

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV051923\  
 Data File : VV031133.D  
 Acq On : 20 May 2023 02:41  
 Operator : SY/MD  
 Sample : 02865-07  
 Misc : 5.0mL/MSVOA\_V/WATER  
 ALS Vial : 44 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 GBX62

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\_V\Method\SFAMVLM051923WMA.M  
 Title : VOC Analysis

Signal : TIC: VV031133.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         | 1.281       | 69            | 75          | 88           | rVB      | 134517         | 149090        | 14.68%          | 1.736%        |
| 2         | 1.532       | 147           | 153         | 169          | rVB      | 126363         | 154835        | 15.24%          | 1.803%        |
| 3         | 2.063       | 309           | 318         | 328          | rBV      | 256705         | 368193        | 36.24%          | 4.288%        |
| 4         | 2.577       | 473           | 478         | 479          | rBV5     | 3728           | 3022          | 0.30%           | 0.035%        |
| 5         | 2.651       | 499           | 501         | 503          | rVB3     | 2445           | 992           | 0.10%           | 0.012%        |
| 6         | 2.670       | 505           | 507         | 510          | rBV4     | 1441           | 879           | 0.09%           | 0.010%        |
| 7         | 2.847       | 557           | 562         | 563          | rBV5     | 1640           | 1350          | 0.13%           | 0.016%        |
| 8         | 2.873       | 568           | 570         | 571          | rBV2     | 665            | 166           | 0.02%           | 0.002%        |
| 9         | 2.889       | 571           | 575         | 577          | rBV4     | 1447           | 1118          | 0.11%           | 0.013%        |
| 10        | 2.921       | 583           | 585         | 586          | rBV2     | 1245           | 401           | 0.04%           | 0.005%        |
| 11        | 2.976       | 599           | 602         | 606          | rBV5     | 2145           | 1820          | 0.18%           | 0.021%        |
| 12        | 2.995       | 606           | 608         | 609          | rBV2     | 1862           | 882           | 0.09%           | 0.010%        |
| 13        | 3.027       | 615           | 618         | 622          | rVB5     | 1921           | 1264          | 0.12%           | 0.015%        |
| 14        | 3.056       | 622           | 627         | 629          | rBV6     | 2676           | 2379          | 0.23%           | 0.028%        |
| 15        | 3.162       | 658           | 660         | 662          | rBV3     | 1570           | 735           | 0.07%           | 0.009%        |
| 16        | 3.175       | 662           | 664         | 666          | rBV3     | 1117           | 387           | 0.04%           | 0.005%        |
| 17        | 3.314       | 704           | 707         | 711          | rBV5     | 2043           | 1645          | 0.16%           | 0.019%        |
| 18        | 3.596       | 793           | 795         | 799          | rBV5     | 2131           | 1461          | 0.14%           | 0.017%        |
| 19        | 3.683       | 819           | 822         | 823          | rBV2     | 1304           | 823           | 0.08%           | 0.010%        |
| 20        | 3.796       | 847           | 857         | 882          | rBV      | 77526          | 221047        | 21.76%          | 2.574%        |
| 21        | 4.172       | 969           | 974         | 976          | rBV6     | 2171           | 1866          | 0.18%           | 0.022%        |
| 22        | 4.256       | 984           | 1000        | 1020         | rBV      | 171858         | 441913        | 43.50%          | 5.147%        |
| 23        | 4.465       | 1063          | 1065        | 1067         | rVB3     | 1767           | 589           | 0.06%           | 0.007%        |
| 24        | 4.616       | 1110          | 1112        | 1114         | rBV3     | 1486           | 848           | 0.08%           | 0.010%        |
| 25        | 4.731       | 1145          | 1148        | 1150         | rBV4     | 1896           | 1322          | 0.13%           | 0.015%        |
| 26        | 4.780       | 1161          | 1163        | 1167         | rBV4     | 2446           | 1423          | 0.14%           | 0.017%        |
| 27        | 4.796       | 1167          | 1168        | 1171         | rVB3     | 1796           | 720           | 0.07%           | 0.008%        |
| 28        | 4.815       | 1171          | 1174        | 1175         | rBV4     | 1385           | 871           | 0.09%           | 0.010%        |
| 29        | 4.873       | 1190          | 1192        | 1193         | rBV2     | 1762           | 801           | 0.08%           | 0.009%        |
| 30        | 4.963       | 1204          | 1220        | 1244         | rBV2     | 383152         | 1015885       | 100.00%         | 11.831%       |
| 31        | 5.336       | 1330          | 1336        | 1337         | rBV5     | 2381           | 2371          | 0.23%           | 0.028%        |
| 32        | 5.542       | 1389          | 1400        | 1426         | rBV      | 308114         | 622034        | 61.23%          | 7.244%        |
| 33        | 5.995       | 1531          | 1541        | 1565         | rVB      | 228100         | 462218        | 45.50%          | 5.383%        |
| 34        | 6.448       | 1680          | 1682        | 1684         | rBV3     | 1526           | 643           | 0.06%           | 0.007%        |
| 35        | 6.712       | 1761          | 1764        | 1767         | rBV5     | 2099           | 1334          | 0.13%           | 0.016%        |
| 36        | 6.805       | 1788          | 1793        | 1795         | rBV5     | 1989           | 1747          | 0.17%           | 0.020%        |

