

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011316\  
 Data File : BF084453.D  
 Acq On : 13 Jan 2016 20:40  
 Operator : SJ/UM  
 Sample : PB87806BL  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB87806BL

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON Filtering: 5  
 Sampling : 1 Min Area: 3 % 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:\HPCHEM1\BNA\_F\METHODS\8270-BF123115.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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         | 4.361       | 196           | 199         | 203          | rBV      | 188557         | 232711        | 3.73%           | 0.425%        |
| 2         | 5.024       | 254           | 257         | 268          | rBV      | 1820554        | 2832904       | 45.36%          | 5.172%        |
| 3         | 5.173       | 268           | 270         | 279          | rBV5     | 40500          | 105320        | 1.69%           | 0.192%        |
| 4         | 5.447       | 291           | 294         | 296          | rBV      | 5416655        | 5632627       | 90.19%          | 10.283%       |
| 5         | 5.836       | 326           | 328         | 331          | rBV      | 167087         | 170805        | 2.73%           | 0.312%        |
| 6         | 6.476       | 381           | 384         | 386          | rBV      | 5658539        | 5655679       | 90.56%          | 10.325%       |
| 7         | 6.602       | 392           | 395         | 397          | rBV      | 5844916        | 5281376       | 84.56%          | 9.642%        |
| 8         | 6.830       | 413           | 415         | 417          | rVB      | 1828316        | 1481435       | 23.72%          | 2.705%        |
| 9         | 6.990       | 426           | 429         | 431          | rBV      | 4694154        | 4446505       | 71.20%          | 8.118%        |
| 10        | 7.390       | 462           | 464         | 467          | rBV      | 2505143        | 3578360       | 57.30%          | 6.533%        |
| 11        | 8.122       | 525           | 528         | 530          | rBV      | 1533432        | 1901598       | 30.45%          | 3.472%        |
| 12        | 9.196       | 619           | 622         | 624          | rBV      | 6427007        | 6231266       | 99.77%          | 11.376%       |
| 13        | 9.870       | 678           | 681         | 683          | rBV      | 2367168        | 2137737       | 34.23%          | 3.903%        |
| 14        | 10.659      | 747           | 750         | 752          | rBV      | 3821964        | 3740931       | 59.90%          | 6.830%        |
