

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU031920\  
 Data File : VU037342.D  
 Acq On : 19 Mar 2020 17:28  
 Operator : JC/MD  
 Sample : L1983-04RE  
 Misc : 25.0mL/MSVOA U/WATER  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AA8RE

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\SOMUTR031620WMA.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         | 1.475       | 35            | 42          | 55           | rBV      | 35451          | 57996         | 13.11%          | 1.390%        |
| 2         | 1.536       | 57            | 61          | 69           | rVV2     | 8235           | 11937         | 2.70%           | 0.286%        |
| 3         | 1.929       | 176           | 183         | 196          | rVB      | 42593          | 56846         | 12.85%          | 1.363%        |
| 4         | 2.591       | 378           | 389         | 400          | rVB      | 34569          | 56549         | 12.78%          | 1.356%        |
| 5         | 2.658       | 403           | 410         | 421          | rVB2     | 5083           | 8254          | 1.87%           | 0.198%        |
| 6         | 2.806       | 443           | 456         | 472          | rBV3     | 6946           | 19269         | 4.36%           | 0.462%        |
| 7         | 3.073       | 527           | 539         | 548          | rBV5     | 3082           | 5401          | 1.22%           | 0.129%        |
| 8         | 3.404       | 629           | 642         | 659          | rBV3     | 12457          | 28445         | 6.43%           | 0.682%        |
| 9         | 4.671       | 1018          | 1036        | 1061         | rBV      | 72088          | 173657        | 39.25%          | 4.163%        |
| 10        | 5.121       | 1155          | 1176        | 1200         | rBV3     | 140057         | 428598        | 96.87%          | 10.275%       |
| 11        | 5.761       | 1354          | 1375        | 1400         | rBV3     | 155846         | 403765        | 91.26%          | 9.680%        |
| 12        | 6.282       | 1522          | 1537        | 1556         | rBV      | 182551         | 344067        | 77.77%          | 8.248%        |
| 13        | 6.726       | 1658          | 1675        | 1691         | rBV      | 101581         | 199100        | 45.00%          | 4.773%        |
| 14        | 7.137       | 1791          | 1803        | 1817         | rVB2     | 40744          | 75457         | 17.05%          | 1.809%        |
| 15        | 7.594       | 1934          | 1945        | 1958         | rBV3     | 27080          | 45836         | 10.36%          | 1.099%        |
| 16        | 7.925       | 2036          | 2048        | 2062         | rBV      | 46273          | 78257         | 17.69%          | 1.876%        |
| 17        | 8.208       | 2124          | 2136        | 2145         | rBV2     | 20984          | 34452         | 7.79%           | 0.826%        |
| 18        | 8.661       | 2265          | 2277        | 2302         | rBV      | 240350         | 421866        | 95.35%          | 10.114%       |
| 19        | 8.835       | 2317          | 2331        | 2343         | rVB      | 31699          | 55515         | 12.55%          | 1.331%        |
| 20        | 9.440       | 2504          | 2519        | 2537         | rBV      | 266701         | 442443        | 100.00%         | 10.607%       |
| 21        | 9.513       | 2537          | 2542        | 2553         | rVB7     | 5369           | 8424          | 1.90%           | 0.202%        |
| 22        | 10.311      | 2782          | 2790        | 2799         | rVB3     | 3883           | 5800          | 1.31%           | 0.139%        |
| 23        | 10.777      | 2922          | 2935        | 2948         | rBV      | 86474          | 138346        | 31.27%          | 3.317%        |
| 24        | 10.947      | 2978          | 2988        | 3004         | rVB2     | 90243          | 142805        | 32.28%          | 3.424%        |
| 25        | 11.063      | 3013          | 3024        | 3038         | rVB      | 38769          | 60217         | 13.61%          | 1.444%        |
| 26        | 11.378      | 3114          | 3122        | 3135         | rVB3     | 3933           | 5708          | 1.29%           | 0.137%        |
| 27        | 11.491      | 3146          | 3157        | 3170         | rVB3     | 4236           | 6732          | 1.52%           | 0.161%        |
| 28        | 11.828      | 3250          | 3262        | 3277         | rBV      | 272109         | 438157        | 99.03%          | 10.504%       |
| 29        | 12.082      | 3330          | 3341        | 3348         | rBV4     | 10547          | 18183         | 4.11%           | 0.436%        |
| 30        | 12.128      | 3348          | 3355        | 3366         | rVV2     | 11913          | 19704         | 4.45%           | 0.472%        |
| 31        | 12.208      | 3368          | 3380        | 3403         | rVB      | 214196         | 379509        | 85.78%          | 9.098%        |