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 ALS Vial : 44 Sample Multiplier: 1

Instrument :  
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 ClientSampleId :  
 GBX62

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\_V\Method\SFAMVLM051923WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 6.921  | 1819 | 1829 | 1844 | rBV  | 108507 | 202542 | 19.94% | 2.359% |
| 38 | 7.095  | 1879 | 1883 | 1884 | rBV3 | 2052   | 1339   | 0.13%  | 0.016% |
| 39 | 7.249  | 1920 | 1931 | 1949 | rBV  | 430796 | 754102 | 74.23% | 8.783% |
| 40 | 7.558  | 2019 | 2027 | 2047 | rBV  | 80465  | 139683 | 13.75% | 1.627% |
| 41 | 7.866  | 2120 | 2123 | 2128 | rBV7 | 2471   | 2564   | 0.25%  | 0.030% |
| 42 | 7.924  | 2139 | 2141 | 2147 | rBV6 | 1782   | 1881   | 0.19%  | 0.022% |
| 43 | 8.034  | 2165 | 2175 | 2187 | rBV  | 265268 | 475349 | 46.79% | 5.536% |
| 44 | 8.612  | 2353 | 2355 | 2357 | rVB3 | 1755   | 552    | 0.05%  | 0.006% |
| 45 | 8.628  | 2357 | 2360 | 2363 | rBV4 | 1603   | 1238   | 0.12%  | 0.014% |
| 46 | 8.712  | 2385 | 2386 | 2387 | rBV  | 1291   | 317    | 0.03%  | 0.004% |
| 47 | 8.789  | 2399 | 2410 | 2431 | rBV  | 469583 | 785120 | 77.28% | 9.144% |
| 48 | 9.654  | 2670 | 2679 | 2695 | rBV  | 28493  | 52800  | 5.20%  | 0.615% |
| 49 | 10.159 | 2826 | 2836 | 2854 | rVB  | 330071 | 525568 | 51.73% | 6.121% |
| 50 | 10.529 | 2947 | 2951 | 2953 | rBV5 | 1816   | 1359   | 0.13%  | 0.016% |
| 51 | 10.542 | 2953 | 2955 | 2956 | rVV2 | 1563   | 537    | 0.05%  | 0.006% |
| 52 | 10.587 | 2967 | 2969 | 2972 | rBV3 | 2219   | 1177   | 0.12%  | 0.014% |
| 53 | 10.673 | 2993 | 2996 | 2999 | rBV5 | 2576   | 1726   | 0.17%  | 0.020% |
| 54 | 10.786 | 3029 | 3031 | 3032 | rBV2 | 1720   | 648    | 0.06%  | 0.008% |
| 55 | 11.191 | 3147 | 3157 | 3179 | rVB  | 442599 | 698411 | 68.75% | 8.134% |
| 56 | 11.487 | 3238 | 3249 | 3264 | rBV  | 316314 | 600443 | 59.11% | 6.993% |
| 57 | 11.567 | 3266 | 3274 | 3298 | rVB  | 504670 | 807154 | 79.45% | 9.400% |
| 58 | 13.554 | 3886 | 3892 | 3893 | rBV6 | 1694   | 1603   | 0.16%  | 0.019% |
| 59 | 13.570 | 3895 | 3897 | 3899 | rVV3 | 2300   | 852    | 0.08%  | 0.010% |
| 60 | 13.586 | 3899 | 3902 | 3905 | rVV5 | 1679   | 1489   | 0.15%  | 0.017% |
| 61 | 13.741 | 3948 | 3950 | 3951 | rBV2 | 1358   | 674    | 0.07%  | 0.008% |
| 62 | 13.770 | 3953 | 3959 | 3960 | rBV4 | 2580   | 2114   | 0.21%  | 0.025% |
| 63 | 13.953 | 4013 | 4016 | 4020 | rBV6 | 2754   | 2542   | 0.25%  | 0.030% |
| 64 | 14.062 | 4047 | 4050 | 4053 | rBV5 | 2049   | 1607   | 0.16%  | 0.019% |
| 65 | 14.168 | 4078 | 4083 | 4084 | rBV5 | 1980   | 1771   | 0.17%  | 0.021% |
| 66 | 14.291 | 4119 | 4121 | 4125 | rBV4 | 2132   | 1488   | 0.15%  | 0.017% |
| 67 | 14.837 | 4287 | 4291 | 4292 | rBV3 | 2482   | 1922   | 0.19%  | 0.022% |
| 68 | 15.985 | 4645 | 4648 | 4651 | rBV5 | 3079   | 2613   | 0.26%  | 0.030% |
| 69 | 16.258 | 4727 | 4733 | 4744 | rVB  | 30796  | 44127  | 4.34%  | 0.514% |