| 15        | 11.356      | 808           | 811         | 813          | rBV      | 2019847        | 2139925       | 34.26%          | 3.907%        |
| 16        | 12.945      | 947           | 950         | 952          | rBV      | 5540295        | 6245495       | 100.00%         | 11.402%       |
| 17        | 13.985      | 1039          | 1041        | 1044         | rBV      | 1974531        | 1781725       | 28.53%          | 3.253%        |
| 18        | 15.402      | 1162          | 1165        | 1168         | rBV      | 892802         | 1178520       | 18.87%          | 2.152%        |

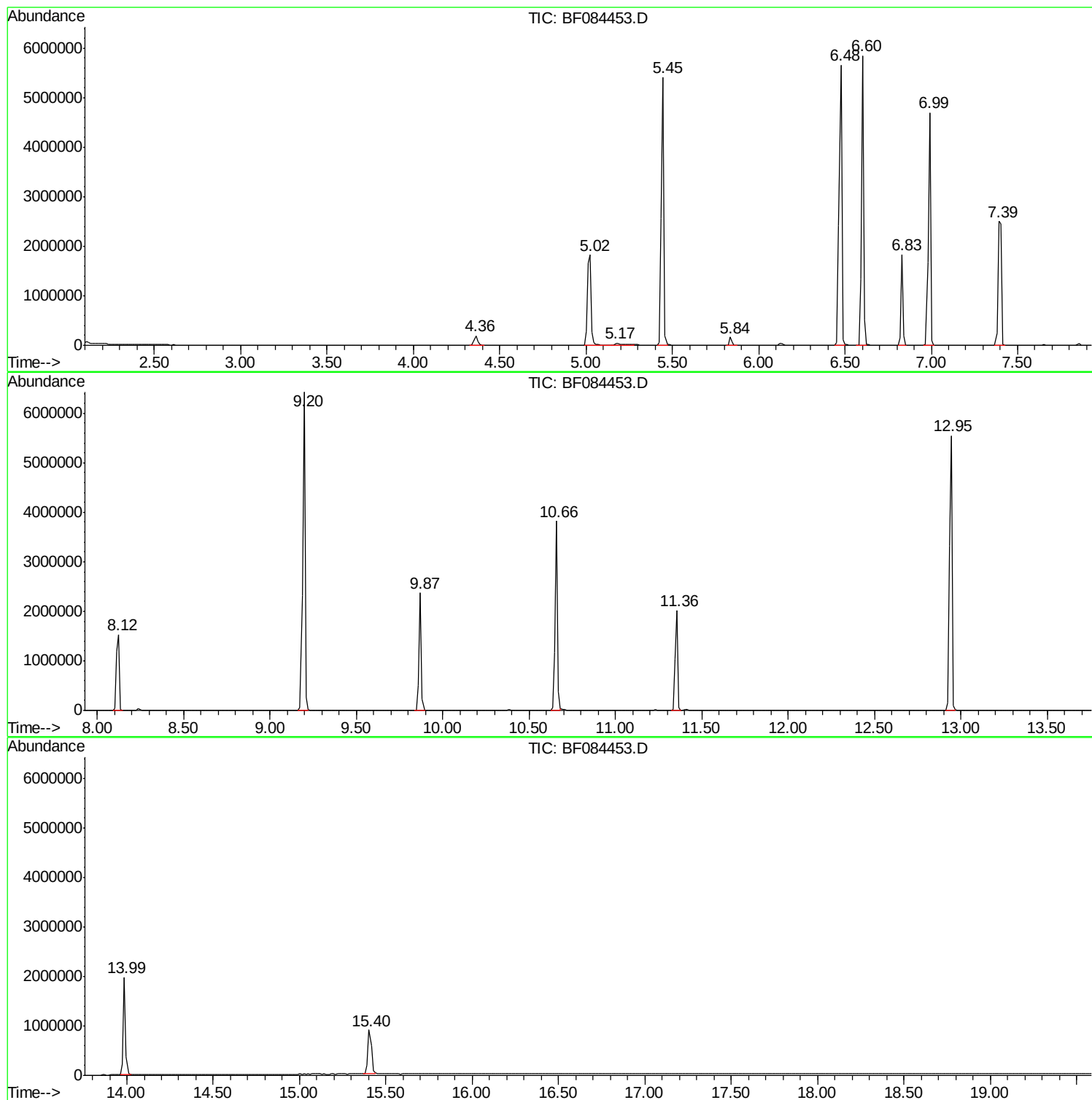
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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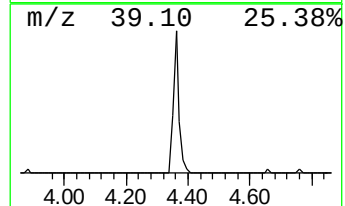
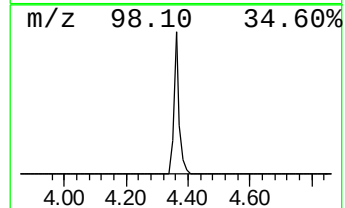
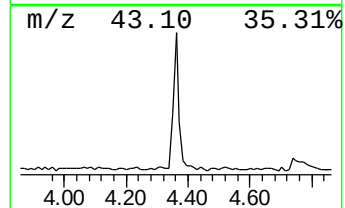
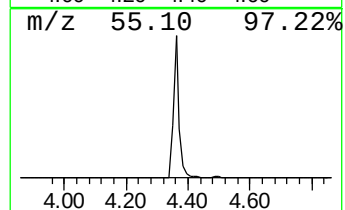
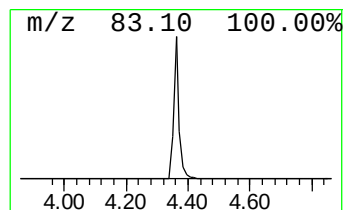
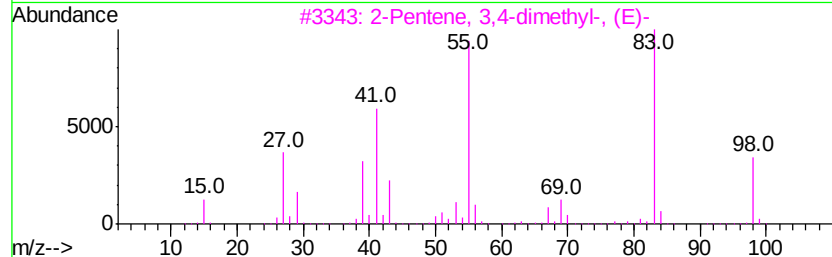
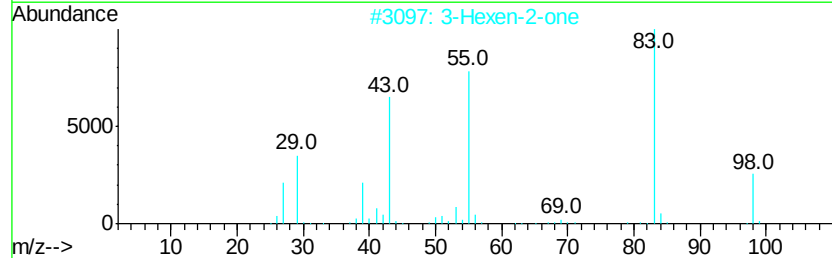
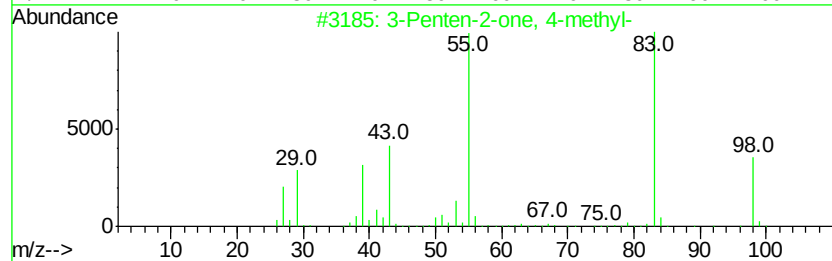
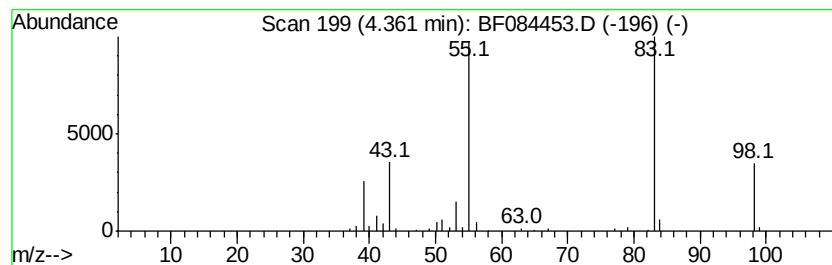
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF123115.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.36 | 3.14 ng | 232711 | 1,4-Dichlorobenzene-d4 | 6.83 |

| Hit# | of | 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|----|---------|-------------|------|
