

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU120721\  
 Data File : VU046158.D  
 Acq On : 07 Dec 2021 22:33  
 Operator : SY/MD  
 Sample : M4960-06 10X  
 Misc : 6.25g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 42 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGKS1

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\_U\Method\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046168.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         | 1.601       | 74            | 81          | 93           | rVB      | 113110         | 125838        | 14.75%          | 1.804%        |
| 2         | 1.919       | 171           | 180         | 196          | rVB      | 80343          | 102608        | 12.03%          | 1.471%        |
| 3         | 2.215       | 267           | 272         | 276          | rVB2     | 406            | 383           | 0.04%           | 0.005%        |
| 4         | 2.340       | 308           | 311         | 317          | rVB2     | 250            | 265           | 0.03%           | 0.004%        |
| 5         | 2.572       | 369           | 383         | 413          | rBV      | 184698         | 310349        | 36.38%          | 4.449%        |
| 6         | 2.790       | 449           | 451         | 456          | rVB      | 194            | 174           | 0.02%           | 0.002%        |
| 7         | 2.935       | 494           | 496         | 499          | rBV      | 154            | 131           | 0.02%           | 0.002%        |
| 8         | 2.970       | 502           | 507         | 511          | rVB3     | 356            | 329           | 0.04%           | 0.005%        |
| 9         | 3.051       | 523           | 532         | 542          | rVB3     | 1638           | 2993          | 0.35%           | 0.043%        |
| 10        | 3.189       | 558           | 575         | 595          | rBV2     | 13315          | 32443         | 3.80%           | 0.465%        |
| 11        | 3.314       | 606           | 614         | 617          | rBB      | 211            | 282           | 0.03%           | 0.004%        |
| 12        | 3.340       | 617           | 622         | 627          | rBB      | 194            | 274           | 0.03%           | 0.004%        |
| 13        | 3.417       | 641           | 646         | 647          | rBV      | 153            | 132           | 0.02%           | 0.002%        |
| 14        | 3.491       | 667           | 669         | 676          | rBV      | 152            | 211           | 0.02%           | 0.003%        |
| 15        | 3.556       | 686           | 689         | 691          | rBV      | 142            | 121           | 0.01%           | 0.002%        |
| 16        | 3.639       | 711           | 715         | 719          | rBV      | 156            | 199           | 0.02%           | 0.003%        |
| 17        | 3.729       | 740           | 743         | 745          | rBV      | 178            | 146           | 0.02%           | 0.002%        |
| 18        | 3.900       | 793           | 796         | 798          | rBV      | 162            | 140           | 0.02%           | 0.002%        |
| 19        | 4.163       | 874           | 878         | 881          | rBB      | 159            | 156           | 0.02%           | 0.002%        |
| 20        | 4.301       | 917           | 921         | 927          | rBB      | 151            | 228           | 0.03%           | 0.003%        |
| 21        | 4.639       | 1010          | 1026        | 1068         | rBV      | 73744          | 229931        | 26.95%          | 3.296%        |
| 22        | 4.848       | 1088          | 1091        | 1095         | rVB2     | 360            | 310           | 0.04%           | 0.004%        |
| 23        | 4.871       | 1095          | 1098        | 1101         | rBV      | 328            | 291           | 0.03%           | 0.004%        |
| 24        | 4.906       | 1106          | 1109        | 1111         | rVV      | 225            | 131           | 0.02%           | 0.002%        |
| 25        | 5.067       | 1142          | 1159        | 1180         | rBV      | 141445         | 323869        | 37.96%          | 4.643%        |
| 26        | 5.199       | 1197          | 1200        | 1201         | rBV      | 243            | 140           | 0.02%           | 0.002%        |
| 27        | 5.289       | 1225          | 1228        | 1230         | rVB      | 230            | 151           | 0.02%           | 0.002%        |
| 28        | 5.388       | 1255          | 1259        | 1261         | rBB      | 191            | 157           | 0.02%           | 0.002%        |
| 29        | 5.449       | 1275          | 1278        | 1283         | rBV      | 169            | 215           | 0.03%           | 0.003%        |
| 30        | 5.543       | 1305          | 1307        | 1311         | rBV      | 141            | 146           | 0.02%           | 0.002%        |
| 31        | 5.594       | 1319          | 1323        | 1327         | rBV      | 171            | 221           | 0.03%           | 0.003%        |
| 32        | 5.729       | 1342          | 1365        | 1386         | rVV2     | 318570         | 853170        | 100.00%         | 12.231%       |
| 33        | 5.970       | 1436          | 1440        | 1443         | rBV2     | 686            | 731           | 0.09%           | 0.010%        |
| 34        | 6.121       | 1484          | 1487        | 1493         | rBV2     | 299            | 321           | 0.04%           | 0.005%        |
| 35        | 6.250       | 1512          | 1527        | 1555         | rBV      | 284950         | 543382        | 63.69%          | 7.790%        |
| 36        | 6.420       | 1577          | 1580        | 1583         | rVV2     | 232            | 172           | 0.02%           | 0.002%        |

