

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX072424\  
 Data File : VX042468.D  
 Acq On : 23 Jul 2024 13:48  
 Operator : JC/MD  
 Sample : P3263-16ME  
 Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 A4CK4ME

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\_X\Method\SFAMXML070324WMA.M  
 Title : VOC Analysis

Signal : TIC: VX042468.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         | 1.239       | 21            | 25          | 27           | rBV      | 31294          | 37613         | 6.25%           | 0.706%        |
| 2         | 1.605       | 70            | 85          | 87           | rBV8     | 7837           | 27133         | 4.51%           | 0.509%        |
| 3         | 1.654       | 89            | 93          | 94           | rBV      | 6019           | 7548          | 1.25%           | 0.142%        |
| 4         | 2.270       | 189           | 194         | 212          | rBV      | 59868          | 122958        | 20.44%          | 2.307%        |
| 5         | 2.727       | 263           | 269         | 275          | rBV2     | 7421           | 16499         | 2.74%           | 0.310%        |
| 6         | 2.952       | 298           | 306         | 318          | rVB2     | 3982           | 10375         | 1.72%           | 0.195%        |
| 7         | 4.501       | 552           | 560         | 577          | rBV      | 31509          | 108556        | 18.04%          | 2.037%        |
| 8         | 5.062       | 642           | 652         | 668          | rVV2     | 66175          | 200384        | 33.30%          | 3.759%        |
| 9         | 5.556       | 726           | 733         | 741          | rBV2     | 860            | 2456          | 0.41%           | 0.046%        |
| 10        | 5.964       | 790           | 800         | 823          | rBV2     | 181129         | 525436        | 87.33%          | 9.857%        |
| 11        | 6.604       | 898           | 905         | 913          | rBV6     | 1175           | 3091          | 0.51%           | 0.058%        |
| 12        | 6.763       | 922           | 931         | 951          | rBV      | 180648         | 440642        | 73.23%          | 8.266%        |
| 13        | 7.232       | 1003          | 1008        | 1013         | rBV2     | 509            | 1120          | 0.19%           | 0.021%        |
| 14        | 7.311       | 1013          | 1021        | 1041         | rBV2     | 107749         | 252812        | 42.02%          | 4.743%        |
| 15        | 7.964       | 1122          | 1128        | 1133         | rBV4     | 1102           | 2336          | 0.39%           | 0.044%        |
| 16        | 8.275       | 1173          | 1179        | 1182         | rBV4     | 1301           | 2157          | 0.36%           | 0.040%        |
| 17        | 8.329       | 1182          | 1188        | 1202         | rBV      | 71145          | 121929        | 20.26%          | 2.287%        |
| 18        | 8.598       | 1227          | 1232        | 1234         | rBV3     | 1207           | 1819          | 0.30%           | 0.034%        |
| 19        | 8.653       | 1234          | 1241        | 1248         | rVV      | 307902         | 506929        | 84.25%          | 9.510%        |
| 20        | 8.720       | 1248          | 1252        | 1264         | rVB      | 42360          | 70805         | 11.77%          | 1.328%        |
| 21        | 8.909       | 1279          | 1283        | 1286         | rVV      | 5588           | 7899          | 1.31%           | 0.148%        |
| 22        | 8.957       | 1286          | 1291        | 1304         | rVV      | 47559          | 79460         | 13.21%          | 1.491%        |
| 23        | 9.274       | 1339          | 1343        | 1350         | rVB2     | 7670           | 11809         | 1.96%           | 0.222%        |
| 24        | 9.396       | 1357          | 1363        | 1376         | rBV      | 158578         | 332522        | 55.26%          | 6.238%        |
| 25        | 9.561       | 1387          | 1390        | 1396         | rVB5     | 2176           | 3684          | 0.61%           | 0.069%        |
| 26        | 9.616       | 1396          | 1399        | 1411         | rVB5     | 1644           | 3027          | 0.50%           | 0.057%        |
| 27        | 9.713       | 1411          | 1415        | 1425         | rVB4     | 1453           | 2628          | 0.44%           | 0.049%        |
| 28        | 9.817       | 1429          | 1432        | 1438         | rVB4     | 1078           | 1601          | 0.27%           | 0.030%        |
| 29        | 9.902       | 1441          | 1446        | 1451         | rVB3     | 2857           | 4192          | 0.70%           | 0.079%        |
| 30        | 10.012      | 1458          | 1464        | 1466         | rBV2     | 2408           | 3320          | 0.55%           | 0.062%        |
| 31        | 10.055      | 1466          | 1471        | 1485         | rVB      | 438264         | 601688        | 100.00%         | 11.288%       |
| 32        | 10.201      | 1490          | 1495        | 1499         | rVV2     | 1697           | 2591          | 0.43%           | 0.049%        |
| 33        | 10.268      | 1503          | 1506        | 1508         | rVV3     | 672            | 1147          | 0.19%           | 0.022%        |
| 34        | 10.305      | 1508          | 1512        | 1517         | rVV2     | 6666           | 11098         | 1.84%           | 0.208%        |
| 35        | 10.360      | 1517          | 1521        | 1528         | rVB2     | 10526          | 14761         | 2.45%           | 0.277%        |
| 36        | 10.585      | 1553          | 1558        | 1564         | rBV4     | 998            | 1789          | 0.30%           | 0.034%        |