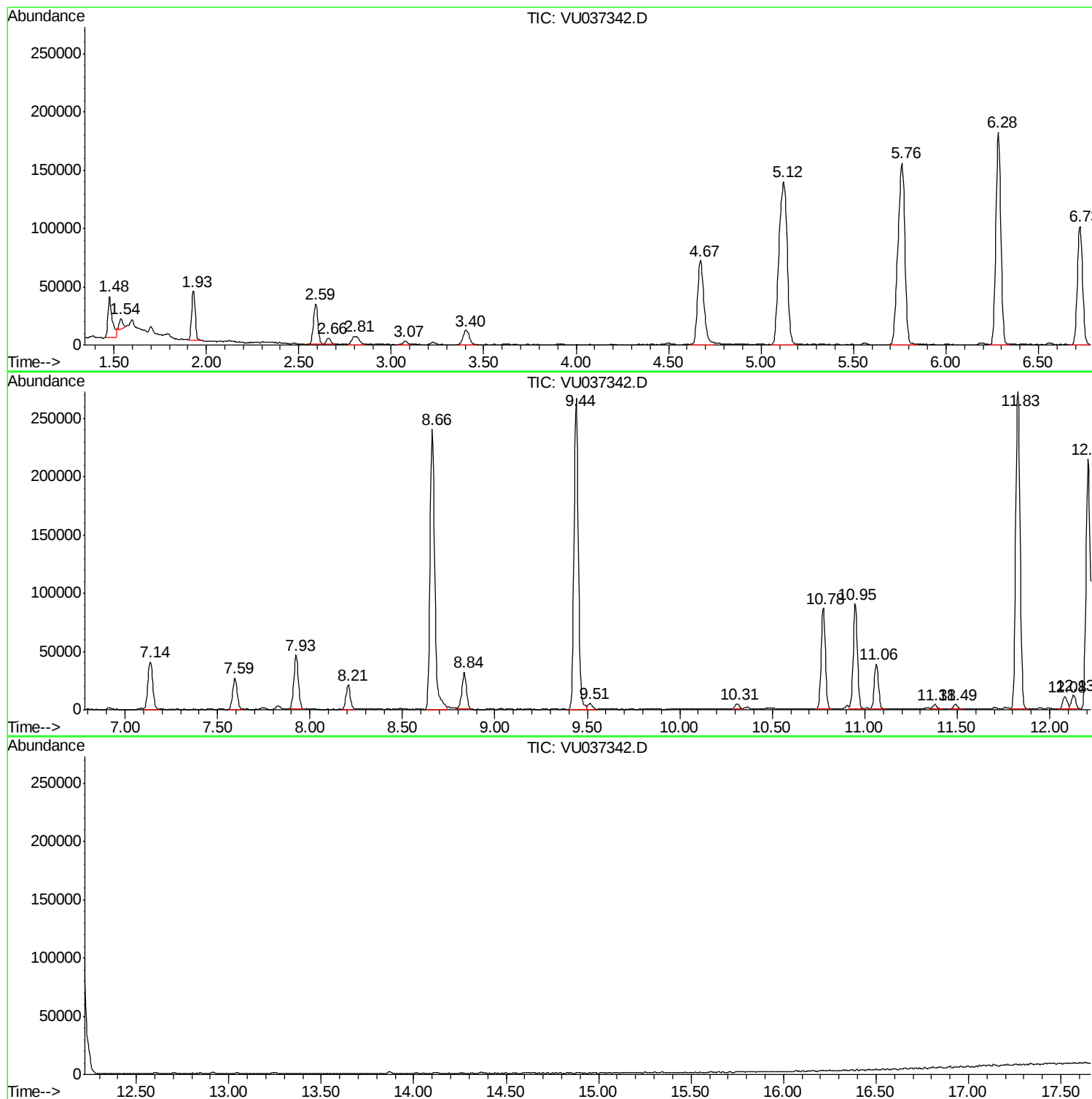
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MSVOA\_U  
ClientSampleId :  
C0AA8RE