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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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\_U\Method\SFAMULM112921WMA.M  
 Title : VOC Analysis

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 37 | 6.436  | 1583 | 1585 | 1588 | rVB  | 242    | 159    | 0.02%  | 0.002%  |
| 38 | 6.459  | 1589 | 1592 | 1595 | rBB2 | 255    | 185    | 0.02%  | 0.003%  |
| 39 | 6.530  | 1605 | 1614 | 1631 | rVV4 | 4156   | 8371   | 0.98%  | 0.120%  |
| 40 | 6.633  | 1642 | 1646 | 1649 | rBV  | 181    | 202    | 0.02%  | 0.003%  |
| 41 | 6.694  | 1649 | 1665 | 1687 | rVV  | 191280 | 367751 | 43.10% | 5.272%  |
| 42 | 6.864  | 1715 | 1718 | 1721 | rBV  | 165    | 161    | 0.02%  | 0.002%  |
| 43 | 7.044  | 1769 | 1774 | 1777 | rBV2 | 243    | 261    | 0.03%  | 0.004%  |
| 44 | 7.182  | 1814 | 1817 | 1820 | rBV2 | 216    | 160    | 0.02%  | 0.002%  |
| 45 | 7.279  | 1845 | 1847 | 1851 | rBV  | 121    | 133    | 0.02%  | 0.002%  |
| 46 | 7.417  | 1887 | 1890 | 1893 | rBB  | 142    | 119    | 0.01%  | 0.002%  |
| 47 | 7.494  | 1910 | 1914 | 1917 | rBV  | 154    | 182    | 0.02%  | 0.003%  |
| 48 | 7.568  | 1923 | 1937 | 1954 | rBV  | 109052 | 188482 | 22.09% | 2.702%  |
| 49 | 7.684  | 1969 | 1973 | 1980 | rVB2 | 415    | 487    | 0.06%  | 0.007%  |
| 50 | 7.790  | 1997 | 2006 | 2014 | rBV2 | 1426   | 2320   | 0.27%  | 0.033%  |
| 51 | 7.899  | 2025 | 2040 | 2056 | rBV  | 415440 | 715697 | 83.89% | 10.260% |
| 52 | 8.179  | 2116 | 2127 | 2145 | rBV  | 74524  | 122998 | 14.42% | 1.763%  |
| 53 | 8.247  | 2145 | 2148 | 2151 | rVV2 | 369    | 300    | 0.04%  | 0.004%  |
| 54 | 8.395  | 2191 | 2194 | 2196 | rBV  | 157    | 132    | 0.02%  | 0.002%  |
| 55 | 8.452  | 2209 | 2212 | 2216 | rBV  | 114    | 126    | 0.01%  | 0.002%  |
