

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV051923\  
 Data File : VV031127.D  
 Acq On : 20 May 2023 00:14  
 Operator : SY/MD  
 Sample : 02865-01  
 Misc : 5.0mL/MSVOA\_V/WATER  
 ALS Vial : 38 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 GBX56

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: VV031127.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         | 1.282       | 69            | 75          | 93           | rVB      | 144942         | 168894        | 16.57%          | 2.213%        |
| 2         | 1.536       | 148           | 154         | 169          | rVB      | 159505         | 187925        | 18.44%          | 2.463%        |
| 3         | 2.063       | 309           | 318         | 332          | rBV      | 270353         | 386152        | 37.88%          | 5.061%        |
| 4         | 3.024       | 613           | 617         | 620          | rBV5     | 3062           | 2358          | 0.23%           | 0.031%        |
| 5         | 3.175       | 663           | 664         | 665          | rBV      | 1523           | 524           | 0.05%           | 0.007%        |
| 6         | 3.349       | 714           | 718         | 722          | rBV4     | 2266           | 1897          | 0.19%           | 0.025%        |
| 7         | 3.526       | 771           | 773         | 774          | rBV2     | 1872           | 758           | 0.07%           | 0.010%        |
| 8         | 3.548       | 778           | 780         | 785          | rBV5     | 2568           | 1670          | 0.16%           | 0.022%        |
| 9         | 3.603       | 795           | 797         | 799          | rBV3     | 1967           | 1154          | 0.11%           | 0.015%        |
| 10        | 3.671       | 816           | 818         | 819          | rBV2     | 1357           | 372           | 0.04%           | 0.005%        |
| 11        | 3.802       | 850           | 859         | 887          | rBV2     | 64611          | 200525        | 19.67%          | 2.628%        |
| 12        | 4.661       | 1122          | 1126        | 1127         | rBV4     | 2998           | 2176          | 0.21%           | 0.029%        |
| 13        | 4.761       | 1155          | 1157        | 1160         | rBV4     | 1744           | 1048          | 0.10%           | 0.014%        |
| 14        | 4.963       | 1204          | 1220        | 1244         | rBV2     | 384126         | 1019328       | 100.00%         | 13.358%       |
| 15        | 5.539       | 1388          | 1399        | 1423         | rBV      | 310584         | 647754        | 63.55%          | 8.489%        |
| 16        | 5.841       | 1482          | 1493        | 1510         | rBV2     | 160226         | 314829        | 30.89%          | 4.126%        |
| 17        | 5.995       | 1530          | 1541        | 1560         | rBV      | 223484         | 449961        | 44.14%          | 5.897%        |
| 18        | 6.346       | 1648          | 1650        | 1651         | rBV3     | 1528           | 630           | 0.06%           | 0.008%        |
| 19        | 6.918       | 1819          | 1828        | 1848         | rBV      | 111594         | 205135        | 20.12%          | 2.688%        |
| 20        | 7.249       | 1920          | 1931        | 1950         | rBV      | 426928         | 755100        | 74.08%          | 9.896%        |
| 21        | 7.558       | 2019          | 2027        | 2044         | rBV      | 80709          | 141089        | 13.84%          | 1.849%        |
| 22        | 8.034       | 2166          | 2175        | 2190         | rBV      | 215646         | 416100        | 40.82%          | 5.453%        |
| 23        | 8.789       | 2399          | 2410        | 2427         | rBV      | 479125         | 798984        | 78.38%          | 10.471%       |
| 24        | 9.735       | 2700          | 2704        | 2705         | rBV3     | 1328           | 960           | 0.09%           | 0.013%        |
| 25        | 9.754       | 2708          | 2710        | 2712         | rBV3     | 2189           | 1105          | 0.11%           | 0.014%        |
| 26        | 9.950       | 2765          | 2771        | 2774         | rBV8     | 1739           | 2258          | 0.22%           | 0.030%        |
| 27        | 9.989       | 2778          | 2783        | 2784         | rBV4     | 1886           | 1675          | 0.16%           | 0.022%        |
| 28        | 10.053      | 2801          | 2803        | 2805         | rBV3     | 1493           | 789           | 0.08%           | 0.010%        |
| 29        | 10.095      | 2814          | 2816        | 2820         | rBV6     | 2319           | 1702          | 0.17%           | 0.022%        |
| 30        | 10.159      | 2826          | 2836        | 2852         | rVB2     | 311935         | 492710        | 48.34%          | 6.457%        |
| 31        | 10.593      | 2968          | 2971        | 2974         | rBV5     | 1834           | 1187          | 0.12%           | 0.016%        |
| 32        | 10.857      | 3048          | 3053        | 3054         | rBV5     | 2333           | 1627          | 0.16%           | 0.021%        |
| 33        | 11.191      | 3147          | 3157        | 3175         | rBV      | 436485         | 694757        | 68.16%          | 9.105%        |
| 34        | 11.500      | 3244          | 3253        | 3263         | rBV4     | 16946          | 35267         | 3.46%           | 0.462%        |
| 35        | 11.567      | 3264          | 3274        | 3290         | rVB      | 421633         | 667990        | 65.53%          | 8.754%        |
| 36        | 11.924      | 3382          | 3385        | 3388         | rBV4     | 1959           | 1666          | 0.16%           | 0.022%        |

