

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030317\  
 Data File : BF093366.D  
 Acq On : 3 Mar 2017 18:44  
 Operator : SJ/MA  
 Sample : PB97309BL  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB97309BL

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         | 4.956       | 248           | 251         | 262          | rBV      | 574561         | 997388        | 18.92%          | 2.418%        |
| 2         | 5.390       | 286           | 289         | 291          | rBV      | 3768322        | 4745982       | 90.01%          | 11.505%       |
| 3         | 6.442       | 378           | 381         | 383          | rBV      | 2993387        | 4432916       | 84.07%          | 10.746%       |
| 4         | 6.556       | 388           | 391         | 393          | rBV      | 4386211        | 4241532       | 80.44%          | 10.282%       |
| 5         | 6.785       | 408           | 411         | 413          | rBV      | 1122655        | 1036049       | 19.65%          | 2.512%        |
| 6         | 6.945       | 422           | 425         | 427          | rBV      | 2742655        | 3464794       | 65.71%          | 8.399%        |
| 7         | 7.356       | 458           | 461         | 464          | rBV      | 2542545        | 2711611       | 51.43%          | 6.573%        |
| 8         | 8.076       | 521           | 524         | 526          | rBV      | 1308862        | 1483466       | 28.13%          | 3.596%        |
| 9         | 9.150       | 614           | 618         | 620          | rBV      | 4553481        | 5272848       | 100.00%         | 12.782%       |
| 10        | 9.825       | 674           | 677         | 679          | rBV      | 1315230        | 1556952       | 29.53%          | 3.774%        |
| 11        | 10.614      | 743           | 746         | 749          | rBV      | 2485689        | 2627944       | 49.84%          | 6.371%        |
| 12        | 11.299      | 804           | 806         | 809          | rBV      | 1220870        | 1572996       | 29.83%          | 3.813%        |
| 13        | 12.888      | 942           | 945         | 948          | rBV      | 3826085        | 4498633       | 85.32%          | 10.905%       |
| 14        | 13.940      | 1035          | 1037        | 1040         | rBV      | 1520358        | 1491974       | 28.30%          | 3.617%        |
