

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV052720\  
 Data File : VV016245.D  
 Acq On : 27 May 2020 22:34  
 Operator : SY/MD  
 Sample : L2766-02  
 Misc : 25.0mL/MSVOA V/WATER  
 ALS Vial : 33 Sample Multiplier: 1

Instrument :  
 MSVOA\_V  
 ClientSampleId :  
 BE4Y6

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % 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\_V\METHOD\SOMVTR052620WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

| 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         | 1.222       | 36            | 41          | 54           | rVB3     | 9726           | 11190         | 2.16%           | 0.288%        |
| 2         | 1.306       | 59            | 67          | 79           | rBV2     | 62336          | 97664         | 18.89%          | 2.513%        |
| 3         | 1.399       | 88            | 96          | 108          | rVB      | 13063          | 17764         | 3.44%           | 0.457%        |
| 4         | 1.582       | 145           | 153         | 166          | rBV      | 37567          | 45431         | 8.78%           | 1.169%        |
| 5         | 2.126       | 311           | 322         | 335          | rBV      | 70057          | 103539        | 20.02%          | 2.664%        |
| 6         | 2.209       | 335           | 348         | 368          | rVV      | 25466          | 74304         | 14.37%          | 1.912%        |
| 7         | 2.749       | 487           | 516         | 521          | rBV4     | 25576          | 102480        | 19.82%          | 2.637%        |
| 8         | 2.978       | 580           | 587         | 598          | rVB6     | 3499           | 6743          | 1.30%           | 0.173%        |
| 9         | 3.717       | 797           | 817         | 845          | rBV      | 191922         | 517146        | 100.00%         | 13.306%       |
| 10        | 3.936       | 872           | 885         | 905          | rBV2     | 36412          | 116843        | 22.59%          | 3.006%        |
| 11        | 4.380       | 1007          | 1023        | 1045         | rBV      | 54016          | 134479        | 26.00%          | 3.460%        |
| 12        | 4.704       | 1109          | 1124        | 1136         | rBV7     | 3470           | 9034          | 1.75%           | 0.232%        |
| 13        | 5.074       | 1223          | 1239        | 1262         | rBV2     | 121504         | 295121        | 57.07%          | 7.593%        |
| 14        | 5.643       | 1402          | 1416        | 1436         | rBV      | 115595         | 235333        | 45.51%          | 6.055%        |
| 15        | 5.817       | 1461          | 1470        | 1485         | rBV3     | 5403           | 12791         | 2.47%           | 0.329%        |
| 16        | 6.097       | 1542          | 1557        | 1573         | rBV2     | 71017          | 142580        | 27.57%          | 3.668%        |
| 17        | 6.563       | 1687          | 1702        | 1710         | rBV      | 165748         | 336857        | 65.14%          | 8.667%        |
| 18        | 7.010       | 1830          | 1841        | 1859         | rBV2     | 32420          | 58129         | 11.24%          | 1.496%        |
| 19        | 7.338       | 1932          | 1943        | 1959         | rBV      | 145466         | 250500        | 48.44%          | 6.445%        |
| 20        | 7.415       | 1959          | 1967        | 1983         | rVB3     | 9492           | 17773         | 3.44%           | 0.457%        |
| 21        | 7.646       | 2028          | 2039        | 2054         | rBV3     | 20109          | 35398         | 6.84%           | 0.911%        |
| 22        | 8.116       | 2175          | 2185        | 2222         | rBV      | 159039         | 306652        | 59.30%          | 7.890%        |
| 23        | 8.270       | 2224          | 2233        | 2243         | rVV6     | 5269           | 9341          | 1.81%           | 0.240%        |
| 24        | 8.875       | 2409          | 2421        | 2444         | rBV      | 180223         | 291456        | 56.36%          | 7.499%        |
| 25        | 9.833       | 2709          | 2719        | 2735         | rBV5     | 5179           | 9464          | 1.83%           | 0.243%        |
| 26        | 9.920       | 2735          | 2746        | 2758         | rVB2     | 3720           | 7493          | 1.45%           | 0.193%        |
| 27        | 10.238      | 2834          | 2845        | 2858         | rBV      | 51249          | 77497         | 14.99%          | 1.994%        |
| 28        | 11.270      | 3156          | 3166        | 3184         | rVB      | 177829         | 286129        | 55.33%          | 7.362%        |
| 29        | 11.646      | 3272          | 3283        | 3301         | rVB      | 141576         | 217229        | 42.01%          | 5.589%        |
| 30        | 13.527      | 3858          | 3868        | 3882         | rBV      | 18871          | 28819         | 5.57%           | 0.741%        |
| 31        | 13.778      | 3935          | 3946        | 3960         | rBV2     | 20097          | 31475         | 6.09%           | 0.810%        |