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR031620WMA.M  
Quant Title : TRACE VOA SOM01.0

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



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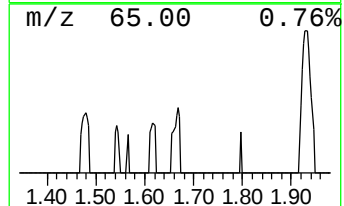
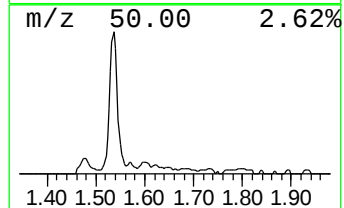
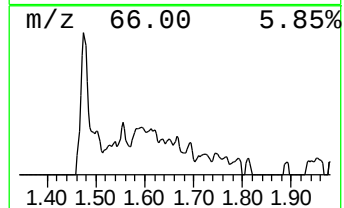
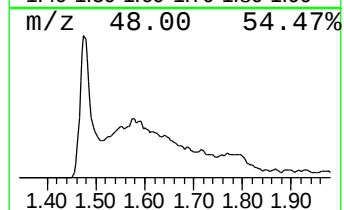
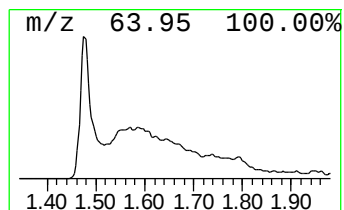
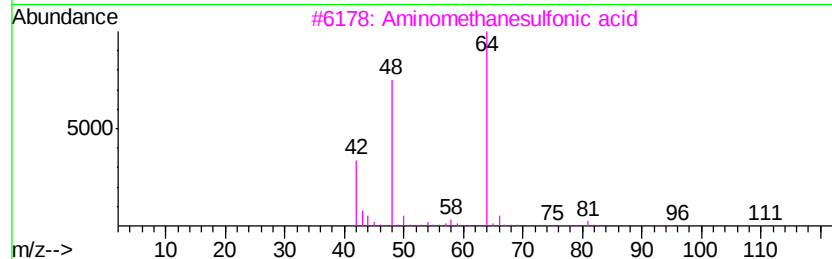
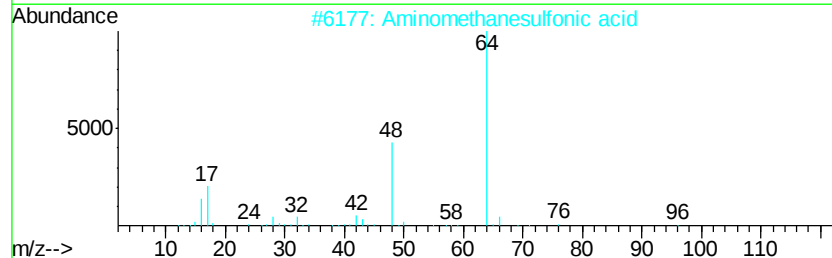
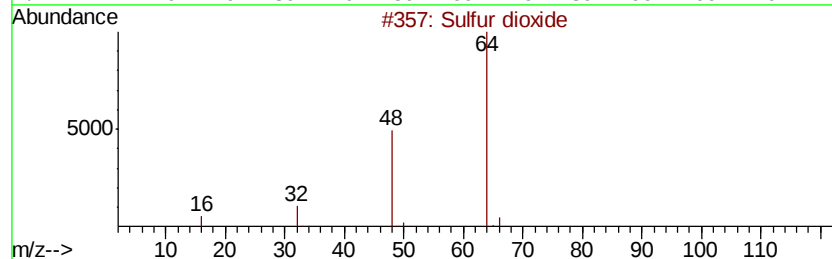
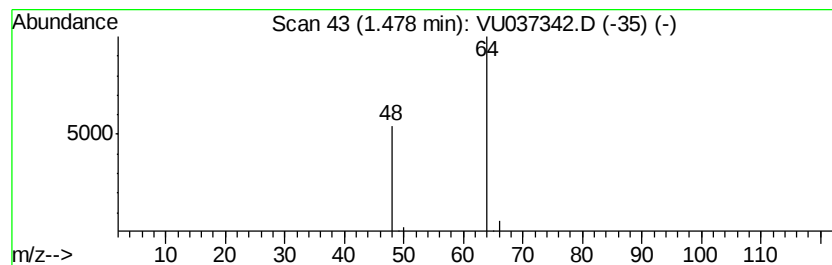
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR031620WMA.M  
Quant Title : TRACE VOA SOM01.0

