

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU050720\  
 Data File : VU038050.D  
 Acq On : 07 May 2020 19:41  
 Operator : JC/MD  
 Sample : L2527-13  
 Misc : 25.0mL/MSVOA U/WATER  
 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFSK0

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\_U\METHOD\SOMUTR050720WMA.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         | 1.369       | 3             | 9           | 23           | rBV      | 112313         | 117970        | 7.85%           | 0.850%        |
| 2         | 1.610       | 74            | 84          | 98           | rBV      | 220449         | 245538        | 16.34%          | 1.769%        |
| 3         | 1.928       | 175           | 183         | 194          | rVB      | 168616         | 216002        | 14.37%          | 1.556%        |
| 4         | 2.591       | 376           | 389         | 401          | rBV      | 291934         | 474723        | 31.59%          | 3.421%        |
| 5         | 2.655       | 401           | 409         | 427          | rVB      | 21076          | 36540         | 2.43%           | 0.263%        |
| 6         | 2.784       | 436           | 449         | 469          | rBV      | 59486          | 114732        | 7.64%           | 0.827%        |
| 7         | 3.215       | 569           | 583         | 602          | rVB      | 21568          | 48604         | 3.23%           | 0.350%        |
| 8         | 3.395       | 623           | 639         | 655          | rBV3     | 20621          | 48301         | 3.21%           | 0.348%        |
| 9         | 3.732       | 729           | 744         | 761          | rBV3     | 28196          | 65666         | 4.37%           | 0.473%        |
| 10        | 4.565       | 989           | 1003        | 1019         | rBV2     | 25196          | 61331         | 4.08%           | 0.442%        |
| 11        | 4.665       | 1019          | 1034        | 1077         | rBV3     | 283670         | 787971        | 52.44%          | 5.678%        |
| 12        | 4.845       | 1077          | 1090        | 1106         | rVB      | 62530          | 133359        | 8.87%           | 0.961%        |
| 13        | 5.099       | 1153          | 1169        | 1194         | rBV3     | 272981         | 682817        | 45.44%          | 4.920%        |
| 14        | 5.423       | 1256          | 1270        | 1288         | rVB3     | 24893          | 54152         | 3.60%           | 0.390%        |
| 15        | 5.758       | 1351          | 1374        | 1399         | rBV2     | 520888         | 1342930       | 89.37%          | 9.676%        |
| 16        | 6.279       | 1522          | 1536        | 1569         | rBV      | 457559         | 872165        | 58.04%          | 6.284%        |
| 17        | 6.571       | 1609          | 1627        | 1644         | rBV      | 360099         | 678728        | 45.17%          | 4.891%        |
| 18        | 6.719       | 1658          | 1673        | 1690         | rBV      | 327120         | 634070        | 42.20%          | 4.569%        |
| 19        | 7.066       | 1769          | 1781        | 1797         | rBV2     | 53139          | 95671         | 6.37%           | 0.689%        |
| 20        | 7.591       | 1932          | 1944        | 1964         | rBV      | 167122         | 289797        | 19.29%          | 2.088%        |
| 21        | 7.922       | 2033          | 2047        | 2084         | rBV      | 644423         | 1164985       | 77.53%          | 8.394%        |
| 22        | 8.201       | 2121          | 2134        | 2150         | rBV      | 102303         | 173373        | 11.54%          | 1.249%        |
| 23        | 8.574       | 2238          | 2250        | 2262         | rBV      | 167888         | 290452        | 19.33%          | 2.093%        |
| 24        | 8.655       | 2262          | 2275        | 2309         | rVV      | 802781         | 1502645       | 100.00%         | 10.827%       |
| 25        | 9.436       | 2505          | 2518        | 2554         | rVB      | 644163         | 1108517       | 73.77%          | 7.987%        |
| 26        | 10.771      | 2920          | 2933        | 2956         | rBV      | 226532         | 364540        | 24.26%          | 2.627%        |
| 27        | 11.825      | 3248          | 3261        | 3279         | rVB      | 668776         | 1054541       | 70.18%          | 7.598%        |
| 28        | 12.205      | 3363          | 3379        | 3395         | rBV      | 608995         | 971967        | 64.68%          | 7.003%        |
| 29        | 17.378      | 4976          | 4988        | 5001         | rBV2     | 133101         | 246247        | 16.39%          | 1.774%        |

