

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082119\  
 Data File : VU033896.D  
 Acq On : 22 Aug 2019 00:53  
 Operator : JC/SP  
 Sample : K4454-06  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 36 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 F2B91

## Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM081619WMA.M  
 Title : VOC Analysis

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|--------|----------|------------|----------|-----------|-------|-------------|------------|--------------|------------|
| 1      | 1.148    | 12         | 18       | 57        | rBV   | 1588543     | 2350302    | 100.00%      | 15.478%    |
| 2      | 1.389    | 87         | 93       | 105       | rVB2  | 267239      | 292185     | 12.43%       | 1.924%     |
| 3      | 1.547    | 136        | 142      | 170       | rVB   | 1113256     | 1400761    | 59.60%       | 9.225%     |
| 4      | 1.669    | 174        | 180      | 197       | rVB   | 192902      | 236957     | 10.08%       | 1.561%     |
| 5      | 2.170    | 330        | 336      | 347       | rVB   | 38324       | 53962      | 2.30%        | 0.355%     |
| 6      | 2.254    | 353        | 362      | 373       | rVB   | 341990      | 518101     | 22.04%       | 3.412%     |
| 7      | 2.360    | 388        | 395      | 408       | rVB   | 32230       | 50607      | 2.15%        | 0.333%     |
| 8      | 2.463    | 423        | 427      | 434       | rVB   | 3354        | 3743       | 0.16%        | 0.025%     |
| 9      | 2.836    | 540        | 543      | 544       | rBV   | 910         | 567        | 0.02%        | 0.004%     |
| 10     | 2.965    | 572        | 583      | 597       | rVB   | 18356       | 33253      | 1.41%        | 0.219%     |
| 11     | 3.508    | 750        | 752      | 756       | rVB2  | 415         | 316        | 0.01%        | 0.002%     |
| 12     | 3.556    | 762        | 767      | 770       | rBV3  | 407         | 411        | 0.02%        | 0.003%     |
| 13     | 3.576    | 770        | 773      | 777       | rBV2  | 455         | 343        | 0.01%        | 0.002%     |
| 14     | 3.691    | 805        | 809      | 813       | rBV3  | 320         | 361        | 0.02%        | 0.002%     |
| 15     | 3.736    | 817        | 823      | 830       | rVV4  | 420         | 504        | 0.02%        | 0.003%     |
| 16     | 3.926    | 879        | 882      | 884       | rBV   | 529         | 354        | 0.02%        | 0.002%     |
| 17     | 4.042    | 916        | 918      | 923       | rVB3  | 374         | 310        | 0.01%        | 0.002%     |
| 18     | 4.148    | 939        | 951      | 962       | rBV   | 124027      | 321954     | 13.70%       | 2.120%     |
| 19     | 4.389    | 1024       | 1026     | 1028      | rBV2  | 523         | 288        | 0.01%        | 0.002%     |
| 20     | 4.479    | 1050       | 1054     | 1057      | rBV3  | 484         | 475        | 0.02%        | 0.003%     |
| 21     | 4.620    | 1080       | 1098     | 1120      | rBV   | 269022      | 634038     | 26.98%       | 4.176%     |
| 22     | 4.842    | 1163       | 1167     | 1170      | rBV2  | 1015        | 880        | 0.04%        | 0.006%     |
| 23     | 4.948    | 1195       | 1200     | 1201      | rBV2  | 565         | 518        | 0.02%        | 0.003%     |
| 24     | 4.958    | 1201       | 1203     | 1206      | rVV2  | 682         | 540        | 0.02%        | 0.004%     |
| 25     | 4.974    | 1206       | 1208     | 1214      | rVB3  | 923         | 495        | 0.02%        | 0.003%     |
| 26     | 5.010    | 1214       | 1219     | 1221      | rBV2  | 365         | 310        | 0.01%        | 0.002%     |
| 27     | 5.222    | 1280       | 1285     | 1289      | rBV   | 490         | 471        | 0.02%        | 0.003%     |
| 28     | 5.315    | 1289       | 1314     | 1340      | rBV2  | 510300      | 1526692    | 64.96%       | 10.054%    |
| 29     | 5.524    | 1377       | 1379     | 1382      | rBV3  | 667         | 384        | 0.02%        | 0.003%     |
| 30     | 5.556    | 1387       | 1389     | 1393      | rBV3  | 558         | 420        | 0.02%        | 0.003%     |
| 31     | 5.749    | 1446       | 1449     | 1451      | rBV2  | 450         | 384        | 0.02%        | 0.003%     |
| 32     | 5.865    | 1471       | 1485     | 1510      | rBV   | 462858      | 915474     | 38.95%       | 6.029%     |
| 33     | 6.112    | 1560       | 1562     | 1566      | rVB4  | 661         | 335        | 0.01%        | 0.002%     |
| 34     | 6.164    | 1566       | 1578     | 1597      | rVB6  | 26029       | 55885      | 2.38%        | 0.368%     |

