

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX081022\  
 Data File : VX030553.D  
 Acq On : 10 Aug 2022 15:34  
 Operator : JC/MD  
 Sample : N4076-03  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 DBUT8

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\SFAMXML080422WMA.M  
 Title : VOC Analysis

Signal : TIC: VX030553.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         | 1.252       | 23            | 27          | 38           | rBV      | 72299          | 151180        | 9.88%           | 1.514%        |
| 2         | 1.367       | 42            | 46          | 51           | rVV      | 116605         | 119476        | 7.81%           | 1.196%        |
| 3         | 1.666       | 91            | 95          | 104          | rVB      | 111358         | 137444        | 8.99%           | 1.376%        |
| 4         | 2.306       | 194           | 200         | 210          | rVV      | 192965         | 300916        | 19.67%          | 3.013%        |
| 5         | 2.404       | 211           | 216         | 225          | rVB3     | 4699           | 9986          | 0.65%           | 0.100%        |
| 6         | 2.843       | 286           | 288         | 290          | rVB2     | 477            | 377           | 0.02%           | 0.004%        |
| 7         | 2.867       | 290           | 292         | 295          | rBV2     | 461            | 582           | 0.04%           | 0.006%        |
| 8         | 3.056       | 321           | 323         | 324          | rBV      | 556            | 398           | 0.03%           | 0.004%        |
| 9         | 3.099       | 324           | 330         | 345          | rVV4     | 12115          | 39132         | 2.56%           | 0.392%        |
| 10        | 3.318       | 364           | 366         | 368          | rBV2     | 436            | 422           | 0.03%           | 0.004%        |