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 ALS Vial : 38 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 GBX56

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 | 12.008 | 3408 | 3411 | 3413 | rBV4 | 1994 | 1096 | 0.11% | 0.014% |
| 38 | 12.108 | 3440 | 3442 | 3444 | rBV3 | 1410 | 713  | 0.07% | 0.009% |
| 39 | 12.159 | 3455 | 3458 | 3459 | rBV4 | 922  | 384  | 0.04% | 0.005% |
| 40 | 12.169 | 3459 | 3461 | 3463 | rBV3 | 936  | 488  | 0.05% | 0.006% |
| 41 | 12.326 | 3507 | 3510 | 3514 | rBV6 | 1647 | 1504 | 0.15% | 0.020% |
| 42 | 12.342 | 3514 | 3515 | 3519 | rVB4 | 1579 | 1011 | 0.10% | 0.013% |
| 43 | 12.371 | 3519 | 3524 | 3525 | rBV4 | 2453 | 1740 | 0.17% | 0.023% |
| 44 | 12.432 | 3541 | 3543 | 3544 | rBV2 | 1024 | 403  | 0.04% | 0.005% |
| 45 | 12.628 | 3602 | 3604 | 3607 | rVB5 | 2598 | 1570 | 0.15% | 0.021% |
| 46 | 12.754 | 3640 | 3643 | 3644 | rBV3 | 1782 | 1069 | 0.10% | 0.014% |
| 47 | 12.812 | 3656 | 3661 | 3666 | rBV8 | 2930 | 2630 | 0.26% | 0.034% |
| 48 | 12.873 | 3675 | 3680 | 3682 | rBV6 | 2105 | 1810 | 0.18% | 0.024% |
| 49 | 12.911 | 3689 | 3692 | 3695 | rVB5 | 2258 | 1572 | 0.15% | 0.021% |
| 50 | 12.934 | 3695 | 3699 | 3700 | rBV4 | 2028 | 1514 | 0.15% | 0.020% |
| 51 | 13.165 | 3769 | 3771 | 3774 | rBV3 | 1411 | 1170 | 0.11% | 0.015% |
| 52 | 13.268 | 3800 | 3803 | 3805 | rBV4 | 1783 | 1140 | 0.11% | 0.015% |
| 53 | 13.358 | 3829 | 3831 | 3833 | rBV3 | 1505 | 786  | 0.08% | 0.010% |
| 54 | 13.474 | 3865 | 3867 | 3870 | rVB3 | 1564 | 797  | 0.08% | 0.010% |
| 55 | 14.931 | 4318 | 4320 | 4322 | rBV3 | 2324 | 1180 | 0.12% | 0.015% |

