

Data Path : U:\HPCHEM1\BNA\_F\DATA\BF020518\  
 Data File : BF102755.D  
 Acq On : 5 Feb 2018 23:57  
 Operator : SJ/JU  
 Sample : PB106322BL  
 Misc :  
 ALS Vial : 28 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB106322BL

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-BF020318.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         | 2.216       | 18            | 22          | 28           | rVB      | 56328          | 84518         | 1.50%           | 0.189%        |
| 2         | 5.122       | 506           | 516         | 528          | rBV      | 359822         | 497883        | 8.85%           | 1.111%        |
| 3         | 5.504       | 575           | 581         | 584          | rBV      | 4975209        | 5489389       | 97.58%          | 12.248%       |
| 4         | 6.510       | 745           | 752         | 754          | rBV      | 4377122        | 5245972       | 93.25%          | 11.705%       |
| 5         | 6.651       | 771           | 776         | 779          | rBV      | 5068097        | 5308127       | 94.36%          | 11.844%       |
| 6         | 6.881       | 811           | 815         | 818          | rBV      | 1484358        | 1208839       | 21.49%          | 2.697%        |
| 7         | 7.040       | 837           | 842         | 845          | rVB      | 4380722        | 4120649       | 73.25%          | 9.194%        |
| 8         | 7.445       | 904           | 911         | 914          | rBV      | 3220061        | 3519205       | 62.56%          | 7.852%        |
| 9         | 8.163       | 1028          | 1033        | 1036         | rBV      | 1867232        | 1642864       | 29.20%          | 3.666%        |
| 10        | 9.239       | 1210          | 1216        | 1219         | rBV      | 5519006        | 5625610       | 100.00%         | 12.552%       |
| 11        | 9.916       | 1326          | 1331        | 1335         | rBV2     | 1847834        | 1667058       | 29.63%          | 3.720%        |
| 12        | 10.704      | 1460          | 1465        | 1469         | rBV      | 2748734        | 2895971       | 51.48%          | 6.462%        |
| 13        | 11.404      | 1580          | 1584        | 1587         | rBV      | 1752244        | 1427868       | 25.38%          | 3.186%        |
| 14        | 12.804      | 1819          | 1822        | 1825         | rBV      | 107962         | 82517         | 1.47%           | 0.184%        |
| 15        | 12.992      | 1849          | 1854        | 1857         | rBV      | 4081819        | 3929741       | 69.85%          | 8.768%        |
| 16        | 13.510      | 1939          | 1942        | 1946         | rVB      | 73342          | 56734         | 1.01%           | 0.127%        |
| 17        | 14.039      | 2028          | 2032        | 2036         | rBV      | 1108468        | 960651        | 17.08%          | 2.143%        |
| 18        | 15.516      | 2278          | 2283        | 2294         | rBV      | 661315         | 935903        | 16.64%          | 2.088%        |
| 19        | 15.986      | 2359          | 2363        | 2369         | rVB      | 34003          | 57183         | 1.02%           | 0.128%        |
| 20        | 16.504      | 2447          | 2451        | 2456         | rVB3     | 37444          | 61002         | 1.08%           | 0.136%        |

