

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF101717\  
 Data File : BF099591.D  
 Acq On : 17 Oct 2017 19:56  
 Operator : SJ/JU  
 Sample : I5869-08  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 DUP-01-10-11-17

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-BF092317.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         | 2.469       | 55            | 65          | 73           | rVB      | 138736         | 213334        | 6.22%           | 0.990%        |
| 2         | 5.051       | 501           | 504         | 518          | rBV      | 117873         | 155746        | 4.54%           | 0.722%        |
| 3         | 5.451       | 568           | 572         | 587          | rBV      | 1467344        | 1422536       | 41.46%          | 6.599%        |
| 4         | 6.457       | 740           | 743         | 755          | rBV      | 888509         | 943255        | 27.49%          | 4.376%        |
| 5         | 6.598       | 763           | 767         | 770          | rBV      | 2604555        | 2459918       | 71.70%          | 11.411%       |
| 6         | 6.828       | 802           | 806         | 813          | rBB      | 706951         | 644872        | 18.80%          | 2.991%        |
| 7         | 6.981       | 828           | 832         | 836          | rBV      | 2409895        | 2409024       | 70.22%          | 11.175%       |
| 8         | 7.398       | 897           | 903         | 906          | rBV      | 1669448        | 1894093       | 55.21%          | 8.786%        |
| 9         | 8.104       | 1019          | 1023        | 1027         | rBV      | 937532         | 883637        | 25.76%          | 4.099%        |
| 10        | 9.181       | 1200          | 1206        | 1210         | rBV      | 3136193        | 3430757       | 100.00%         | 15.914%       |
| 11        | 9.575       | 1270          | 1273        | 1276         | rBV      | 76487          | 56892         | 1.66%           | 0.264%        |
| 12        | 9.863       | 1317          | 1322        | 1325         | rBV      | 1082557        | 950961        | 27.72%          | 4.411%        |
| 13        | 10.651      | 1452          | 1456        | 1460         | rBV      | 1454924        | 1492989       | 43.52%          | 6.926%        |
| 14        | 11.351      | 1571          | 1575        | 1578         | rBV      | 943937         | 862050        | 25.13%          | 3.999%        |
| 15        | 12.933      | 1839          | 1844        | 1847         | rBV      | 2607291        | 2439124       | 71.10%          | 11.314%       |
| 16        | 13.810      | 1990          | 1993        | 1998         | rBV      | 49421          | 52715         | 1.54%           | 0.245%        |
| 17        | 13.986      | 2020          | 2023        | 2028         | rBV      | 624954         | 609530        | 17.77%          | 2.827%        |