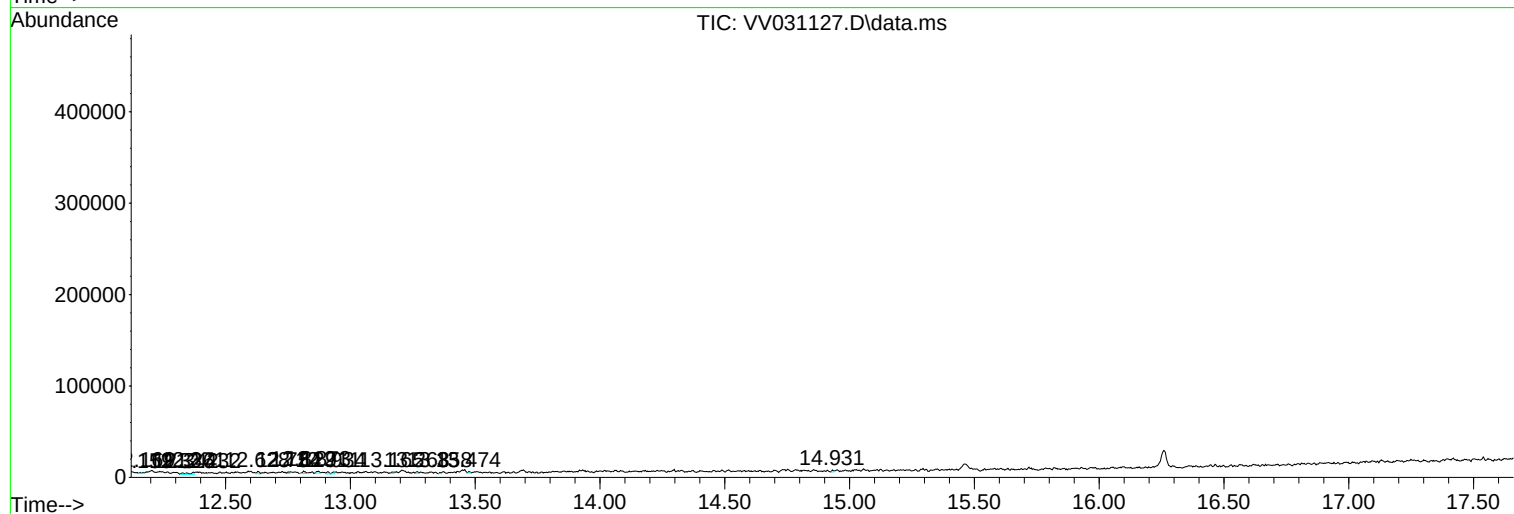
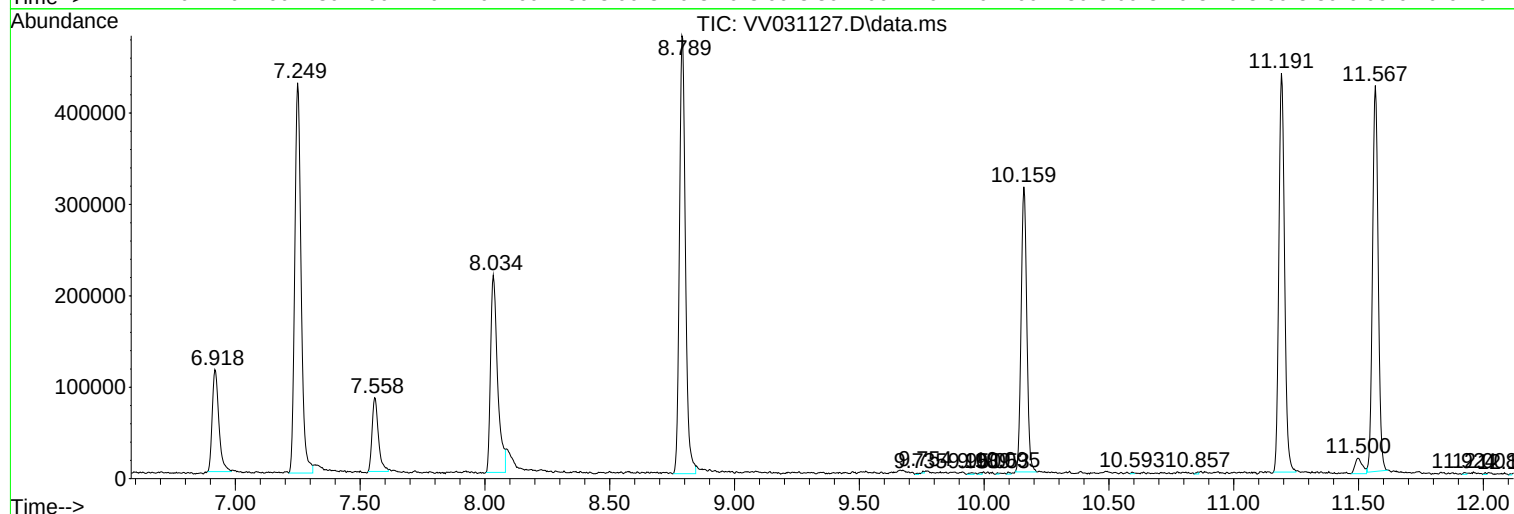
