

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF092317\  
 Data File : BF098754.D  
 Acq On : 23 Sep 2017 22:23  
 Operator : SJ/JU  
 Sample : I5360-03 10X  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SP-1-B-COMP

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 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         | 5.133       | 515           | 518         | 526          | rBV      | 36848          | 40516         | 3.88%           | 0.454%        |
| 2         | 5.527       | 581           | 585         | 588          | rBV      | 314357         | 255879        | 24.52%          | 2.866%        |
| 3         | 6.527       | 751           | 755         | 760          | rBV      | 315105         | 249544        | 23.92%          | 2.795%        |
| 4         | 6.680       | 778           | 781         | 785          | rVB      | 305390         | 263039        | 25.21%          | 2.946%        |
| 5         | 6.922       | 818           | 822         | 825          | rBV      | 1053770        | 845670        | 81.05%          | 9.472%        |
| 6         | 7.074       | 844           | 848         | 851          | rBV      | 256054         | 201341        | 19.30%          | 2.255%        |
| 7         | 7.474       | 912           | 916         | 919          | rVB      | 177234         | 138586        | 13.28%          | 1.552%        |
| 8         | 8.204       | 1035          | 1040        | 1043         | rBV      | 1282112        | 1043449       | 100.00%         | 11.687%       |
| 9         | 9.274       | 1218          | 1222        | 1225         | rBV      | 332948         | 252569        | 24.21%          | 2.829%        |
| 10        | 9.351       | 1232          | 1235        | 1238         | rBV3     | 23994          | 24682         | 2.37%           | 0.276%        |
| 11        | 9.668       | 1286          | 1289        | 1292         | rBV2     | 51742          | 47732         | 4.57%           | 0.535%        |
| 12        | 9.821       | 1312          | 1315        | 1317         | rBV2     | 27777          | 28741         | 2.75%           | 0.322%        |
| 13        | 9.868       | 1321          | 1323        | 1327         | rVB3     | 21781          | 21012         | 2.01%           | 0.235%        |
| 14        | 9.957       | 1333          | 1338        | 1342         | rBV      | 1072350        | 903101        | 86.55%          | 10.115%       |
| 15        | 9.986       | 1342          | 1343        | 1348         | rVB      | 34328          | 27419         | 2.63%           | 0.307%        |
| 16        | 10.157      | 1368          | 1372        | 1376         | rBV2     | 20689          | 22919         | 2.20%           | 0.257%        |
| 17        | 10.262      | 1384          | 1390        | 1391         | rBV2     | 11841          | 17335         | 1.66%           | 0.194%        |
| 18        | 10.362      | 1404          | 1407        | 1411         | rVB4     | 14403          | 18377         | 1.76%           | 0.206%        |
| 19        | 10.504      | 1428          | 1431        | 1436         | rVB      | 26560          | 24123         | 2.31%           | 0.270%        |
| 20        | 10.598      | 1444          | 1447        | 1453         | rVB5     | 13207          | 21067         | 2.02%           | 0.236%        |
| 21        | 10.739      | 1468          | 1471        | 1478         | rBV      | 127627         | 107665        | 10.32%          | 1.206%        |
| 22        | 10.868      | 1488          | 1493        | 1496         | rBV      | 38795          | 43209         | 4.14%           | 0.484%        |
| 23        | 11.245      | 1554          | 1557        | 1561         | rVB3     | 16116          | 14908         | 1.43%           | 0.167%        |
| 24        | 11.333      | 1569          | 1572        | 1578         | rVB4     | 29635          | 35867         | 3.44%           | 0.402%        |
| 25        | 11.392      | 1579          | 1582        | 1587         | rVB2     | 13047          | 14151         | 1.36%           | 0.158%        |
| 26        | 11.445      | 1587          | 1591        | 1593         | rBV      | 931624         | 768485        | 73.65%          | 8.608%        |
| 27        | 11.468      | 1593          | 1595        | 1598         | rVV      | 219438         | 163623        | 15.68%          | 1.833%        |
| 28        | 11.515      | 1601          | 1603        | 1606         | rVB      | 58362          | 48018         | 4.60%           | 0.538%        |
| 29        | 11.551      | 1606          | 1609        | 1612         | rBV3     | 10726          | 14389         | 1.38%           | 0.161%        |
| 30        | 11.668      | 1627          | 1629        | 1635         | rVB2     | 22061          | 27095         | 2.60%           | 0.303%        |
| 31        | 11.945      | 1673          | 1676        | 1678         | rBV      | 28344          | 31871         | 3.05%           | 0.357%        |
| 32        | 11.974      | 1678          | 1681        | 1684         | rVV      | 39339          | 38729         | 3.71%           | 0.434%        |
| 33        | 12.015      | 1686          | 1688        | 1692         | rVV2     | 15510          | 18448         | 1.77%           | 0.207%        |
| 34        | 12.056      | 1692          | 1695        | 1697         | rVV      | 49337          | 52908         | 5.07%           | 0.593%        |