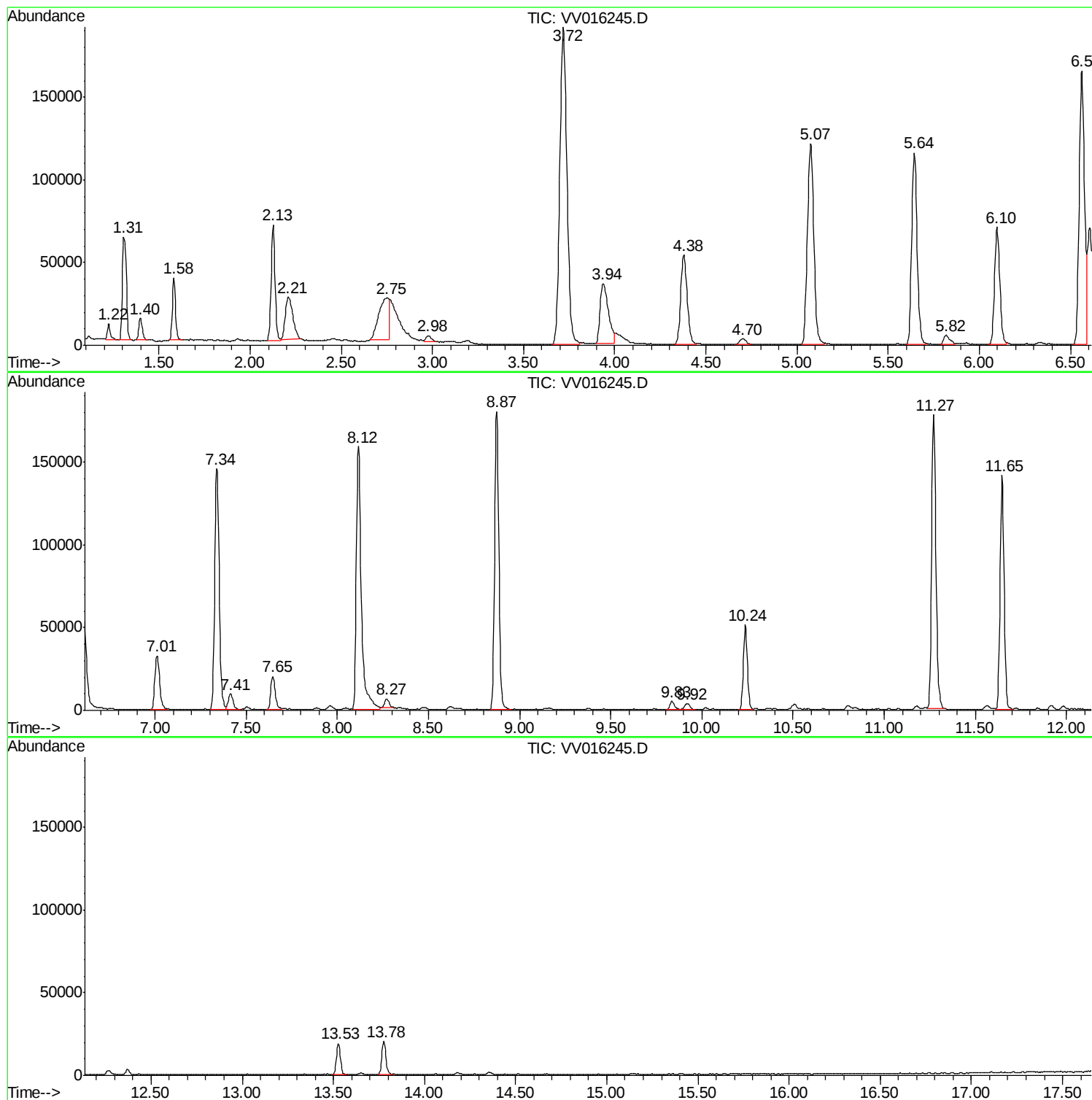
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MSVOA\_V  
ClientSampleId :  
BE4Y6