| 56 | 8.475  | 2216 | 2219 | 2222 | rVV2 | 199    | 147    | 0.02%  | 0.002%  |
| 57 | 8.636  | 2256 | 2269 | 2301 | rBV  | 242669 | 453429 | 53.15% | 6.500%  |
| 58 | 8.915  | 2348 | 2356 | 2367 | rBV4 | 2528   | 4103   | 0.48%  | 0.059%  |
| 59 | 9.263  | 2459 | 2464 | 2465 | rBV  | 197    | 199    | 0.02%  | 0.003%  |
| 60 | 9.330  | 2479 | 2485 | 2488 | rBV  | 165    | 247    | 0.03%  | 0.004%  |
| 61 | 9.417  | 2499 | 2512 | 2538 | rBV  | 407021 | 673359 | 78.92% | 9.653%  |
| 62 | 9.568  | 2555 | 2559 | 2561 | rBV2 | 259    | 226    | 0.03%  | 0.003%  |
| 63 | 9.690  | 2593 | 2597 | 2605 | rBV2 | 767    | 988    | 0.12%  | 0.014%  |
| 64 | 9.803  | 2628 | 2632 | 2634 | rBV2 | 231    | 189    | 0.02%  | 0.003%  |
| 65 | 9.909  | 2661 | 2665 | 2670 | rVB  | 161    | 138    | 0.02%  | 0.002%  |
| 66 | 9.983  | 2679 | 2688 | 2692 | rBV  | 109    | 187    | 0.02%  | 0.003%  |
| 67 | 10.063 | 2709 | 2713 | 2718 | rVB2 | 147    | 140    | 0.02%  | 0.002%  |
| 68 | 10.671 | 2895 | 2902 | 2909 | rVB3 | 2579   | 3290   | 0.39%  | 0.047%  |
| 69 | 10.758 | 2917 | 2929 | 2947 | rVB  | 281557 | 451636 | 52.94% | 6.475%  |
| 70 | 10.838 | 2950 | 2954 | 2957 | rBV  | 208    | 151    | 0.02%  | 0.002%  |
| 71 | 10.867 | 2958 | 2963 | 2967 | rBV3 | 293    | 282    | 0.03%  | 0.004%  |
| 72 | 10.922 | 2977 | 2980 | 2981 | rBV  | 234    | 152    | 0.02%  | 0.002%  |
| 73 | 11.095 | 3029 | 3034 | 3037 | rBV2 | 192    | 229    | 0.03%  | 0.003%  |
| 74 | 11.115 | 3037 | 3040 | 3042 | rBV2 | 412    | 281    | 0.03%  | 0.004%  |
| 75 | 11.208 | 3066 | 3069 | 3072 | rBV  | 266    | 146    | 0.02%  | 0.002%  |
| 76 | 11.375 | 3119 | 3121 | 3127 | rVB2 | 204    | 208    | 0.02%  | 0.003%  |

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 BGKS1

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\_U\Method\SFAMULM112921WMA.M  
 Title : VOC Analysis