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Misc :  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SP-1-B-COMP

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

|    |        |      |      |      |      |        |        |        |         |
|----|--------|------|------|------|------|--------|--------|--------|---------|
| 35 | 12.080 | 1697 | 1699 | 1702 | rVB  | 18884  | 15311  | 1.47%  | 0.171%  |
| 36 | 12.239 | 1724 | 1726 | 1728 | rBV  | 24320  | 19182  | 1.84%  | 0.215%  |
| 37 | 12.262 | 1728 | 1730 | 1733 | rVB4 | 15948  | 14131  | 1.35%  | 0.158%  |
| 38 | 12.492 | 1766 | 1769 | 1772 | rVB3 | 21152  | 24545  | 2.35%  | 0.275%  |
| 39 | 12.527 | 1772 | 1775 | 1777 | rBV3 | 16901  | 19591  | 1.88%  | 0.219%  |
| 40 | 12.574 | 1781 | 1783 | 1786 | rBV2 | 15986  | 15423  | 1.48%  | 0.173%  |
| 41 | 12.656 | 1793 | 1797 | 1800 | rBV  | 331149 | 266504 | 25.54% | 2.985%  |
| 42 | 12.745 | 1810 | 1812 | 1815 | rVB3 | 14905  | 15744  | 1.51%  | 0.176%  |
| 43 | 12.803 | 1820 | 1822 | 1825 | rBV3 | 14172  | 15100  | 1.45%  | 0.169%  |
| 44 | 12.886 | 1833 | 1836 | 1841 | rVB  | 300641 | 264657 | 25.36% | 2.964%  |
| 45 | 13.021 | 1856 | 1859 | 1866 | rVB  | 231596 | 231125 | 22.15% | 2.589%  |
| 46 | 13.098 | 1868 | 1872 | 1876 | rBV5 | 25902  | 47870  | 4.59%  | 0.536%  |
| 47 | 13.186 | 1885 | 1887 | 1888 | rBV2 | 18170  | 15764  | 1.51%  | 0.177%  |
| 48 | 13.209 | 1889 | 1891 | 1895 | rVB2 | 53337  | 48621  | 4.66%  | 0.545%  |
| 49 | 13.280 | 1900 | 1903 | 1905 | rVB  | 30292  | 25907  | 2.48%  | 0.290%  |
| 50 | 13.315 | 1906 | 1909 | 1912 | rBV2 | 34695  | 34665  | 3.32%  | 0.388%  |
| 51 | 14.080 | 2035 | 2039 | 2042 | rBV2 | 851602 | 903523 | 86.59% | 10.120% |
| 52 | 14.109 | 2042 | 2044 | 2050 | rVB  | 136768 | 118827 | 11.39% | 1.331%  |
| 53 | 15.133 | 2215 | 2218 | 2226 | rVB  | 119878 | 233737 | 22.40% | 2.618%  |
| 54 | 15.574 | 2289 | 2293 | 2306 | rVB  | 515512 | 771384 | 73.93% | 8.640%  |