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 Sample : P3263-16ME  
 Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 A4CK4ME

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\_X\Method\SFAMXML070324WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 10.646 | 1564 | 1568 | 1576 | rBV2 | 2732   | 4890   | 0.81%  | 0.092%  |
| 38 | 10.780 | 1586 | 1590 | 1596 | rVB3 | 2724   | 3873   | 0.64%  | 0.073%  |
| 39 | 10.853 | 1599 | 1602 | 1606 | rBV4 | 3210   | 5145   | 0.86%  | 0.097%  |
| 40 | 10.890 | 1606 | 1608 | 1614 | rVB3 | 2495   | 3490   | 0.58%  | 0.065%  |
| 41 | 10.969 | 1614 | 1621 | 1627 | rBV4 | 2173   | 3830   | 0.64%  | 0.072%  |
| 42 | 11.030 | 1628 | 1631 | 1634 | rBV4 | 1361   | 1541   | 0.26%  | 0.029%  |
| 43 | 11.085 | 1634 | 1640 | 1642 | rBV3 | 4254   | 6333   | 1.05%  | 0.119%  |
| 44 | 11.195 | 1652 | 1658 | 1669 | rVB  | 268951 | 350107 | 58.19% | 6.568%  |
| 45 | 11.305 | 1672 | 1676 | 1681 | rBV2 | 1504   | 2359   | 0.39%  | 0.044%  |
| 46 | 11.384 | 1686 | 1689 | 1693 | rBV4 | 2308   | 3594   | 0.60%  | 0.067%  |
| 47 | 11.433 | 1693 | 1697 | 1700 | rBV3 | 3111   | 4641   | 0.77%  | 0.087%  |
| 48 | 11.475 | 1701 | 1704 | 1714 | rVB2 | 22109  | 29596  | 4.92%  | 0.555%  |
| 49 | 11.579 | 1717 | 1721 | 1723 | rBV2 | 696    | 1083   | 0.18%  | 0.020%  |
| 50 | 11.628 | 1725 | 1729 | 1735 | rVB5 | 1359   | 2475   | 0.41%  | 0.046%  |
| 51 | 11.683 | 1735 | 1738 | 1740 | rBV4 | 877    | 1182   | 0.20%  | 0.022%  |
| 52 | 11.713 | 1740 | 1743 | 1747 | rBV  | 4860   | 5577   | 0.93%  | 0.105%  |
| 53 | 11.756 | 1747 | 1750 | 1759 | rVB  | 6876   | 11490  | 1.91%  | 0.216%  |
| 54 | 11.841 | 1759 | 1764 | 1766 | rBV3 | 1055   | 1591   | 0.26%  | 0.030%  |
| 55 | 11.890 | 1769 | 1772 | 1776 | rVB5 | 2005   | 2445   | 0.41%  | 0.046%  |
| 56 | 11.945 | 1776 | 1781 | 1784 | rBV4 | 6226   | 8460   | 1.41%  | 0.159%  |
| 57 | 11.975 | 1784 | 1786 | 1788 | rVB3 | 1314   | 1242   | 0.21%  | 0.023%  |
| 58 | 12.024 | 1788 | 1794 | 1800 | rBV  | 465682 | 594023 | 98.73% | 11.144% |
| 59 | 12.176 | 1815 | 1819 | 1823 | rVB3 | 2680   | 3872   | 0.64%  | 0.073%  |
| 60 | 12.249 | 1823 | 1831 | 1832 | rBV6 | 1781   | 2676   | 0.44%  | 0.050%  |
| 61 | 12.268 | 1832 | 1834 | 1837 | rVV  | 3032   | 3399   | 0.56%  | 0.064%  |
| 62 | 12.323 | 1837 | 1843 | 1851 | rVV  | 392078 | 499184 | 82.96% | 9.365%  |
| 63 | 12.426 | 1855 | 1860 | 1864 | rVV  | 22549  | 30440  | 5.06%  | 0.571%  |
| 64 | 12.469 | 1864 | 1867 | 1874 | rVB4 | 3493   | 5137   | 0.85%  | 0.096%  |
| 65 | 12.560 | 1874 | 1882 | 1885 | rBV4 | 2371   | 5547   | 0.92%  | 0.104%  |
| 66 | 12.615 | 1889 | 1891 | 1898 | rVB2 | 1830   | 2742   | 0.46%  | 0.051%  |
| 67 | 12.682 | 1899 | 1902 | 1905 | rBV2 | 1790   | 2284   | 0.38%  | 0.043%  |
| 68 | 12.731 | 1905 | 1910 | 1913 | rVB3 | 1117   | 1689   | 0.28%  | 0.032%  |
| 69 | 12.768 | 1913 | 1916 | 1919 | rBV5 | 1129   | 1530   | 0.25%  | 0.029%  |
| 70 | 12.816 | 1922 | 1924 | 1927 | rVB3 | 1474   | 1612   | 0.27%  | 0.030%  |
| 71 | 12.884 | 1927 | 1935 | 1942 | rBV8 | 5483   | 13946  | 2.32%  | 0.262%  |
| 72 | 12.975 | 1947 | 1950 | 1955 | rVB4 | 2567   | 3786   | 0.63%  | 0.071%  |
| 73 | 13.036 | 1955 | 1960 | 1964 | rBV3 | 1784   | 2984   | 0.50%  | 0.056%  |
| 74 | 13.164 | 1976 | 1981 | 1985 | rVB4 | 3684   | 4931   | 0.82%  | 0.093%  |
| 75 | 13.213 | 1985 | 1989 | 1992 | rBV4 | 2133   | 3132   | 0.52%  | 0.059%  |
| 76 | 13.268 | 1994 | 1998 | 2001 | rBV  | 9684   | 11821  | 1.96%  | 0.222%  |