|     |        |      |      |      |      |        |        |        |         |
|-----|--------|------|------|------|------|--------|--------|--------|---------|
| 77  | 11.456 | 3139 | 3146 | 3157 | rVB3 | 1757   | 2977   | 0.35%  | 0.043%  |
| 78  | 11.578 | 3180 | 3184 | 3189 | rVV  | 369    | 325    | 0.04%  | 0.005%  |
| 79  | 11.693 | 3214 | 3220 | 3227 | rVV4 | 1025   | 1230   | 0.14%  | 0.018%  |
| 80  | 11.812 | 3244 | 3257 | 3276 | rBV  | 477939 | 740205 | 86.76% | 10.611% |
| 81  | 11.935 | 3287 | 3295 | 3297 | rBV2 | 594    | 628    | 0.07%  | 0.009%  |
| 82  | 11.973 | 3302 | 3307 | 3316 | rVB3 | 1957   | 2643   | 0.31%  | 0.038%  |
| 83  | 12.195 | 3360 | 3376 | 3395 | rBV  | 427634 | 692763 | 81.20% | 9.931%  |
| 84  | 12.330 | 3413 | 3418 | 3422 | rBV3 | 404    | 371    | 0.04%  | 0.005%  |
| 85  | 12.639 | 3507 | 3514 | 3520 | rBV2 | 330    | 401    | 0.05%  | 0.006%  |
| 86  | 13.057 | 3641 | 3644 | 3649 | rBV  | 206    | 153    | 0.02%  | 0.002%  |
| 87  | 13.144 | 3669 | 3671 | 3673 | rVV  | 322    | 201    | 0.02%  | 0.003%  |
| 88  | 13.156 | 3673 | 3675 | 3678 | rVB  | 388    | 218    | 0.03%  | 0.003%  |
| 89  | 13.279 | 3710 | 3713 | 3718 | rBV  | 130    | 132    | 0.02%  | 0.002%  |
| 90  | 14.092 | 3960 | 3966 | 3970 | rBV2 | 411    | 506    | 0.06%  | 0.007%  |
| 91  | 14.491 | 4088 | 4090 | 4098 | rVB  | 282    | 256    | 0.03%  | 0.004%  |
| 92  | 14.578 | 4108 | 4117 | 4123 | rBV2 | 1292   | 1975   | 0.23%  | 0.028%  |
| 93  | 14.780 | 4178 | 4180 | 4183 | rBV2 | 250    | 140    | 0.02%  | 0.002%  |
| 94  | 14.841 | 4195 | 4199 | 4203 | rBV2 | 216    | 218    | 0.03%  | 0.003%  |
| 95  | 14.918 | 4219 | 4223 | 4227 | rBV2 | 277    | 258    | 0.03%  | 0.004%  |
| 96  | 15.053 | 4262 | 4265 | 4271 | rVB2 | 325    | 316    | 0.04%  | 0.005%  |
| 97  | 15.150 | 4292 | 4295 | 4297 | rBV2 | 180    | 121    | 0.01%  | 0.002%  |
| 98  | 15.330 | 4344 | 4351 | 4354 | rBV  | 353    | 505    | 0.06%  | 0.007%  |
| 99  | 15.947 | 4540 | 4543 | 4545 | rBV2 | 309    | 178    | 0.02%  | 0.003%  |
| 100 | 16.356 | 4668 | 4670 | 4672 | rBV2 | 362    | 189    | 0.02%  | 0.003%  |