| 11        | 3.611       | 410           | 414         | 422          | rVB4     | 2273           | 4792          | 0.31%           | 0.048%        |
| 12        | 3.696       | 427           | 428         | 431          | rVB      | 607            | 447           | 0.03%           | 0.004%        |
| 13        | 3.843       | 449           | 452         | 453          | rBV2     | 445            | 426           | 0.03%           | 0.004%        |
| 14        | 4.184       | 505           | 508         | 509          | rBV2     | 580            | 629           | 0.04%           | 0.006%        |
| 15        | 4.495       | 547           | 559         | 574          | rBV2     | 532095         | 1529572       | 100.00%         | 15.314%       |
| 16        | 5.068       | 641           | 653         | 667          | rBV      | 158111         | 474012        | 30.99%          | 4.746%        |
| 17        | 5.702       | 754           | 757         | 758          | rBV2     | 383            | 327           | 0.02%           | 0.003%        |
| 18        | 5.751       | 763           | 765         | 768          | rBV2     | 409            | 563           | 0.04%           | 0.006%        |
| 19        | 5.873       | 784           | 785         | 787          | rBV2     | 523            | 354           | 0.02%           | 0.004%        |
| 20        | 5.976       | 790           | 802         | 819          | rVV2     | 401317         | 1161422       | 75.93%          | 11.628%       |
| 21        | 6.306       | 853           | 856         | 859          | rBV3     | 500            | 685           | 0.04%           | 0.007%        |
| 22        | 6.769       | 921           | 932         | 947          | rBV      | 250843         | 594528        | 38.87%          | 5.953%        |