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 Sample : P3263-16ME  
 Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 A4CK4ME

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\_X\Method\SFAMXML070324WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |       |       |       |        |
|-----|--------|------|------|------|------|-------|-------|-------|--------|
| 77  | 13.335 | 2007 | 2009 | 2013 | rVB4 | 1132  | 1341  | 0.22% | 0.025% |
| 78  | 13.383 | 2013 | 2017 | 2021 | rBV4 | 2379  | 4672  | 0.78% | 0.088% |
| 79  | 13.591 | 2046 | 2051 | 2055 | rBV6 | 1236  | 2327  | 0.39% | 0.044% |
| 80  | 13.694 | 2062 | 2068 | 2072 | rBV7 | 1645  | 3966  | 0.66% | 0.074% |
| 81  | 13.731 | 2072 | 2074 | 2077 | rVV4 | 1601  | 2223  | 0.37% | 0.042% |
| 82  | 13.780 | 2077 | 2082 | 2088 | rVV  | 22539 | 30831 | 5.12% | 0.578% |
| 83  | 13.841 | 2088 | 2092 | 2095 | rVV4 | 1276  | 1758  | 0.29% | 0.033% |
| 84  | 13.944 | 2105 | 2109 | 2115 | rVB3 | 1148  | 2457  | 0.41% | 0.046% |
| 85  | 14.042 | 2121 | 2125 | 2129 | rVB4 | 4055  | 5140  | 0.85% | 0.096% |
| 86  | 14.213 | 2151 | 2153 | 2158 | rVB4 | 894   | 1156  | 0.19% | 0.022% |
| 87  | 14.432 | 2185 | 2189 | 2192 | rBV4 | 1991  | 2395  | 0.40% | 0.045% |
| 88  | 14.639 | 2216 | 2223 | 2227 | rBV  | 14070 | 17748 | 2.95% | 0.333% |
| 89  | 14.780 | 2239 | 2246 | 2253 | rVB  | 7982  | 14085 | 2.34% | 0.264% |
| 90  | 14.853 | 2253 | 2258 | 2261 | rBV4 | 1038  | 1544  | 0.26% | 0.029% |
| 91  | 15.139 | 2302 | 2305 | 2307 | rVV3 | 869   | 1119  | 0.19% | 0.021% |
| 92  | 15.182 | 2309 | 2312 | 2314 | rVV4 | 1336  | 1846  | 0.31% | 0.035% |
| 93  | 15.206 | 2314 | 2316 | 2323 | rVB  | 2566  | 3494  | 0.58% | 0.066% |
| 94  | 15.383 | 2338 | 2345 | 2356 | rBV7 | 2362  | 6697  | 1.11% | 0.126% |
| 95  | 15.481 | 2356 | 2361 | 2366 | rBV3 | 6215  | 9678  | 1.61% | 0.182% |
| 96  | 15.615 | 2378 | 2383 | 2386 | rBV2 | 5451  | 8666  | 1.44% | 0.163% |
| 97  | 15.956 | 2435 | 2439 | 2443 | rBV3 | 3647  | 5067  | 0.84% | 0.095% |
| 98  | 16.090 | 2456 | 2461 | 2465 | rBV4 | 1730  | 2582  | 0.43% | 0.048% |
| 99  | 16.334 | 2495 | 2501 | 2502 | rBV5 | 1563  | 2867  | 0.48% | 0.054% |
| 100 | 16.651 | 2549 | 2553 | 2555 | rBV4 | 949   | 1332  | 0.22% | 0.025% |