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_V\METHOD\SOMVTR052620WMA.M  
Quant Title : TRACE VOA SOM01.0

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



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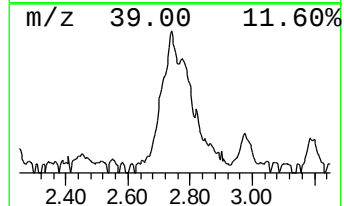
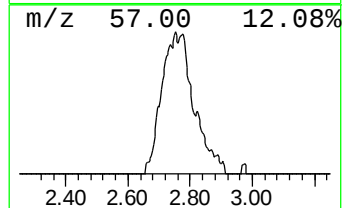
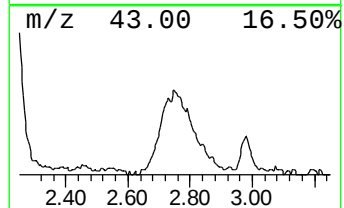
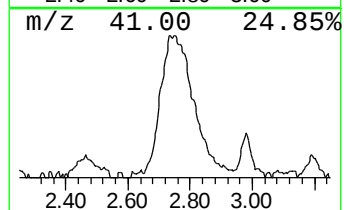
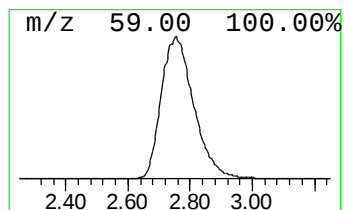
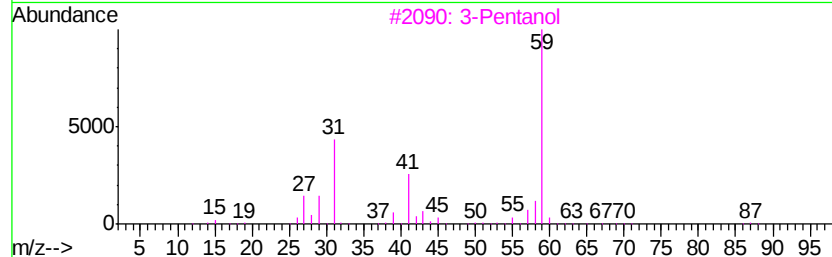
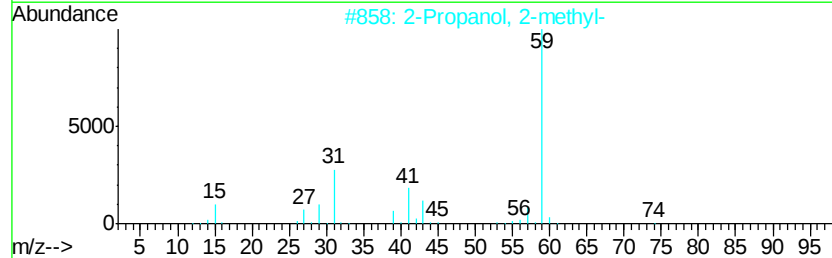
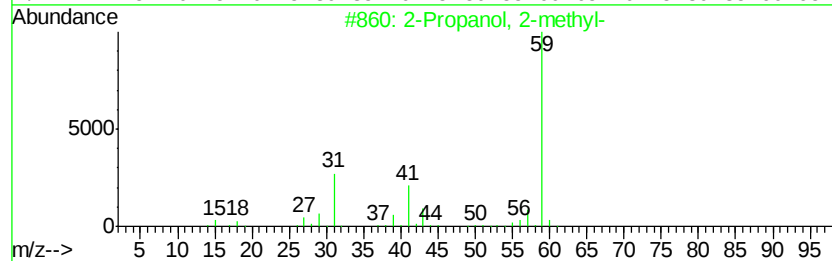
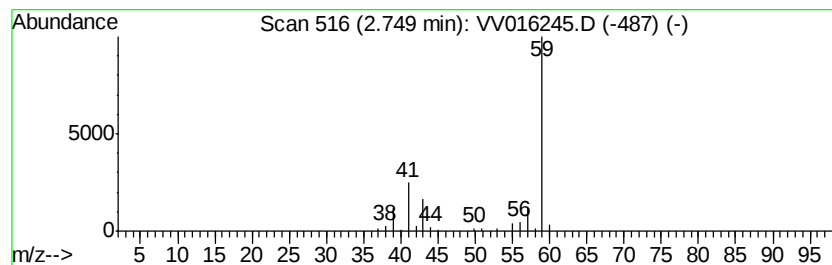
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_V\METHOD\SOMVTR052620WMA.M  
Quant Title : TRACE VOA SOM01.0