| 23        | 7.019       | 971           | 973         | 974          | rBV2     | 505            | 359           | 0.02%           | 0.004%        |
| 24        | 7.037       | 974           | 976         | 979          | rVB2     | 398            | 380           | 0.02%           | 0.004%        |
| 25        | 7.110       | 981           | 988         | 989          | rBV4     | 7564           | 11292         | 0.74%           | 0.113%        |
| 26        | 7.312       | 1013          | 1021        | 1035         | rVB      | 243874         | 538665        | 35.22%          | 5.393%        |
| 27        | 7.537       | 1056          | 1058        | 1062         | rVV2     | 948            | 642           | 0.04%           | 0.006%        |
| 28        | 7.622       | 1070          | 1072        | 1075         | rVB3     | 421            | 368           | 0.02%           | 0.004%        |
| 29        | 7.848       | 1107          | 1109        | 1110         | rBV      | 382            | 367           | 0.02%           | 0.004%        |
| 30        | 7.879       | 1112          | 1114        | 1117         | rVB2     | 617            | 498           | 0.03%           | 0.005%        |
| 31        | 7.982       | 1129          | 1131        | 1133         | rBV2     | 450            | 400           | 0.03%           | 0.004%        |
| 32        | 8.330       | 1181          | 1188        | 1202         | rBV      | 167862         | 280055        | 18.31%          | 2.804%        |
| 33        | 8.561       | 1223          | 1226        | 1228         | rBV3     | 693            | 887           | 0.06%           | 0.009%        |
| 34        | 8.653       | 1234          | 1241        | 1257         | rBV      | 570992         | 875775        | 57.26%          | 8.768%        |
