

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF022317\  
 Data File : BF093143.D  
 Acq On : 24 Feb 2017 11:07  
 Operator : SJ/MA  
 Sample : I1947-02  
 Misc :  
 ALS Vial : 39 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 022117-PRRT-E-U-M

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-BF013017.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         | 5.001       | 253           | 255         | 265          | rBV      | 265443         | 448870        | 10.73%          | 1.869%        |
| 2         | 5.424       | 291           | 292         | 295          | rBV      | 856545         | 1208036       | 28.87%          | 5.031%        |
| 3         | 6.476       | 381           | 384         | 393          | rBV      | 770505         | 831550        | 19.87%          | 3.463%        |
| 4         | 6.602       | 393           | 395         | 398          | rBV      | 1964189        | 2126303       | 50.81%          | 8.856%        |
| 5         | 6.842       | 413           | 416         | 418          | rBV      | 964684         | 918862        | 21.96%          | 3.827%        |
| 6         | 7.002       | 427           | 430         | 432          | rBV      | 2683999        | 3194951       | 76.34%          | 13.306%       |
| 7         | 7.413       | 463           | 466         | 468          | rBV      | 2683173        | 2599746       | 62.12%          | 10.827%       |
| 8         | 8.133       | 526           | 529         | 531          | rBV      | 834550         | 1097275       | 26.22%          | 4.570%        |
| 9         | 9.208       | 620           | 623         | 625          | rBV      | 4029314        | 4185113       | 100.00%         | 17.430%       |
| 10        | 9.596       | 655           | 657         | 661          | rBV      | 59471          | 59264         | 1.42%           | 0.247%        |
| 11        | 9.882       | 679           | 682         | 684          | rBV      | 1040372        | 1052839       | 25.16%          | 4.385%        |
| 12        | 10.671      | 748           | 751         | 753          | rBV      | 905253         | 1108972       | 26.50%          | 4.619%        |
| 13        | 10.785      | 759           | 761         | 765          | rBV      | 46816          | 68212         | 1.63%           | 0.284%        |
| 14        | 11.356      | 809           | 811         | 814          | rBV2     | 692081         | 823042        | 19.67%          | 3.428%        |
| 15        | 12.945      | 947           | 950         | 952          | rBV      | 2918204        | 2629775       | 62.84%          | 10.953%       |
| 16        | 13.848      | 1026          | 1029        | 1037         | rBV2     | 17329          | 45751         | 1.09%           | 0.191%        |
| 17        | 13.997      | 1039          | 1042        | 1045         | rBV      | 959011         | 867163        | 20.72%          | 3.612%        |
| 18        | 15.425      | 1164          | 1167        | 1170         | rBV      | 613139         | 744888        | 17.80%          | 3.102%        |