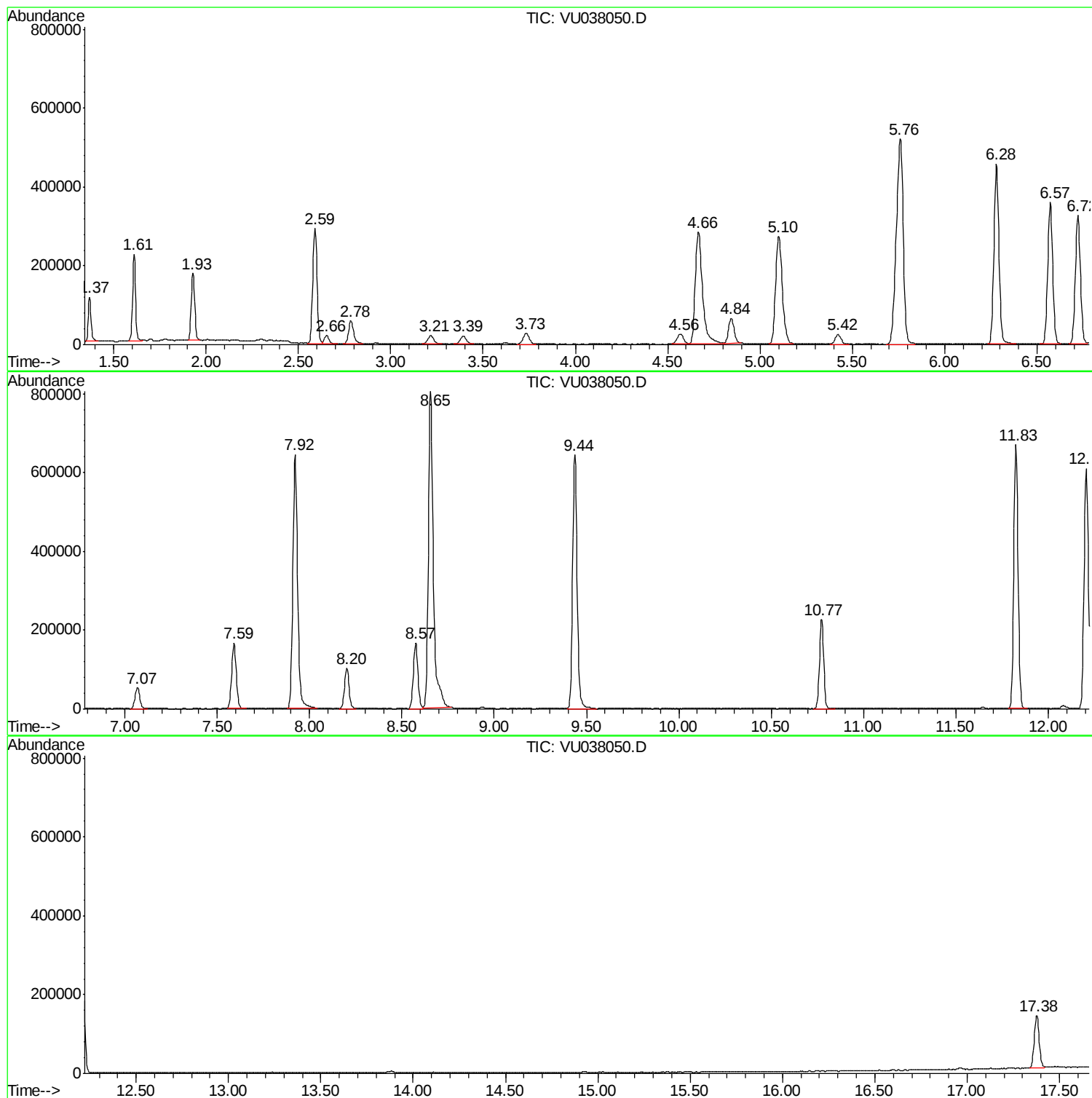
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR050720WMA.M  
Quant Title : TRACE VOA SOM01.0