| 35        | 8.811       | 1266          | 1267        | 1269         | rBV      | 658            | 589           | 0.04%           | 0.006%        |
| 36        | 8.951       | 1285          | 1290        | 1299         | rVV      | 121299         | 183073        | 11.97%          | 1.833%        |

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 MSVOA\_X  
 ClientSampleId :  
 DBUT8

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\SFAMXML080422WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 37 | 9.177  | 1323 | 1327 | 1332 | rVB4 | 2135   | 3748   | 0.25%  | 0.038% |
| 38 | 9.244  | 1333 | 1338 | 1353 | rVB  | 15351  | 25661  | 1.68%  | 0.257% |
| 39 | 9.348  | 1353 | 1355 | 1356 | rBV2 | 504    | 384    | 0.03%  | 0.004% |
| 40 | 9.390  | 1356 | 1362 | 1372 | rBV  | 500415 | 699004 | 45.70% | 6.999% |
| 41 | 9.707  | 1412 | 1414 | 1418 | rBV3 | 481    | 610    | 0.04%  | 0.006% |
| 42 | 9.860  | 1436 | 1439 | 1441 | rBV2 | 460    | 399    | 0.03%  | 0.004% |
| 43 | 9.945  | 1451 | 1453 | 1456 | rBV2 | 368    | 441    | 0.03%  | 0.004% |
| 44 | 10.018 | 1460 | 1465 | 1466 | rBV3 | 2054   | 3219   | 0.21%  | 0.032% |
| 45 | 10.055 | 1466 | 1471 | 1481 | rVB  | 526993 | 721807 | 47.19% | 7.227% |
| 46 | 10.152 | 1486 | 1487 | 1489 | rBV2 | 887    | 684    | 0.04%  | 0.007% |
| 47 | 10.378 | 1519 | 1524 | 1533 | rBV  | 39089  | 55145  | 3.61%  | 0.552% |
| 48 | 10.561 | 1552 | 1554 | 1556 | rBV2 | 692    | 539    | 0.04%  | 0.005% |
| 49 | 10.646 | 1567 | 1568 | 1571 | rVB3 | 653    | 542    | 0.04%  | 0.005% |
| 50 | 10.677 | 1571 | 1573 | 1575 | rBV3 | 332    | 325    | 0.02%  | 0.003% |
| 51 | 10.835 | 1595 | 1599 | 1601 | rBV3 | 548    | 648    | 0.04%  | 0.006% |
| 52 | 10.860 | 1601 | 1603 | 1606 | rVB3 | 605    | 596    | 0.04%  | 0.006% |
| 53 | 10.915 | 1610 | 1612 | 1613 | rBV2 | 596    | 357    | 0.02%  | 0.004% |
| 54 | 10.957 | 1618 | 1619 | 1623 | rVB3 | 657    | 705    | 0.05%  | 0.007% |