| 15        | 15.357      | 1158          | 1161        | 1166         | rVB      | 900984         | 1116478       | 21.17%          | 2.707%        |

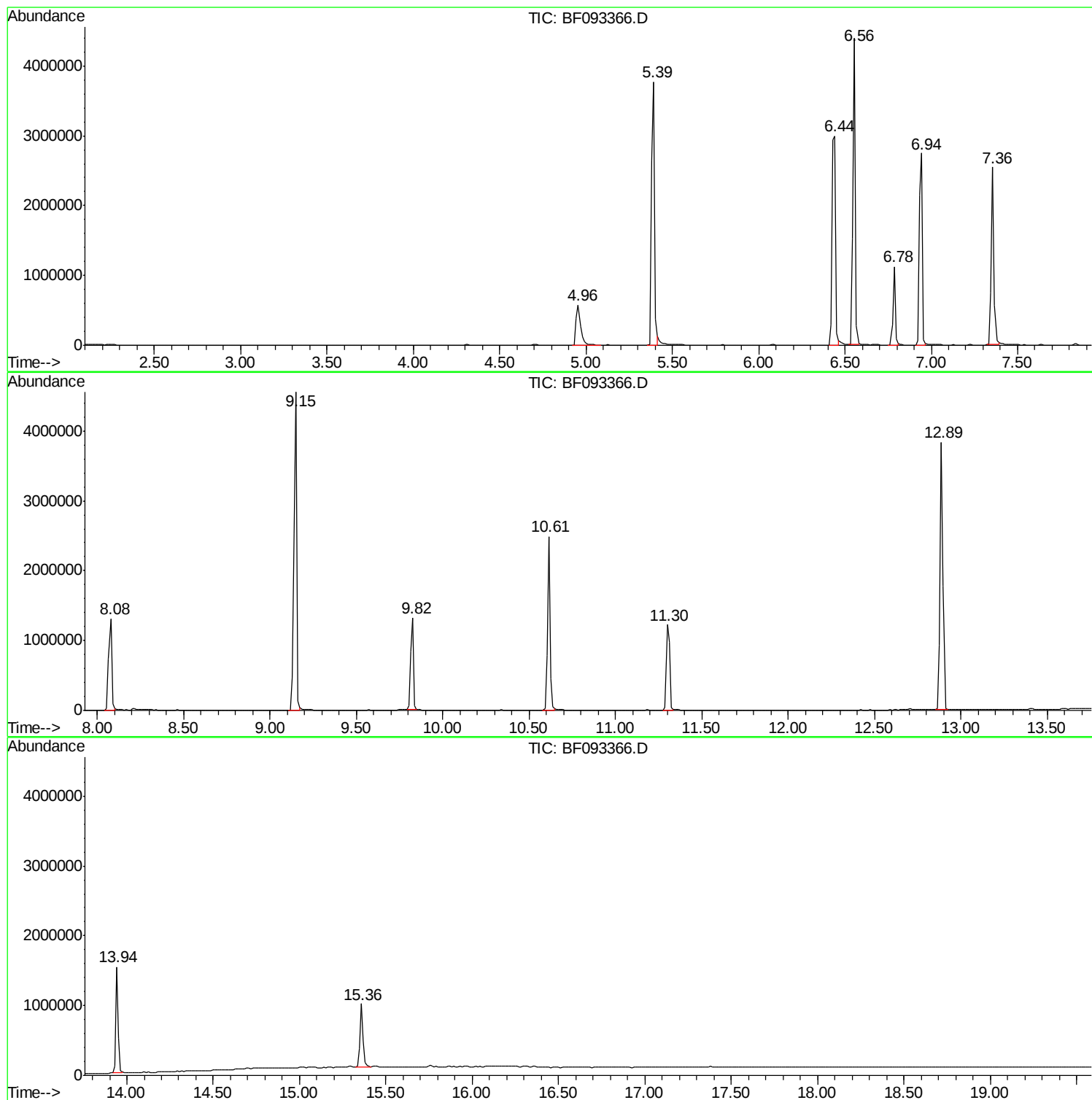
Sum of corrected areas: 41251563

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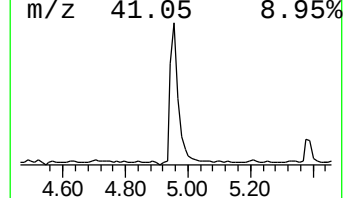
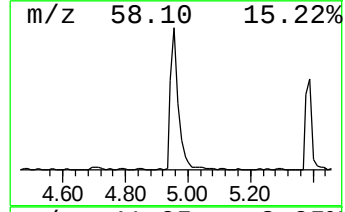
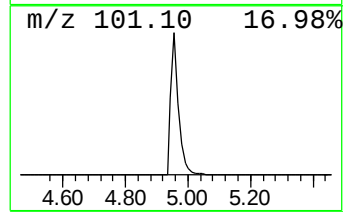
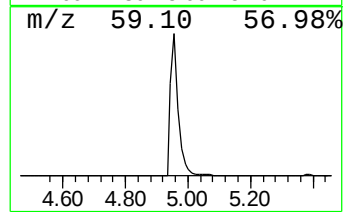
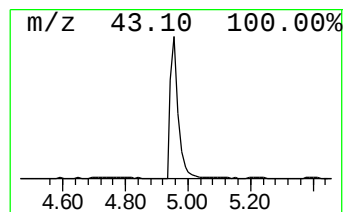
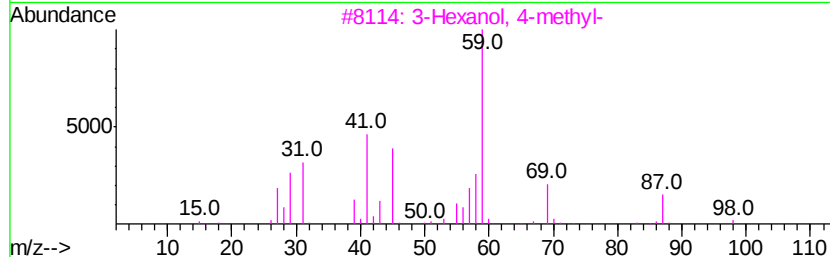
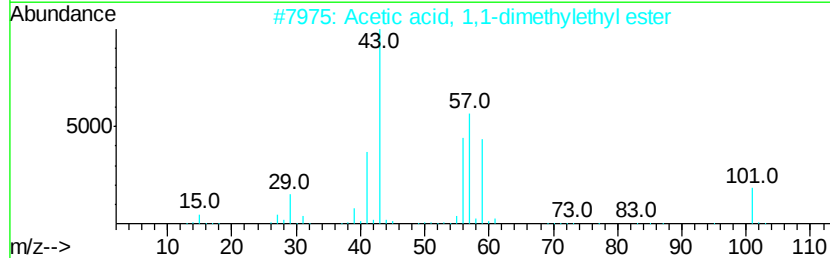
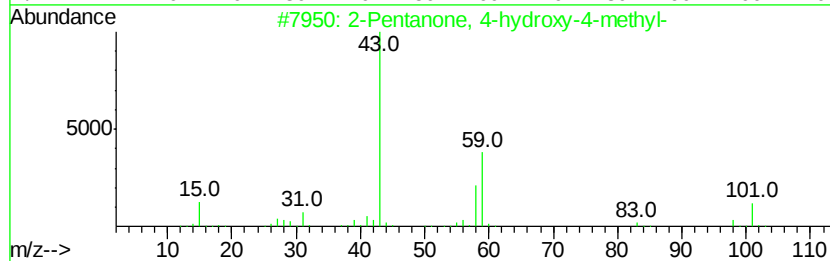
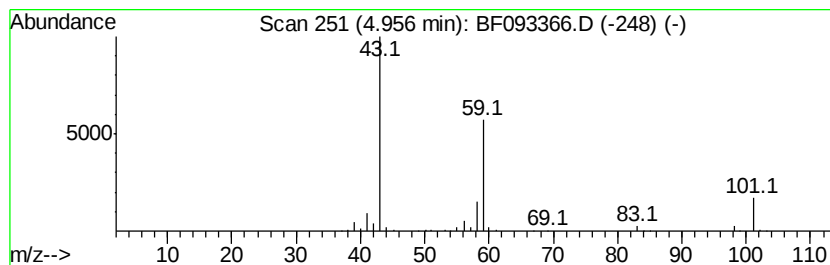
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|--------|------------------------|------|
| 4.96 | 19.25 ng | 997388 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 64   |
| 2    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 39   |
| 3    |    | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 33   |
| 4    |    | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 33   |
| 5    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |



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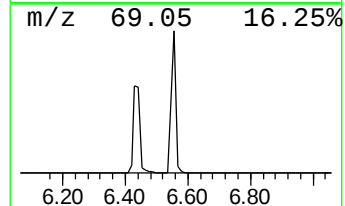