| 1    |    |   | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |    |   | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 91   |
| 3    |    |   | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 90   |
| 4    |    |   | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14   | 000690-08-4 | 86   |
| 5    |    |   | 2-Pentene, 2,4-dimethyl-       | 98 | C7H14   | 000625-65-0 | 86   |



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ClientSampled :  
PB87806BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

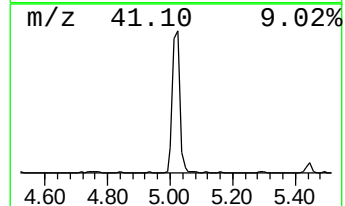
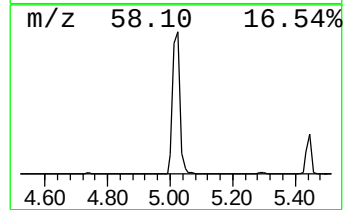
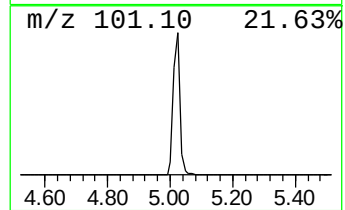
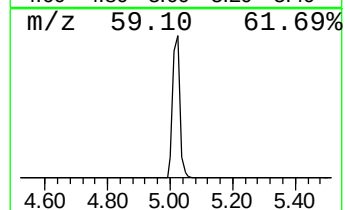
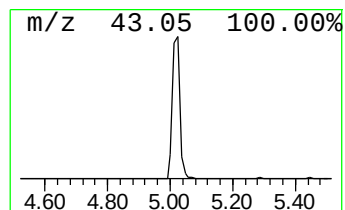
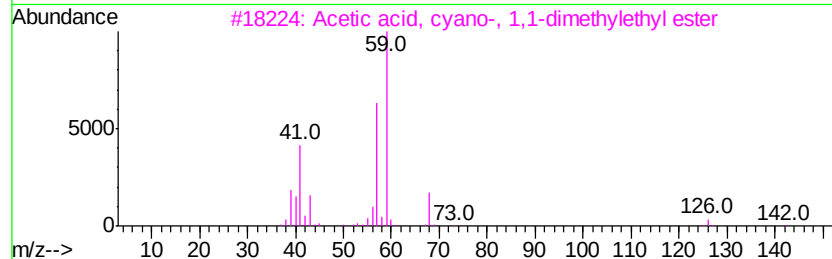
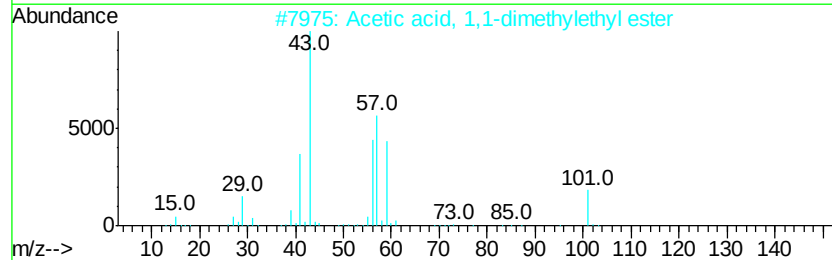
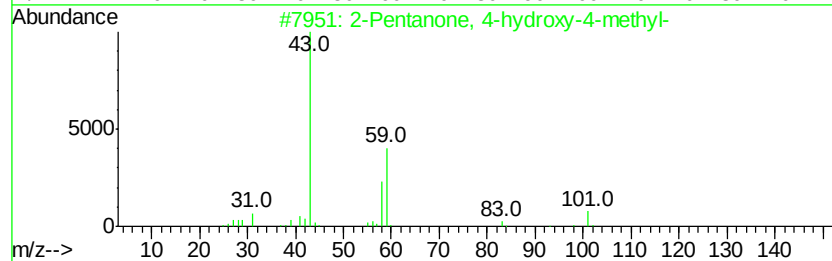
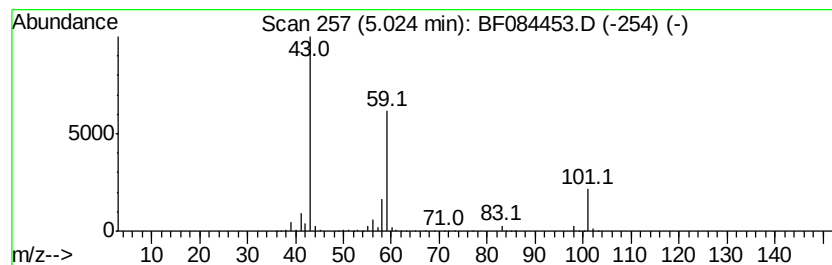
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 5.02 | 38.25 ng | 2832900 | 1,4-Dichlorobenzene-d4 | 6.83 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 39   |
| 3    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 4    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 5    |    | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |



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ClientSampled :  
