

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\  
 Data File : VU038424.D  
 Acq On : 30 May 2020 19:29  
 Operator : JC/MD  
 Sample : L2787-03  
 Misc : 25.0mL/MSVOA U/WATER  
 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFX73

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\SOMUTR053120WMA.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           | 20           | rVB      | 128859         | 126541        | 8.02%           | 1.063%        |
| 2         | 1.610       | 73            | 84          | 95           | rBV      | 154915         | 204691        | 12.98%          | 1.720%        |
| 3         | 1.932       | 176           | 184         | 199          | rVB      | 119699         | 152072        | 9.64%           | 1.278%        |
| 4         | 2.591       | 376           | 389         | 404          | rBV      | 250018         | 411510        | 26.09%          | 3.457%        |
| 5         | 2.674       | 405           | 415         | 421          | rBV      | 9146           | 18359         | 1.16%           | 0.154%        |
| 6         | 2.874       | 448           | 477         | 479          | rBV4     | 8929           | 27779         | 1.76%           | 0.233%        |
| 7         | 3.221       | 566           | 585         | 596          | rBV2     | 6999           | 16153         | 1.02%           | 0.136%        |
| 8         | 3.398       | 626           | 640         | 656          | rVB5     | 9271           | 21747         | 1.38%           | 0.183%        |
| 9         | 3.732       | 736           | 744         | 759          | rVB4     | 8474           | 18662         | 1.18%           | 0.157%        |
| 10        | 4.571       | 987           | 1005        | 1020         | rVB3     | 17251          | 41417         | 2.63%           | 0.348%        |
| 11        | 4.674       | 1020          | 1037        | 1075         | rBV      | 228893         | 728613        | 46.19%          | 6.122%        |
| 12        | 4.845       | 1075          | 1090        | 1112         | rVB      | 222987         | 501698        | 31.80%          | 4.215%        |
| 13        | 5.102       | 1153          | 1170        | 1195         | rBV      | 264991         | 615005        | 38.99%          | 5.167%        |
| 14        | 5.423       | 1254          | 1270        | 1284         | rBV4     | 9254           | 19902         | 1.26%           | 0.167%        |
| 15        | 5.761       | 1352          | 1375        | 1396         | rBV3     | 441322         | 1160554       | 73.57%          | 9.751%        |
| 16        | 6.279       | 1522          | 1536        | 1572         | rBV      | 375867         | 727083        | 46.09%          | 6.109%        |
| 17        | 6.568       | 1615          | 1626        | 1643         | rVB5     | 23834          | 47590         | 3.02%           | 0.400%        |
| 18        | 6.722       | 1656          | 1674        | 1693         | rBV      | 269493         | 527682        | 33.45%          | 4.434%        |
| 19        | 7.066       | 1767          | 1781        | 1800         | rBV      | 196706         | 350043        | 22.19%          | 2.941%        |
| 20        | 7.591       | 1931          | 1944        | 1958         | rBV      | 145235         | 254298        | 16.12%          | 2.137%        |
| 21        | 7.922       | 2033          | 2047        | 2063         | rBV      | 519943         | 919112        | 58.26%          | 7.722%        |
| 22        | 7.989       | 2064          | 2068        | 2081         | rVB      | 13023          | 21462         | 1.36%           | 0.180%        |
| 23        | 8.201       | 2119          | 2134        | 2150         | rBV      | 90264          | 156996        | 9.95%           | 1.319%        |
| 24        | 8.655       | 2260          | 2275        | 2305         | rBV      | 860111         | 1577510       | 100.00%         | 13.254%       |
| 25        | 9.436       | 2504          | 2518        | 2537         | rBV      | 547242         | 924265        | 58.59%          | 7.766%        |
| 26        | 10.770      | 2921          | 2933        | 2950         | rBV      | 224422         | 357145        | 22.64%          | 3.001%        |
| 27        | 11.825      | 3245          | 3261        | 3275         | rBV      | 581186         | 926481        | 58.73%          | 7.784%        |
| 28        | 12.079      | 3330          | 3340        | 3353         | rBV4     | 9463           | 20150         | 1.28%           | 0.169%        |
| 29        | 12.205      | 3366          | 3379        | 3394         | rVB      | 555680         | 891632        | 56.52%          | 7.491%        |
| 30        | 17.384      | 4980          | 4990        | 5001         | rBV2     | 73067          | 135907        | 8.62%           | 1.142%        |