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



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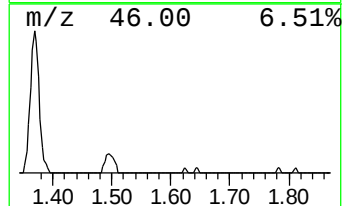
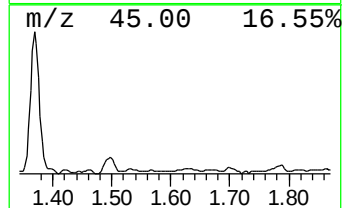
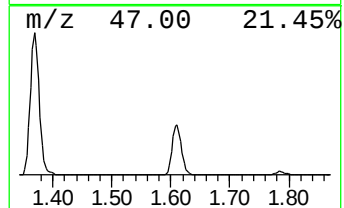
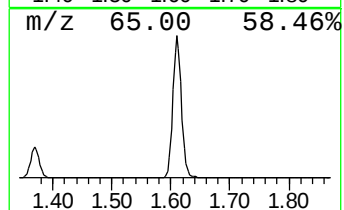
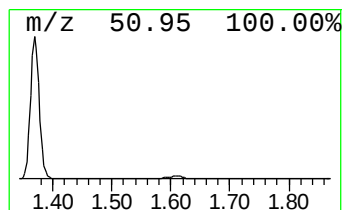
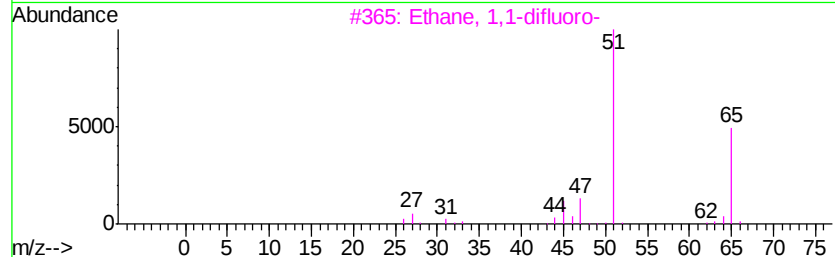
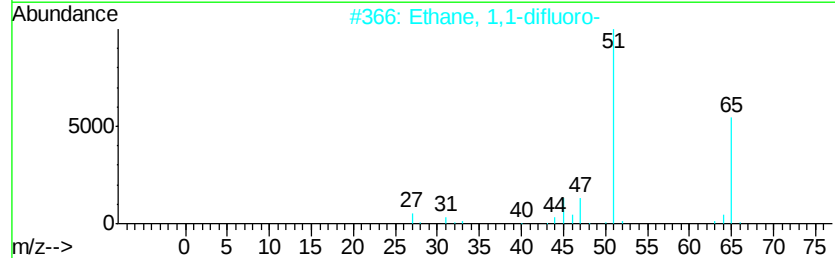
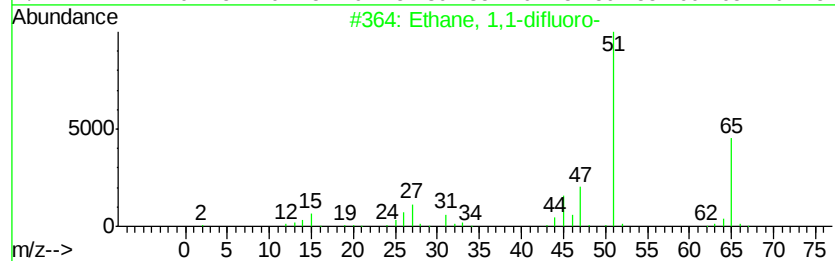
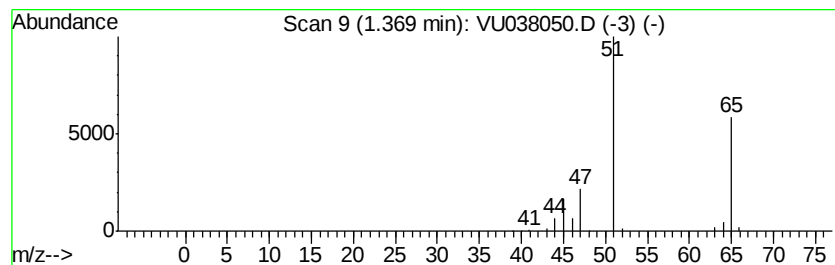
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Quant Title : TRACE VOA SOM01.0

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

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Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 4

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 1.37 | 0.68 ug/L | 117970 | 1,4-Difluorobenzene | 6.28 |

| Hit# | of | 5 | Tentative ID           | MW | MolForm | CAS#        | Qual |
|------|----|---|------------------------|----|---------|-------------|------|
| 1    |    |   | Ethane, 1,1-difluoro-  | 66 | C2H4F2  | 000075-37-6 | 91   |
| 2    |    |   | Ethane, 1,1-difluoro-  | 66 | C2H4F2  | 000075-37-6 | 90   |
| 3    |    |   | Ethane, 1,1-difluoro-  | 66 | C2H4F2  | 000075-37-6 | 90   |
| 4    |    |   | Propiolonitrile        | 51 | C3HN    | 001070-71-9 | 3    |
| 5    |    |   | Propane, 2,2-difluoro- | 80 | C3H6F2  | 000420-45-1 | 2    |



