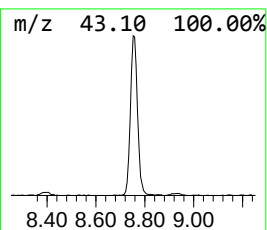
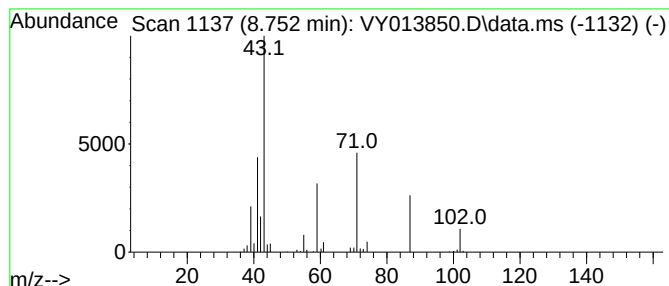
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y052323S.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 Methyl isobutyrate Concentration Rank 2

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 8.752 | 19.55 ug/l | 244362 | 1,4-Difluorobenzene | 8.685 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Methyl isobutyrate                  | 102 | C5H10O2  | 000547-63-7  | 91   |
| 2    |    |   | Butanoic acid, methyl ester         | 102 | C5H10O2  | 000623-42-7  | 50   |
| 3    |    |   | Sulfurous acid, pentyl 2-propyl ... | 194 | C8H18O3S | 1000309-11-5 | 23   |
| 4    |    |   | 4-Methyl-2-pentyl acetate           | 144 | C8H16O2  | 000108-84-9  | 17   |
| 5    |    |   | 2-Oxo-n-valeric acid                | 116 | C5H8O3   | 001821-02-9  | 17   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_Y\Data\VY052423\  
Data File : VY013850.D  
Acq On : 24 May 2023 16:45  
Operator : KP/MD  
Sample : 02848-01  
Misc : 4.10g/5.0mL/MSVOA\_Y/SOIL  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_Y  
ClientSampleId :  
TP4

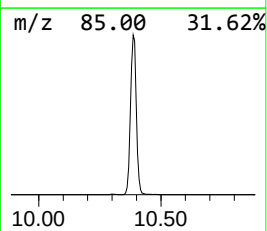
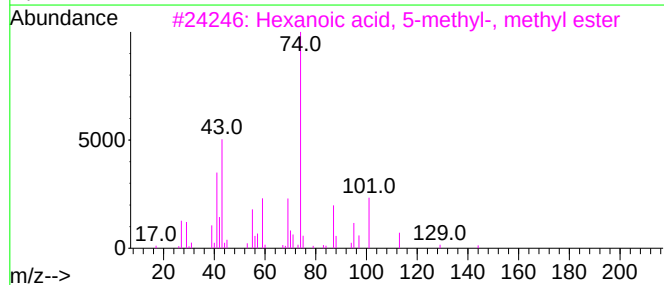
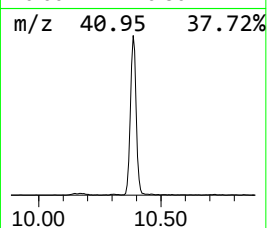
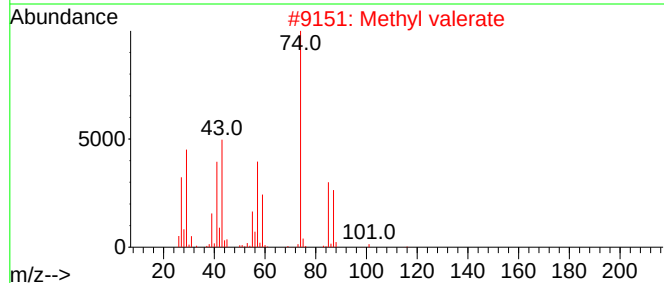
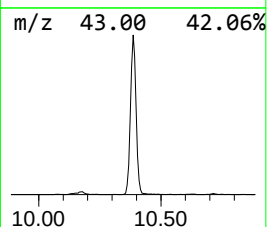
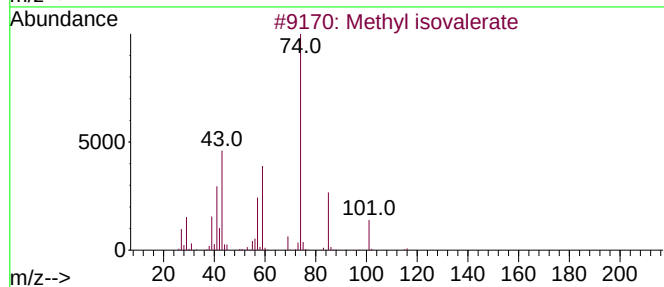
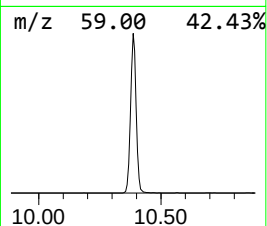
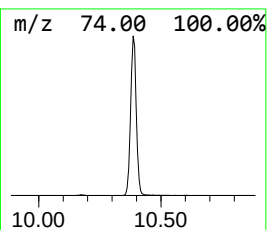
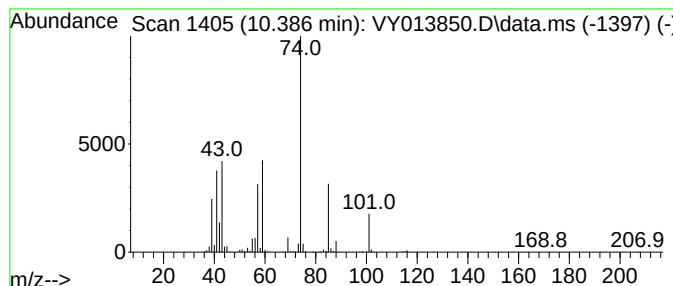
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y052323S.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 Methyl isovalerate Concentration Rank 1