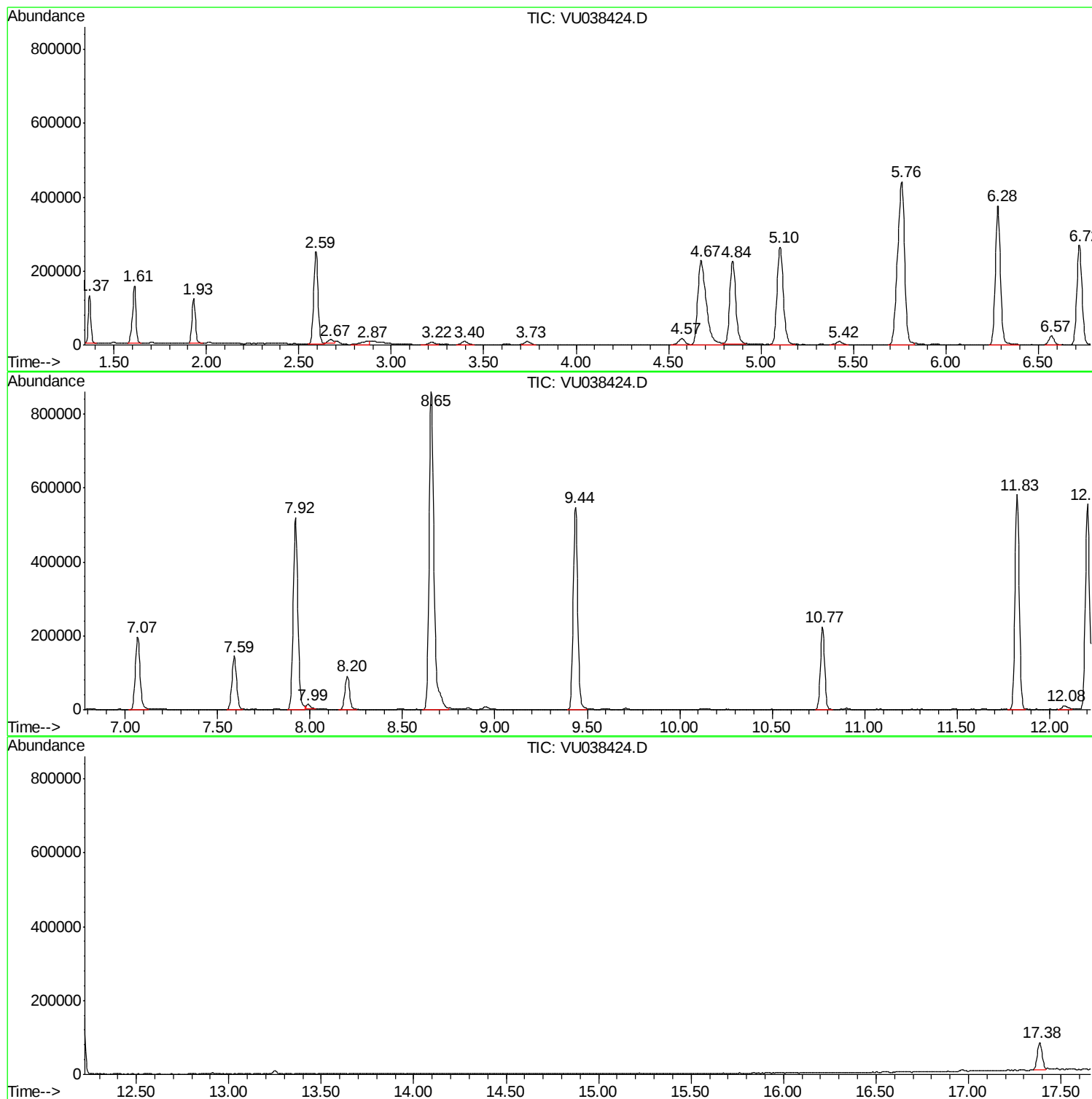
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ClientSampleId :  
BFX73