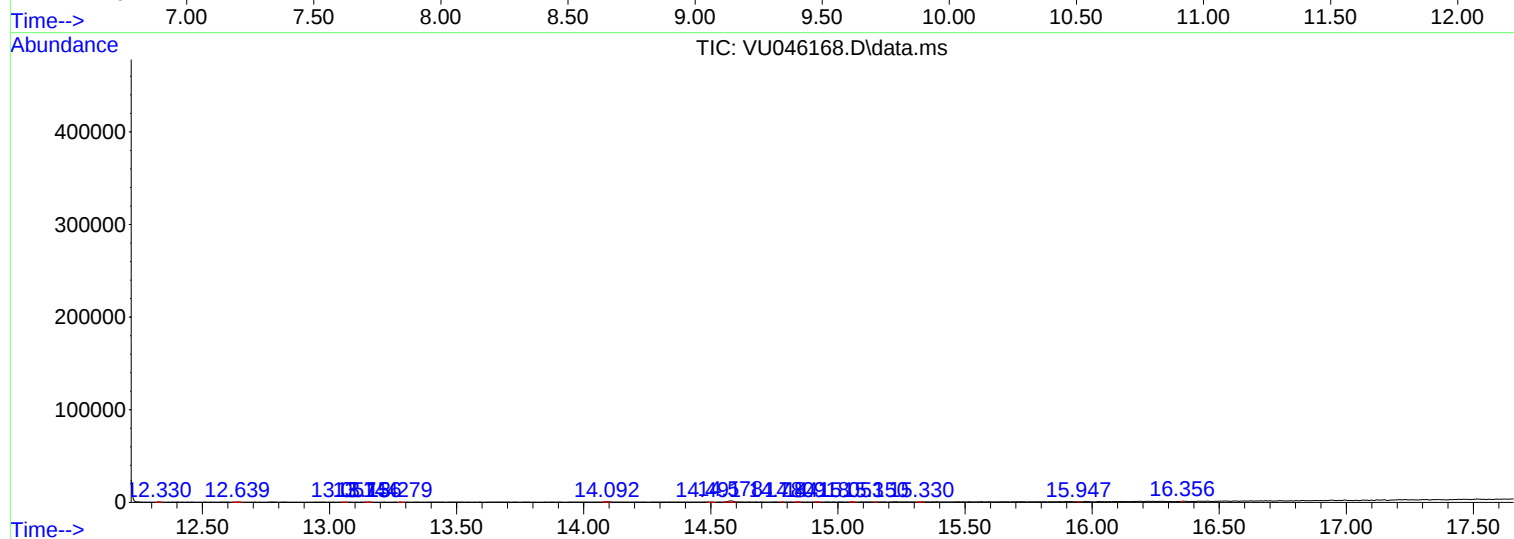
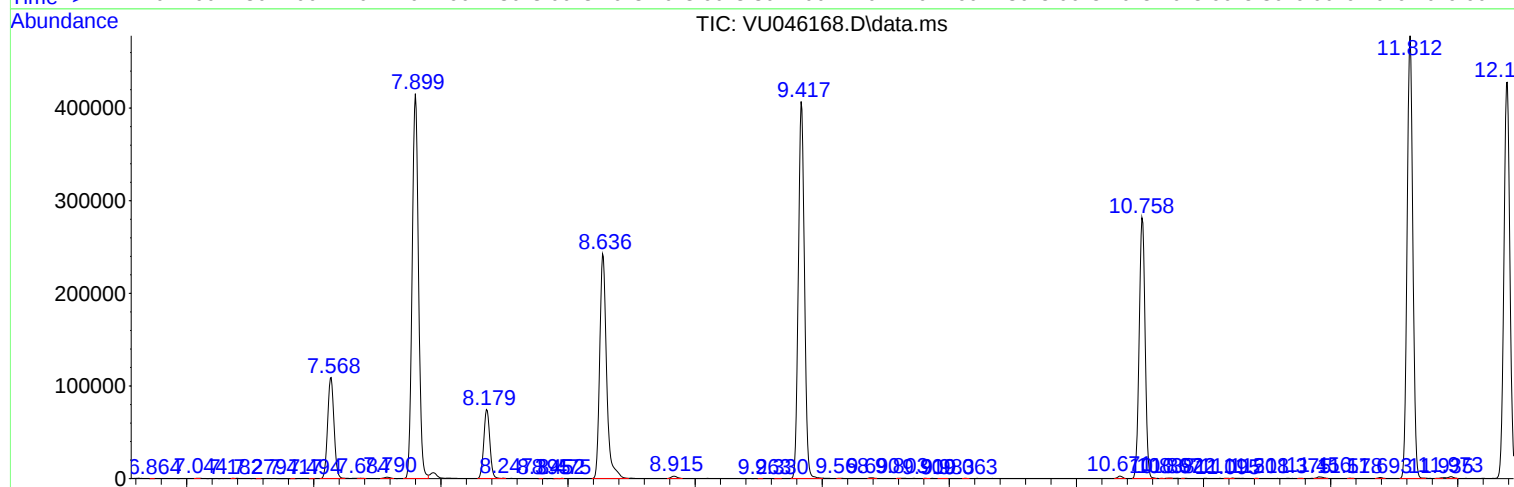