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

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Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 3

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 2.75 | 2.18 ug/L | 102480 | 1,4-Difluorobenzene | 5.64 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Propanol, 2-methyl-               | 74  | C4H10O  | 000075-65-0 | 78   |
| 2    |    |   | 2-Propanol, 2-methyl-               | 74  | C4H10O  | 000075-65-0 | 40   |
| 3    |    |   | 3-Pentanol                          | 88  | C5H12O  | 000584-02-1 | 40   |
| 4    |    |   | Propanoic acid, 2-hydroxy-2-methyl- | 104 | C4H8O3  | 000594-61-6 | 38   |
| 5    |    |   | Guanidine                           | 59  | CH5N3   | 000113-00-8 | 9    |



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MSVOA\_V  
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BE4Y6

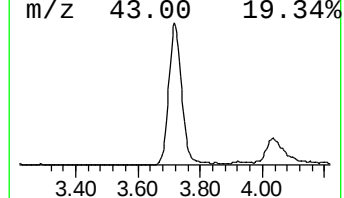
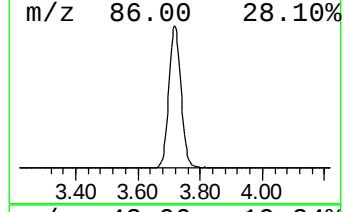
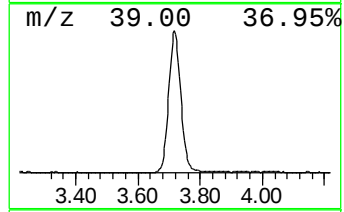
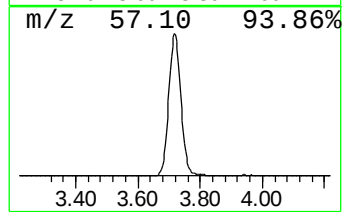
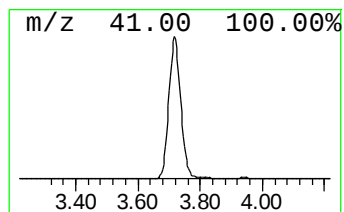
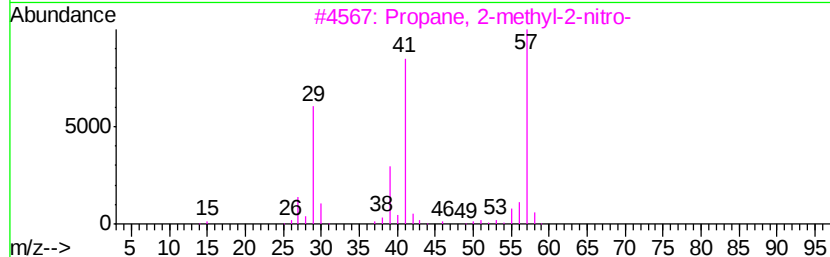