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR053120WMA.M  
Quant Title : TRACE VOA SOM01.0

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



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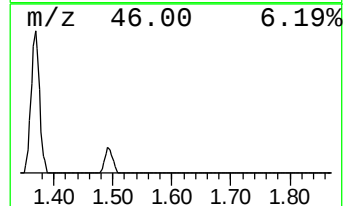
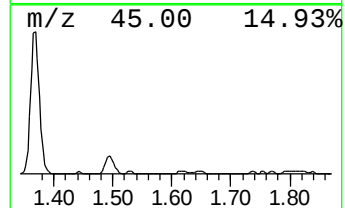
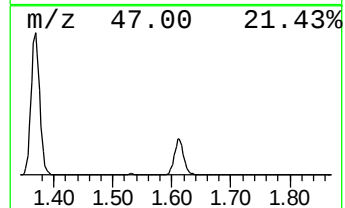
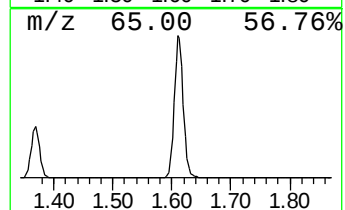
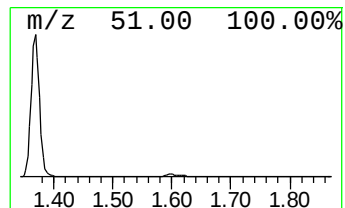
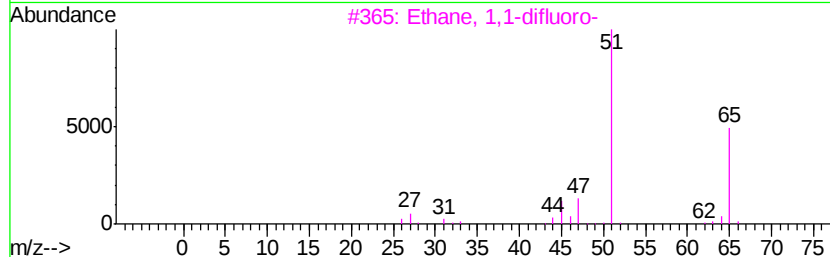
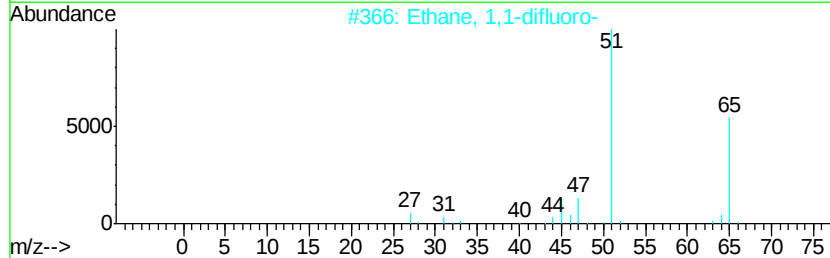
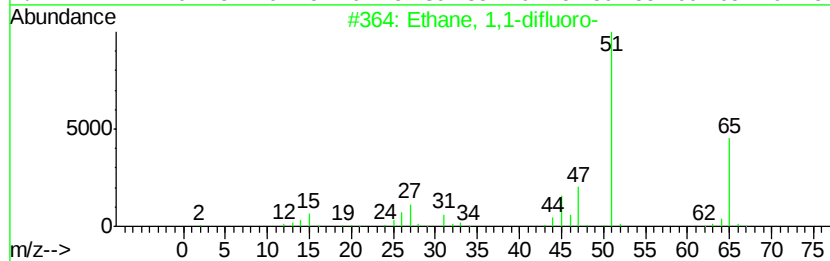
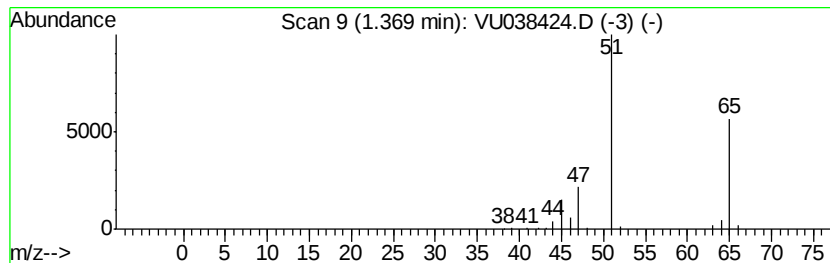
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Quant Title : TRACE VOA SOM01.0

