

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF013118\  
 Data File : BF102662.D  
 Acq On : 31 Jan 2018 18:42  
 Operator : SJ/JU  
 Sample : PB106208BL  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB106208BL

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-BF012218.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         | 4.910       | 475           | 480         | 489          | rBV      | 152328         | 241244        | 5.84%           | 0.746%        |
| 2         | 5.322       | 546           | 550         | 573          | rBV      | 3131094        | 3575506       | 86.50%          | 11.051%       |
| 3         | 6.351       | 721           | 725         | 742          | rBV      | 3014411        | 3537567       | 85.58%          | 10.933%       |
| 4         | 6.475       | 742           | 746         | 750          | rBV      | 3643241        | 3506288       | 84.83%          | 10.837%       |
| 5         | 6.698       | 781           | 784         | 794          | rBV      | 879341         | 792180        | 19.16%          | 2.448%        |
| 6         | 6.857       | 807           | 811         | 814          | rBV      | 3146326        | 2771257       | 67.04%          | 8.565%        |
| 7         | 7.269       | 876           | 881         | 903          | rBV      | 2089475        | 2327906       | 56.32%          | 7.195%        |
| 8         | 7.981       | 998           | 1002        | 1017         | rBV      | 1049442        | 1121251       | 27.13%          | 3.465%        |
| 9         | 9.057       | 1180          | 1185        | 1200         | rBV      | 3684523        | 4133538       | 100.00%         | 12.775%       |
| 10        | 9.733       | 1295          | 1300        | 1310         | rBV2     | 1282530        | 1245800       | 30.14%          | 3.850%        |
| 11        | 10.527      | 1431          | 1435        | 1454         | rBV      | 2142940        | 2226421       | 53.86%          | 6.881%        |
| 12        | 11.222      | 1549          | 1553        | 1569         | rVB      | 1282112        | 1230214       | 29.76%          | 3.802%        |
| 13        | 12.804      | 1817          | 1822        | 1826         | rBV      | 3490082        | 3728665       | 90.21%          | 11.524%       |
| 14        | 13.857      | 1997          | 2001        | 2010         | rBV      | 992596         | 1018048       | 24.63%          | 3.146%        |
| 15        | 15.280      | 2238          | 2243        | 2254         | rBV      | 608741         | 855543        | 20.70%          | 2.644%        |