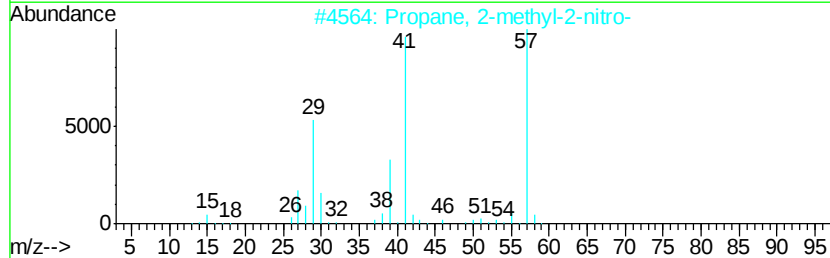
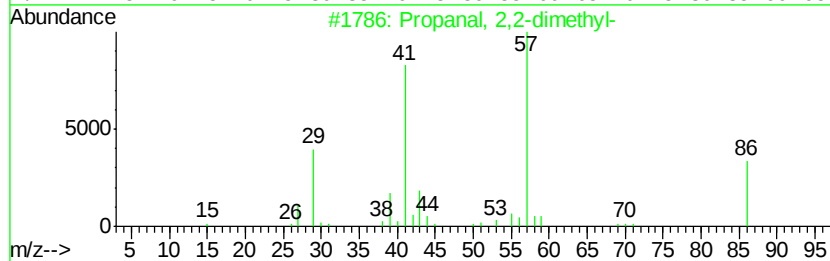
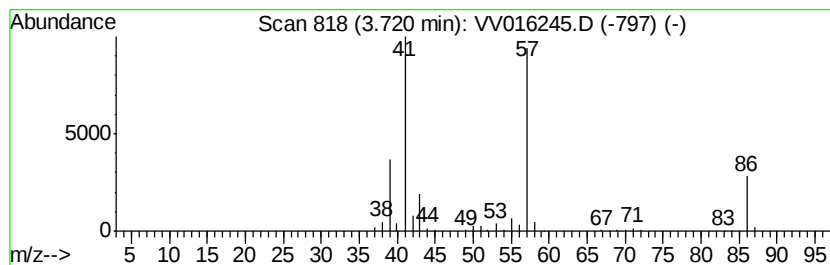
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_V\METHOD\SOMVTR052620WMA.M  
Quant Title : TRACE VOA SOM01.0

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

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Peak Number 2 Propanal, 2,2-dimethyl- Concentration Rank 1

| R.T. | EstConc    | Area   | Relative to ISTD    | R.T. |
|------|------------|--------|---------------------|------|
| 3.72 | 10.99 ug/L | 517146 | 1,4-Difluorobenzene | 5.64 |

| Hit# | of | Tentative ID               | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------------|-----|---------|-------------|------|
| 1    | 5  | Propanal, 2,2-dimethyl-    | 86  | C5H10O  | 000630-19-3 | 58   |
| 2    |    | Propane, 2-methyl-2-nitro- | 103 | C4H9NO2 | 000594-70-7 | 45   |
| 3    |    | Propane, 2-methyl-2-nitro- | 103 | C4H9NO2 | 000594-70-7 | 43   |
| 4    |    | Butane, 2-nitro-           | 103 | C4H9NO2 | 000600-24-8 | 40   |
| 5    |    | 3-Pentanone                | 86  | C5H10O  | 000096-22-0 | 40   |