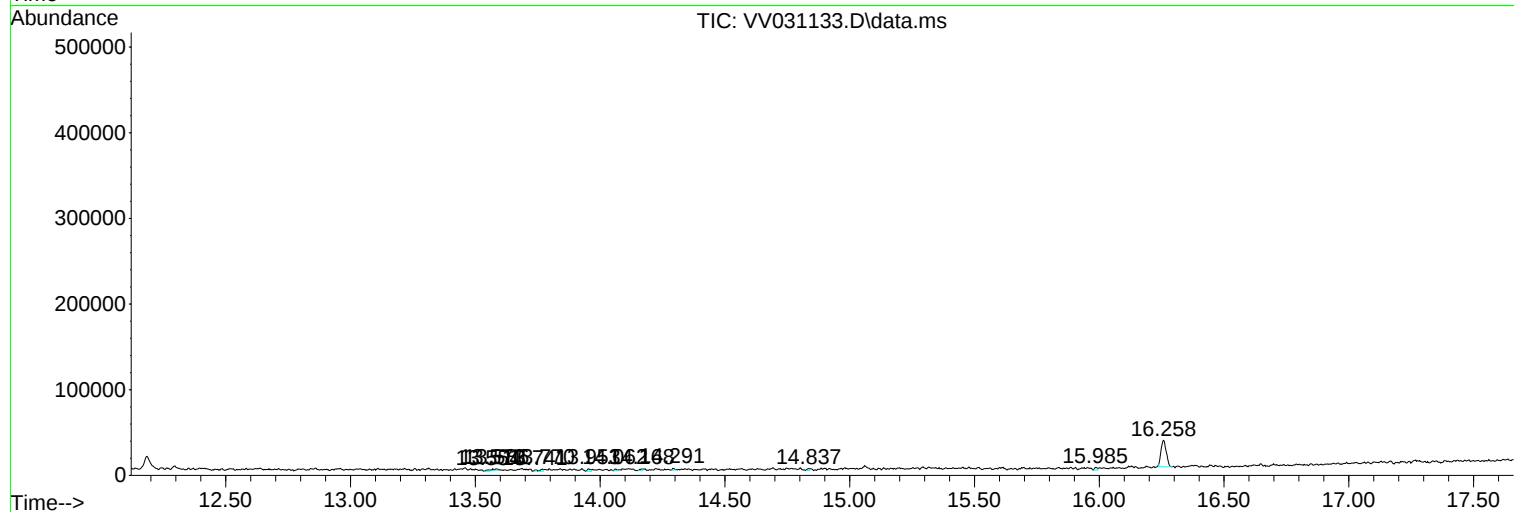
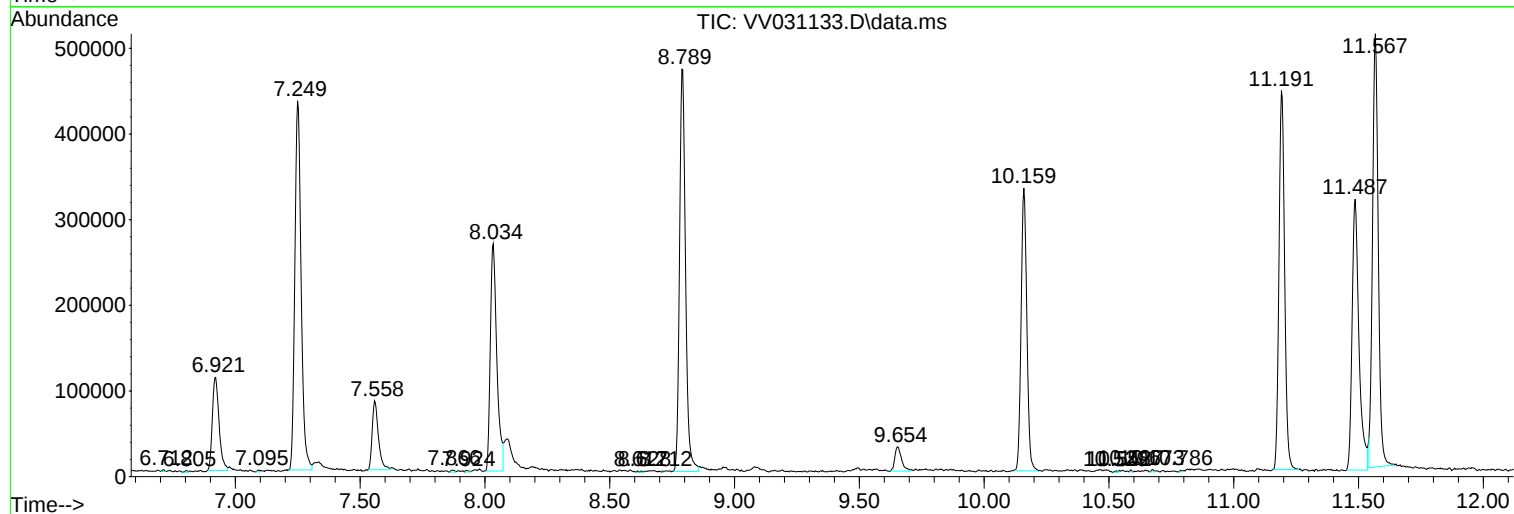
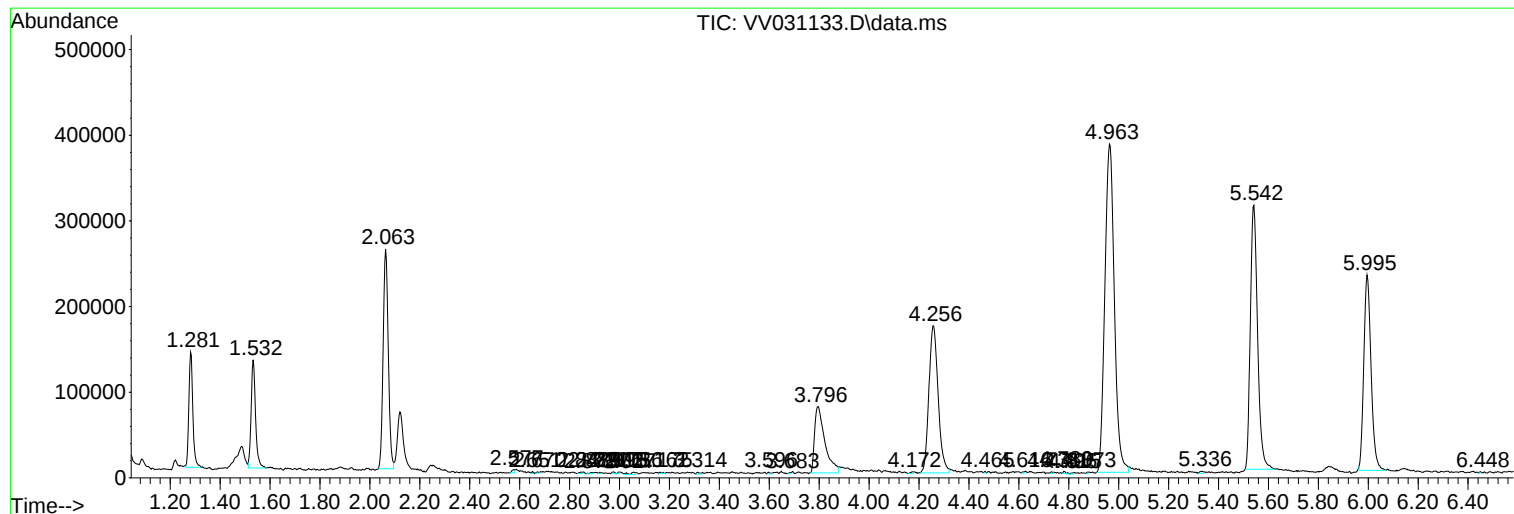
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ALS Vial : 44 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
GBX62