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Filtering: 5  
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 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM081619WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 35 | 6.309  | 1609 | 1623 | 1647 | rBV  | 351366 | 711059  | 30.25% | 4.683% |
| 36 | 6.524  | 1686 | 1690 | 1691 | rBV2 | 495    | 342     | 0.01%  | 0.002% |
| 37 | 6.582  | 1700 | 1708 | 1710 | rBV3 | 488    | 663     | 0.03%  | 0.004% |
| 38 | 6.688  | 1738 | 1741 | 1748 | rVB3 | 629    | 578     | 0.02%  | 0.004% |
| 39 | 6.727  | 1748 | 1753 | 1756 | rBV3 | 401    | 303     | 0.01%  | 0.002% |
| 40 | 6.842  | 1785 | 1789 | 1790 | rBV2 | 983    | 567     | 0.02%  | 0.004% |
| 41 | 6.874  | 1795 | 1799 | 1801 | rVV4 | 767    | 553     | 0.02%  | 0.004% |
| 42 | 6.916  | 1810 | 1812 | 1817 | rBV3 | 514    | 394     | 0.02%  | 0.003% |
| 43 | 7.106  | 1866 | 1871 | 1875 | rBV4 | 436    | 536     | 0.02%  | 0.004% |
| 44 | 7.225  | 1904 | 1908 | 1909 | rVV2 | 531    | 295     | 0.01%  | 0.002% |
| 45 | 7.370  | 1949 | 1953 | 1957 | rVV5 | 558    | 482     | 0.02%  | 0.003% |
| 46 | 7.431  | 1970 | 1972 | 1979 | rVB4 | 501    | 517     | 0.02%  | 0.003% |
| 47 | 7.546  | 1994 | 2008 | 2027 | rBV  | 634865 | 1118339 | 47.58% | 7.365% |
| 48 | 7.842  | 2089 | 2100 | 2105 | rBV7 | 1701   | 2884    | 0.12%  | 0.019% |
| 49 | 7.939  | 2127 | 2130 | 2135 | rVB2 | 441    | 391     | 0.02%  | 0.003% |
| 50 | 8.090  | 2171 | 2177 | 2179 | rBV2 | 352    | 349     | 0.01%  | 0.002% |
| 51 | 8.212  | 2206 | 2215 | 2223 | rBV4 | 5970   | 9406    | 0.40%  | 0.062% |
| 52 | 8.296  | 2229 | 2241 | 2277 | rBV  | 377960 | 736856  | 31.35% | 4.853% |
| 53 | 8.505  | 2297 | 2306 | 2321 | rVB  | 4819   | 10922   | 0.46%  | 0.072% |
| 54 | 8.559  | 2321 | 2323 | 2326 | rVB2 | 1016   | 616     | 0.03%  | 0.004% |
| 55 | 8.579  | 2326 | 2329 | 2331 | rBV3 | 748    | 490     | 0.02%  | 0.003% |
| 56 | 8.733  | 2372 | 2377 | 2381 | rVV4 | 471    | 487     | 0.02%  | 0.003% |
| 57 | 8.833  | 2404 | 2408 | 2413 | rBV2 | 386    | 491     | 0.02%  | 0.003% |
| 58 | 8.990  | 2452 | 2457 | 2462 | rVB2 | 400    | 378     | 0.02%  | 0.002% |
| 59 | 9.070  | 2469 | 2482 | 2524 | rBV  | 703071 | 1181333 | 50.26% | 7.780% |
| 60 | 9.328  | 2555 | 2562 | 2567 | rVB5 | 634    | 836     | 0.04%  | 0.006% |
| 61 | 9.415  | 2587 | 2589 | 2598 | rVB3 | 496    | 683     | 0.03%  | 0.004% |
| 62 | 9.453  | 2598 | 2601 | 2606 | rBV3 | 411    | 440     | 0.02%  | 0.003% |
| 63 | 9.498  | 2613 | 2615 | 2620 | rBV3 | 393    | 385     | 0.02%  | 0.003% |
| 64 | 9.640  | 2656 | 2659 | 2663 | rVV3 | 660    | 526     | 0.02%  | 0.003% |
| 65 | 9.759  | 2694 | 2696 | 2701 | rVV3 | 438    | 321     | 0.01%  | 0.002% |
| 66 | 9.871  | 2727 | 2731 | 2734 | rBV3 | 566    | 488     | 0.02%  | 0.003% |
| 67 | 9.913  | 2738 | 2744 | 2745 | rBV3 | 432    | 397     | 0.02%  | 0.003% |
| 68 | 10.093 | 2797 | 2800 | 2805 | rVB3 | 320    | 307     | 0.01%  | 0.002% |
| 69 | 10.199 | 2829 | 2833 | 2835 | rBV3 | 431    | 311     | 0.01%  | 0.002% |
| 70 | 10.292 | 2859 | 2862 | 2866 | rBV3 | 424    | 397     | 0.02%  | 0.003% |
| 71 | 10.334 | 2871 | 2875 | 2879 | rVB3 | 460    | 415     | 0.02%  | 0.003% |

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## Integration Parameters: LSCINT.P

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 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