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

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Peak Number 1 Sulfur dioxide Concentration Rank 2

| R.T. | EstConc   | Area  | Relative to ISTD    | R.T. |
|------|-----------|-------|---------------------|------|
| 1.48 | 0.84 ug/L | 57996 | 1,4-Difluorobenzene | 6.28 |

| Hit# | of | Tentative ID              | MW  | MolForm  | CAS#        | Qual |
|------|----|---------------------------|-----|----------|-------------|------|
| 1    | 5  | Sulfur dioxide            | 64  | O2S      | 007446-09-5 | 90   |
| 2    |    | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 74   |
| 3    |    | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 64   |
| 4    |    | L-Alanine, 3-sulfo-       | 169 | C3H7NO5S | 000498-40-8 | 9    |
| 5    |    | Aminomethanesulfonic acid | 111 | CH5NO3S  | 013881-91-9 | 9    |



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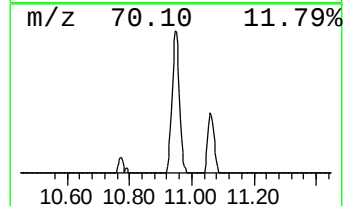
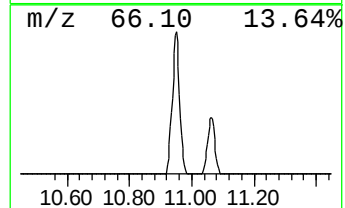
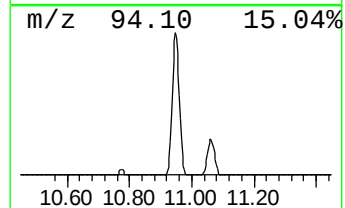
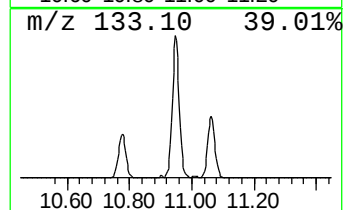
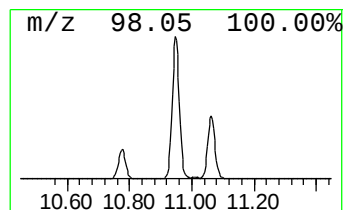
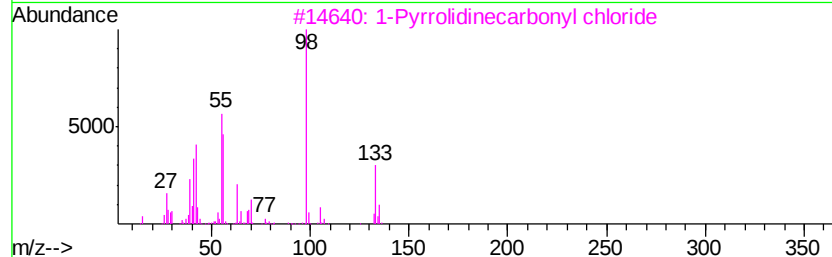
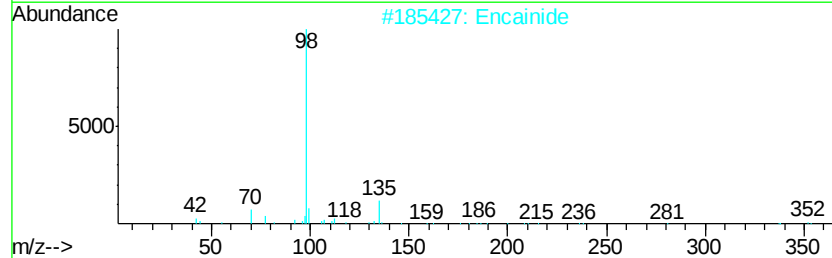
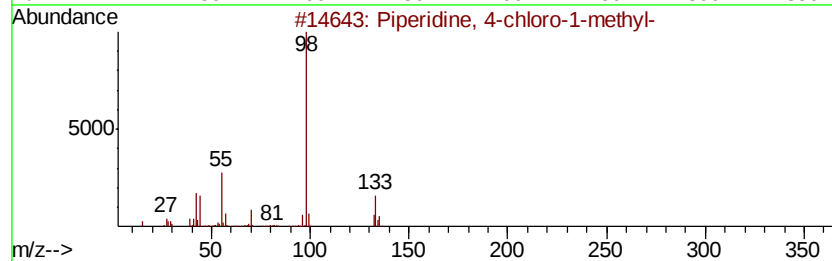
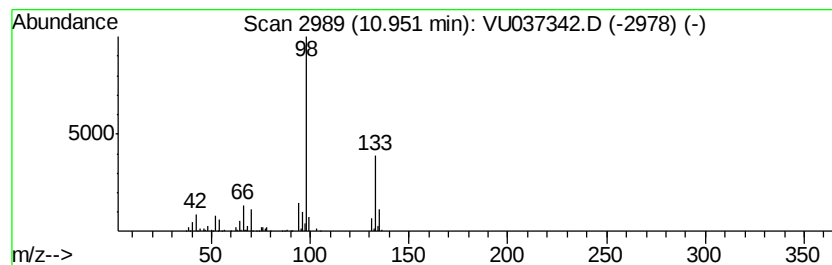
Instrument :  
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Quant Title : TRACE VOA SOM01.0