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM051923WMA.M  
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV051923\  
Data File : VV031133.D  
Acq On : 20 May 2023 02:41  
Operator : SY/MD  
Sample : 02865-07  
Misc : 5.0mL/MSVOA\_V/WATER  
ALS Vial : 44 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
GBX62

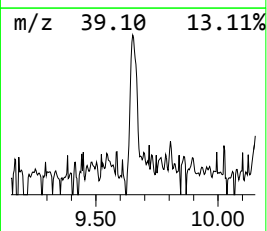
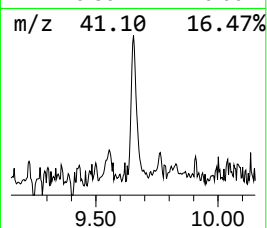
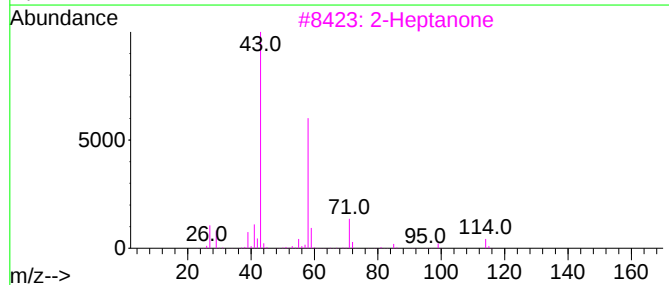
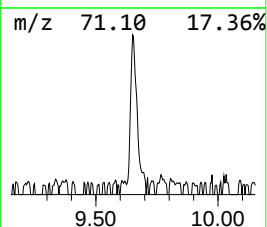
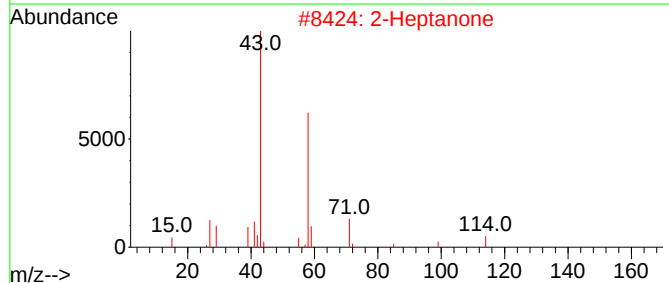
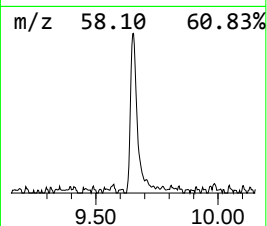
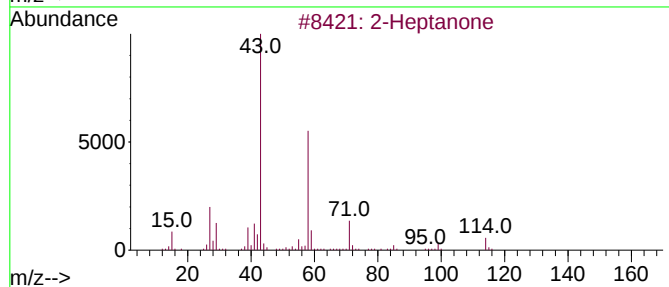
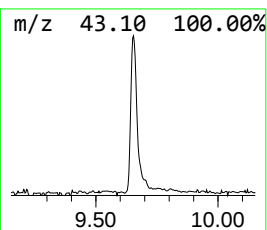
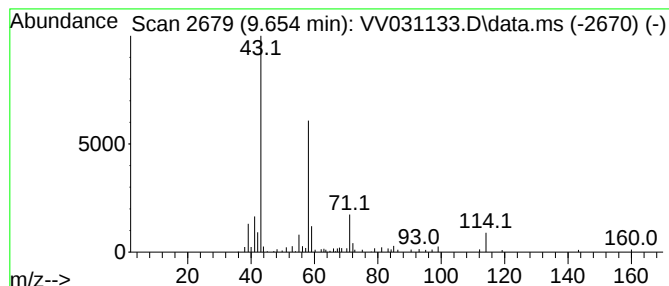
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM051923WMA.M  
Quant Title : VOC Analysis