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ALS Vial : 33 Sample Multiplier: 1

Instrument :  
MSVOA\_V  
ClientSampleId :  
BE4Y6

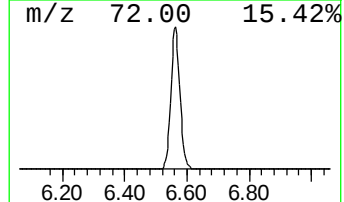
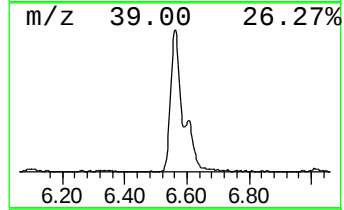
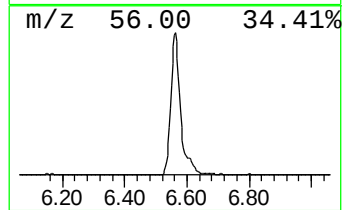
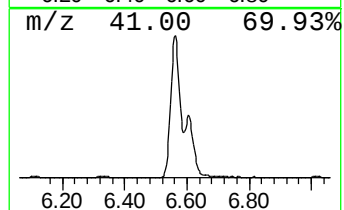
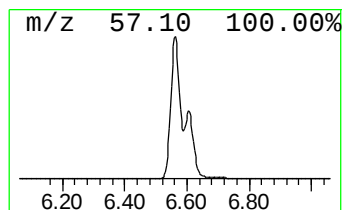
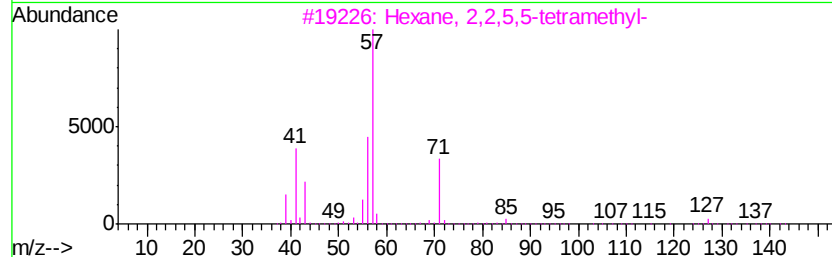
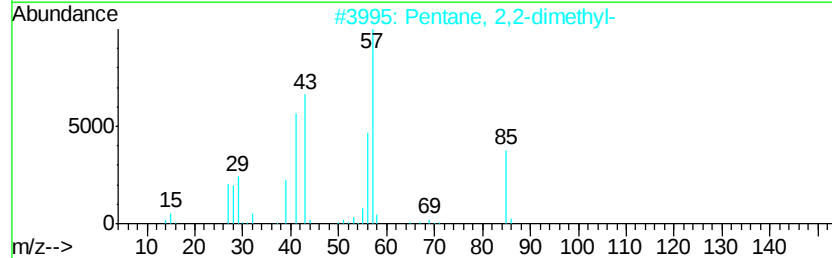
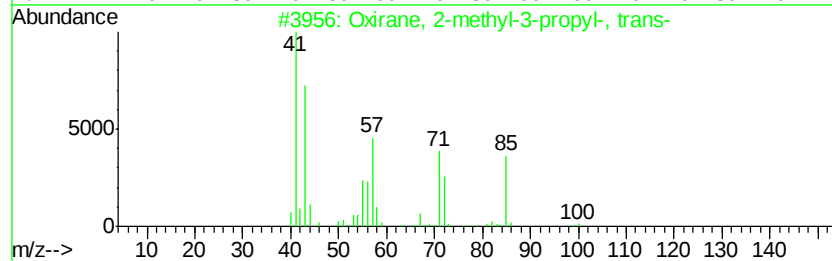
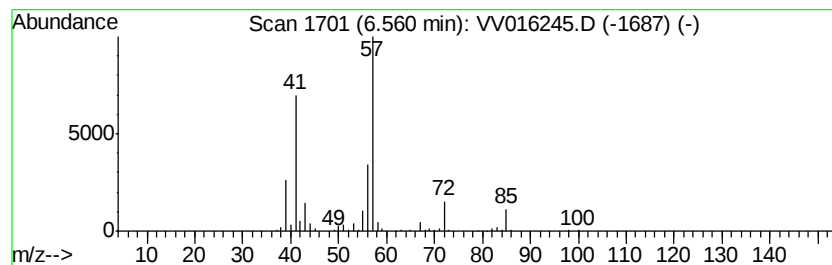
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_V\METHOD\SOMVTR052620WMA.M  
Quant Title : TRACE VOA SOM01.0