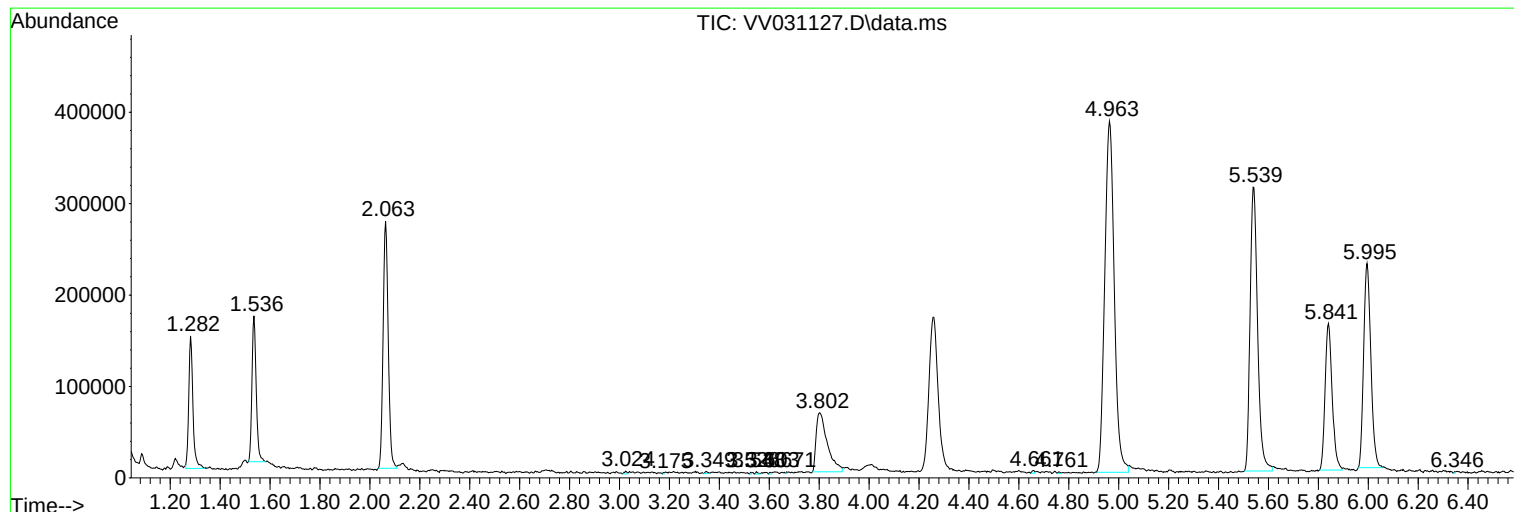
Sum of corrected areas: 7630633