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

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Peak Number 3 Piperidine, 4-chloro-1-methyl- Concentration Rank 1

| R.T.    | EstConc   | Area                           | Relative to ISTD       | R.T.       |             |      |
|---------|-----------|--------------------------------|------------------------|------------|-------------|------|
| 10.95   | 1.63 ug/L | 142805                         | 1,4-Dichlorobenzene-d4 | 11.83      |             |      |
| Hit# of | 5         | Tentative ID                   | MW                     | MolForm    | CAS#        | Qual |
| 1       |           | Piperidine, 4-chloro-1-methyl- | 133                    | C6H12ClN   | 005570-77-4 | 50   |
| 2       |           | Encainide                      | 352                    | C22H28N2O2 | 037612-13-8 | 43   |
| 3       |           | 1-Pyrrolidinecarbonyl chloride | 133                    | C5H8ClNO   | 001192-63-8 | 33   |
| 4       |           | Mepivacaine                    | 246                    | C15H22N2O  | 000096-88-8 | 32   |
| 5       |           | Benzen-d5-amine                | 98                     | C6H2D5N    | 004165-61-1 | 32   |



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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR031620WMA.M  
Quant Title : TRACE VOA SOM01.0

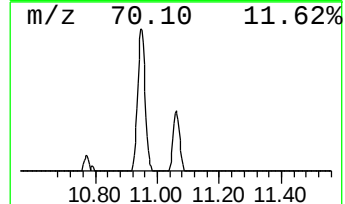
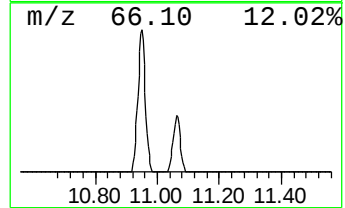
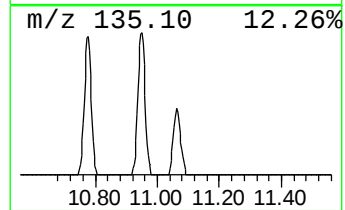
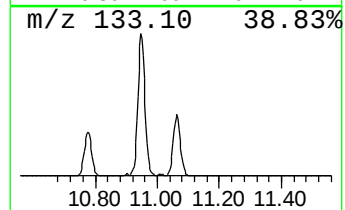
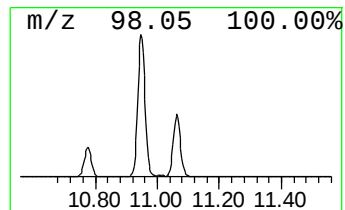