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 Peak Location: TOP

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 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM081619WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |         |        |        |
|-----|--------|------|------|------|------|--------|---------|--------|--------|
| 72  | 10.414 | 2887 | 2900 | 2926 | rBV  | 524667 | 847188  | 36.05% | 5.579% |
| 73  | 10.562 | 2944 | 2946 | 2951 | rVB  | 558    | 359     | 0.02%  | 0.002% |
| 74  | 10.595 | 2951 | 2956 | 2960 | rBV4 | 553    | 661     | 0.03%  | 0.004% |
| 75  | 10.646 | 2967 | 2972 | 2973 | rBV  | 554    | 373     | 0.02%  | 0.002% |
| 76  | 10.797 | 3016 | 3019 | 3024 | rBV3 | 580    | 458     | 0.02%  | 0.003% |
| 77  | 10.842 | 3030 | 3033 | 3036 | rBV2 | 388    | 322     | 0.01%  | 0.002% |
| 78  | 10.913 | 3048 | 3055 | 3056 | rBV  | 461    | 509     | 0.02%  | 0.003% |
| 79  | 10.987 | 3068 | 3078 | 3093 | rVV3 | 11708  | 21679   | 0.92%  | 0.143% |
| 80  | 11.099 | 3110 | 3113 | 3118 | rVB3 | 441    | 312     | 0.01%  | 0.002% |
| 81  | 11.144 | 3118 | 3127 | 3139 | rBV4 | 6061   | 11130   | 0.47%  | 0.073% |
| 82  | 11.234 | 3149 | 3155 | 3161 | rBV4 | 484    | 551     | 0.02%  | 0.004% |
| 83  | 11.289 | 3169 | 3172 | 3177 | rBV3 | 393    | 297     | 0.01%  | 0.002% |
| 84  | 11.334 | 3182 | 3186 | 3189 | rBV2 | 585    | 429     | 0.02%  | 0.003% |
| 85  | 11.353 | 3189 | 3192 | 3195 | rVB2 | 636    | 423     | 0.02%  | 0.003% |
| 86  | 11.376 | 3195 | 3199 | 3203 | rBV2 | 818    | 825     | 0.04%  | 0.005% |
| 87  | 11.466 | 3211 | 3227 | 3247 | rBV  | 634618 | 1022923 | 43.52% | 6.737% |
| 88  | 11.842 | 3331 | 3344 | 3365 | rBV  | 674033 | 1082970 | 46.08% | 7.132% |
| 89  | 11.939 | 3372 | 3374 | 3381 | rVB6 | 1337   | 1032    | 0.04%  | 0.007% |
| 90  | 12.180 | 3445 | 3449 | 3452 | rBV4 | 705    | 588     | 0.03%  | 0.004% |
| 91  | 12.225 | 3461 | 3463 | 3466 | rBV3 | 599    | 309     | 0.01%  | 0.002% |
| 92  | 12.572 | 3567 | 3571 | 3577 | rVB4 | 625    | 584     | 0.02%  | 0.004% |
| 93  | 12.646 | 3591 | 3594 | 3599 | rBV4 | 459    | 377     | 0.02%  | 0.002% |
| 94  | 13.054 | 3718 | 3721 | 3723 | rBV2 | 483    | 310     | 0.01%  | 0.002% |
| 95  | 13.160 | 3751 | 3754 | 3759 | rVB2 | 640    | 475     | 0.02%  | 0.003% |
| 96  | 14.009 | 4016 | 4018 | 4022 | rBV3 | 450    | 363     | 0.02%  | 0.002% |
| 97  | 14.697 | 4230 | 4232 | 4235 | rBV2 | 503    | 303     | 0.01%  | 0.002% |
| 98  | 14.717 | 4235 | 4238 | 4243 | rVV4 | 719    | 729     | 0.03%  | 0.005% |
| 99  | 14.816 | 4267 | 4269 | 4273 | rBV3 | 629    | 369     | 0.02%  | 0.002% |
| 100 | 15.096 | 4354 | 4356 | 4358 | rBV3 | 807    | 425     | 0.02%  | 0.003% |