| 55 | 11.000 | 1623 | 1626 | 1628 | rBV3 | 564    | 539    | 0.04%  | 0.005% |
| 56 | 11.018 | 1628 | 1629 | 1632 | rVB3 | 625    | 577    | 0.04%  | 0.006% |
| 57 | 11.091 | 1635 | 1641 | 1643 | rBV5 | 1145   | 2026   | 0.13%  | 0.020% |
| 58 | 11.195 | 1653 | 1658 | 1669 | rVB  | 474443 | 582728 | 38.10% | 5.834% |
| 59 | 11.341 | 1679 | 1682 | 1685 | rBV4 | 534    | 807    | 0.05%  | 0.008% |
| 60 | 11.451 | 1698 | 1700 | 1703 | rBV2 | 442    | 528    | 0.03%  | 0.005% |
| 61 | 11.482 | 1703 | 1705 | 1708 | rVB3 | 628    | 484    | 0.03%  | 0.005% |
| 62 | 11.640 | 1728 | 1731 | 1735 | rBV3 | 854    | 1309   | 0.09%  | 0.013% |
| 63 | 11.701 | 1737 | 1741 | 1747 | rVB5 | 2775   | 4332   | 0.28%  | 0.043% |
| 64 | 11.756 | 1747 | 1750 | 1751 | rBV3 | 698    | 626    | 0.04%  | 0.006% |
| 65 | 11.829 | 1760 | 1762 | 1764 | rBV2 | 364    | 336    | 0.02%  | 0.003% |
| 66 | 11.890 | 1768 | 1772 | 1778 | rVB4 | 4934   | 7085   | 0.46%  | 0.071% |
| 67 | 12.024 | 1788 | 1794 | 1803 | rBV  | 555997 | 668431 | 43.70% | 6.692% |
| 68 | 12.219 | 1823 | 1826 | 1827 | rBV2 | 984    | 994    | 0.06%  | 0.010% |
| 69 | 12.323 | 1837 | 1843 | 1853 | rBV  | 612534 | 762796 | 49.87% | 7.637% |
| 70 | 12.615 | 1889 | 1891 | 1893 | rBV  | 534    | 424    | 0.03%  | 0.004% |
| 71 | 12.707 | 1904 | 1906 | 1907 | rBV2 | 427    | 373    | 0.02%  | 0.004% |
| 72 | 12.859 | 1930 | 1931 | 1933 | rBV  | 669    | 376    | 0.02%  | 0.004% |
| 73 | 12.945 | 1940 | 1945 | 1946 | rBV3 | 546    | 545    | 0.04%  | 0.005% |
| 74 | 13.000 | 1952 | 1954 | 1960 | rBV3 | 625    | 1123   | 0.07%  | 0.011% |
| 75 | 13.048 | 1960 | 1962 | 1963 | rBV  | 349    | 339    | 0.02%  | 0.003% |
| 76 | 13.091 | 1968 | 1969 | 1971 | rBV  | 443    | 411    | 0.03%  | 0.004% |

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Instrument :  