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 | 0.87 ug/L | 126541 | 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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MSVOA\_U  
ClientSampleId :  
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR053120WMA.M  
Quant Title : TRACE VOA SOM01.0

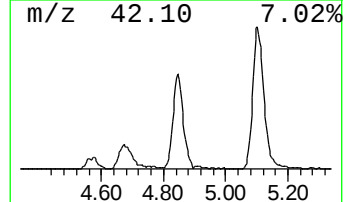
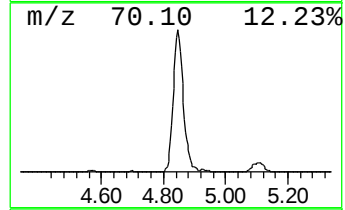
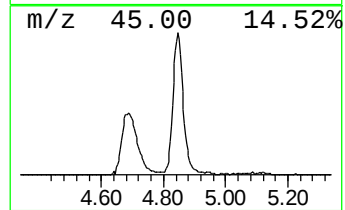
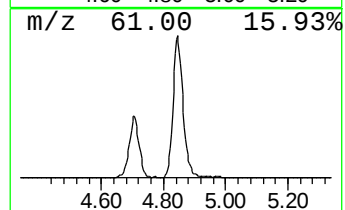
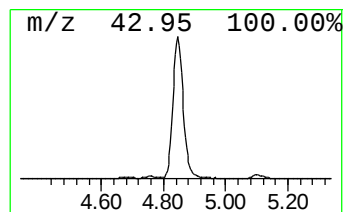
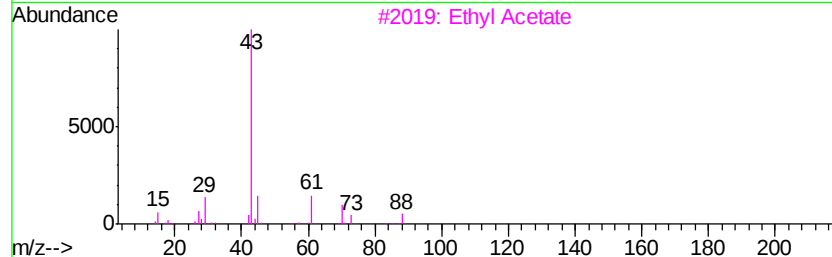
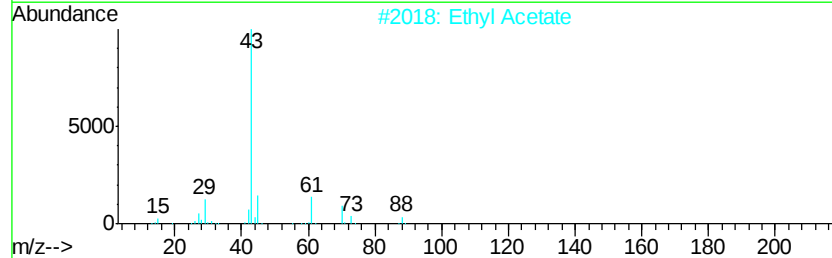
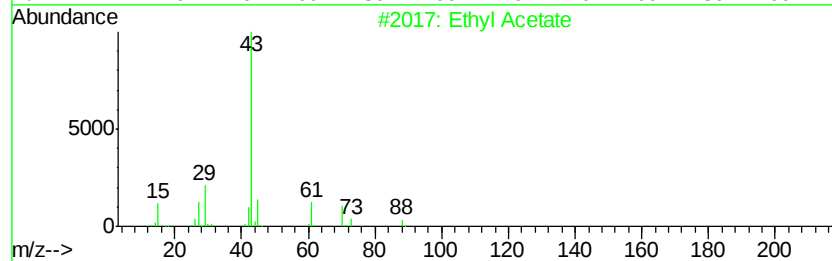
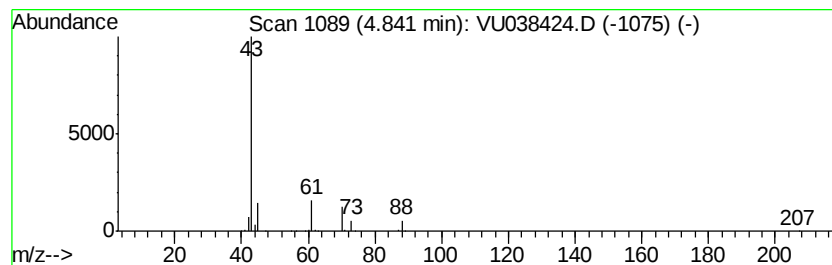
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Ethyl Acetate Concentration Rank 1