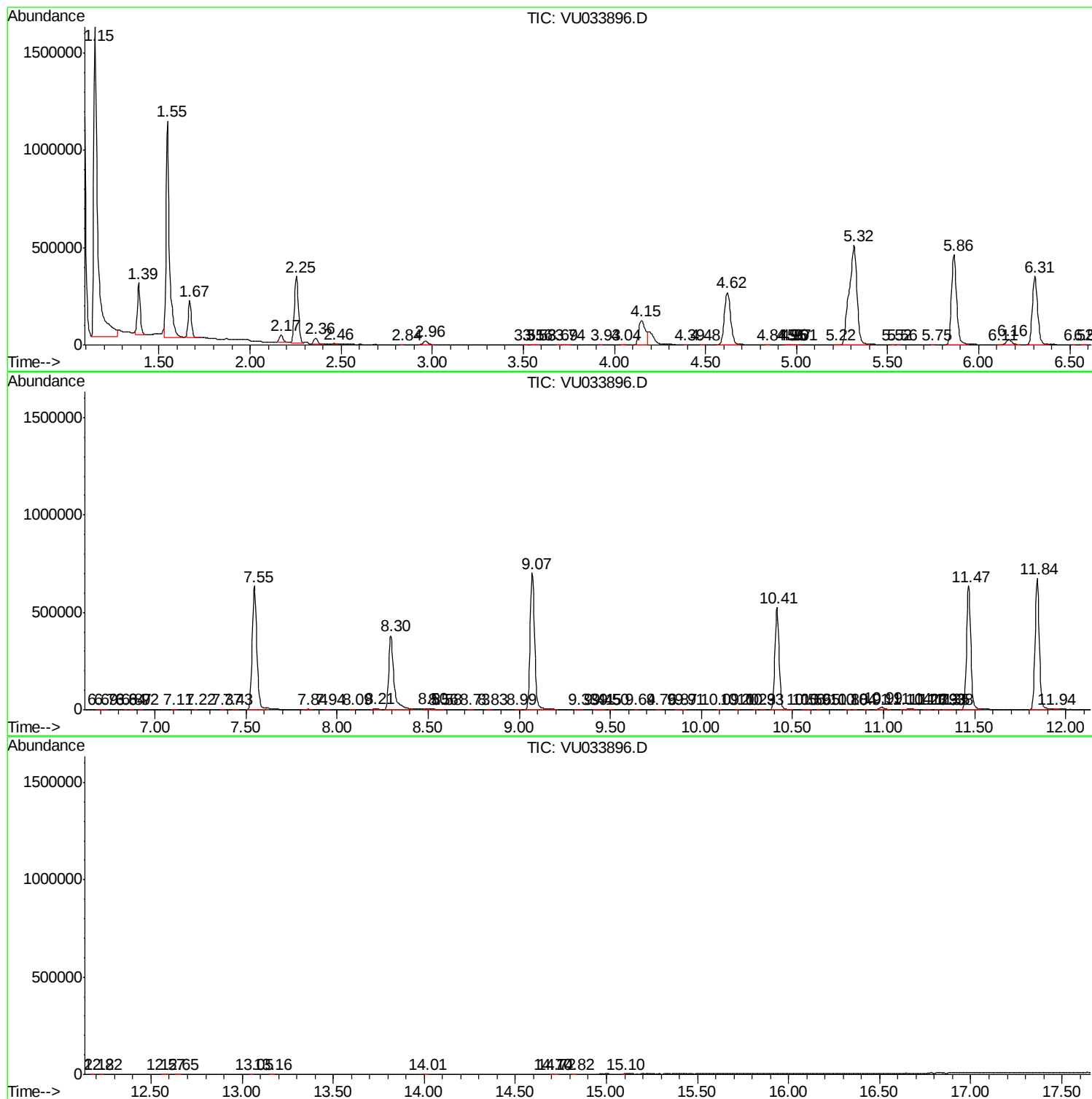
Sum of corrected areas: 15184590

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM081619WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU082119\  
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM081619WMA.M  
Quant Title : VOC Analysis

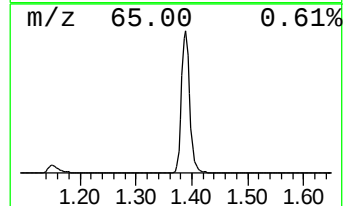
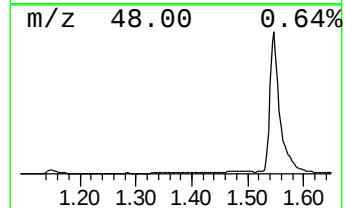