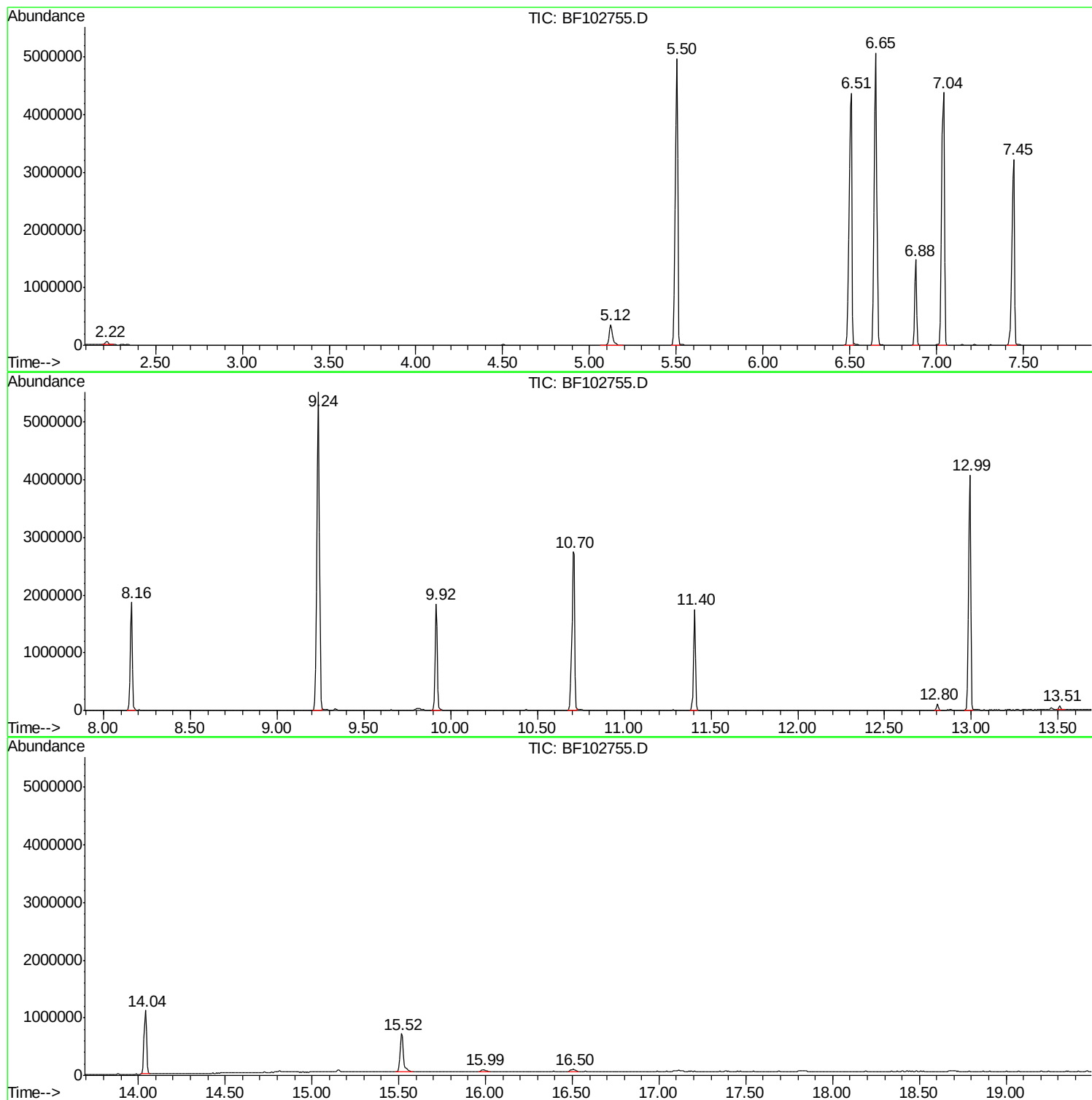
Sum of corrected areas: 44817684

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ClientSampleId :  
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF020318.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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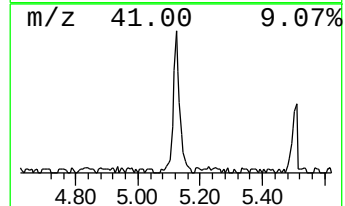
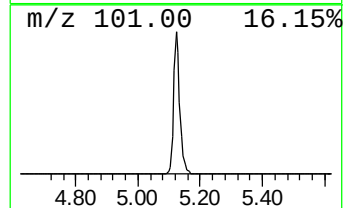
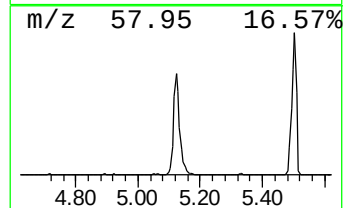
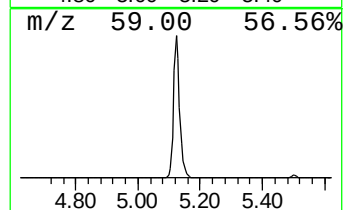
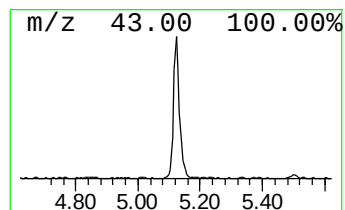
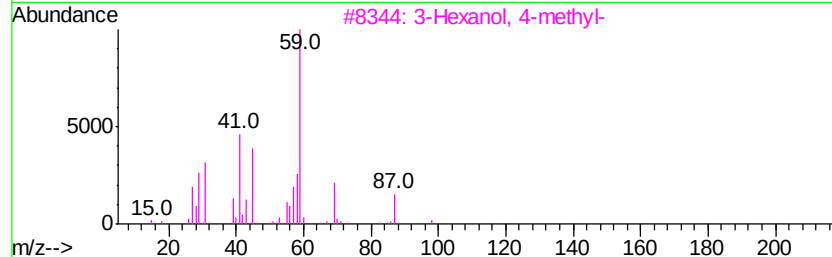