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Instrument :  
MSVOA\_U  
ClientSampleId :  
BFSK0

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR050720WMA.M  
Quant Title : TRACE VOA SOM01.0

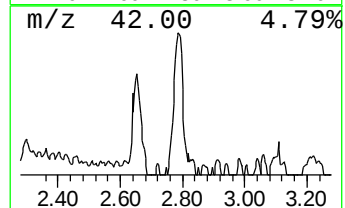
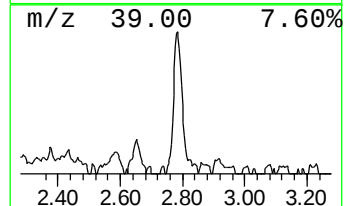
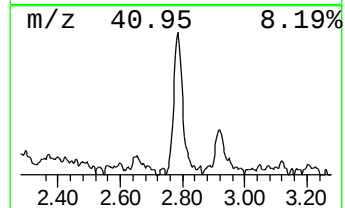
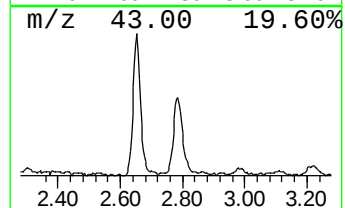
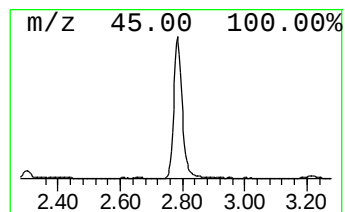
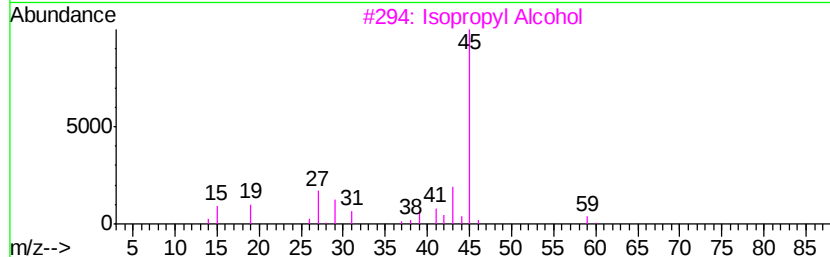
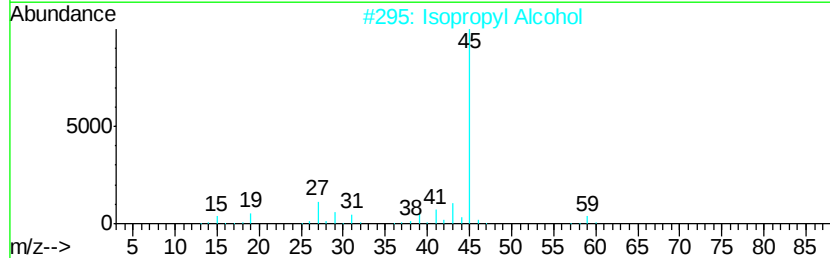
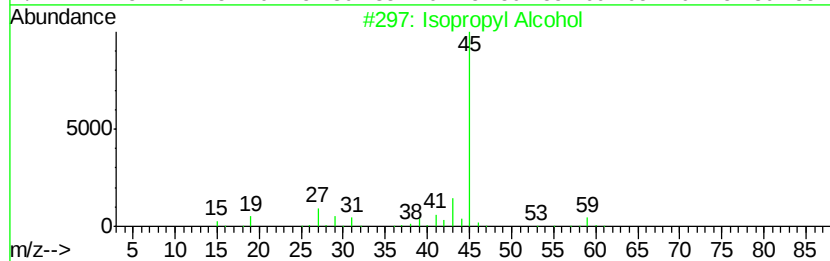
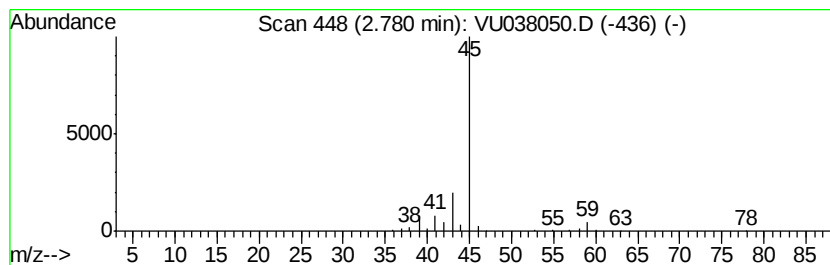
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Isopropyl Alcohol Concentration Rank 5