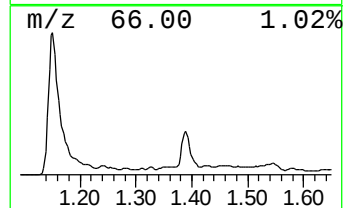
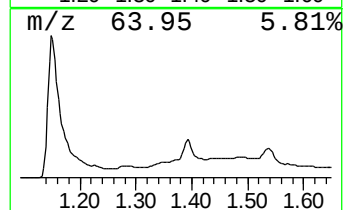
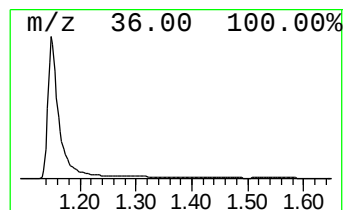
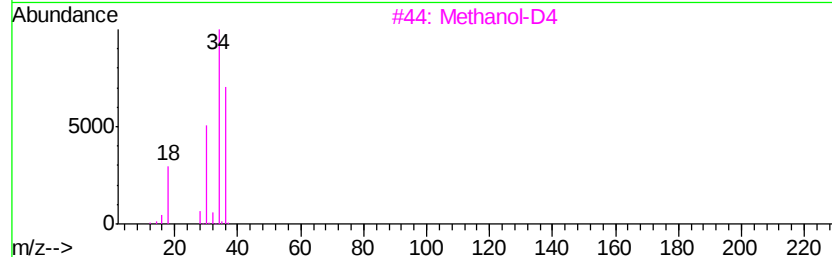
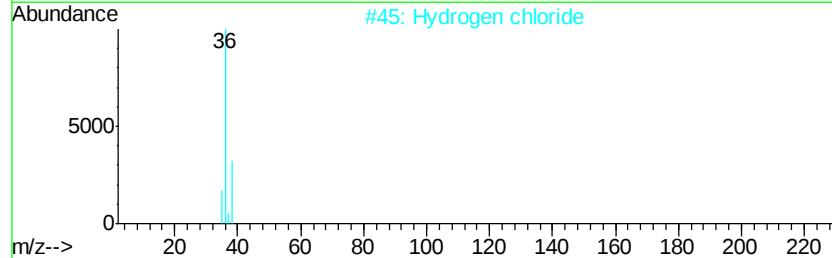
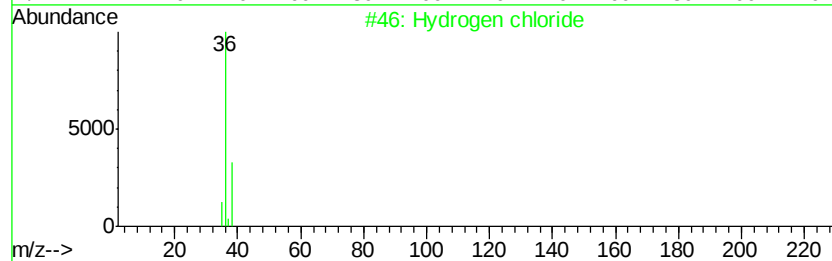
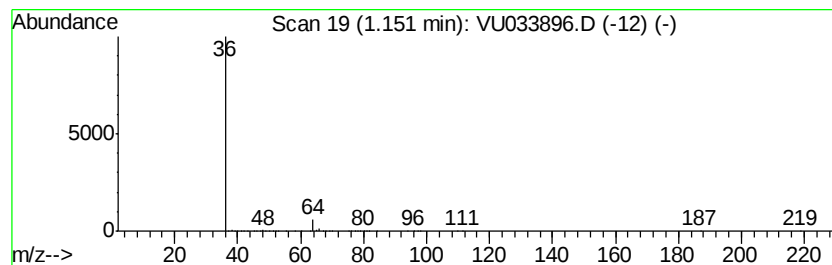
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown-01 Concentration Rank 1