| 16        | 16.139      | 2386          | 2389        | 2396         | rVB4     | 24425          | 44517         | 1.08%           | 0.138%        |

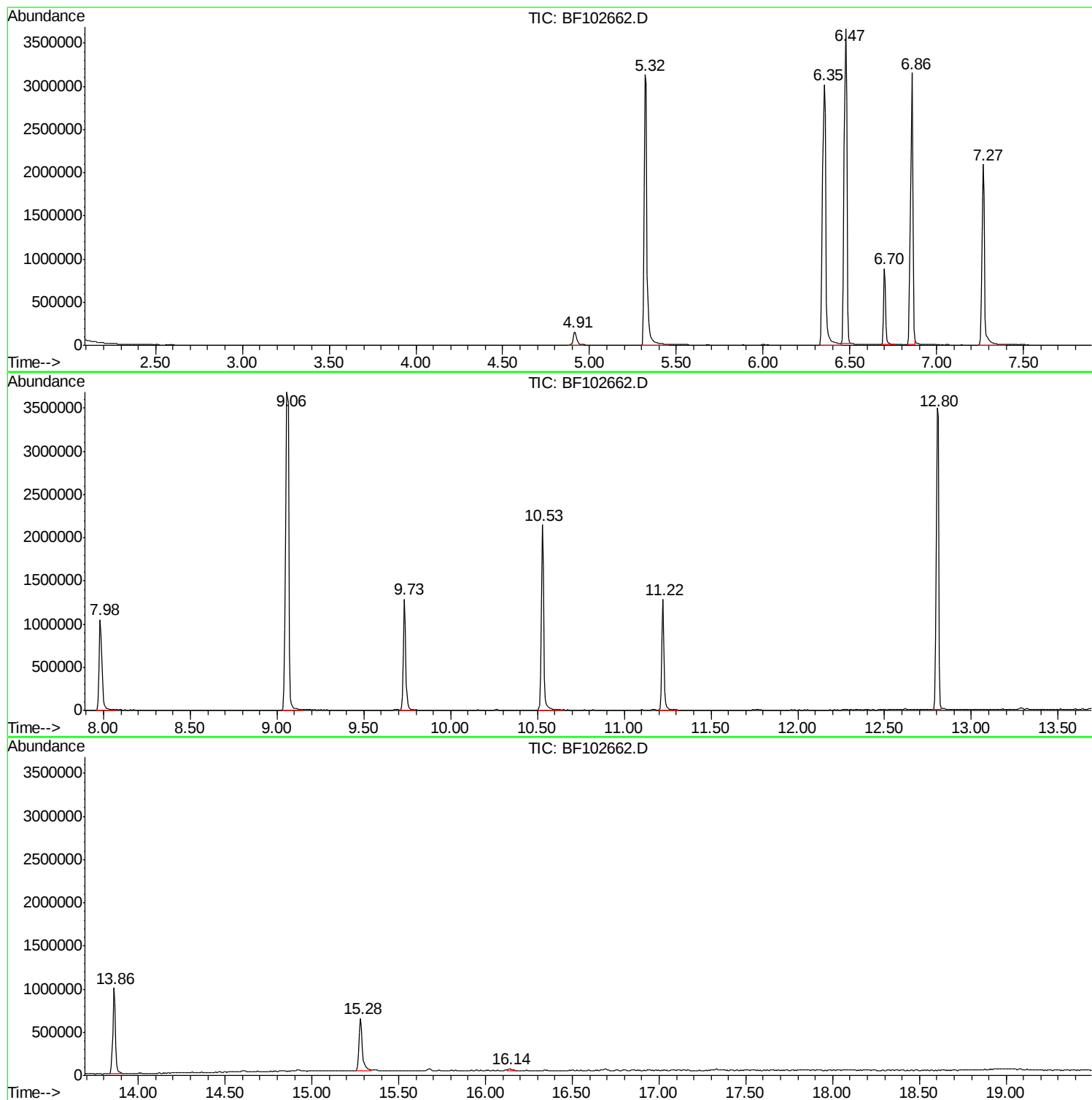
Sum of corrected areas: 32355945

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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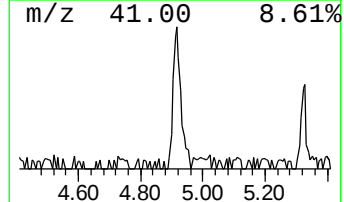
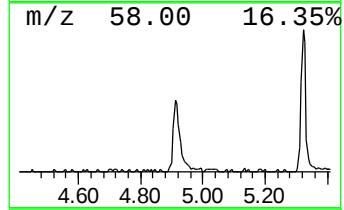
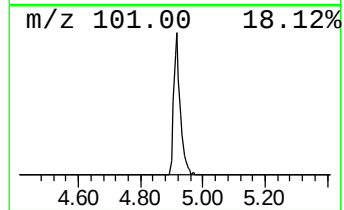
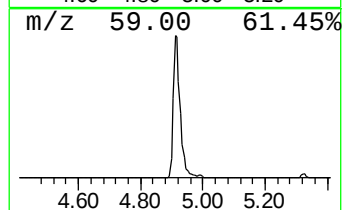
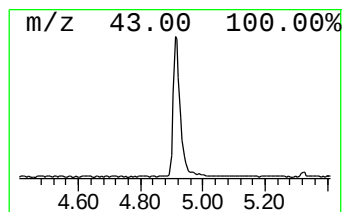
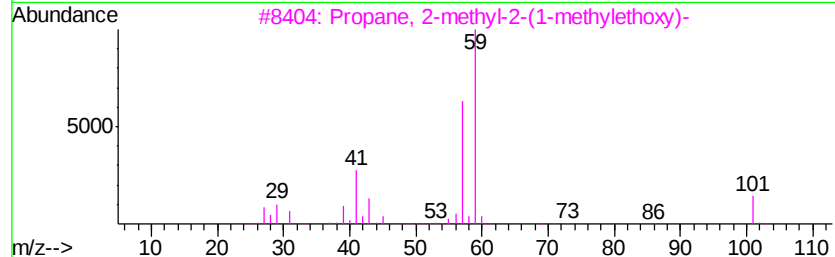
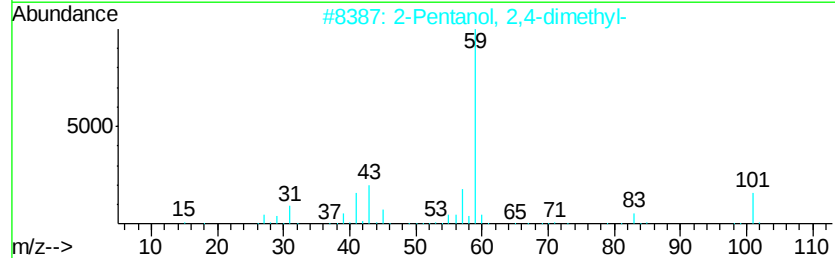
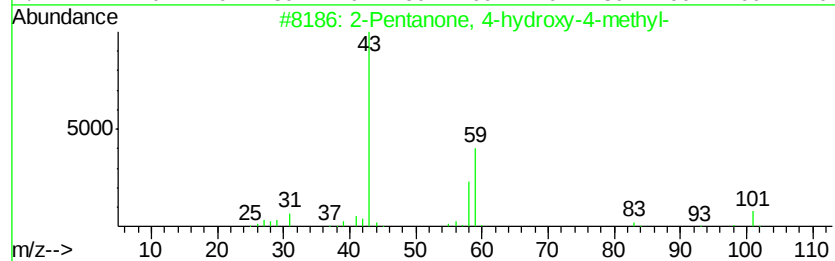
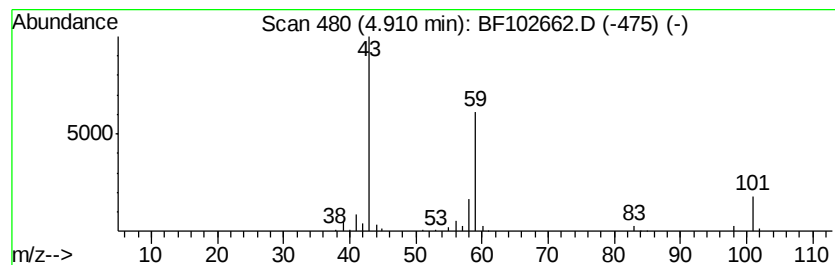
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF012218.M  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|---------|--------|------------------------|------|
| 4.91 | 6.09 ng | 241244 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# | of | 5 | Tentative ID                          | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-      | 116 | C6H12O2 | 000123-42-2 | 64   |
| 2    |    |   | 2-Pentanol, 2,4-dimethyl-             | 116 | C7H16O  | 000625-06-9 | 42   |
| 3    |    |   | Propane, 2-methyl-2-(1-methylethoxy)- | 116 | C7H16O  | 017348-59-3 | 42   |
| 4    |    |   | 2-Hexanol, 2-methyl-                  | 116 | C7H16O  | 000625-23-0 | 38   |