Sum of corrected areas: 5330484



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Data File : VX042468.D  
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Sample : P3263-16ME  
Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
A4CK4ME

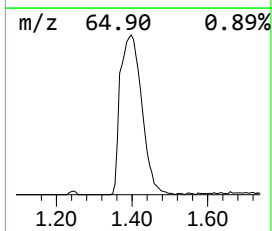
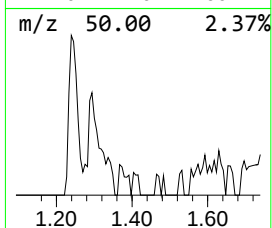
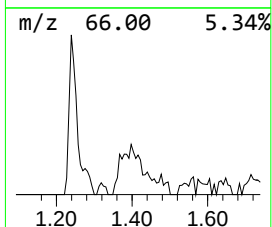
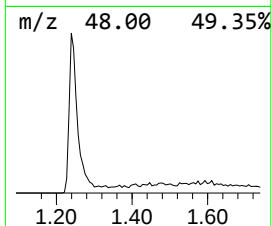
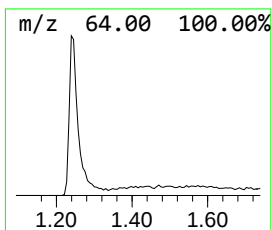
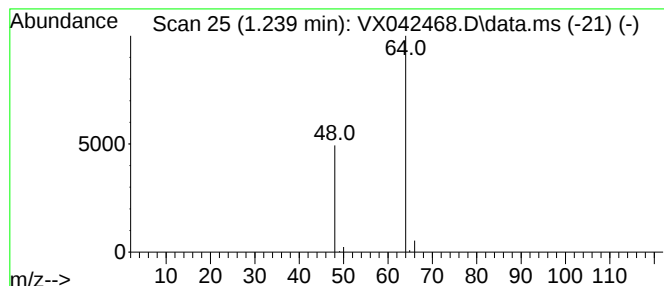
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML070324WMA.M  
Quant Title : VOC Analysis

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

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Peak Number 1 Sulfur dioxide Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 1.239 | 4.27 ug/L | 37613 | 1,4-Difluorobenzene | 6.763 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------|-----|----------|-------------|------|
| 1    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 83   |
| 2    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 74   |
| 3    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |
| 4    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 5    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 5    |



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Sample : P3263-16ME  
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ALS Vial : 5 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
A4CK4ME