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML080422WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |      |      |       |        |
|-----|--------|------|------|------|------|------|------|-------|--------|
| 77  | 13.109 | 1971 | 1972 | 1975 | rVB2 | 654  | 566  | 0.04% | 0.006% |
| 78  | 13.341 | 2008 | 2010 | 2012 | rBV  | 345  | 349  | 0.02% | 0.003% |
| 79  | 13.365 | 2012 | 2014 | 2018 | rVV3 | 507  | 690  | 0.05% | 0.007% |
| 80  | 13.463 | 2028 | 2030 | 2036 | rVB4 | 541  | 1085 | 0.07% | 0.011% |
|     |        |      |      |      |      |      |      |       |        |
| 81  | 13.518 | 2036 | 2039 | 2042 | rBV3 | 691  | 602  | 0.04% | 0.006% |
| 82  | 13.554 | 2042 | 2045 | 2047 | rBV2 | 425  | 474  | 0.03% | 0.005% |
| 83  | 13.585 | 2049 | 2050 | 2052 | rBV2 | 751  | 574  | 0.04% | 0.006% |
| 84  | 13.646 | 2058 | 2060 | 2065 | rVV2 | 449  | 643  | 0.04% | 0.006% |
| 85  | 13.688 | 2065 | 2067 | 2070 | rVB  | 645  | 625  | 0.04% | 0.006% |
|     |        |      |      |      |      |      |      |       |        |
| 86  | 13.780 | 2079 | 2082 | 2085 | rBV3 | 719  | 682  | 0.04% | 0.007% |
| 87  | 13.835 | 2089 | 2091 | 2093 | rVB2 | 504  | 323  | 0.02% | 0.003% |
| 88  | 13.859 | 2093 | 2095 | 2098 | rBV3 | 583  | 761  | 0.05% | 0.008% |
| 89  | 13.890 | 2098 | 2100 | 2103 | rBV3 | 406  | 383  | 0.03% | 0.004% |
| 90  | 13.969 | 2112 | 2113 | 2115 | rVB  | 601  | 425  | 0.03% | 0.004% |
|     |        |      |      |      |      |      |      |       |        |
| 91  | 14.066 | 2127 | 2129 | 2131 | rBV3 | 417  | 424  | 0.03% | 0.004% |
| 92  | 14.170 | 2145 | 2146 | 2147 | rBV  | 549  | 323  | 0.02% | 0.003% |
| 93  | 14.816 | 2250 | 2252 | 2253 | rVB  | 671  | 321  | 0.02% | 0.003% |
| 94  | 15.310 | 2331 | 2333 | 2335 | rBV3 | 697  | 813  | 0.05% | 0.008% |
| 95  | 15.597 | 2378 | 2380 | 2384 | rVB5 | 1540 | 1596 | 0.10% | 0.016% |