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

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Peak Number 2 2-Heptanone Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD | R.T.  |
|-------|-----------|-------|------------------|-------|
| 9.654 | 3.36 ug/L | 52800 | Chlorobenzene-d5 | 8.792 |

| Hit# | of 5        | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|-------------|--------------|-----|---------|-------------|------|
| 1    | 2-Heptanone |              | 114 | C7H14O  | 000110-43-0 | 91   |
| 2    | 2-Heptanone |              | 114 | C7H14O  | 000110-43-0 | 90   |
| 3    | 2-Heptanone |              | 114 | C7H14O  | 000110-43-0 | 90   |
| 4    | 2-Heptanone |              | 114 | C7H14O  | 000110-43-0 | 87   |
| 5    | 2-Heptanone |              | 114 | C7H14O  | 000110-43-0 | 64   |



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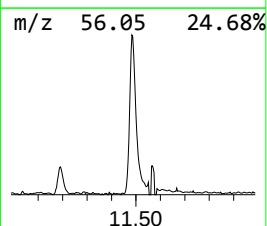
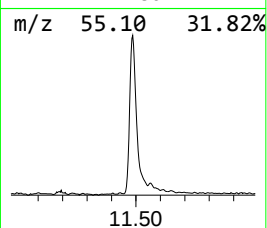
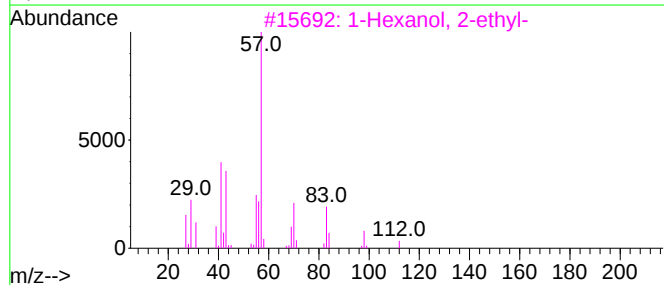
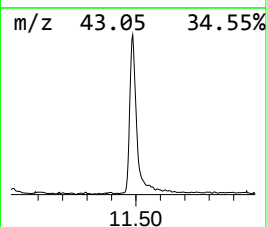
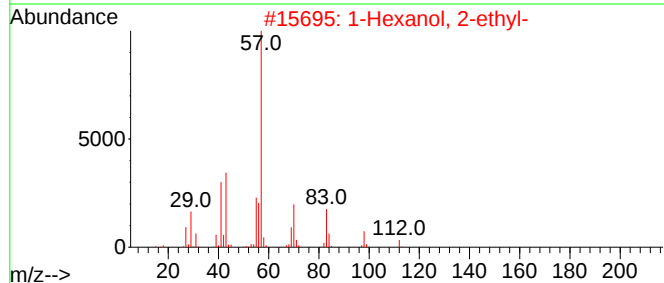
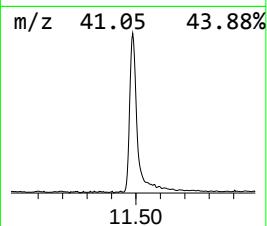
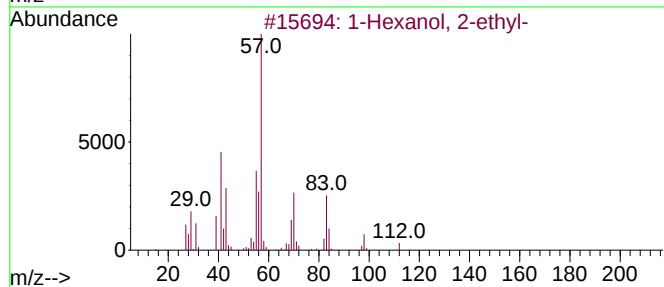
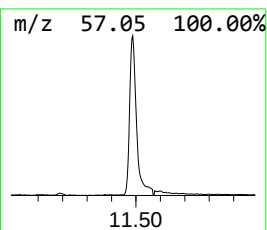
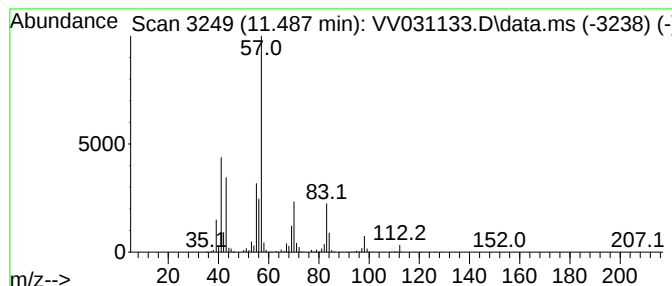
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM051923WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 11.487 | 42.99 ug/L | 600443 | 1,4-Dichlorobenzene-d4 | 11.191 |