| 18        | 15.451      | 2266          | 2272        | 2280         | rVB      | 516487         | 636135        | 18.54%          | 2.951%        |

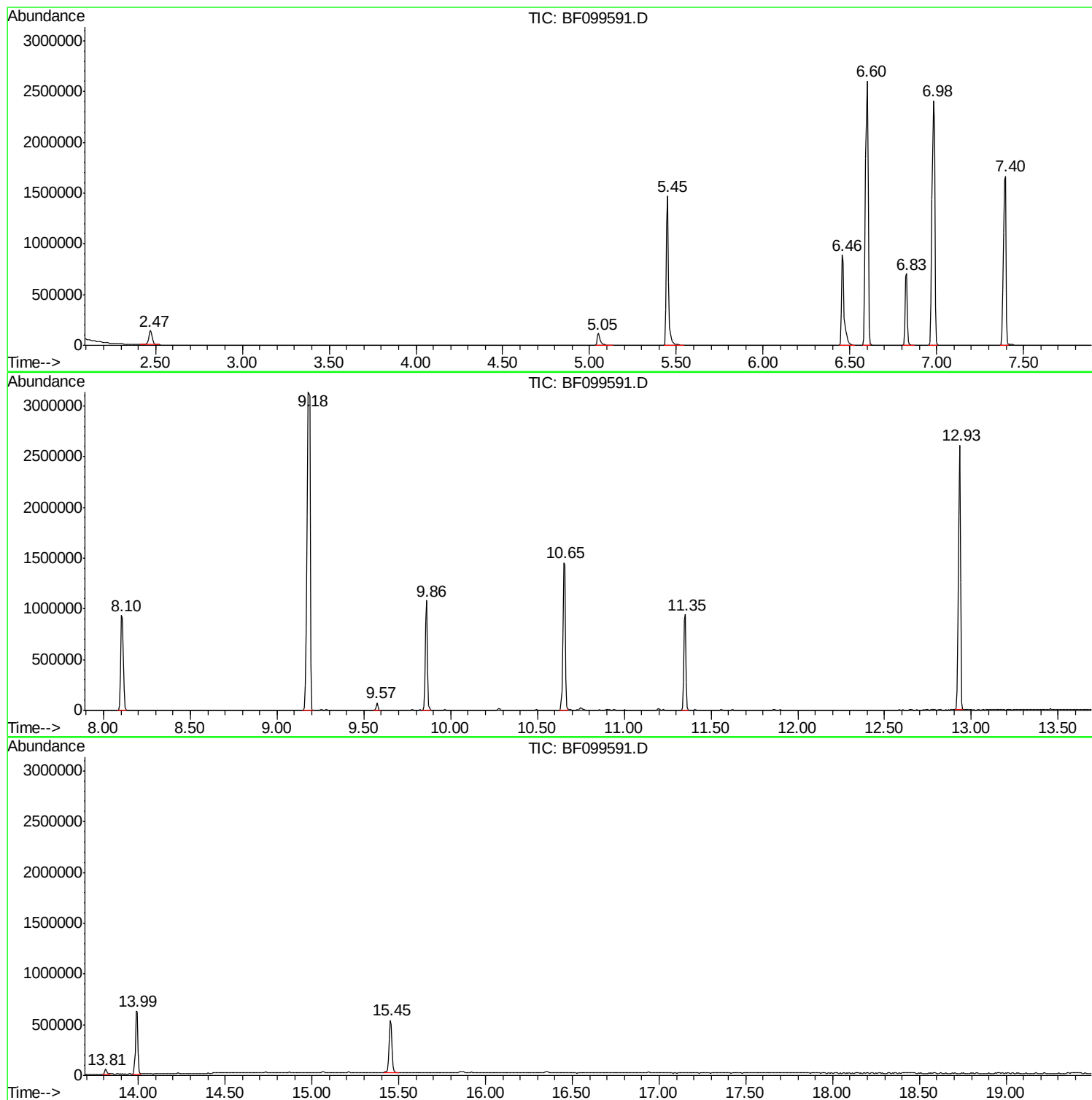
Sum of corrected areas: 21557568

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



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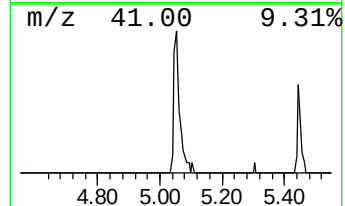
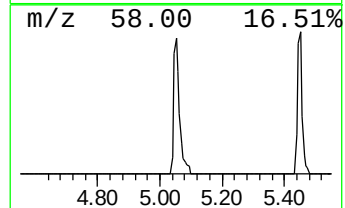
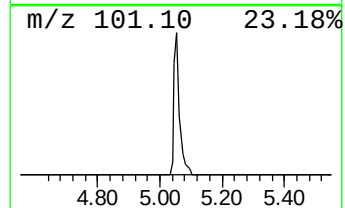
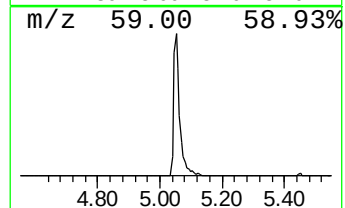
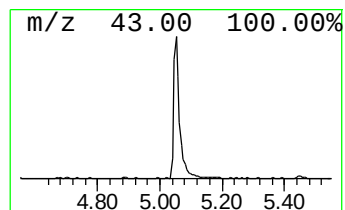
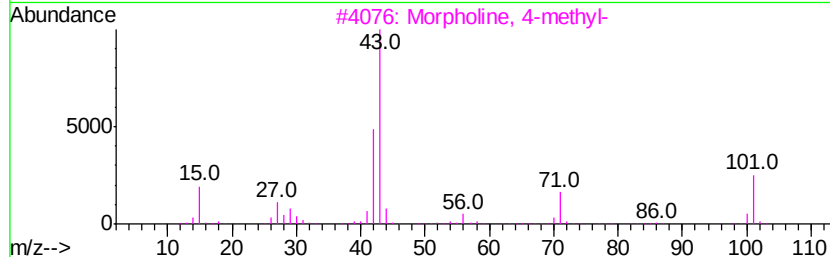
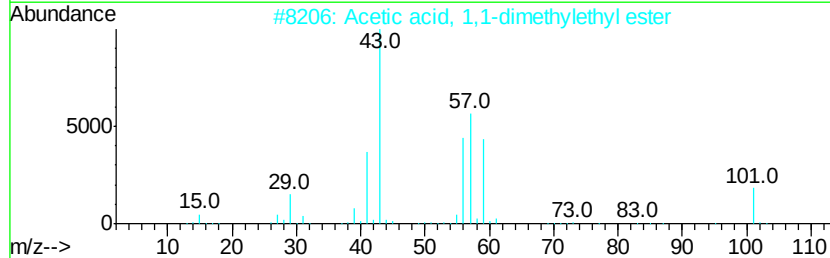
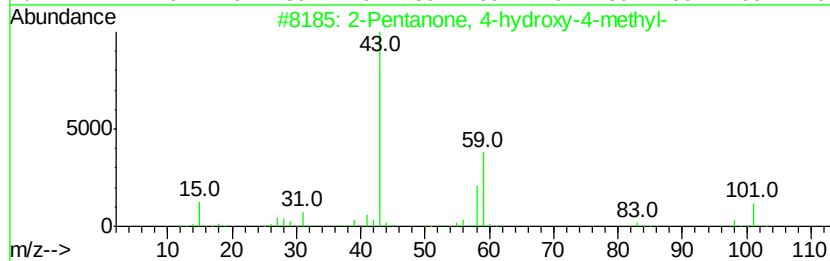
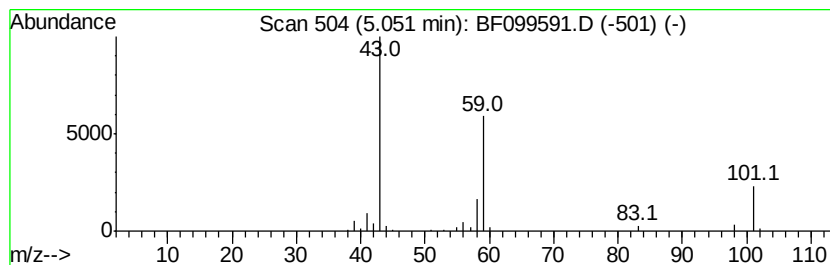
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.    | EstConc                             | Area         | Relative to ISTD       | R.T.        |      |      |
|---------|-------------------------------------|--------------|------------------------|-------------|------|------|
| 5.05    | 4.83 ng                             | 155746       | 1,4-Dichlorobenzene-d4 | 6.83        |      |      |
| Hit# of | 5                                   | Tentative ID | MW                     | MolForm     | CAS# | Qual |
| 1       | 2-Pentanone, 4-hydroxy-4-methyl-    | 116          | C6H12O2                | 000123-42-2 | 72   |      |