| 5    |    |   | 3-Hexanol                             | 102 | C6H14O  | 000623-37-0 | 33   |



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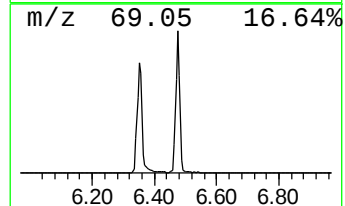
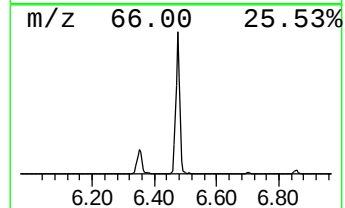
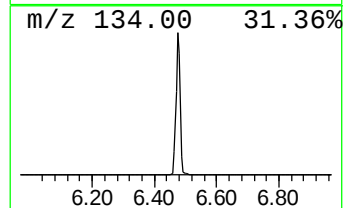
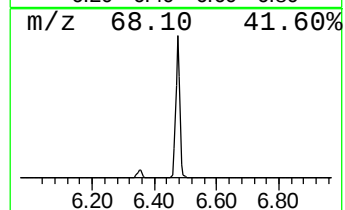
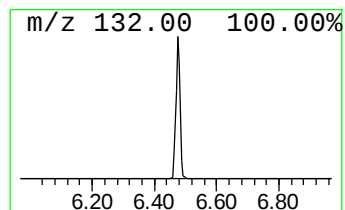
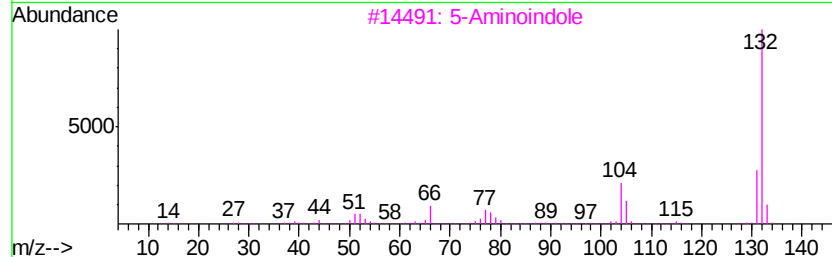
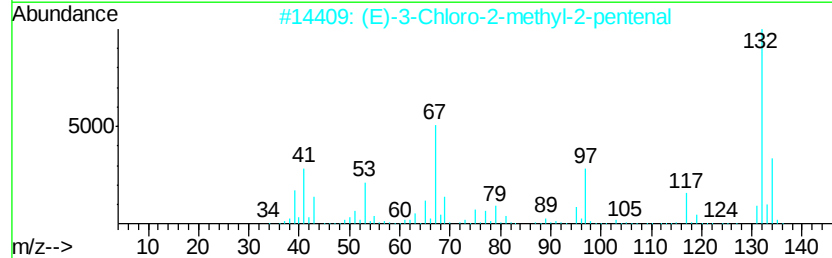
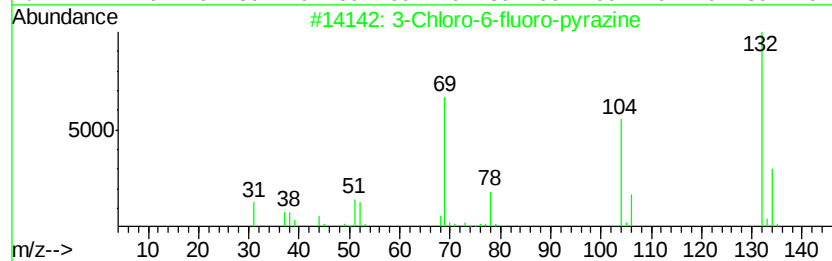
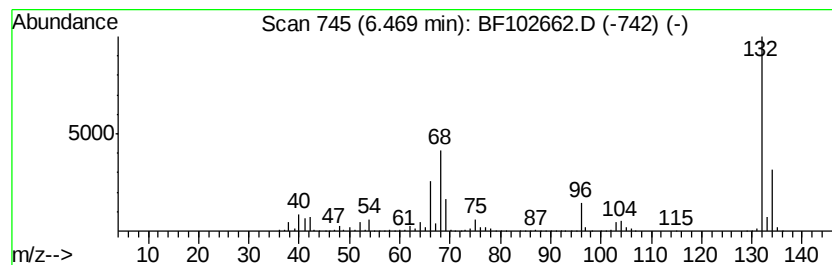
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Peak Number 2 unknown6.47 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.47 | 88.52 ng | 3506290 | 1,4-Dichlorobenzene-d4 | 6.70 |

| 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    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | ---Internal Standard--- |      |        |      |
|----------------------|------|---------|-------|----------|-------------------------|------|--------|------|
|                      |      |         |       |          | #                       | RT   | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.91 | 6.1     | ng    | 241244   | 1                       | 6.70 | 792180 | 20.0 |
| unknown6.47          | 6.47 | 88.5    | ng    | 3506290  | 1                       | 6.70 | 792180 | 20.0 |