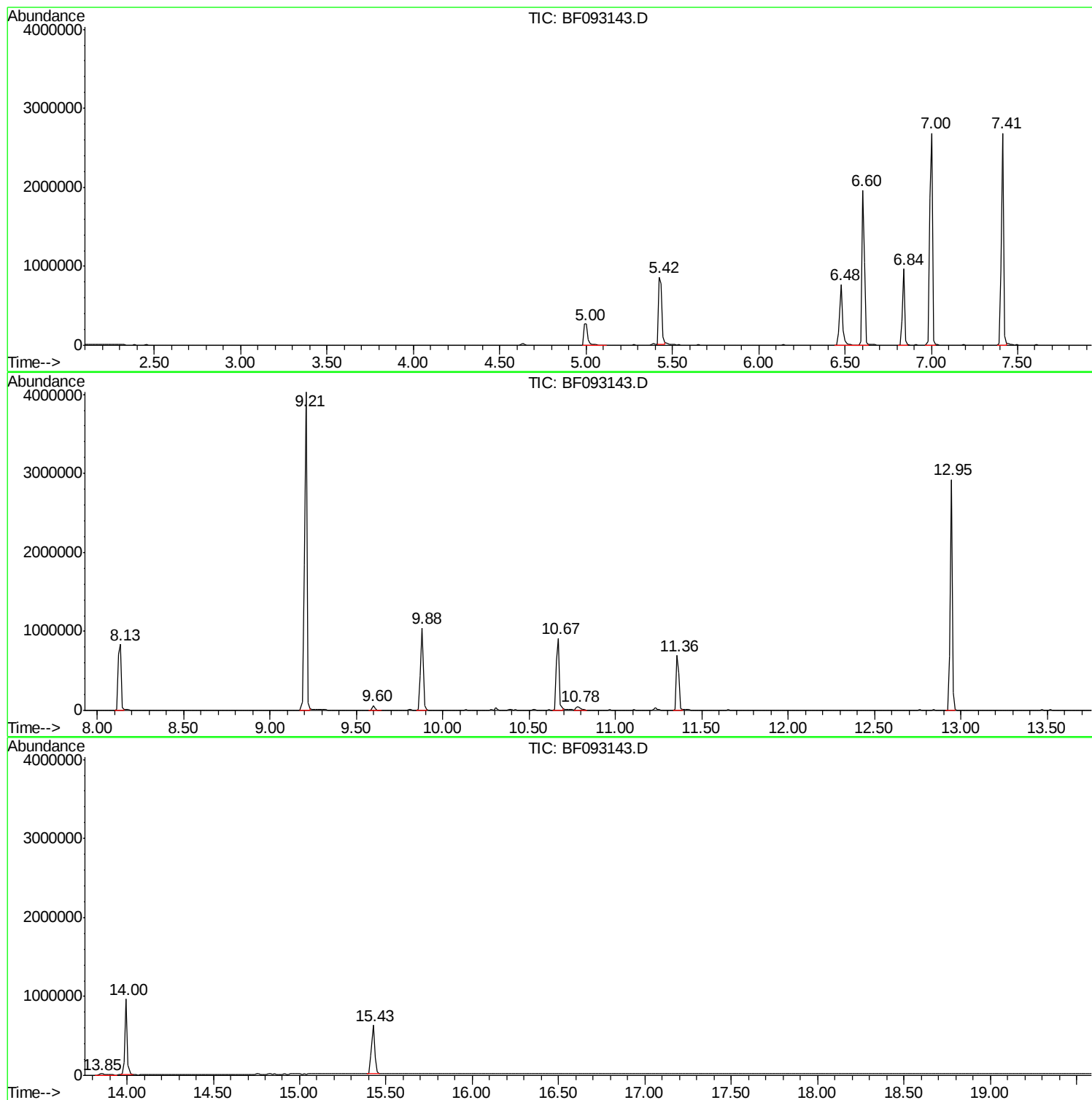
Sum of corrected areas: 24010612

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



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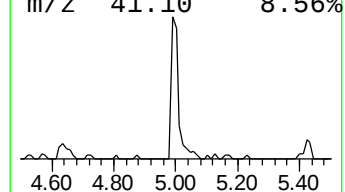
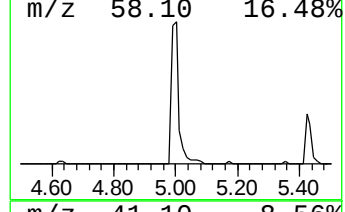
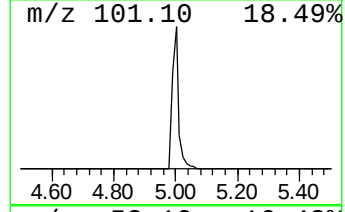
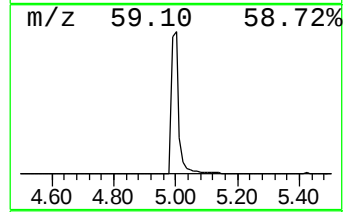
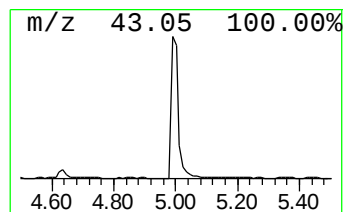
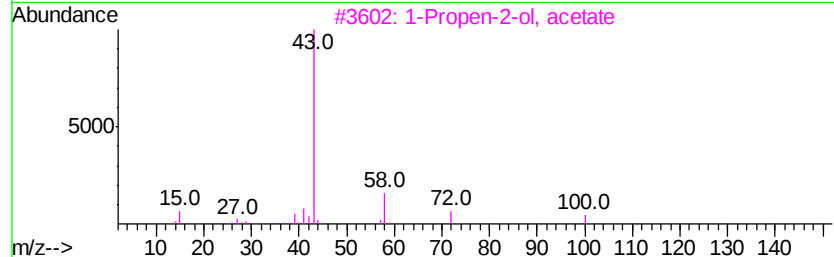
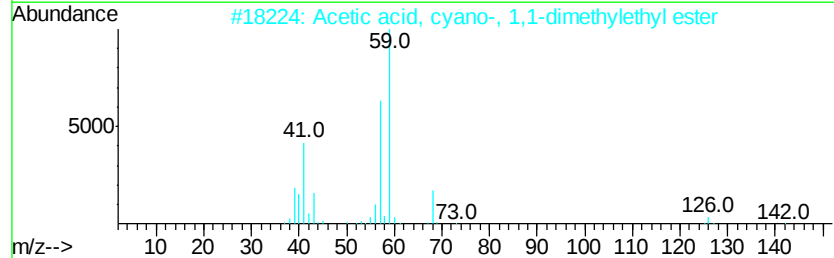
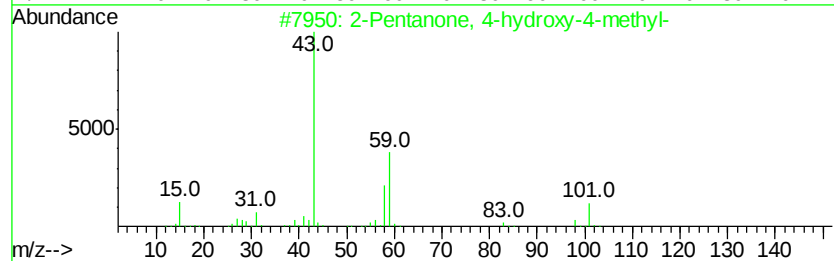
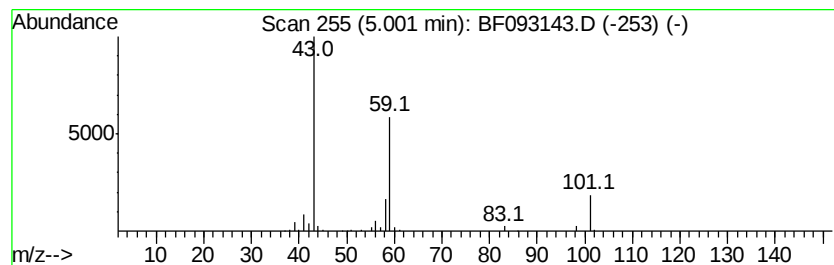
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.00 | 9.77 ng | 448870 | 1,4-Dichlorobenzene-d4 | 6.84 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 64   |
| 2    |    |   | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 3    |    |   | 1-Propen-2-ol, acetate               | 100 | C5H8O2   | 000108-22-5 | 10   |
| 4    |    |   | Acetic acid, 1,1-dimethylethyl e...  | 116 | C6H12O2  | 000540-88-5 | 9    |
| 5    |    |   | Propane, 1-ethoxy-2-methyl-          | 102 | C6H14O   | 000627-02-1 | 9    |