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 4.84 | 3.45 ug/L | 501698 | 1,4-Difluorobenzene | 6.28 |

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



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ClientSampleId :  
BFX73

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR053120WMA.M  
Quant Title : TRACE VOA SOM01.0

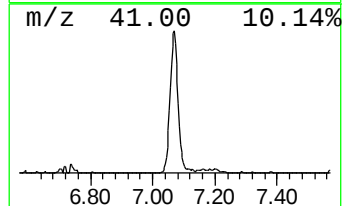
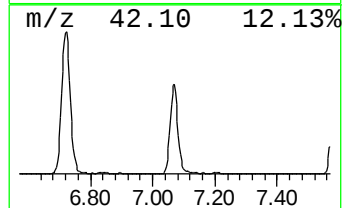
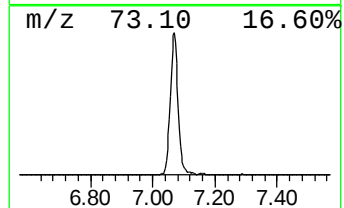
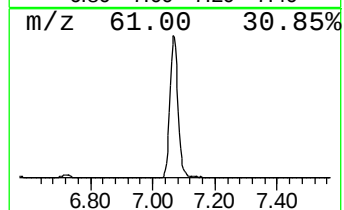
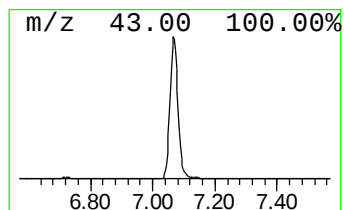
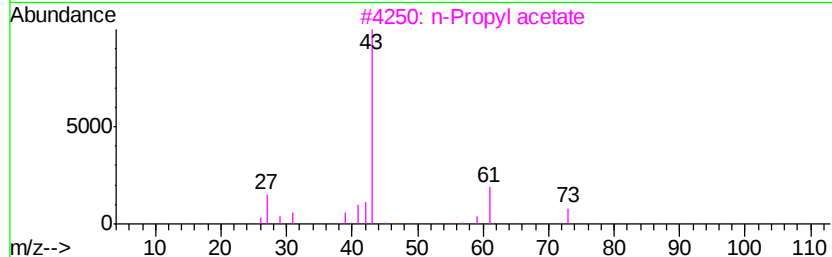
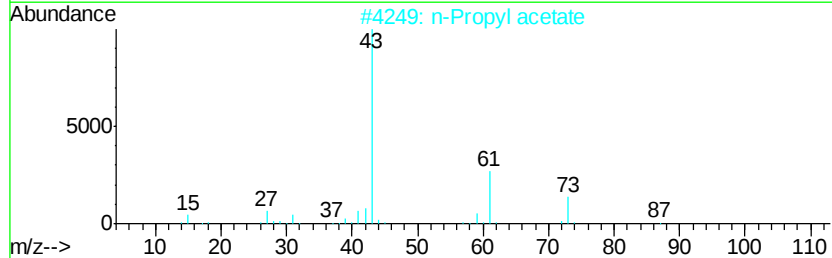
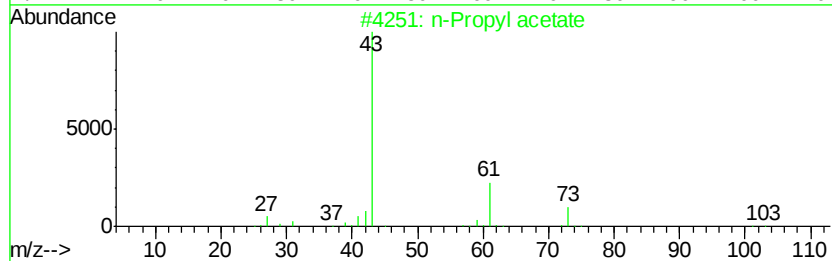
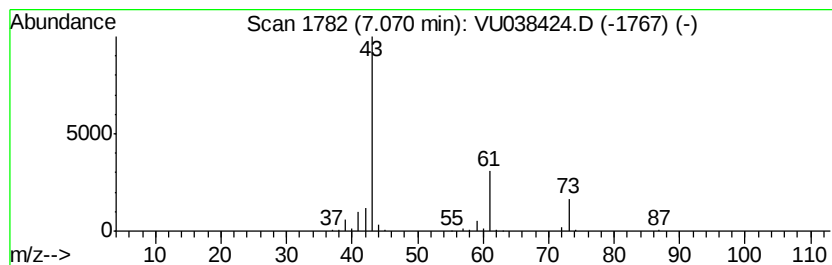
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Propyl acetate Concentration Rank 2