| R.T. | EstConc     | Area    | Relative to ISTD    | R.T. |
|------|-------------|---------|---------------------|------|
| 1.15 | 128.37 ug/L | 2350300 | 1,4-Difluorobenzene | 5.86 |

| Hit# | of | Tentative ID       | MW | MolForm | CAS#        | Qual |
|------|----|--------------------|----|---------|-------------|------|
| 1    | 5  | Hydrogen chloride  | 36 | ClH     | 007647-01-0 | 2    |
| 2    |    | Hydrogen chloride  | 36 | ClH     | 007647-01-0 | 2    |
| 3    |    | Methanol-D4        | 36 | CD4O    | 000811-98-3 | 2    |
| 4    |    | Ammonium Chloride  | 53 | ClH4N   | 012125-02-9 | 1    |
| 5    |    | 2-Chloroethylamine | 79 | C2H6ClN | 000689-98-5 | 1    |



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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM081619WMA.M  
Quant Title : VOC Analysis

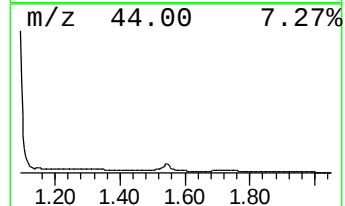
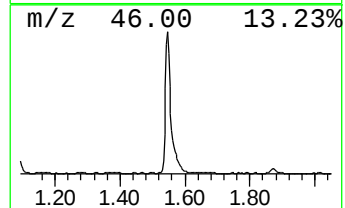
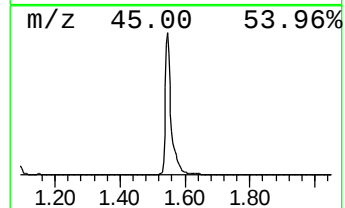
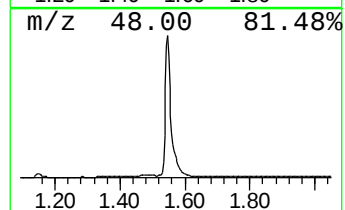
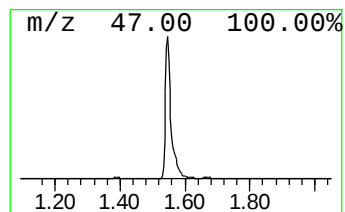
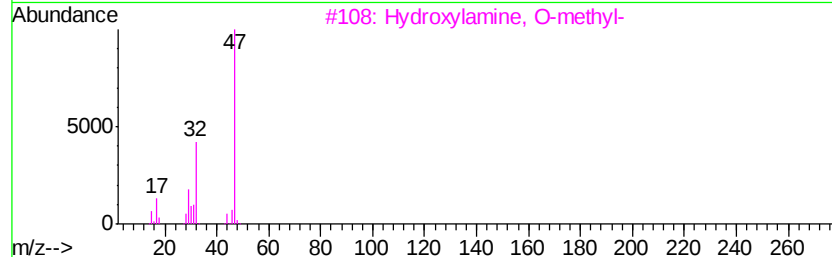
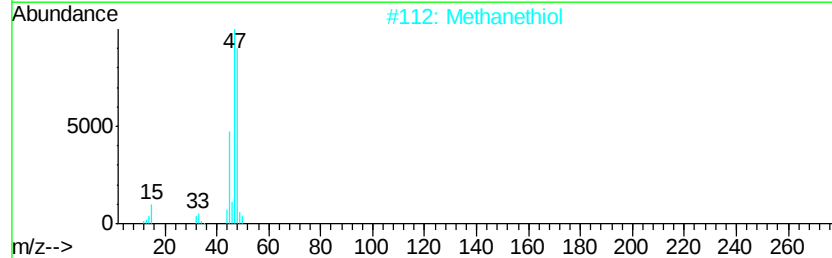
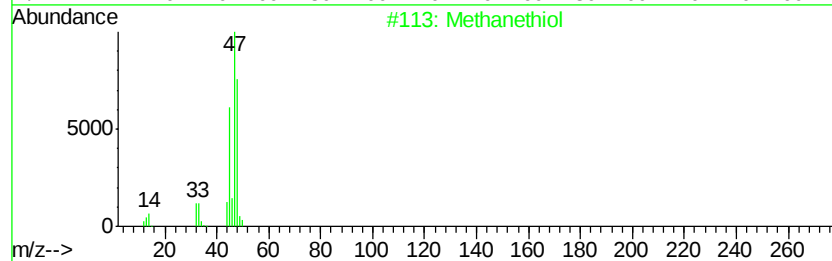
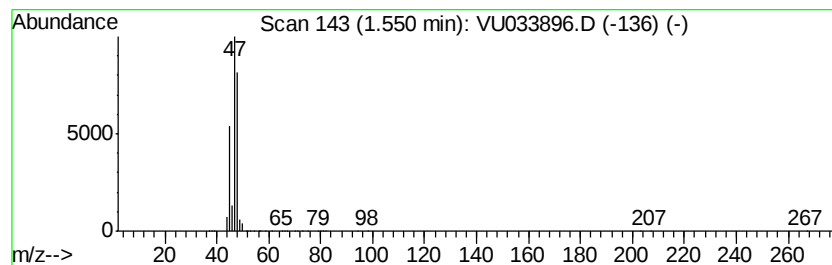
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Methanethiol Concentration Rank 2

| R.T. | EstConc    | Area    | Relative to ISTD    | R.T. |
|------|------------|---------|---------------------|------|
| 1.55 | 76.50 ug/L | 1400760 | 1,4-Difluorobenzene | 5.86 |

| Hit# | of | Tentative ID             | MW | MolForm | CAS#        | Qual |
|------|----|--------------------------|----|---------|-------------|------|
| 1    | 5  | Methanethiol             | 48 | CH4S    | 000074-93-1 | 91   |
| 2    |    | Methanethiol             | 48 | CH4S    | 000074-93-1 | 90   |
| 3    |    | Hvdroxylamine, O-methyl- | 47 | CH5NO   | 000067-62-9 | 7    |
| 4    |    | Hvdroxylamine, O-methyl- | 47 | CH5NO   | 000067-62-9 | 7    |
| 5    |    | Methane, nitroso-        | 45 | CH3NO   | 000865-40-7 | 5    |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU082119\  
Data File : VU033896.D  
Acq On : 22 Aug 2019 00:53  
Operator : JC/SP  
Sample : K4454-06  
Misc : 5.0mL/MSVOA U/WATER  
ALS Vial : 36 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F2B91

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM081619WMA.M  
Quant Title : VOC Analysis