PB87806BL

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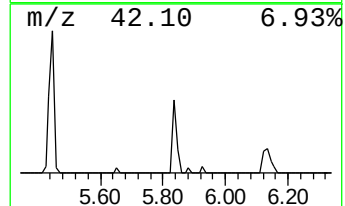
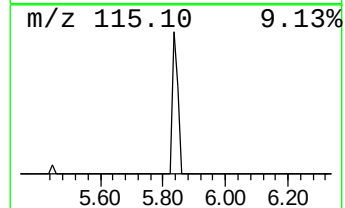
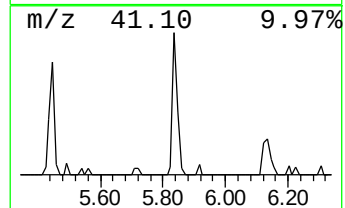
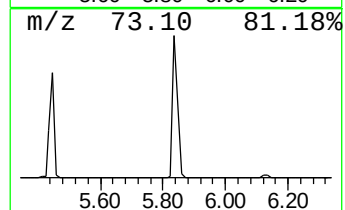
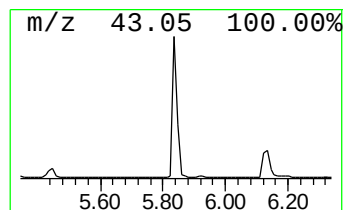
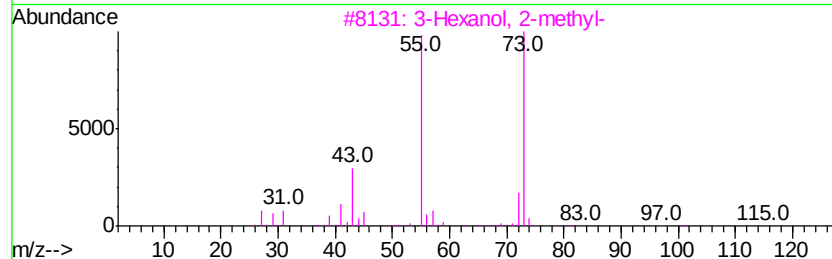
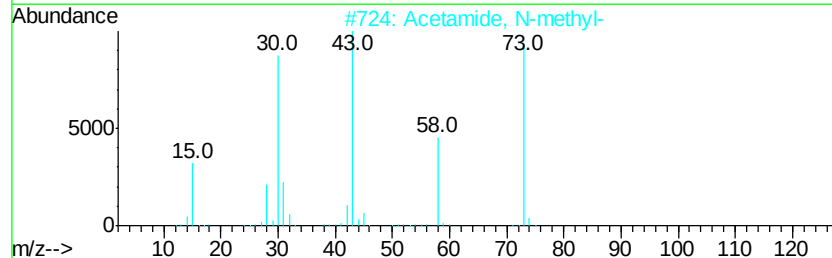
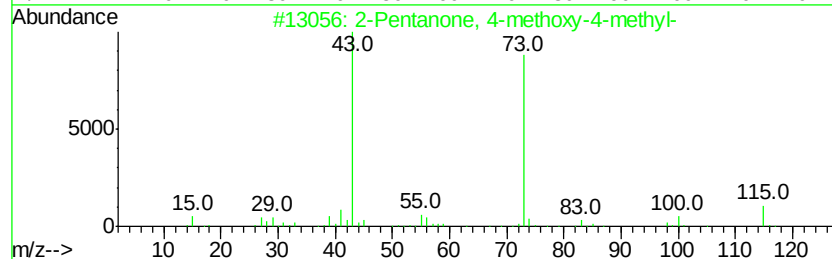
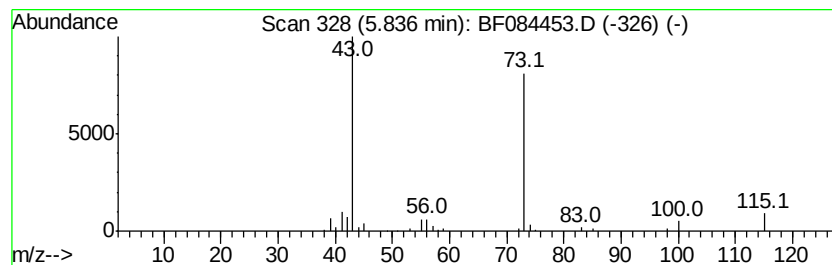
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.84 | 2.31 ng | 170805 | 1,4-Dichlorobenzene-d4 | 6.83 |

| Hit# | of | Tentative ID                      | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-methoxy-4-methyl-  | 130 | C7H14O2 | 000107-70-0 | 83   |
| 2    |    | Acetamide, N-methyl-              | 73  | C3H7NO  | 000079-16-3 | 32   |
| 3    |    | 3-Hexanol, 2-methyl-              | 116 | C7H16O  | 000617-29-8 | 17   |
| 4    |    | 2-Pentanone, 3-methyl-            | 100 | C6H12O  | 000565-61-7 | 16   |
| 5    |    | 1,3-Dioxolane, 2-(1-methylethyl)- | 116 | C6H12O2 | 000822-83-3 | 12   |



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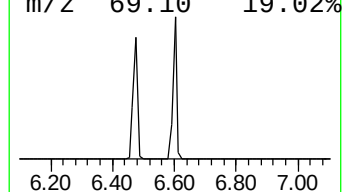
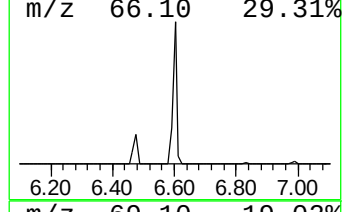
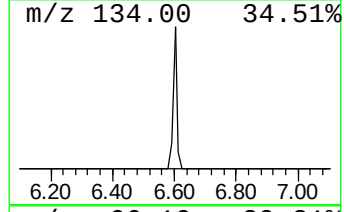
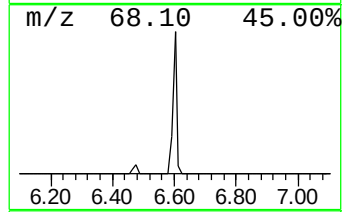
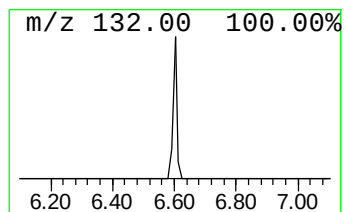
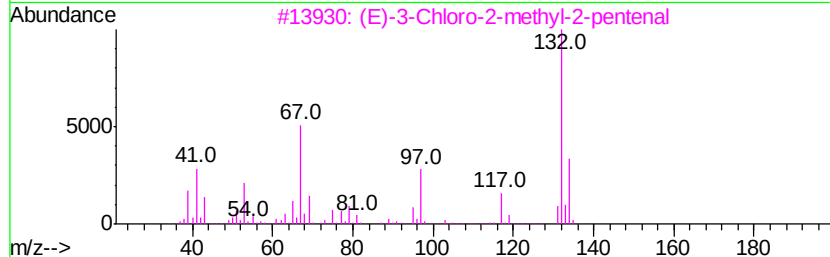