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 2.78 | 0.66 ug/L | 114732 | 1,4-Difluorobenzene | 6.28 |

| Hit# of 5 | Tentative ID      | MW | MolForm | CAS#        | Qual |
|-----------|-------------------|----|---------|-------------|------|
| 1         | Isopropyl Alcohol | 60 | C3H8O   | 000067-63-0 | 78   |
| 2         | Isopropyl Alcohol | 60 | C3H8O   | 000067-63-0 | 78   |
| 3         | Isopropyl Alcohol | 60 | C3H8O   | 000067-63-0 | 78   |
| 4         | Isopropyl Alcohol | 60 | C3H8O   | 000067-63-0 | 56   |
| 5         | Hydrazine, ethyl- | 60 | C2H8N2  | 000624-80-6 | 40   |



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ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFSK0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR050720WMA.M  
Quant Title : TRACE VOA SOM01.0

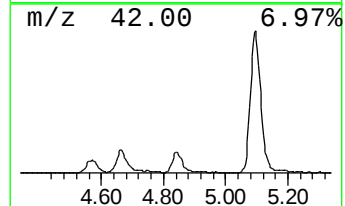
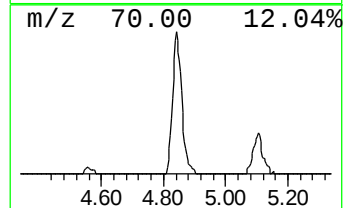
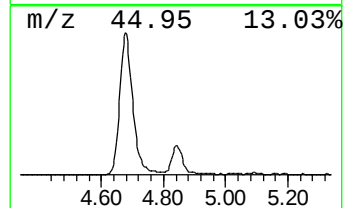
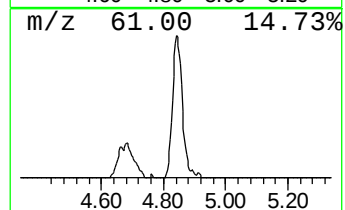
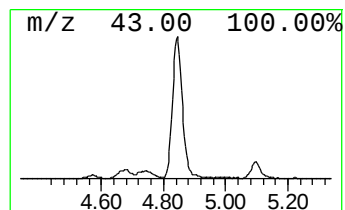
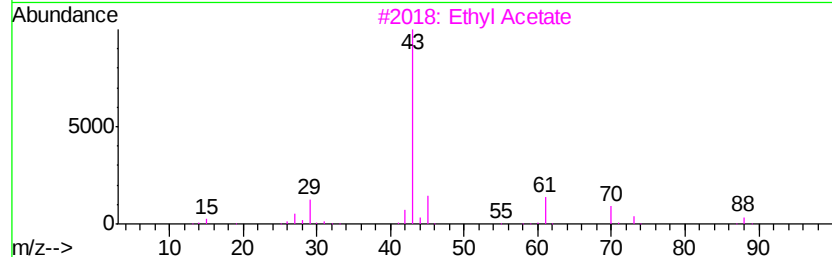
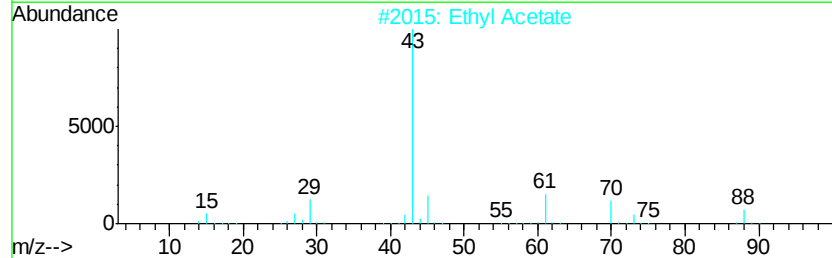
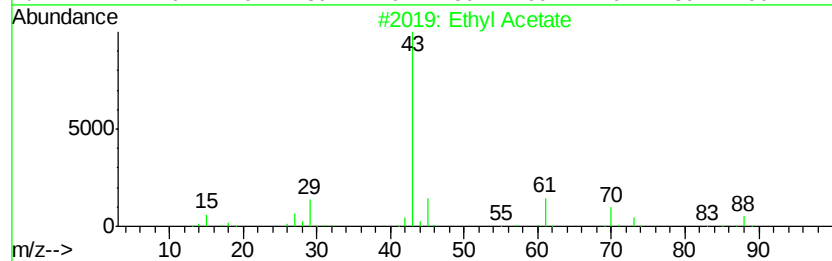
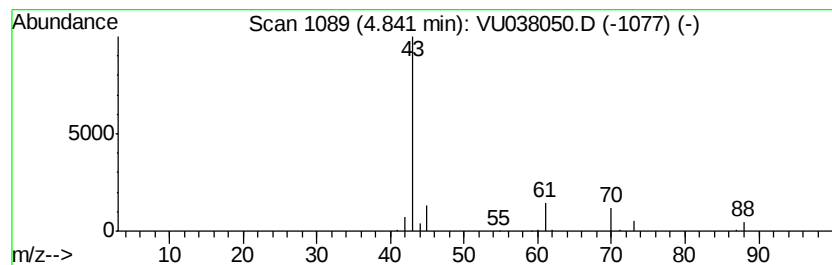
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Ethyl Acetate Concentration Rank 3