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 7.07 | 2.41 ug/L | 350043 | 1,4-Difluorobenzene | 6.28 |

| Hit# | of | Tentative ID      | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------|-----|---------|-------------|------|
| 1    | 5  | n-Propyl acetate  | 102 | C5H10O2 | 000109-60-4 | 83   |
| 2    |    | n-Propyl acetate  | 102 | C5H10O2 | 000109-60-4 | 83   |
| 3    |    | n-Propyl acetate  | 102 | C5H10O2 | 000109-60-4 | 78   |
| 4    |    | Isopropyl acetate | 102 | C5H10O2 | 000108-21-4 | 36   |
| 5    |    | Isopropyl acetate | 102 | C5H10O2 | 000108-21-4 | 9    |



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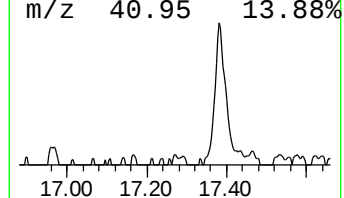
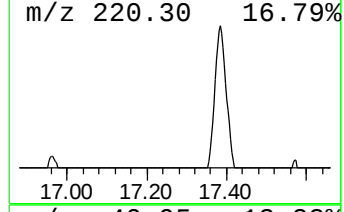
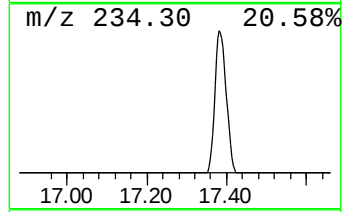
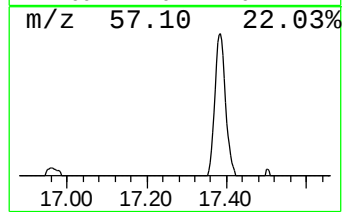
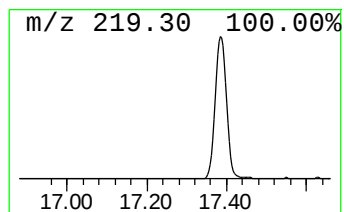
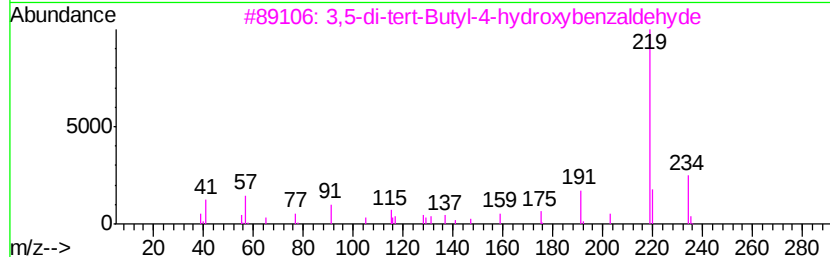
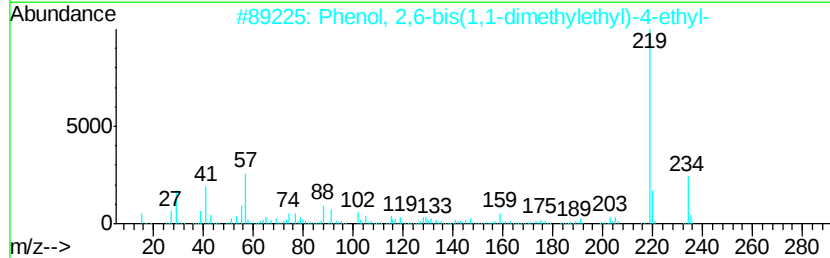
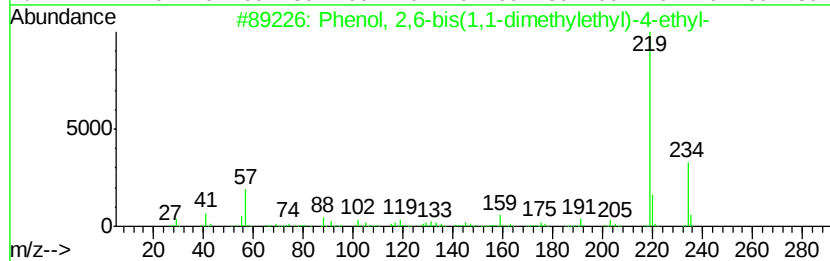
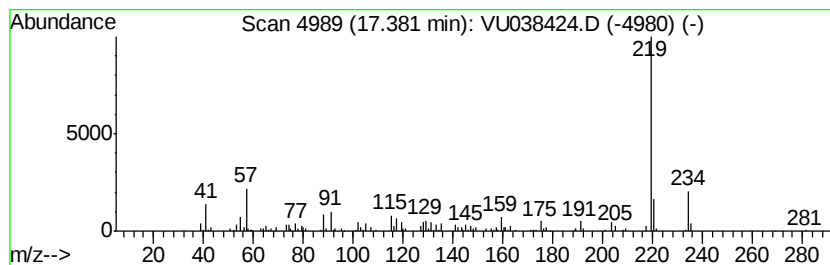
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 5 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 5

| R.T.    | EstConc                             | Area         | Relative to ISTD       | R.T.      |
|---------|-------------------------------------|--------------|------------------------|-----------|