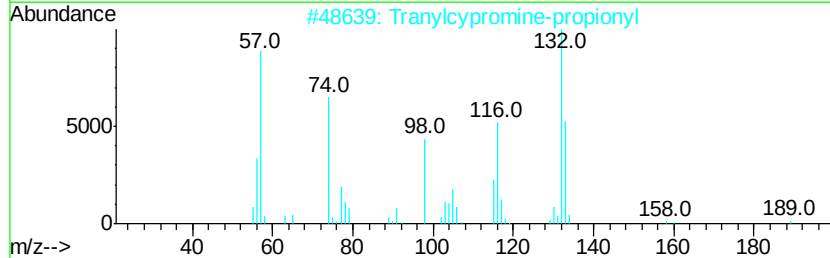
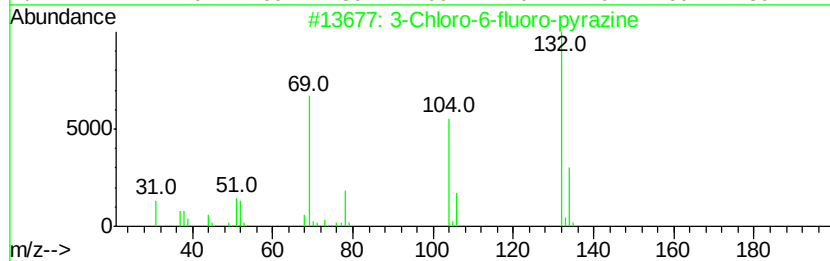
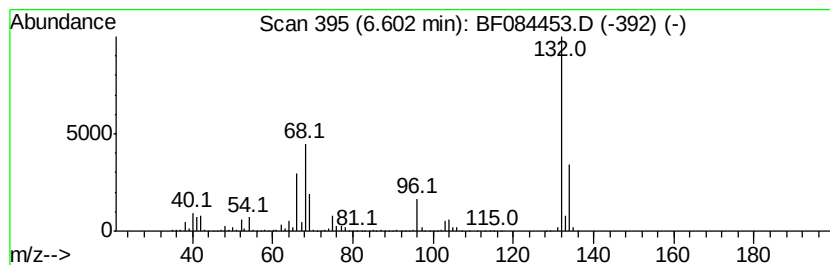
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Peak Number 4 unknown6.60 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.60 | 71.30 ng | 5281380 | 1,4-Dichlorobenzene-d4 | 6.83 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 3    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 9    |
| 4    |    | Benzene, 1,2,4-trifluoro-        | 132 | C6H3F3    | 000367-23-7  | 9    |
| 5    |    | Benzene, 1,3,5-trifluoro-        | 132 | C6H3F3    | 000372-38-3  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |         |      |
|----------------------|------|---------|-------|----------|-----------------------|------|---------|------|
|                      |      |         |       |          | #                     | RT   | Resp    | Conc |
| 3-Penten-2-one, 4... | 4.36 | 3.1 ng  |       | 232711   | 1                     | 6.83 | 1481440 | 20.0 |
| 2-Pentanone, 4-hy... | 5.02 | 38.3 ng |       | 2832900  | 1                     | 6.83 | 1481440 | 20.0 |
| 2-Pentanone, 4-me... | 5.84 | 2.3 ng  |       | 170805   | 1                     | 6.83 | 1481440 | 20.0 |
| unknown6.60          | 6.60 | 71.3 ng |       | 5281380  | 1                     | 6.83 | 1481440 | 20.0 |