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 4.84 | 0.76 ug/L | 133359 | 1,4-Difluorobenzene | 6.28 |

| Hit# of | 5               | Tentative ID | MW | MolForm | CAS#        | Qual |
|---------|-----------------|--------------|----|---------|-------------|------|
| 1       | Ethyl           | Acetate      | 88 | C4H8O2  | 000141-78-6 | 90   |
| 2       | Ethyl           | Acetate      | 88 | C4H8O2  | 000141-78-6 | 90   |
| 3       | Ethyl           | Acetate      | 88 | C4H8O2  | 000141-78-6 | 86   |
| 4       | Ethyl           | Acetate      | 88 | C4H8O2  | 000141-78-6 | 86   |
| 5       | CH3C(O)CH2CH2OH |              | 88 | C4H8O2  | 000590-90-9 | 40   |



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ClientSampleId :  
BFSK0

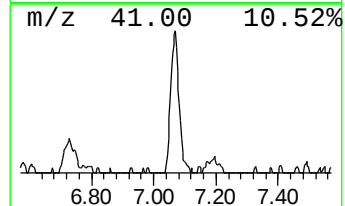
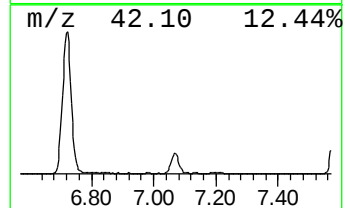
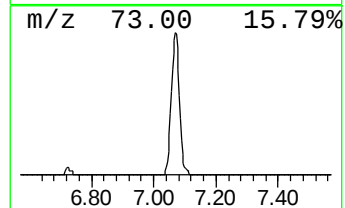
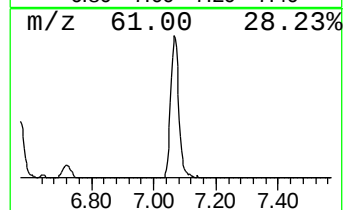
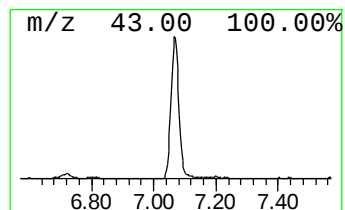
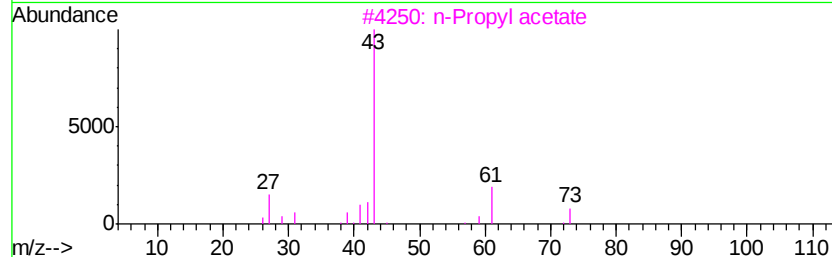
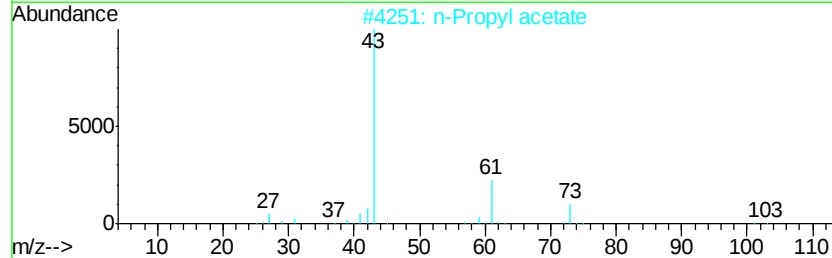
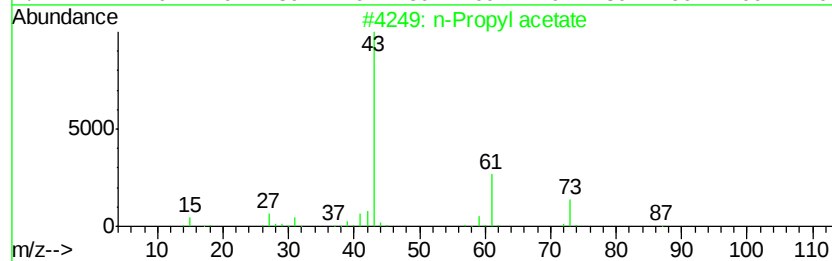
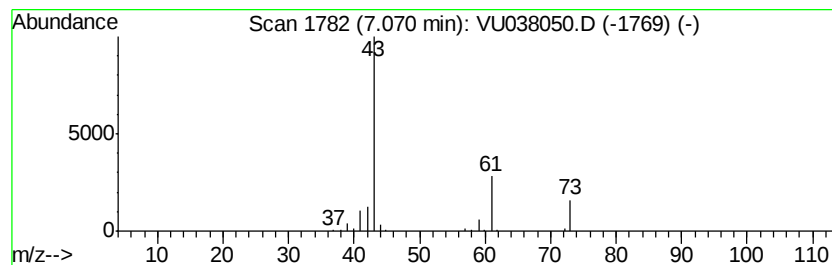
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Peak Number 4 n-Propyl acetate Concentration Rank 6