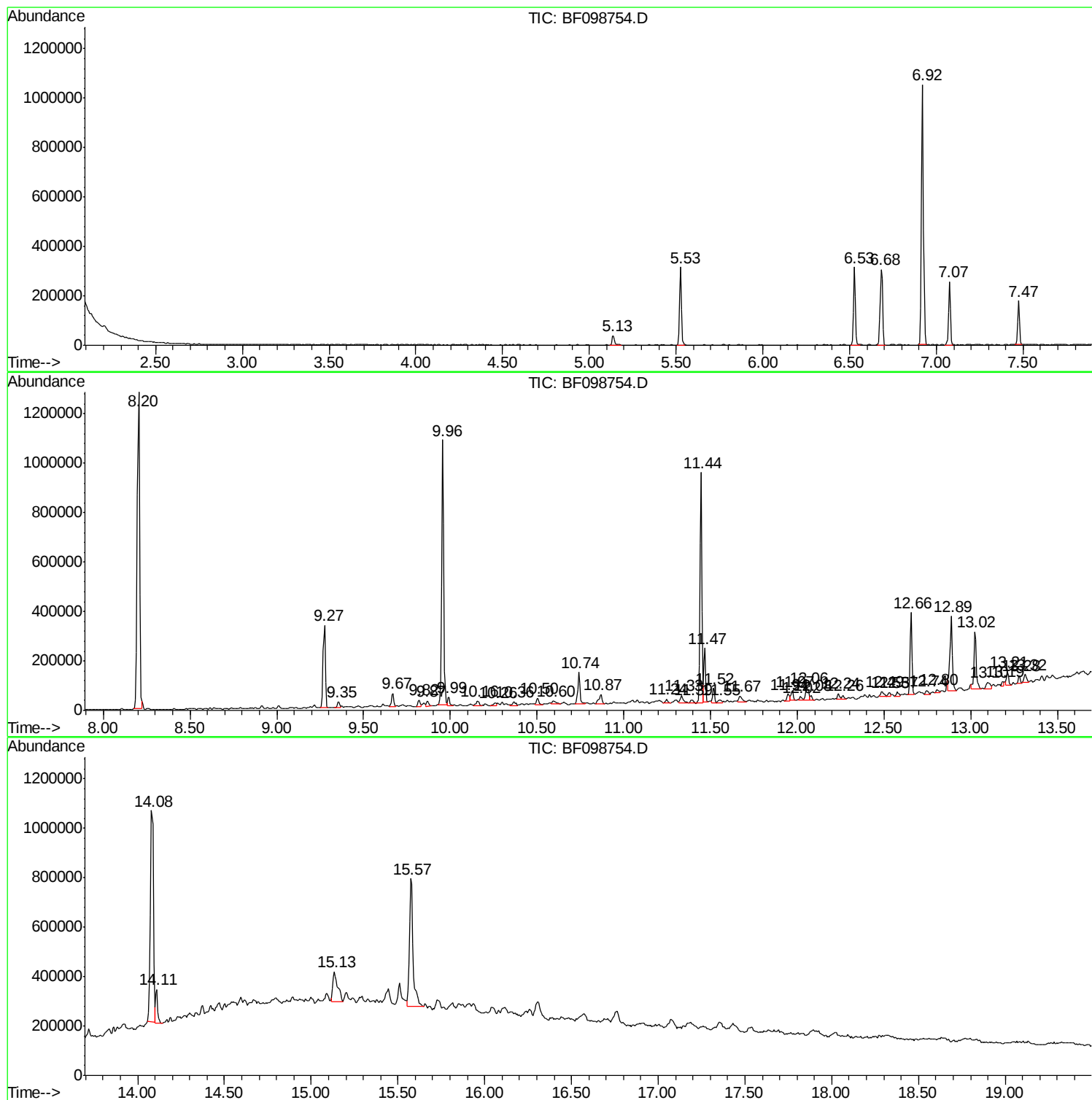
Sum of corrected areas: 8928078

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.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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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092317.M  
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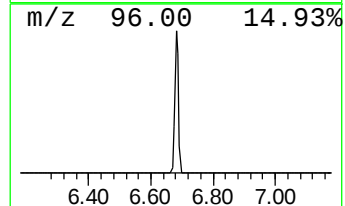
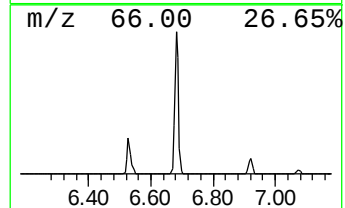
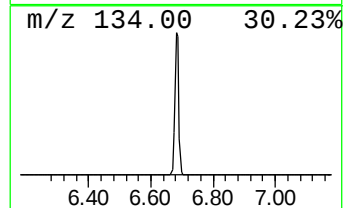
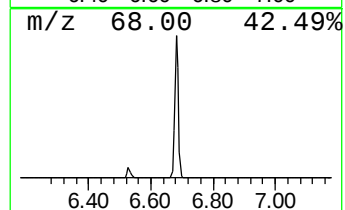
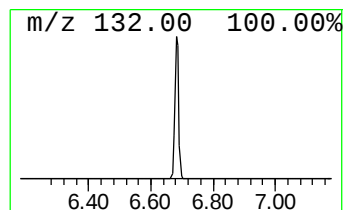
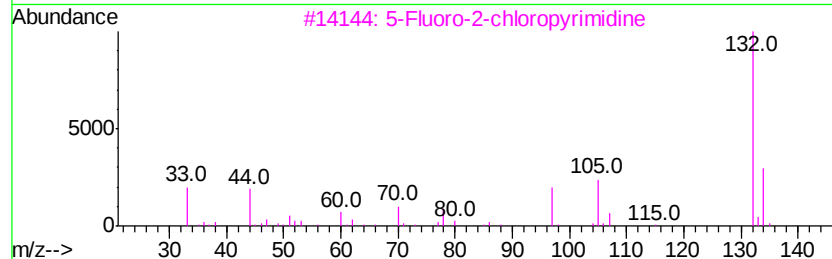
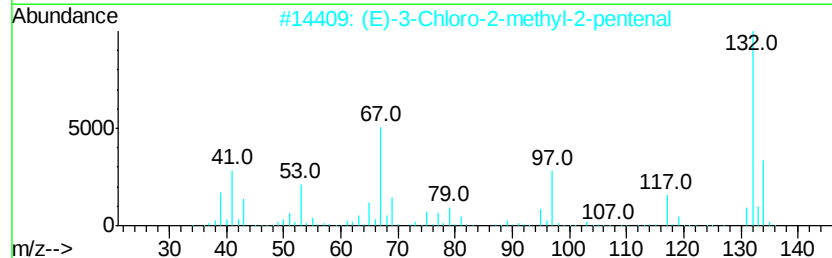
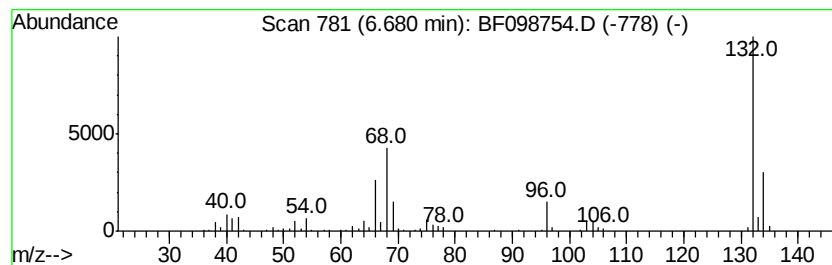
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown6.68 Concentration Rank 1

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 6.68 | 6.22 ng | 263039 | 1,4-Dichlorobenzene-d4 | 6.92 |

| 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-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | 4-Chloro-2-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-00-5  | 9    |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092317.M  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                  |      |         |       |          | #                     | RT   | Resp   | Conc |
| unknown6.68      | 6.68 | 6.2     | ng    | 263039   | 1                     | 6.92 | 845670 | 20.0 |