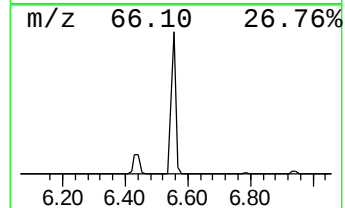
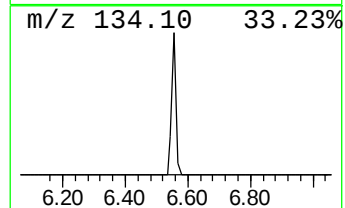
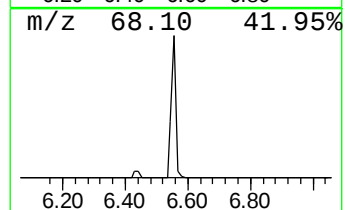
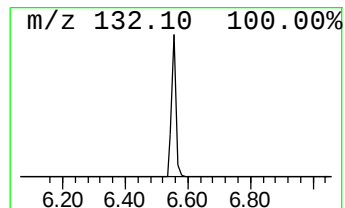
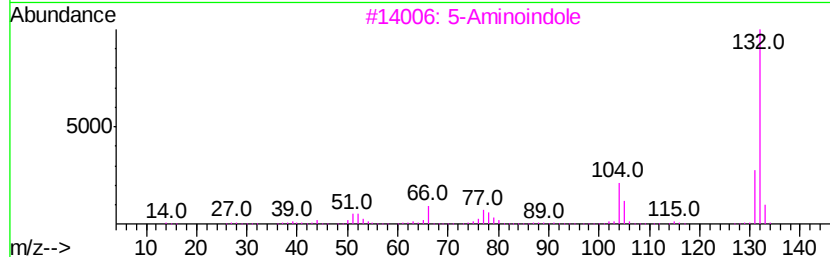
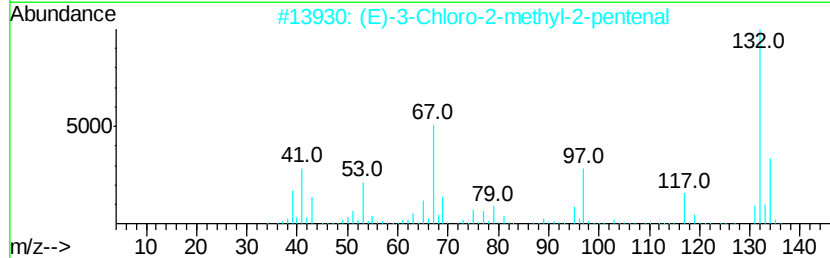
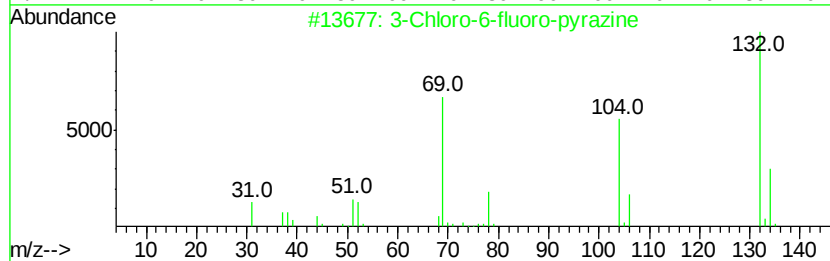
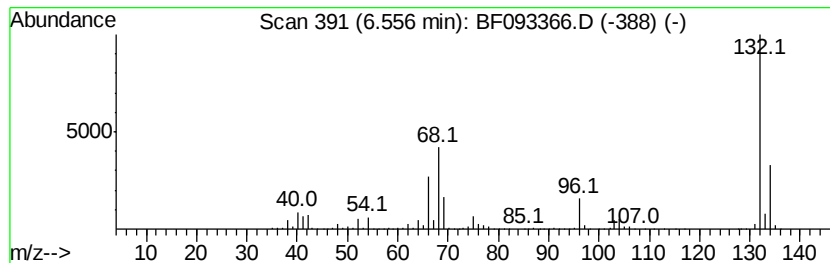
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Peak Number 2 unknown6.56 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.56 | 81.88 ng | 4241530 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 16   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4    | 019485-35-9  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | ---Internal Standard--- |      |         |      |
|----------------------|------|---------|-------|----------|-------------------------|------|---------|------|
|                      |      |         |       |          | #                       | RT   | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.96 | 19.3    | ng    | 997388   | 1                       | 6.78 | 1036050 | 20.0 |
| unknown6.56          | 6.56 | 81.9    | ng    | 4241530  | 1                       | 6.78 | 1036050 | 20.0 |