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Instrument :  
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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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_V\Data\VV051923\  
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Sample : 02865-01  
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ALS Vial : 38 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
GBX56

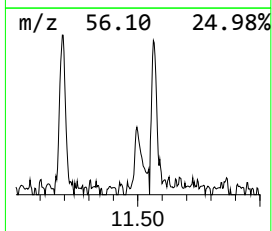
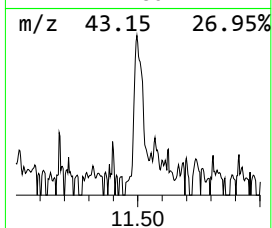
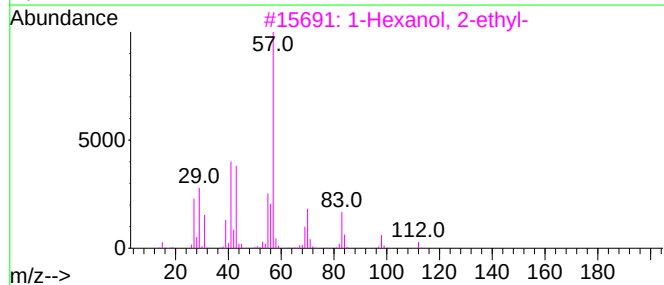
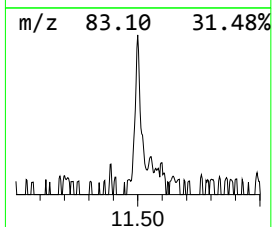
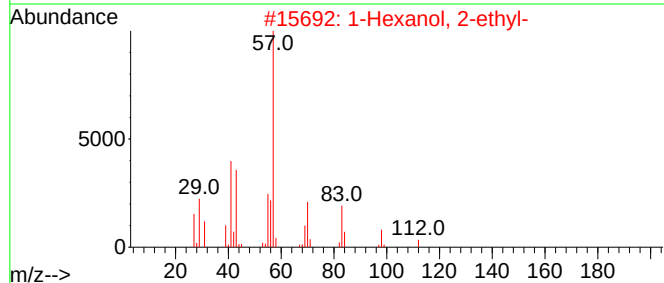
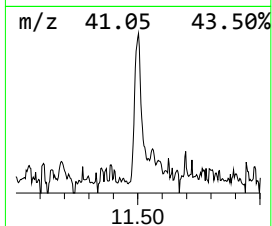
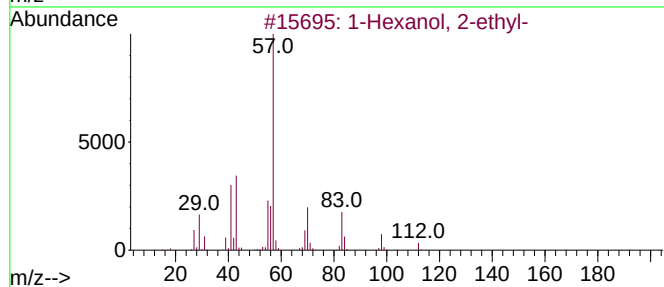
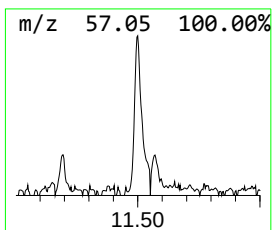
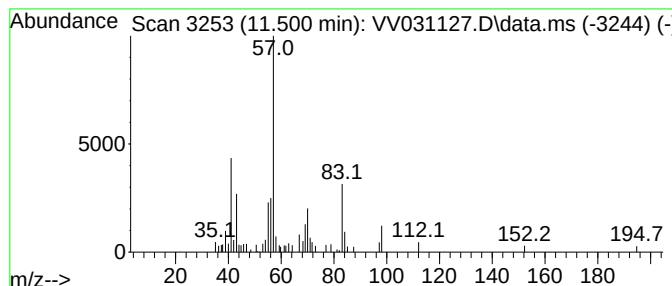
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_V\Method\SFAMVLM051923WMA.M  
Quant Title : VOC Analysis

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

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Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 11.500 | 2.54 ug/L | 35267 | 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 | 59   |
| 2    | 1-Hexanol, 2-ethyl-            |   |              | 130 | C8H18O   | 000104-76-7 | 59   |
| 3    | 1-Hexanol, 2-ethyl-            |   |              | 130 | C8H18O   | 000104-76-7 | 59   |
| 4    | Oxirane, [(dodecyloxy)methyl]- |   |              | 242 | C15H30O2 | 002461-18-9 | 50   |
| 5    | 1-Decene, 2,4-dimethyl-        |   |              | 168 | C12H24   | 055170-80-4 | 50   |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 1-Hexanol, 2-et... | 11.500 | 2.5     | ug/L  | 35267    | 3                     | 11.191 | 694757 | 50.0 |