|     |        |      |      |      |      |      |      |       |        |
| 96  | 15.725 | 2399 | 2401 | 2403 | rVB3 | 726  | 598  | 0.04% | 0.006% |
| 97  | 16.115 | 2463 | 2465 | 2466 | rBV2 | 592  | 366  | 0.02% | 0.004% |
| 98  | 16.170 | 2472 | 2474 | 2478 | rBV3 | 858  | 856  | 0.06% | 0.009% |
| 99  | 16.310 | 2495 | 2497 | 2501 | rBV2 | 619  | 715  | 0.05% | 0.007% |
| 100 | 16.517 | 2529 | 2531 | 2533 | rVB2 | 839  | 560  | 0.04% | 0.006% |

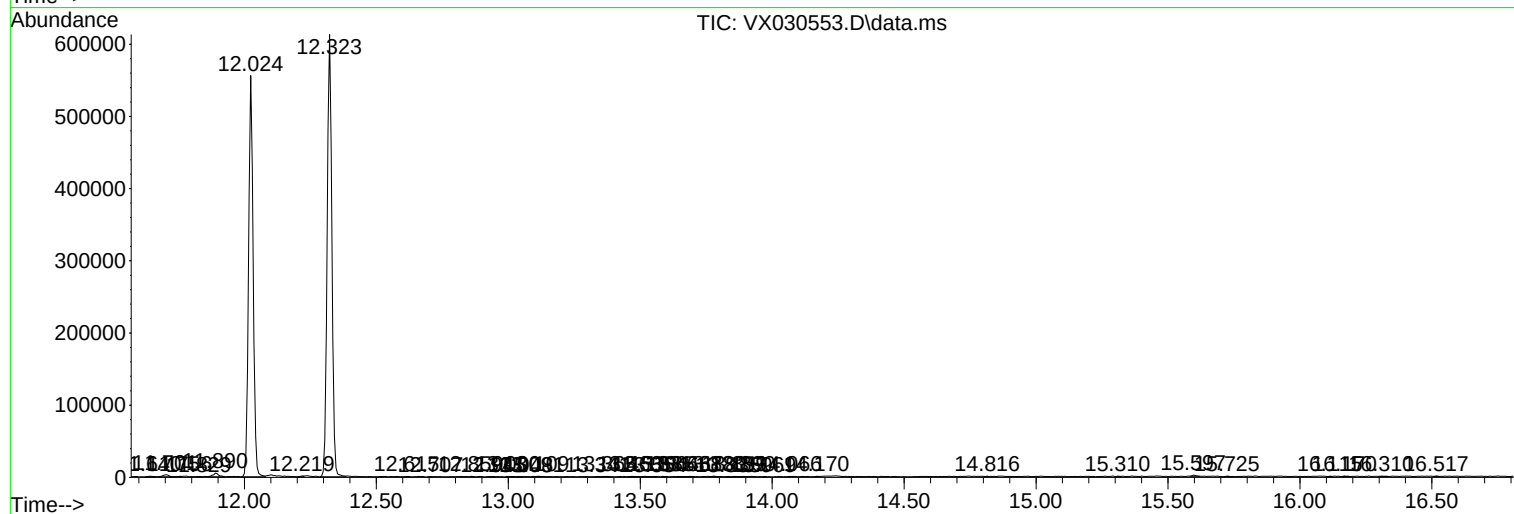
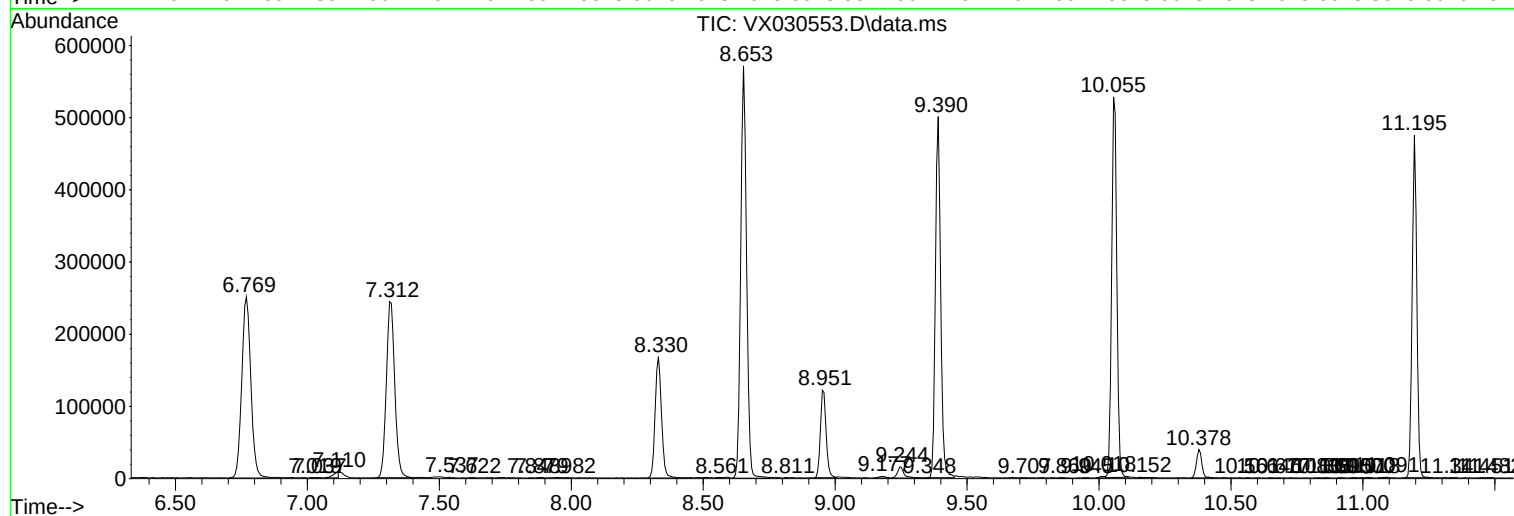
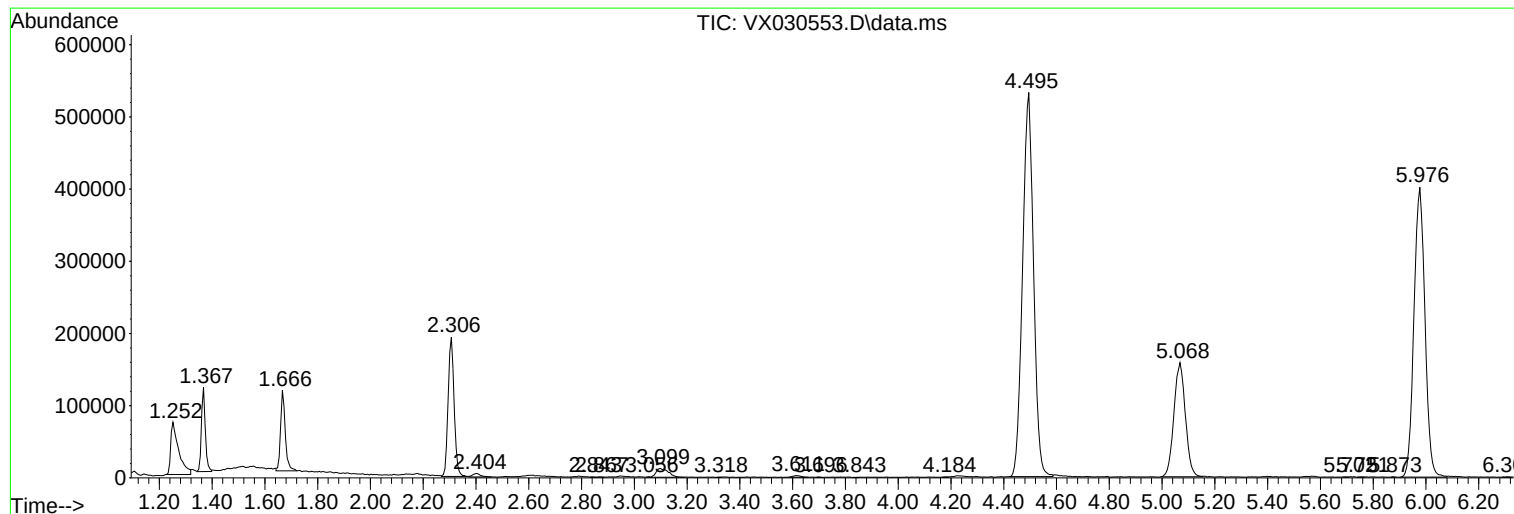
Sum of corrected areas: 9987777

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Instrument :  
MSVOA\_X  
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML080422WMA.M  
Quant Title : VOC Analysis

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



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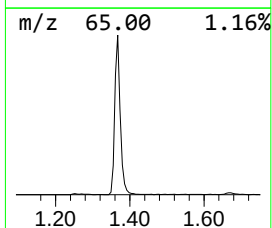
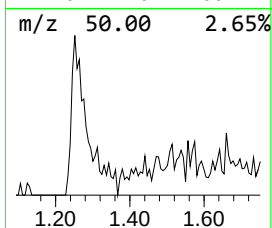
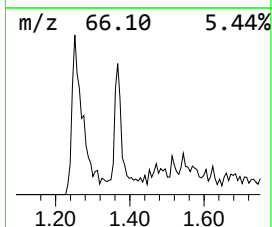
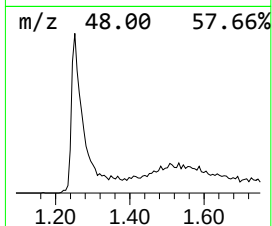
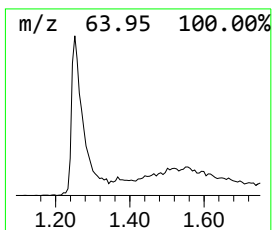
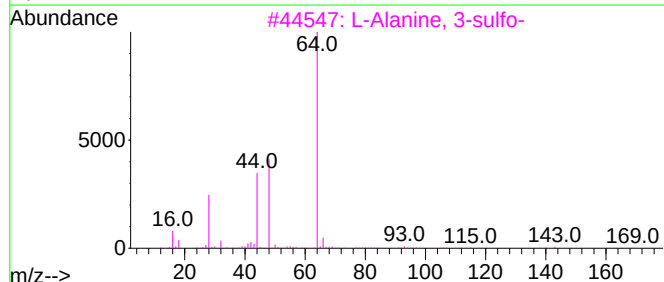
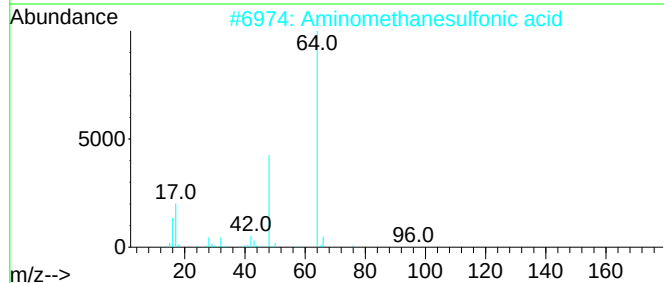
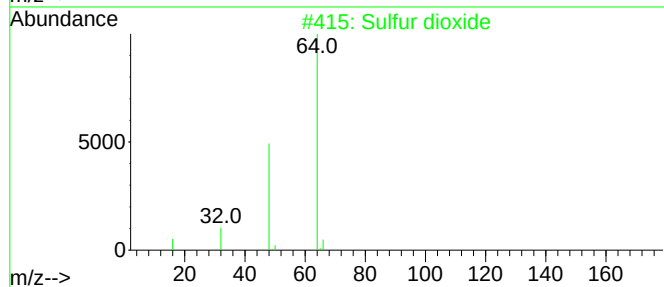
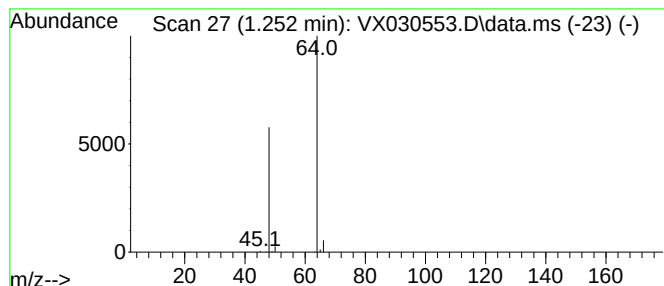
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML080422WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 Sulfur dioxide Concentration Rank 2

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 1.252 | 12.71 ug/L | 151180 | 1,4-Difluorobenzene | 6.769 |

| 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    |    |   | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 4    |    |   | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |
| 5    |    |   | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 5    |