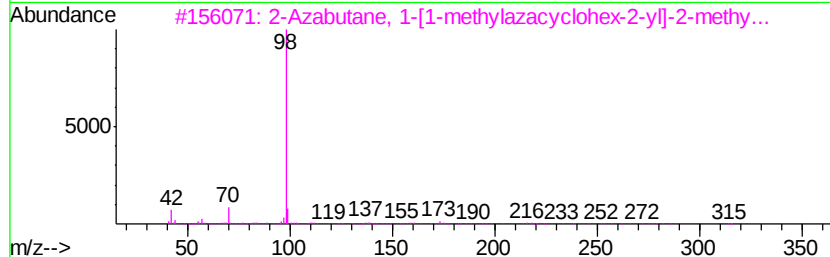
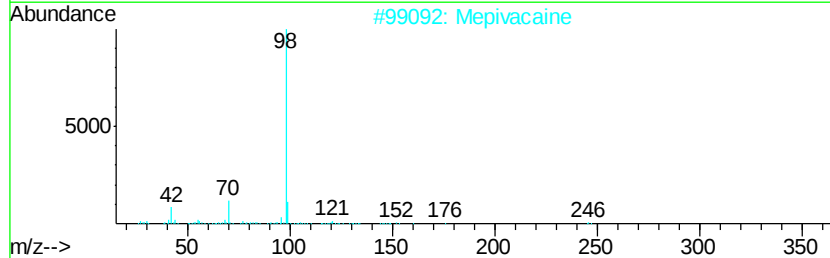
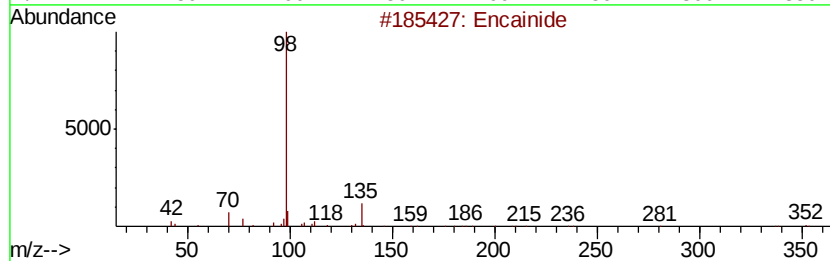
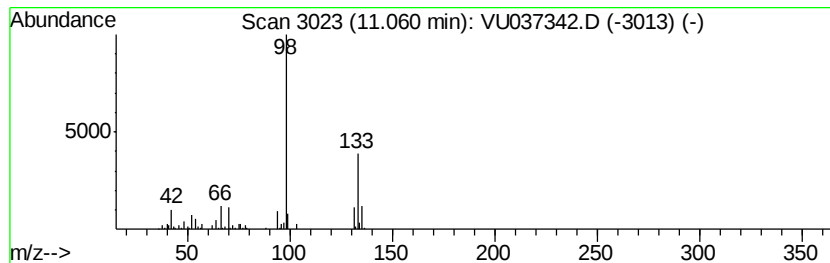
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 unknown-01 Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD       | R.T.  |
|-------|-----------|-------|------------------------|-------|
| 11.06 | 0.69 ug/L | 60217 | 1,4-Dichlorobenzene-d4 | 11.83 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|-------------------------------------|-----|-------------|-------------|------|
| 1    | 5  | Encainide                           | 352 | C22H28N2O2  | 037612-13-8 | 37   |
| 2    |    | Mepivacaine                         | 246 | C15H22N2O   | 000096-88-8 | 35   |
| 3    |    | 2-Azabutane, 1-[1-methylazacyclo... | 314 | C16H24Cl2N2 | 184637-45-4 | 32   |
| 4    |    | Propanamide, N-[1-methyl-2-(1-pi... | 275 | C16H25N3O   | 015686-91-6 | 25   |
| 5    |    | 5-Phenyl-3-piperidin-1-ylmethyl-... | 275 | C14H17N3OS  | 023269-66-1 | 25   |



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TIC Library : C:\DATABASE\NIST11.L  
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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| Sulfur dioxide       | 1.48  | 0.8     | ug/L  | 57996    | 1                     | 6.28  | 344067 | 5.0  |
| Piperidine, 4-chl... | 10.95 | 1.6     | ug/L  | 142805   | 3                     | 11.83 | 438157 | 5.0  |
| unknown-01           | 11.06 | 0.7     | ug/L  | 60217    | 3                     | 11.83 | 438157 | 5.0  |