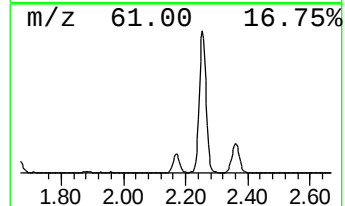
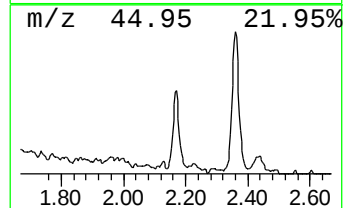
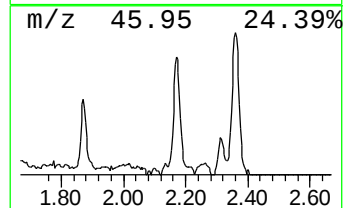
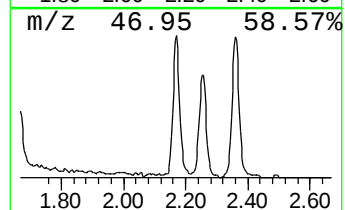
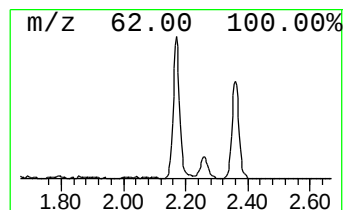
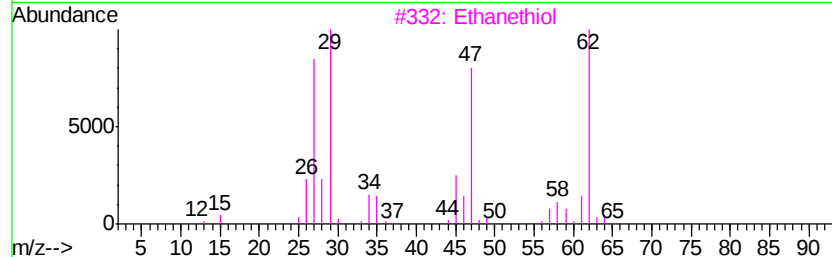
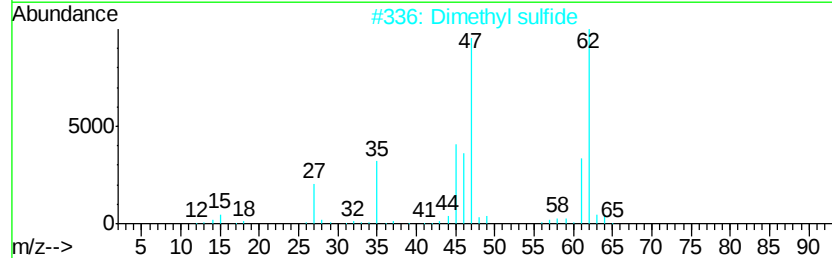
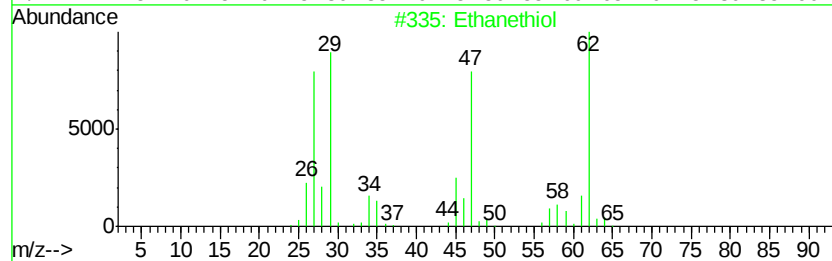
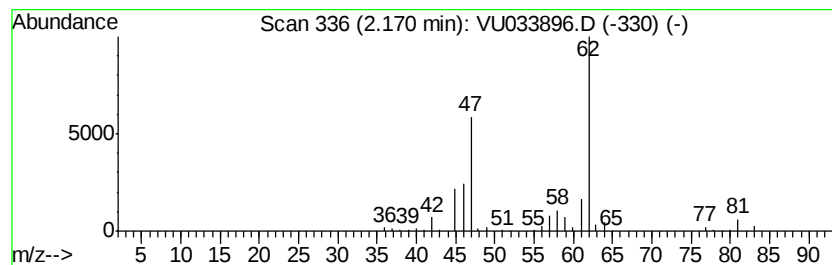
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 Ethanethiol Concentration Rank 3

| R.T. | EstConc   | Area  | Relative to ISTD    | R.T. |
|------|-----------|-------|---------------------|------|
| 2.17 | 2.95 ug/L | 53962 | 1,4-Difluorobenzene | 5.86 |

| Hit# | of | Tentative ID     | MW | MolForm | CAS#        | Qual |
|------|----|------------------|----|---------|-------------|------|
| 1    | 5  | Ethanethiol      | 62 | C2H6S   | 000075-08-1 | 91   |
| 2    |    | Dimethyl sulfide | 62 | C2H6S   | 000075-18-3 | 83   |
| 3    |    | Ethanethiol      | 62 | C2H6S   | 000075-08-1 | 83   |
| 4    |    | Ethanethiol      | 62 | C2H6S   | 000075-08-1 | 78   |
| 5    |    | Dimethyl sulfide | 62 | C2H6S   | 000075-18-3 | 74   |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU082119\  
Data File : VU033896.D  
Acq On : 22 Aug 2019 00:53  
Operator : JC/SP  
Sample : K4454-06  
Misc : 5.0mL/MSVOA U/WATER  
ALS Vial : 36 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F2B91