| R.T.   | EstConc    | Area    | Relative to ISTD | R.T.   |
|--------|------------|---------|------------------|--------|
| 10.386 | 66.54 ug/l | 1074220 | Chlorobenzene-d5 | 11.490 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Methyl isovalerate                  | 116 | C6H12O2  | 000556-24-1 | 95   |
| 2    |    |   | Methyl valerate                     | 116 | C6H12O2  | 000624-24-8 | 50   |
| 3    |    |   | Hexanoic acid, 5-methyl-, methyl... | 144 | C8H16O2  | 002177-83-5 | 33   |
| 4    |    |   | Heptanoic acid, methyl ester        | 144 | C8H16O2  | 000106-73-0 | 28   |
| 5    |    |   | Diethanolamine                      | 105 | C4H11NO2 | 000111-42-2 | 9    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_Y\Data\VY052423\  
Data File : VY013850.D  
Acq On : 24 May 2023 16:45  
Operator : KP/MD  
Sample : 02848-01  
Misc : 4.10g/5.0mL/MSVOA\_Y/SOIL  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_Y  
ClientSampleId :  
TP4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y052323S.M  
Quant Title : SW846 8260

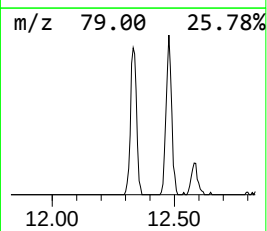
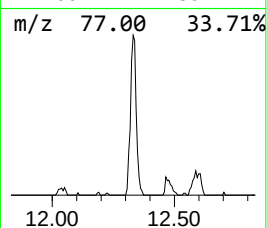
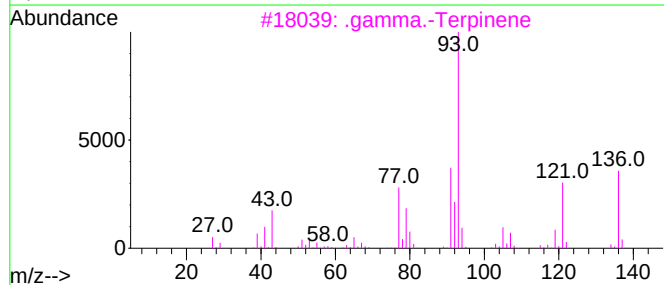
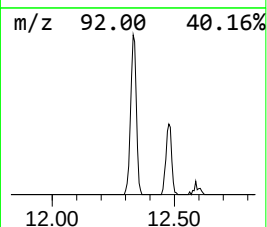
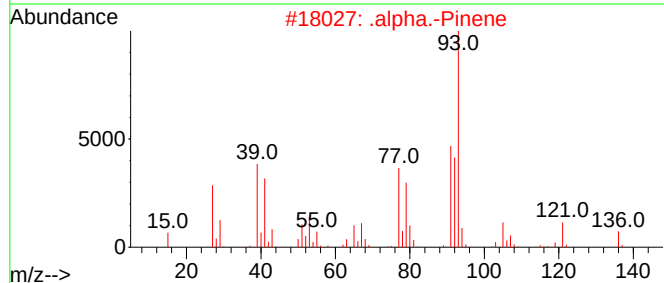
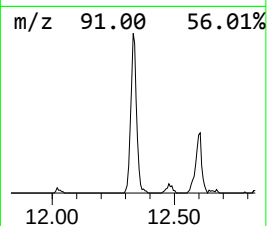
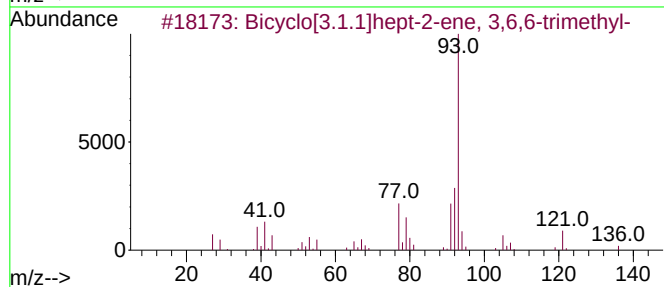
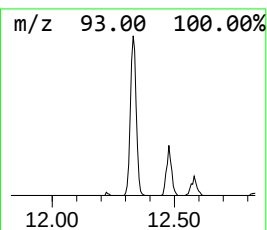
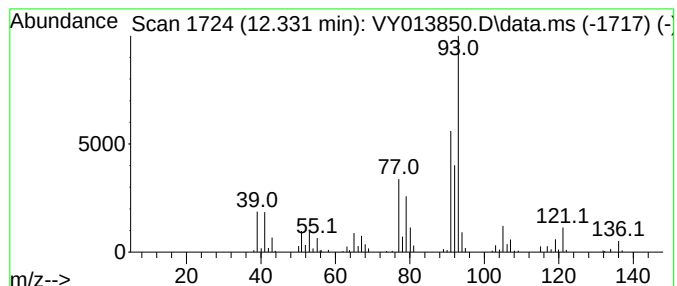