| R.T. | EstConc   | Area  | Relative to ISTD    | R.T. |
|------|-----------|-------|---------------------|------|
| 7.07 | 0.55 ug/L | 95671 | 1,4-Difluorobenzene | 6.28 |

| Hit# | of                | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------|-----|--------------|-------------|---------|------|------|
| 1    | n-Propyl acetate  | 102 | C5H10O2      | 000109-60-4 | 83      |      |      |
| 2    | n-Propyl acetate  | 102 | C5H10O2      | 000109-60-4 | 78      |      |      |
| 3    | n-Propyl acetate  | 102 | C5H10O2      | 000109-60-4 | 72      |      |      |
| 4    | Isopropyl acetate | 102 | C5H10O2      | 000108-21-4 | 38      |      |      |
| 5    | Isobutylamine     | 73  | C4H11N       | 000078-81-9 | 7       |      |      |



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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR050720WMA.M  
Quant Title : TRACE VOA SOM01.0

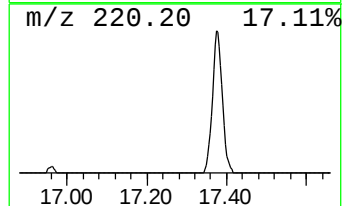
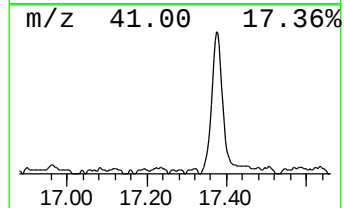
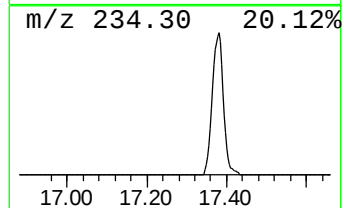
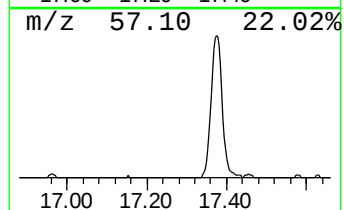
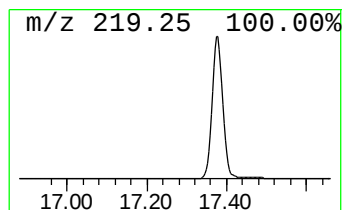
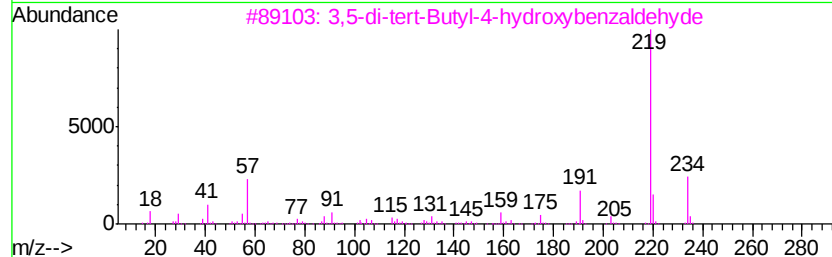
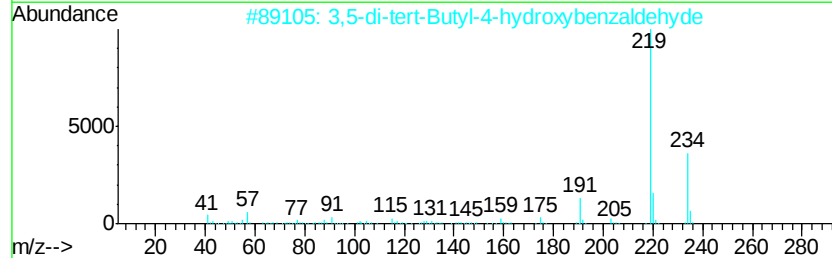
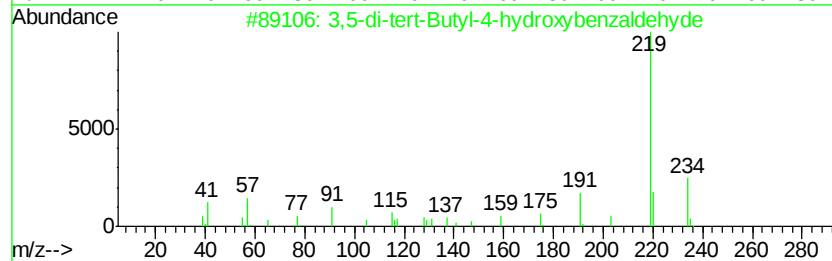
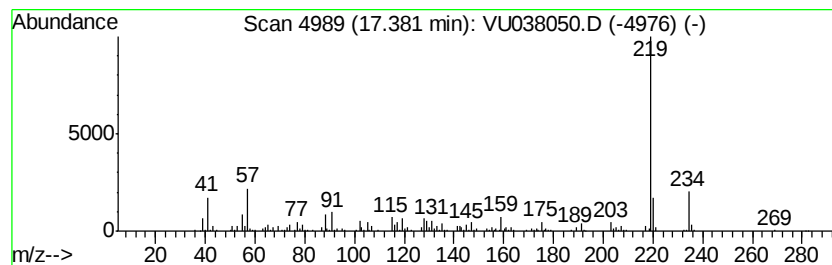
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD       | R.T.  |
|-------|-----------|--------|------------------------|-------|