| Hit# | of                    | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|-----------------------|---|--------------|-----|---------|-------------|------|
| 1    | 1-Hexanol, 2-ethyl-   |   |              | 130 | C8H18O  | 000104-76-7 | 90   |
| 2    | 1-Hexanol, 2-ethyl-   |   |              | 130 | C8H18O  | 000104-76-7 | 90   |
| 3    | 1-Hexanol, 2-ethyl-   |   |              | 130 | C8H18O  | 000104-76-7 | 86   |
| 4    | 1-Hexanol, 2-ethyl-   |   |              | 130 | C8H18O  | 000104-76-7 | 64   |
| 5    | Heptane, 1,1'-oxybis- |   |              | 214 | C14H30O | 000629-64-1 | 53   |



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM051923WMA.M  
Quant Title : VOC Analysis

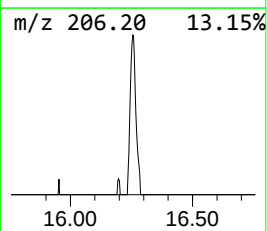
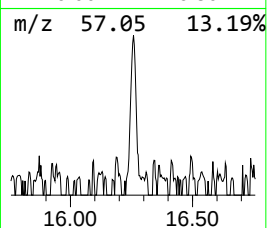
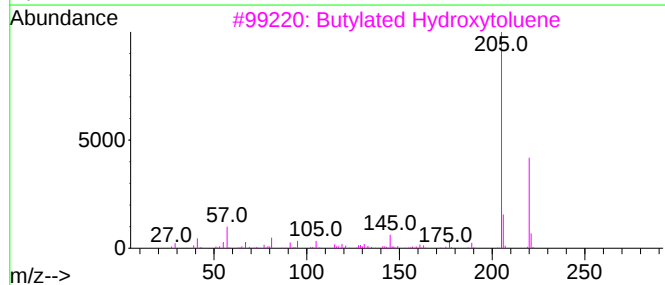
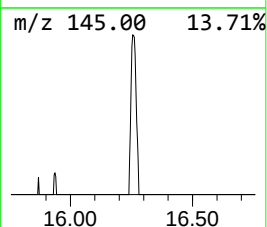
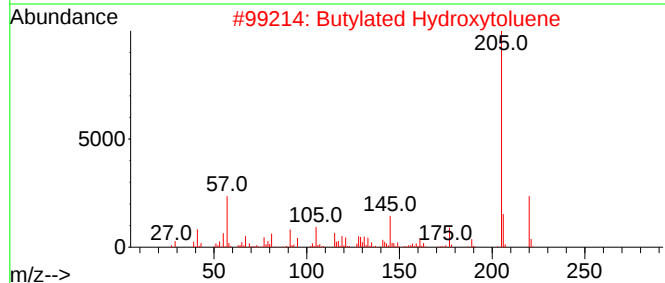
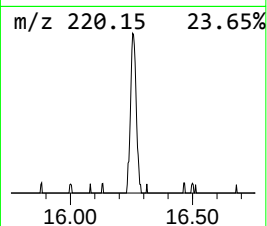
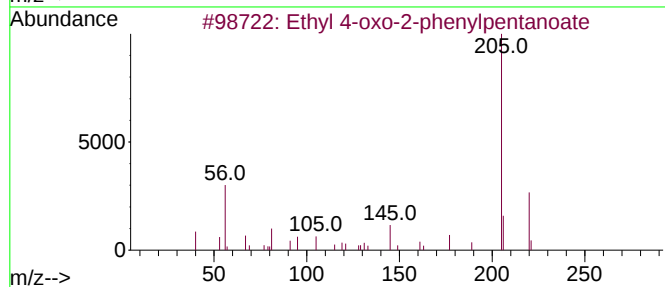
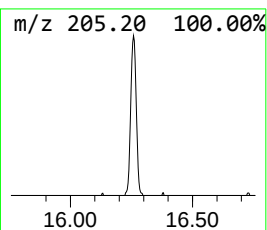
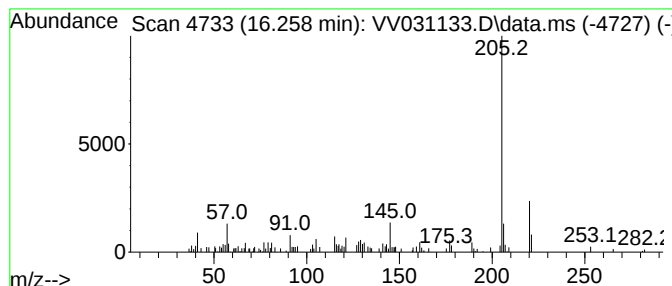
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Ethyl 4-oxo-2-phenylpentanoate Concentration Rank 4

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 16.258 | 3.16 ug/L | 44127 | 1,4-Dichlorobenzene-d4 | 11.191 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm  | CAS#         | Qual |