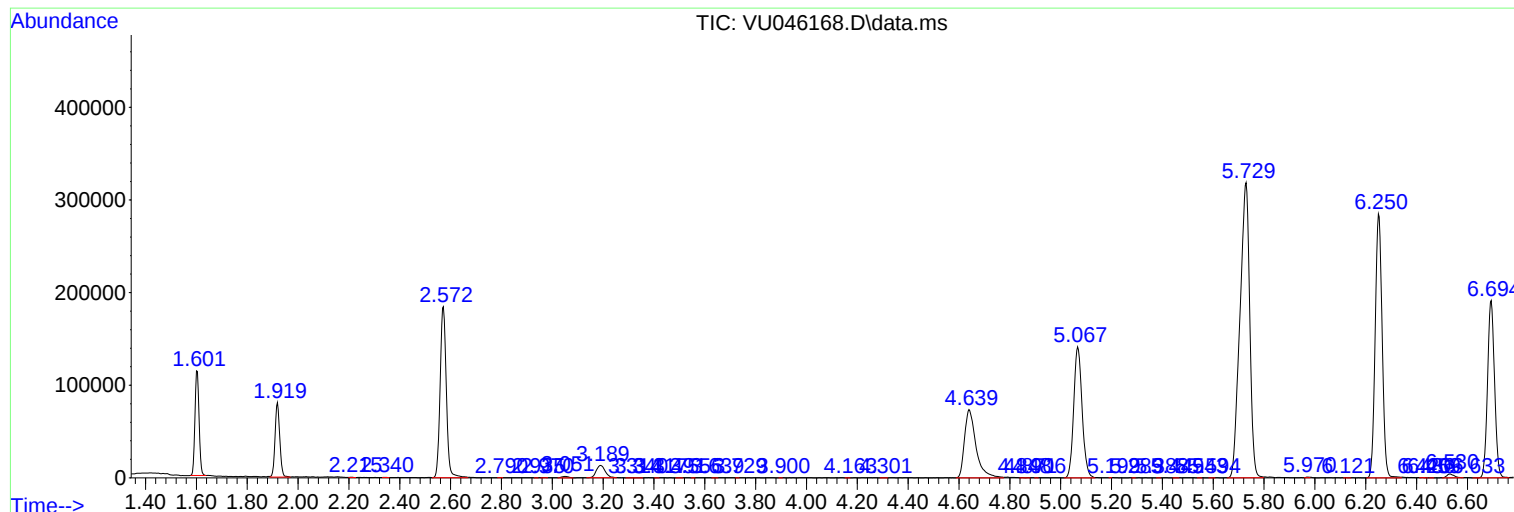
Sum of corrected areas: 6975602