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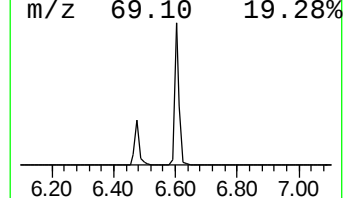
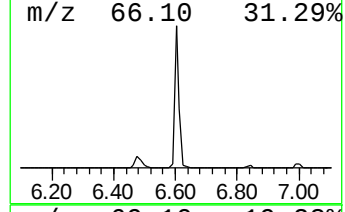
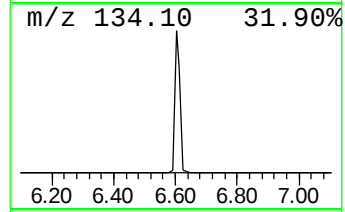
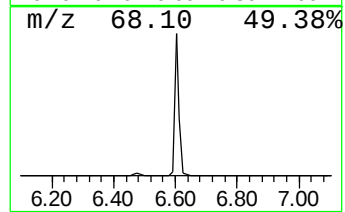
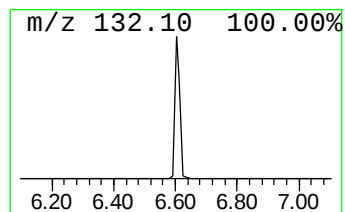
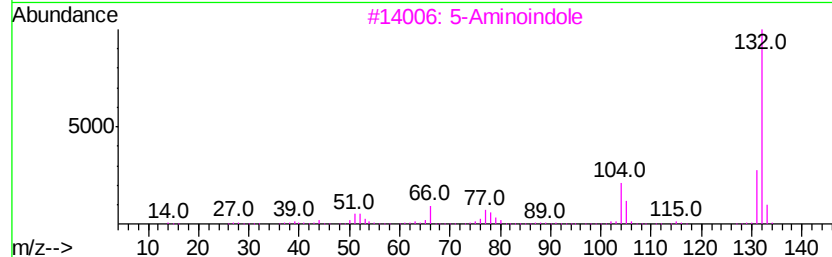
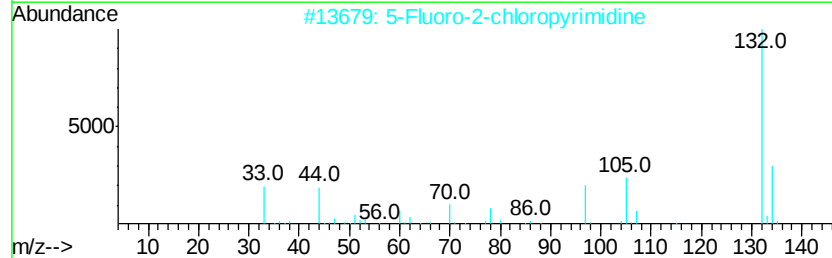
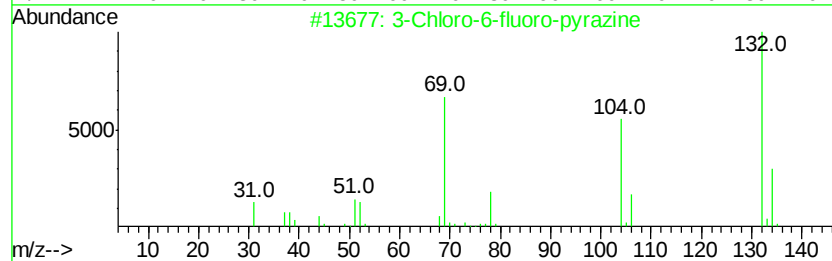
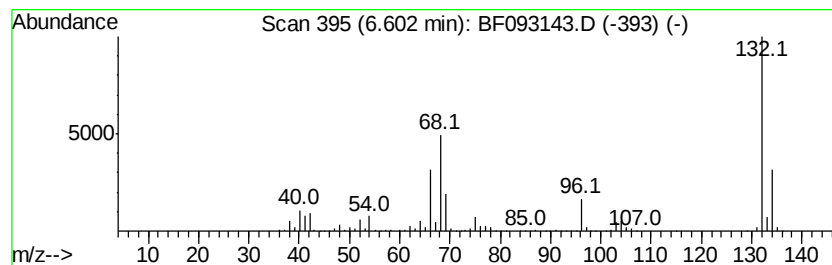
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Peak Number 2 unknown6.60 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.60 | 46.28 ng | 2126300 | 1,4-Dichlorobenzene-d4 | 6.84 |

| Hit# | of | Tentative ID                | MW  | MolForm   | CAS#         | Qual |
|------|----|-----------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine  | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 3    |    | 5-Aminoindole               | 132 | C8H8N2    | 005192-03-0  | 10   |
| 4    |    | Benzene, 1,3,5-trifluoro-   | 132 | C6H3F3    | 000372-38-3  | 9    |
| 5    |    | Tranylcypromine-propionyl   | 189 | C12H15NO  | 1000123-86-3 | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.00 | 9.8     | ng    | 448870   | 1                     | 6.84 | 918862 | 20.0 |
| unknown6.60          | 6.60 | 46.3    | ng    | 2126300  | 1                     | 6.84 | 918862 | 20.0 |