|------|----|---|--------------------------------|-----|----------|--------------|------|
| 1    |    |   | Ethyl 4-oxo-2-phenylpentanoate | 220 | C13H16O3 | 1000427-11-2 | 91   |
| 2    |    |   | Butylated Hydroxytoluene       | 220 | C15H24O  | 000128-37-0  | 90   |
| 3    |    |   | Butylated Hydroxytoluene       | 220 | C15H24O  | 000128-37-0  | 87   |
| 4    |    |   | Butylated Hydroxytoluene       | 220 | C15H24O  | 000128-37-0  | 87   |
| 5    |    |   | Butylated Hydroxytoluene       | 220 | C15H24O  | 000128-37-0  | 87   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV051923\  
Data File : VV031133.D  
Acq On : 20 May 2023 02:41  
Operator : SY/MD  
Sample : 02865-07  
Misc : 5.0mL/MSVOA\_V/WATER  
ALS Vial : 44 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
GBX62

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM051923WMA.M  
Quant Title : VOC Analysis

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Heptanone        | 9.654  | 3.4     | ug/L  | 52800    | 2                     | 8.792  | 785120 | 50.0 |
| 1-Hexanol, 2-et... | 11.487 | 43.0    | ug/L  | 600443   | 3                     | 11.191 | 698411 | 50.0 |
| Ethyl 4-oxo-2-p... | 16.258 | 3.2     | ug/L  | 44127    | 3                     | 11.191 | 698411 | 50.0 |