| 17.38   | 0.73 ug/L                           | 135907       | 1,4-Dichlorobenzene-d4 | 11.83     |
| Hit# of | 5                                   | Tentative ID | MW MolForm             | CAS# Qual |
| 1       | Phenol, 2,6-bis(1,1-dimethylethy... | 234 C16H26O  | 004130-42-1            | 96        |
| 2       | Phenol, 2,6-bis(1,1-dimethylethy... | 234 C16H26O  | 004130-42-1            | 95        |
| 3       | 3,5-di-tert-Butyl-4-hydroxybenza... | 234 C15H22O2 | 001620-98-0            | 93        |
| 4       | 3,5-di-tert-Butyl-4-hydroxybenza... | 234 C15H22O2 | 001620-98-0            | 93        |
| 5       | Phenol, 2,6-bis(1,1-dimethylethy... | 234 C16H26O  | 004130-42-1            | 91        |



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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 |
| Ethane, 1,1-diflu... | 1.37  | 0.9     | ug/L  | 126541   | 1                     | 6.28  | 727083 | 5.0  |
| Ethyl Acetate        | 4.84  | 3.5     | ug/L  | 501698   | 1                     | 6.28  | 727083 | 5.0  |
| n-Propyl acetate     | 7.07  | 2.4     | ug/L  | 350043   | 1                     | 6.28  | 727083 | 5.0  |
| Phenol, 2,6-bis(1... | 17.38 | 0.7     | ug/L  | 135907   | 3                     | 11.83 | 926481 | 5.0  |