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

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Peak Number 3 unknown-01 Concentration Rank 2

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 6.56 | 7.16 ug/L | 336857 | 1,4-Difluorobenzene | 5.64 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Oxirane, 2-methyl-3-propyl-, trans- | 100 | C6H12O  | 006124-91-0 | 43   |
| 2    |    | Pentane, 2,2-dimethyl-              | 100 | C7H16   | 000590-35-2 | 42   |
| 3    |    | Hexane, 2,2,5,5-tetramethyl-        | 142 | C10H22  | 001071-81-4 | 40   |
| 4    |    | 1-Butanol, 3,3-dimethyl-            | 102 | C6H14O  | 000624-95-3 | 40   |
| 5    |    | Butane, 2,2,3,3-tetramethyl-        | 114 | C8H18   | 000594-82-1 | 37   |



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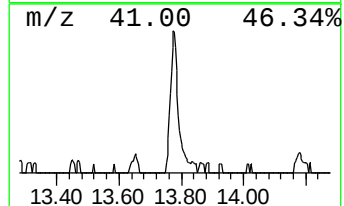
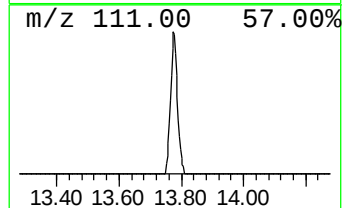
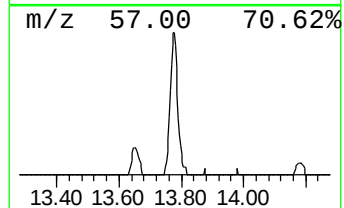
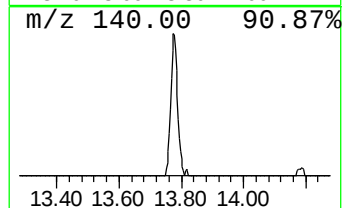
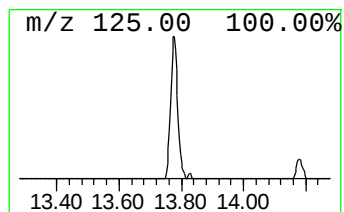
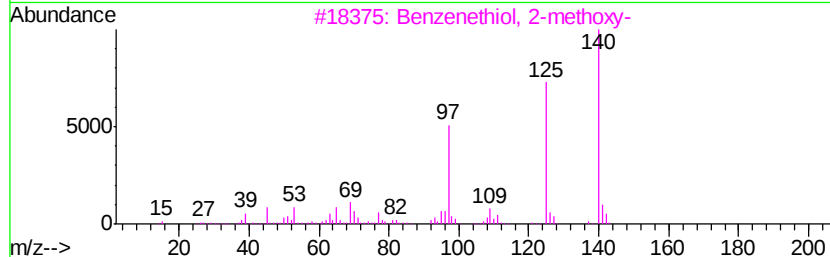
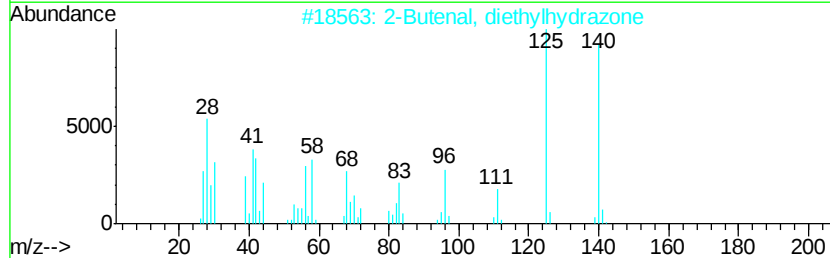
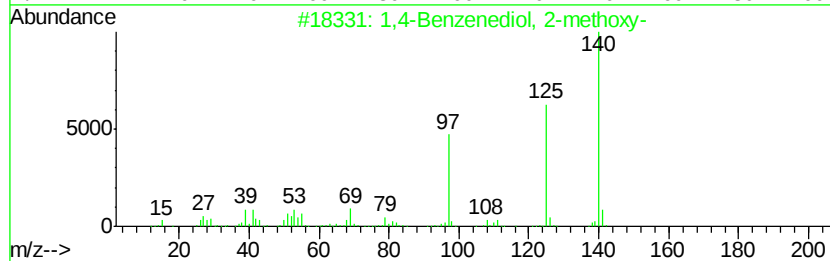
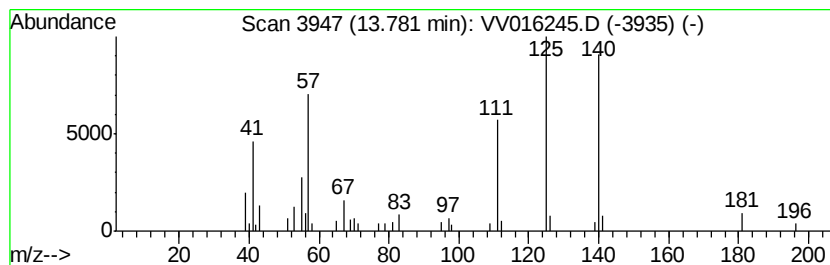
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 1,4-Benzenediol, 2-methoxy- Concentration Rank 5