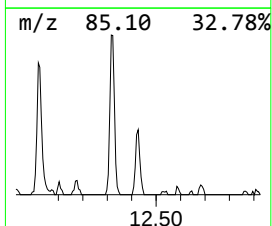
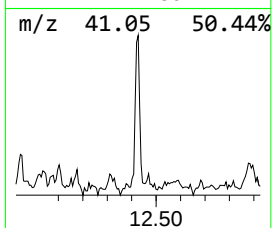
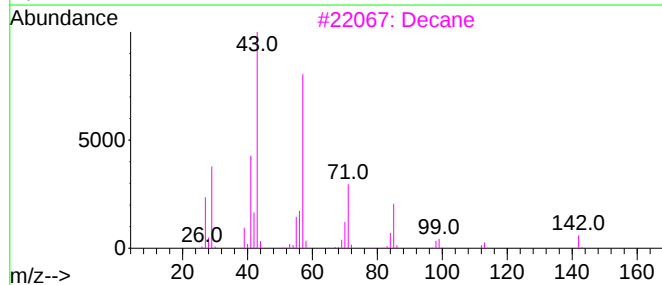
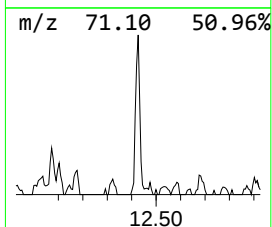
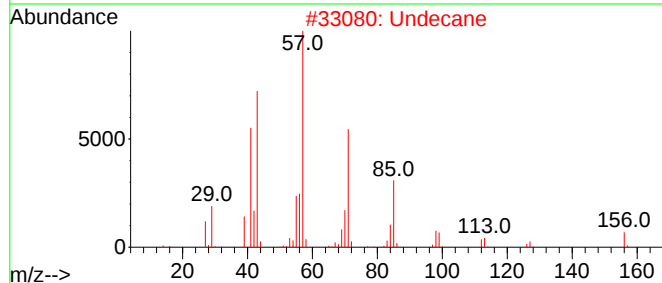
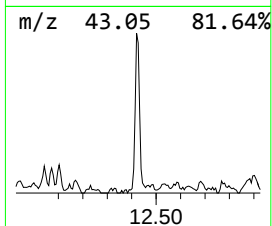
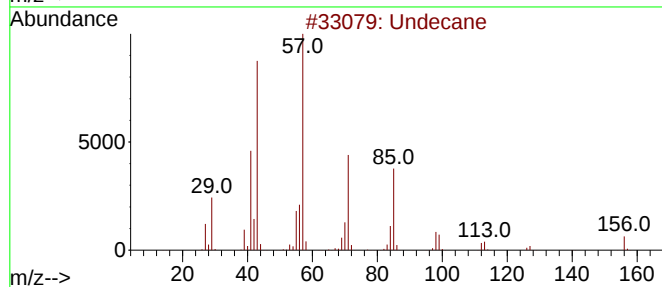
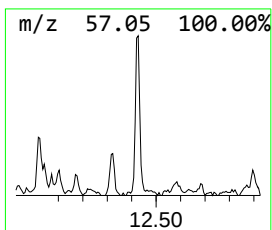
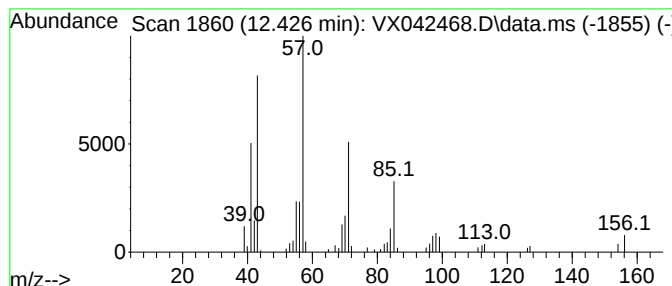
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML070324WMA.M  
Quant Title : VOC Analysis

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

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Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.426 | 2.56 ug/L | 30440 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of          | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|-------------|---|--------------|-----|---------|-------------|------|
| 1    | Undecane    |   |              | 156 | C11H24  | 001120-21-4 | 97   |
| 2    | Undecane    |   |              | 156 | C11H24  | 001120-21-4 | 96   |
| 3    | Decane      |   |              | 142 | C10H22  | 000124-18-5 | 86   |
| 4    | Decane      |   |              | 142 | C10H22  | 000124-18-5 | 86   |
| 5    | Tetradecane |   |              | 198 | C14H30  | 000629-59-4 | 86   |



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ALS Vial : 5 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
A4CK4ME