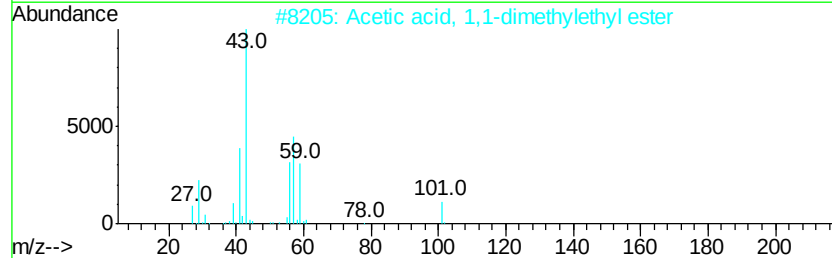
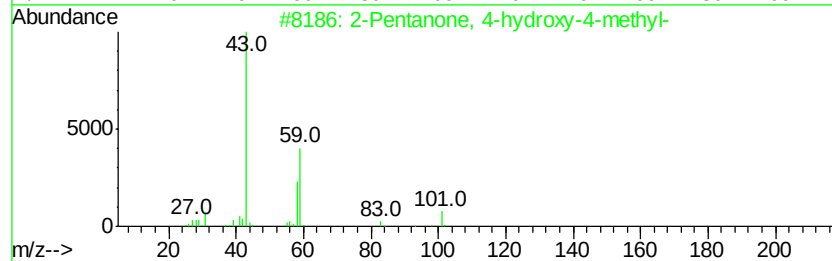
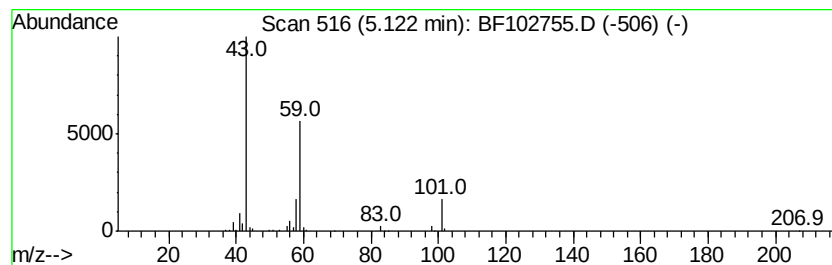
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TIC Integration Parameters: LSCINT.P

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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. |
|------|---------|--------|------------------------|------|
| 5.12 | 8.24 ng | 497883 | 1,4-Dichlorobenzene-d4 | 6.88 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 38   |
| 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 | 25   |