| R.T.  | EstConc   | Area  | Relative to ISTD       | R.T.  |
|-------|-----------|-------|------------------------|-------|
| 13.78 | 0.55 ug/L | 31475 | 1,4-Dichlorobenzene-d4 | 11.27 |

| Hit# | of | Tentative ID                | MW  | MolForm  | CAS#        | Qual |
|------|----|-----------------------------|-----|----------|-------------|------|
| 1    | 5  | 1,4-Benzenediol, 2-methoxy- | 140 | C7H8O3   | 000824-46-4 | 59   |
| 2    |    | 2-Butenal, diethylhydrazone | 140 | C8H16N2  | 025186-07-6 | 59   |
| 3    |    | Benzenethiol, 2-methoxy-    | 140 | C7H8OS   | 007217-59-6 | 59   |
| 4    |    | Uracil, 5-ethyl-            | 140 | C6H8N2O2 | 004212-49-1 | 59   |
| 5    |    | Benzenethiol, 4-methoxy-    | 140 | C7H8OS   | 000696-63-9 | 59   |



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Quant Title : TRACE VOA SOM01.0

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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Propanol, 2-met... | 2.75  | 2.2     | ug/L  | 102480   | 1                     | 5.64  | 235333 | 5.0  |
| Propanal, 2,2-dim... | 3.72  | 11.0    | ug/L  | 517146   | 1                     | 5.64  | 235333 | 5.0  |
| unknown-01           | 6.56  | 7.2     | ug/L  | 336857   | 1                     | 5.64  | 235333 | 5.0  |
| 1,4-Benzenediol, ... | 13.78 | 0.6     | ug/L  | 31475    | 3                     | 11.27 | 286129 | 5.0  |