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Instrument :  
MSVOA\_U  
ClientSampleId :  
BGKS1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
Quant Title : VOC Analysis

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



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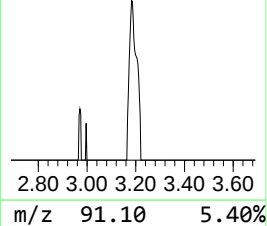
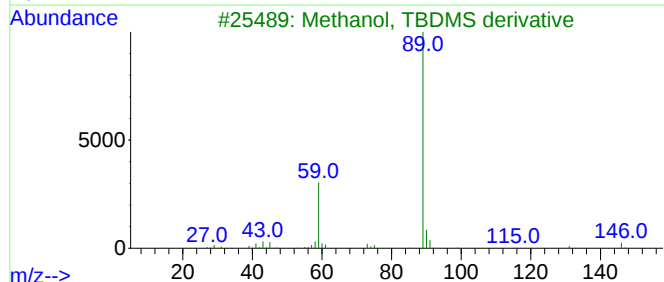
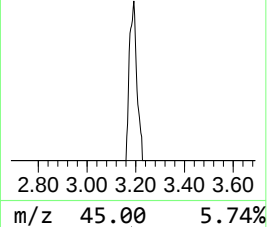
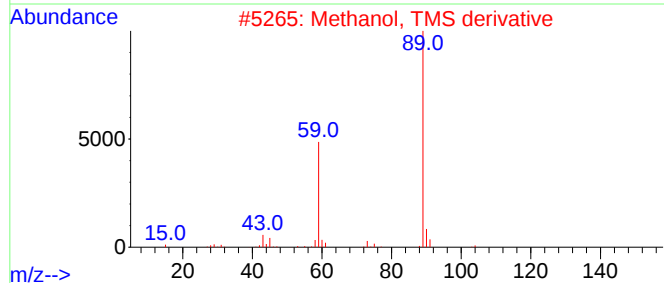
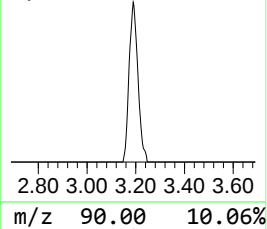
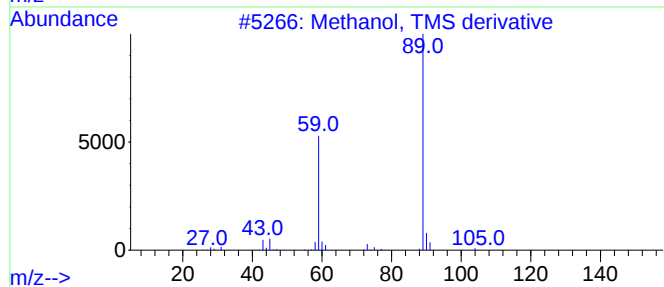
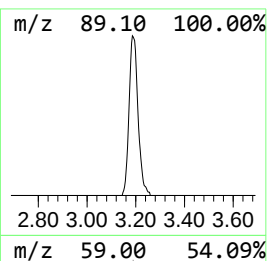
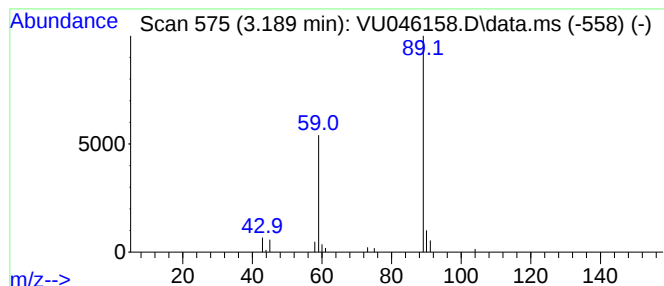
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM112921WMA.M  
Quant Title : VOC Analysis

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

\*\*\*\*\*  
Peak Number 1 Methanol, TMS derivative Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD    | R.T.  |
|-------|-----------|-------|---------------------|-------|
| 3.189 | 2.99 ug/L | 32443 | 1,4-Difluorobenzene | 6.250 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm  | CAS#         | Qual |
|------|----|---|------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Methanol, TMS derivative           | 104 | C4H12OSi | 001825-61-2  | 91   |
| 2    |    |   | Methanol, TMS derivative           | 104 | C4H12OSi | 001825-61-2  | 90   |
| 3    |    |   | Methanol, TBDMS derivative         | 146 | C7H18OSi | 1000364-10-7 | 83   |
| 4    |    |   | Ethyl(dimethyl)methoxysilane       | 118 | C5H14OSi | 052686-75-6  | 74   |
| 5    |    |   | Silane, (2-methoxyethyl)trimethyl- | 132 | C6H16OSi | 018173-63-2  | 64   |



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| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| Methanol, TMS d... | 3.189 | 3.0     | ug/L  | 32443    | 1                     | 6.250 | 543382 | 50.0 |