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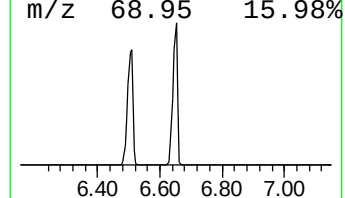
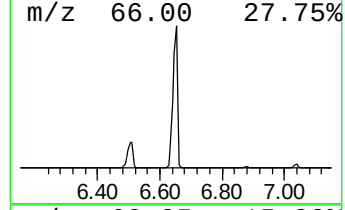
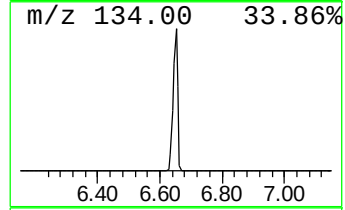
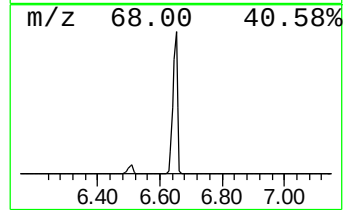
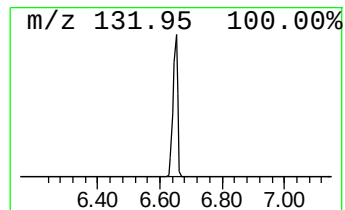
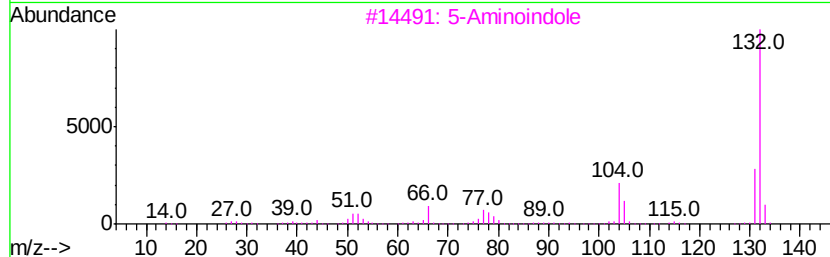
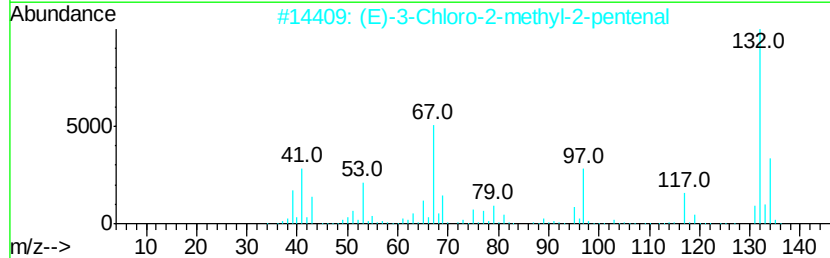
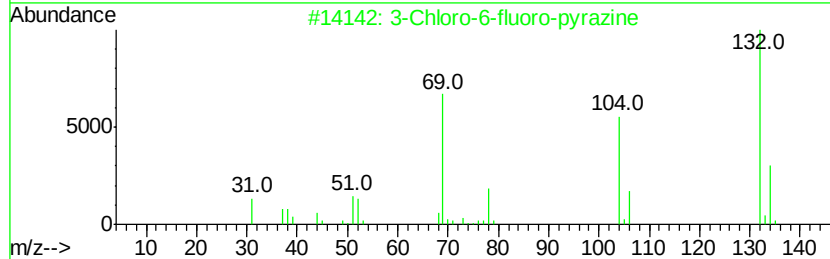
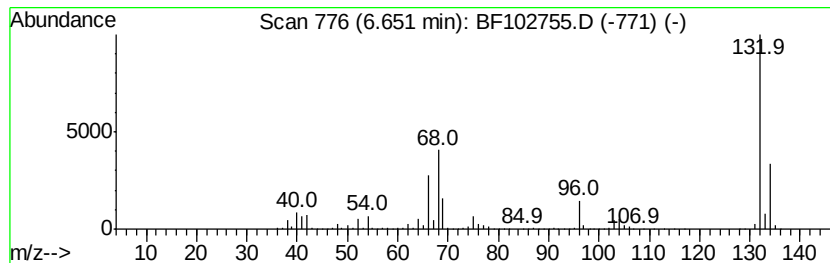
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Peak Number 2 unknown6.65 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.65 | 87.82 ng | 5308130 | 1,4-Dichlorobenzene-d4 | 6.88 |

| 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    |    | Benzene, 1-ethenyl-3,5-dimethyl-    | 132 | C10H12    | 005379-20-4  | 9    |
| 5    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |         |      |
|----------------------|------|---------|-------|----------|-----------------------|------|---------|------|
|                      |      |         |       |          | #                     | RT   | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.12 | 8.2     | ng    | 497883   | 1                     | 6.88 | 1208840 | 20.0 |
| unknown6.65          | 6.65 | 87.8    | ng    | 5308130  | 1                     | 6.88 | 1208840 | 20.0 |