| 17.38 | 1.17 ug/L | 246247 | 1,4-Dichlorobenzene-d4 | 11.83 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 3,5-di-tert-Butyl-4-hydroxybenza... | 234 | C15H22O2 | 001620-98-0 | 94   |
| 2    |    | 3,5-di-tert-Butyl-4-hydroxybenza... | 234 | C15H22O2 | 001620-98-0 | 91   |
| 3    |    | 3,5-di-tert-Butyl-4-hydroxybenza... | 234 | C15H22O2 | 001620-98-0 | 91   |
| 4    |    | 3,5-di-tert-Butyl-4-hydroxybenza... | 234 | C15H22O2 | 001620-98-0 | 91   |
| 5    |    | 3,5-Di-tert-butylbenzoic acid       | 234 | C15H22O2 | 016225-26-6 | 83   |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_U\DATA\VU050720\  
Data File : VU038050.D  
Acq On : 07 May 2020 19:41  
Operator : JC/MD  
Sample : L2527-13  
Misc : 25.0mL/MSVOA\_U/WATER  
ALS Vial : 1 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BFSK0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR050720WMA.M  
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 |
| Ethane, 1,1-diflu... | 1.37  | 0.7     | ug/L  | 117970   | 1                     | 6.28  | 872165  | 5.0  |
| Isopropyl Alcohol    | 2.78  | 0.7     | ug/L  | 114732   | 1                     | 6.28  | 872165  | 5.0  |
| Ethyl Acetate        | 4.84  | 0.8     | ug/L  | 133359   | 1                     | 6.28  | 872165  | 5.0  |
| n-Propyl acetate     | 7.07  | 0.6     | ug/L  | 95671    | 1                     | 6.28  | 872165  | 5.0  |
| 3,5-di-tert-Butyl... | 17.38 | 1.2     | ug/L  | 246247   | 3                     | 11.83 | 1054540 | 5.0  |