| 2       | Acetic acid, 1,1-dimethylethyl e... | 116          | C6H12O2                | 000540-88-5 | 39   |      |
| 3       | Morpholine, 4-methyl-               | 101          | C5H11NO                | 000109-02-4 | 9    |      |
| 4       | Butane, 1-ethoxy-                   | 102          | C6H14O                 | 000628-81-9 | 9    |      |
| 5       | Butanamide, 2-hydroxy-2,N-dimethyl- | 117          | C5H11NO2               | 039961-72-3 | 9    |      |



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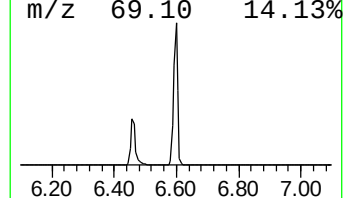
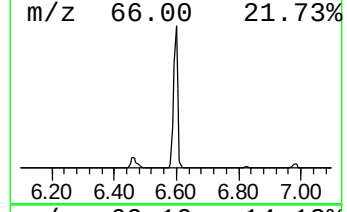
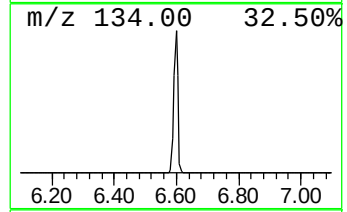
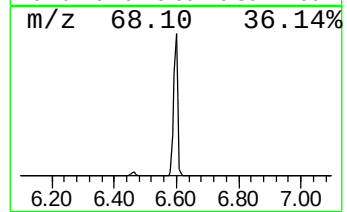
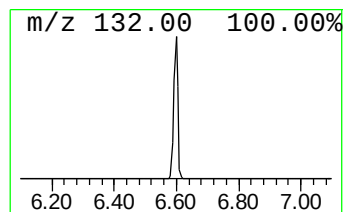
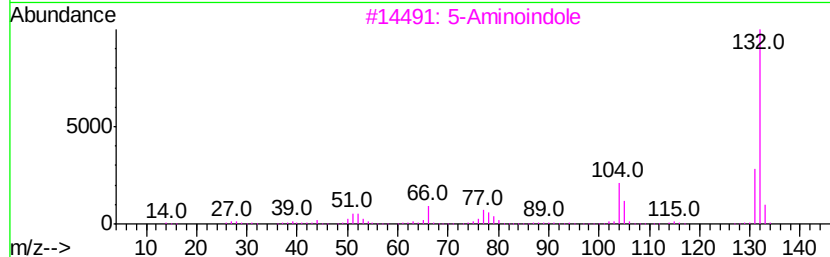
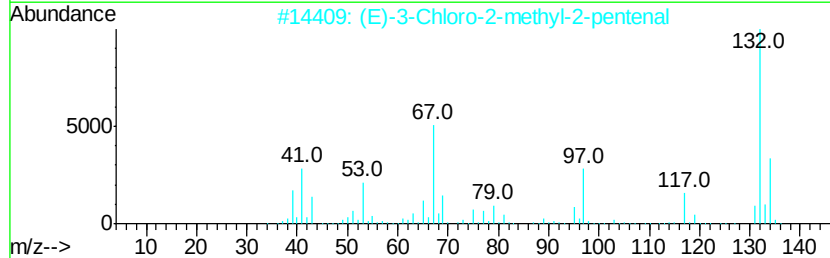
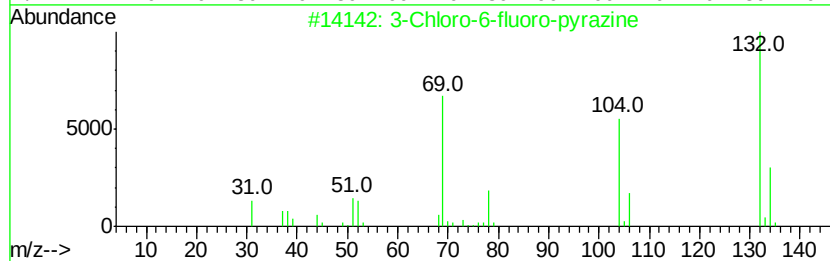
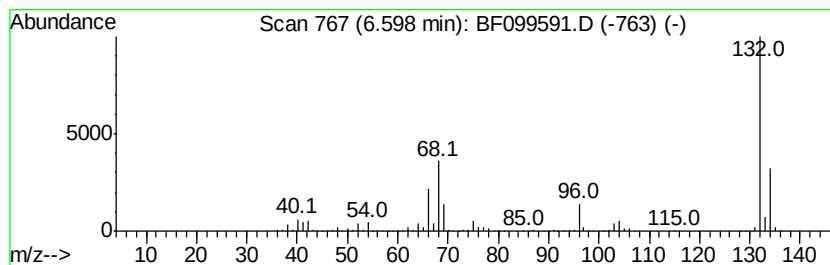
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Peak Number 3 unknown6.60 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.60 | 76.29 ng | 2459920 | 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 | 38   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 25   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 5    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.05 | 4.8     | ng    | 155746   | 1                     | 6.83 | 644872 | 20.0 |
| unknown6.60          | 6.60 | 76.3    | ng    | 2459920  | 1                     | 6.83 | 644872 | 20.0 |