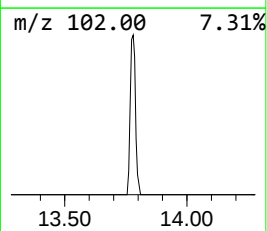
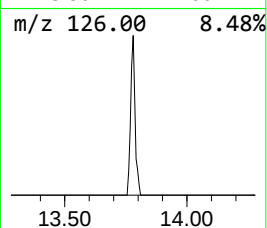
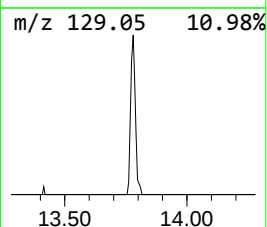
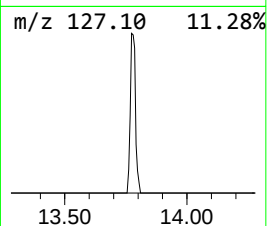
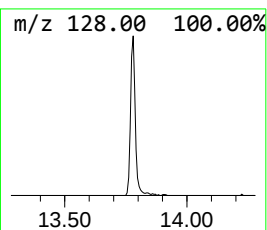
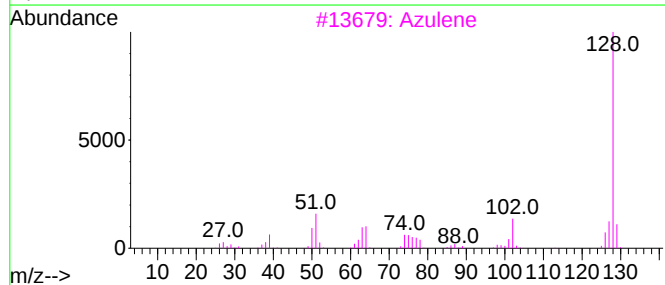
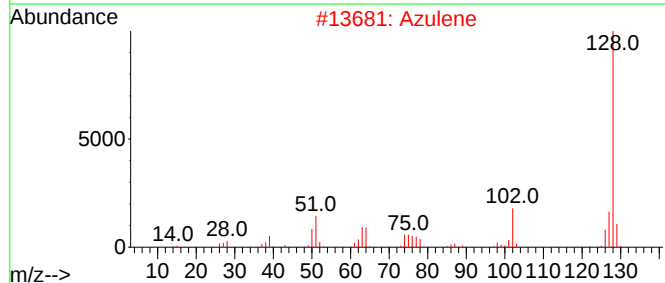
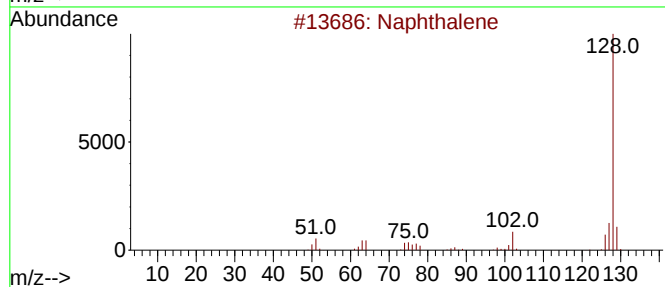
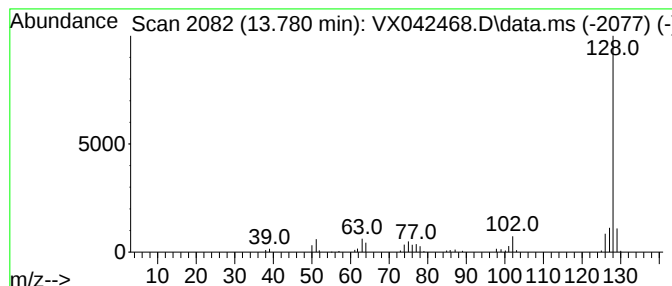
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML070324WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 4 Azulene Concentration Rank 3

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 13.780 | 2.60 ug/L | 30831 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------|-----|---------|-------------|------|
| 1    |    |   | Naphthalene  | 128 | C10H8   | 000091-20-3 | 95   |
| 2    |    |   | Azulene      | 128 | C10H8   | 000275-51-4 | 91   |
| 3    |    |   | Azulene      | 128 | C10H8   | 000275-51-4 | 91   |
| 4    |    |   | Azulene      | 128 | C10H8   | 000275-51-4 | 91   |
| 5    |    |   | Azulene      | 128 | C10H8   | 000275-51-4 | 90   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX072424\  
Data File : VX042468.D  
Acq On : 23 Jul 2024 13:48  
Operator : JC/MD  
Sample : P3263-16ME  
Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA\_X/MEOH  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
A4CK4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML070324WMA.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 |
| Sulfur dioxide     | 1.239  | 4.3     | ug/L  | 37613    | 1                     | 6.763  | 440642 | 50.0 |
| (DEL) Alkane: S... | 12.426 | 2.6     | ug/L  | 30440    | 3                     | 12.024 | 594023 | 50.0 |
| Azulene            | 13.780 | 2.6     | ug/L  | 30831    | 3                     | 12.024 | 594023 | 50.0 |