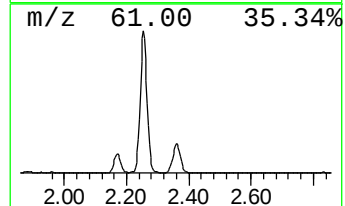
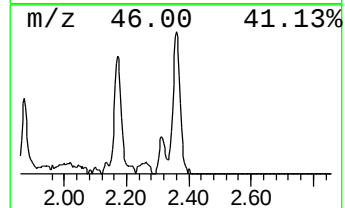
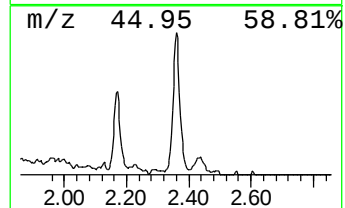
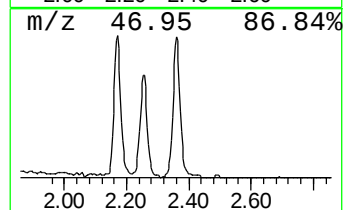
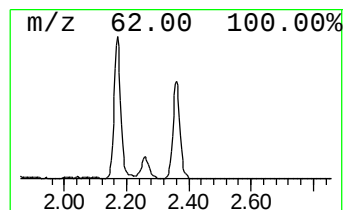
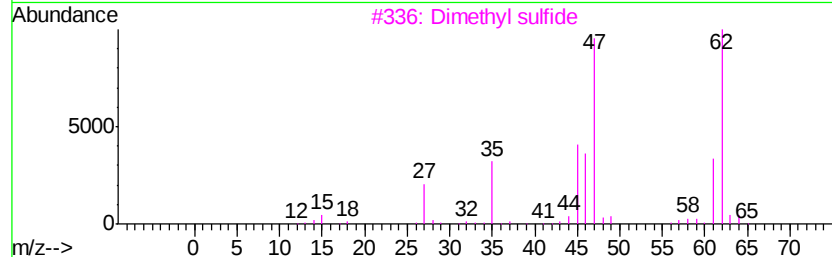
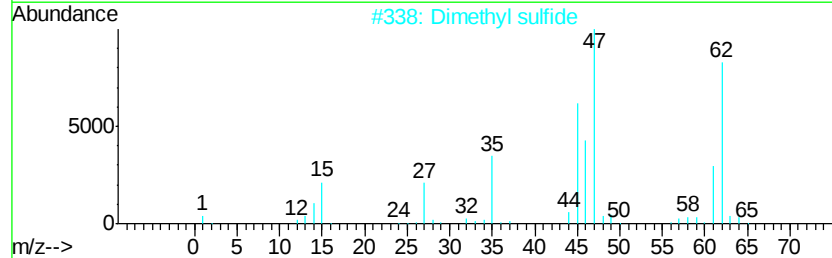
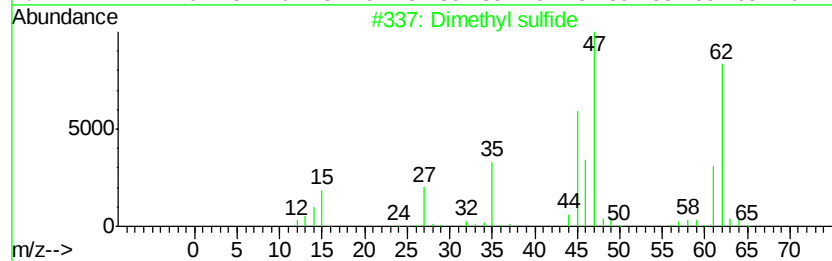
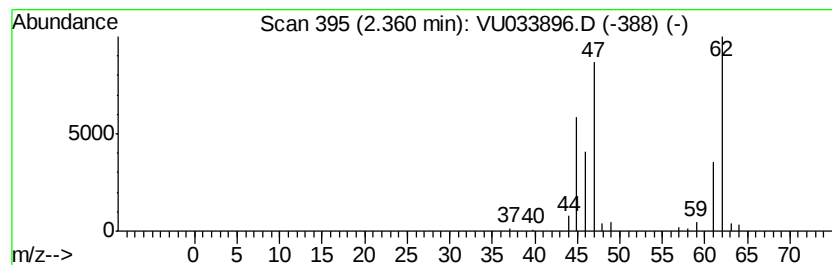
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM081619WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Dimethyl sulfide Concentration Rank 4

| R.T. | EstConc   | Area  | Relative to ISTD    | R.T. |
|------|-----------|-------|---------------------|------|
| 2.36 | 2.76 ug/L | 50607 | 1,4-Difluorobenzene | 5.86 |

| Hit# | of | Tentative ID                  | MW | MolForm | CAS#        | Qual |
|------|----|-------------------------------|----|---------|-------------|------|
| 1    | 5  | Dimethyl sulfide              | 62 | C2H6S   | 000075-18-3 | 94   |
| 2    |    | Dimethyl sulfide              | 62 | C2H6S   | 000075-18-3 | 91   |
| 3    |    | Dimethyl sulfide              | 62 | C2H6S   | 000075-18-3 | 91   |
| 4    |    | Borane-methyl sulfide complex | 76 | C2H9BS  | 013292-87-0 | 90   |
| 5    |    | Dimethyl sulfide              | 62 | C2H6S   | 000075-18-3 | 87   |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_U\DATA\VU082119\  
Data File : VU033896.D  
Acq On : 22 Aug 2019 00:53  
Operator : JC/SP  
Sample : K4454-06  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 36 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
F2B91

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM081619WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                  |      |         |       |          | #                     | RT   | Resp   | Conc |
| unknown-01       | 1.15 | 128.4   | ug/L  | 2350300  | 1                     | 5.86 | 915474 | 50.0 |
| Methanethiol     | 1.55 | 76.5    | ug/L  | 1400760  | 1                     | 5.86 | 915474 | 50.0 |
| Ethanethiol      | 2.17 | 3.0     | ug/L  | 53962    | 1                     | 5.86 | 915474 | 50.0 |
| Dimethyl sulfide | 2.36 | 2.8     | ug/L  | 50607    | 1                     | 5.86 | 915474 | 50.0 |