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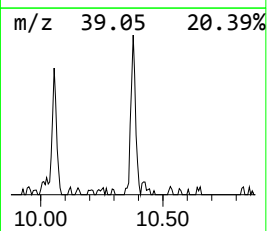
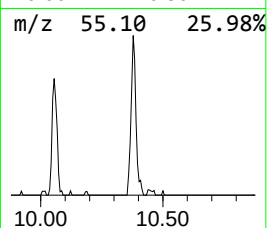
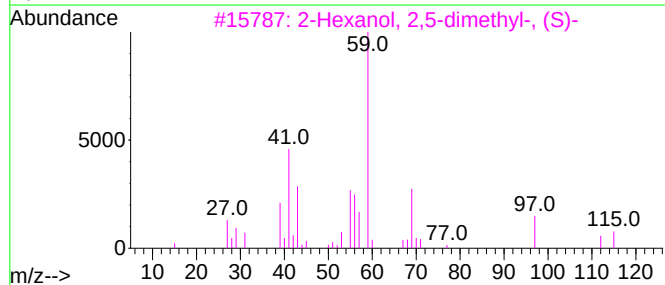
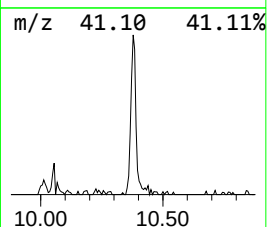
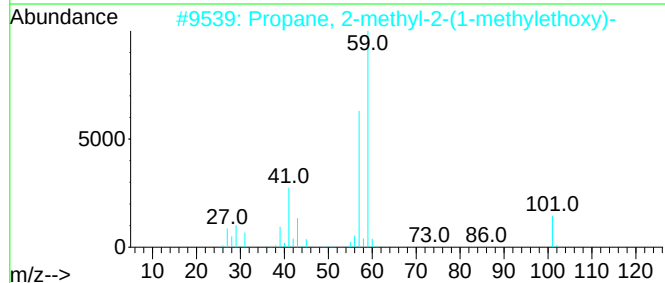
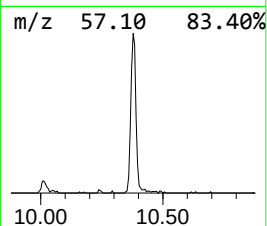
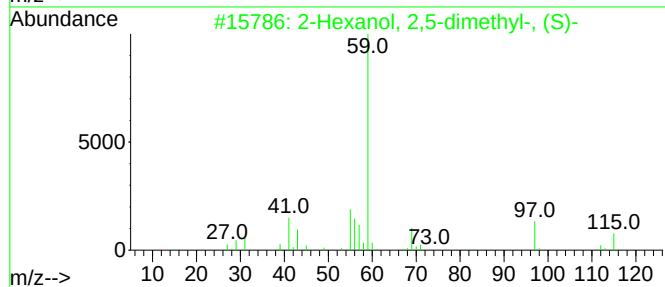
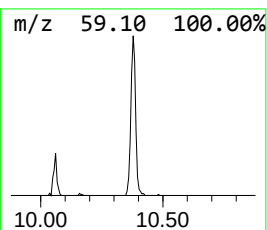
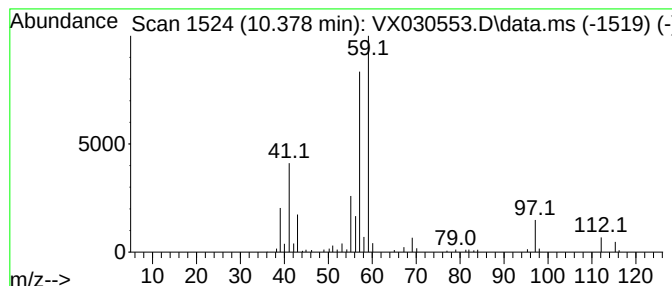
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML080422WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 3 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

| R.T.   | EstConc   | Area  | Relative to ISTD | R.T.   |
|--------|-----------|-------|------------------|--------|
| 10.378 | 3.82 ug/L | 55145 | Chlorobenzene-d5 | 10.061 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Hexanol, 2,5-dimethyl-, (S)-      | 130 | C8H18O       | 003730-60-7 | 56      |      |      |
| 2    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O       | 017348-59-3 | 45      |      |      |
| 3    | 2-Hexanol, 2,5-dimethyl-, (S)-      | 130 | C8H18O       | 003730-60-7 | 38      |      |      |
| 4    | 3-Hexanol, 4-methyl-                | 116 | C7H16O       | 000615-29-2 | 36      |      |      |
| 5    | 3-Pentanol, 2,2-dimethyl-           | 116 | C7H16O       | 003970-62-5 | 36      |      |      |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX081022\  
Data File : VX030553.D  
Acq On : 10 Aug 2022 15:34  
Operator : JC/MD  
Sample : N4076-03  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
DBUT8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML080422WMA.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     | 1.252  | 12.7    | ug/L  | 151180   | 1                     | 6.769  | 594528 | 50.0 |
| 2-Hexanol, 2,5-... | 10.378 | 3.8     | ug/L  | 55145    | 2                     | 10.061 | 721807 | 50.0 |