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 3 Bicyclo[3.1.1]hept-2-ene, 3... Concentration Rank 3

| R.T.   | EstConc   | Area   | Relative to ISTD | R.T.   |
|--------|-----------|--------|------------------|--------|
| 12.331 | 6.32 ug/l | 101968 | Chlorobenzene-d5 | 11.490 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Bicyclo[3.1.1]hept-2-ene, 3,6,6-... | 136 | C10H16  | 004889-83-2 | 94   |
| 2    |    |   | .alpha.-Pinene                      | 136 | C10H16  | 000080-56-8 | 94   |
| 3    |    |   | .gamma.-Terpinene                   | 136 | C10H16  | 000099-85-4 | 87   |
| 4    |    |   | (1S)-2,6,6-Trimethylbicyclo[3.1.... | 136 | C10H16  | 007785-26-4 | 87   |
| 5    |    |   | 3-Carene                            | 136 | C10H16  | 013466-78-9 | 83   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_Y\Data\VY052423\  
Data File : VY013850.D  
Acq On : 24 May 2023 16:45  
Operator : KP/MD  
Sample : 02848-01  
Misc : 4.10g/5.0mL/MSVOA\_Y/SOIL  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_Y  
ClientSampleId :  
TP4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y052323S.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Methyl isobutyrate | 8.752  | 19.6    | ug/l  | 244362   | 2                     | 8.685  | 624827 | 50.0 |
| Methyl isovalerate | 10.386 | 66.5    | ug/l  | 1074220  | 3                     | 11.490 | 807148 | 50.0 |
| Bicyclo[3.1.1]h... | 12.331 | 6.3     | ug/l  | 101968   | 3                     | 11.490 | 807148 | 50.0 |