

Data Path : Z:\HPCHEM1\BNA F\Data\BF081817\  
 Data File : BF097843.D  
 Acq On : 18 Aug 2017 20:06  
 Operator : SJ/JU  
 Sample : I4811-01  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 EP-12

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-BF081517.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         | 4.969       | 485           | 490         | 498          | rVB      | 444963         | 604258        | 18.36%          | 1.902%        |
| 2         | 5.381       | 554           | 560         | 563          | rBV      | 2850845        | 2891974       | 87.87%          | 9.103%        |
| 3         | 6.404       | 728           | 734         | 737          | rBV      | 3113956        | 3291144       | 100.00%         | 10.359%       |
| 4         | 6.539       | 752           | 757         | 760          | rBV      | 3102457        | 3117523       | 94.72%          | 9.813%        |
| 5         | 6.769       | 793           | 796         | 800          | rBV      | 947746         | 758832        | 23.06%          | 2.388%        |
| 6         | 6.928       | 819           | 823         | 826          | rBV      | 2783606        | 2442314       | 74.21%          | 7.687%        |
| 7         | 7.334       | 887           | 892         | 895          | rBV      | 2183065        | 2085118       | 63.36%          | 6.563%        |
| 8         | 8.051       | 1010          | 1014        | 1022         | rBV      | 1114927        | 1023685       | 31.10%          | 3.222%        |
| 9         | 9.133       | 1193          | 1198        | 1201         | rBV      | 3431986        | 3285599       | 99.83%          | 10.342%       |
| 10        | 9.522       | 1261          | 1264        | 1268         | rBV      | 481717         | 422925        | 12.85%          | 1.331%        |
| 11        | 9.804       | 1308          | 1312        | 1316         | rBV      | 1112793        | 1050539       | 31.92%          | 3.307%        |
| 12        | 10.592      | 1441          | 1446        | 1449         | rBV      | 1777103        | 1662900       | 50.53%          | 5.234%        |
| 13        | 10.716      | 1464          | 1467        | 1473         | rBV      | 40760          | 45967         | 1.40%           | 0.145%        |
| 14        | 11.286      | 1560          | 1564        | 1567         | rBV      | 1125255        | 1122689       | 34.11%          | 3.534%        |
| 15        | 11.310      | 1567          | 1568        | 1572         | rVV      | 288101         | 192849        | 5.86%           | 0.607%        |
| 16        | 11.363      | 1572          | 1577        | 1580         | rVB      | 79627          | 76287         | 2.32%           | 0.240%        |
| 17        | 11.786      | 1646          | 1649        | 1652         | rBV      | 42671          | 40470         | 1.23%           | 0.127%        |
| 18        | 11.816      | 1652          | 1654        | 1657         | rVB      | 57913          | 48357         | 1.47%           | 0.152%        |
| 19        | 11.898      | 1665          | 1668        | 1671         | rBV      | 66396          | 72621         | 2.21%           | 0.229%        |
| 20        | 12.339      | 1739          | 1743        | 1746         | rBV      | 33104          | 34744         | 1.06%           | 0.109%        |
| 21        | 12.498      | 1766          | 1770        | 1773         | rVB      | 335701         | 273748        | 8.32%           | 0.862%        |
| 22        | 12.721      | 1803          | 1808        | 1811         | rBV      | 284005         | 314666        | 9.56%           | 0.990%        |
| 23        | 12.880      | 1830          | 1835        | 1838         | rBV      | 3194938        | 3147339       | 95.63%          | 9.906%        |
| 24        | 13.057      | 1862          | 1865        | 1868         | rVB      | 50875          | 47927         | 1.46%           | 0.151%        |
| 25        | 13.121      | 1873          | 1876        | 1879         | rVB2     | 46596          | 39915         | 1.21%           | 0.126%        |
| 26        | 13.157      | 1879          | 1882        | 1885         | rBV      | 42036          | 42789         | 1.30%           | 0.135%        |
| 27        | 13.574      | 1947          | 1953        | 1955         | rVB4     | 30623          | 44892         | 1.36%           | 0.141%        |
| 28        | 13.663      | 1964          | 1968        | 1972         | rBV3     | 47211          | 66870         | 2.03%           | 0.210%        |
| 29        | 13.757      | 1981          | 1984        | 1986         | rBV3     | 191383         | 190445        | 5.79%           | 0.599%        |
| 30        | 13.774      | 1986          | 1987        | 1994         | rVB      | 225574         | 188599        | 5.73%           | 0.594%        |
| 31        | 13.921      | 2004          | 2012        | 2015         | rBV      | 1183464        | 1279682       | 38.88%          | 4.028%        |
| 32        | 13.945      | 2015          | 2016        | 2019         | rVB      | 136431         | 89613         | 2.72%           | 0.282%        |
| 33        | 14.310      | 2074          | 2078        | 2080         | rBV      | 34262          | 35070         | 1.07%           | 0.110%        |
| 34        | 14.410      | 2092          | 2095        | 2101         | rBV6     | 58014          | 82851         | 2.52%           | 0.261%        |

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ClientSampleId :  
EP-12

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-BF081517.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |       |        |        |        |        |
|----|--------|------|------|------|-------|--------|--------|--------|--------|
| 35 | 14.939 | 2181 | 2185 | 2188 | rBV   | 89207  | 131516 | 4.00%  | 0.414% |
| 36 | 15.039 | 2198 | 2202 | 2211 | rVB5  | 40488  | 77620  | 2.36%  | 0.244% |
| 37 | 15.227 | 2231 | 2234 | 2239 | rVB   | 57475  | 68665  | 2.09%  | 0.216% |
| 38 | 15.286 | 2240 | 2244 | 2250 | rVB   | 80311  | 97948  | 2.98%  | 0.308% |
| 39 | 15.351 | 2250 | 2255 | 2262 | rBV   | 699731 | 888054 | 26.98% | 2.795% |
| 40 | 15.821 | 2332 | 2335 | 2339 | rVB3  | 31586  | 40008  | 1.22%  | 0.126% |
| 41 | 15.874 | 2339 | 2344 | 2350 | rVB7  | 28613  | 54348  | 1.65%  | 0.171% |
| 42 | 16.304 | 2413 | 2417 | 2426 | rVB7  | 17616  | 37260  | 1.13%  | 0.117% |
| 43 | 16.733 | 2486 | 2490 | 2499 | rVB2  | 27540  | 55027  | 1.67%  | 0.173% |
| 44 | 17.156 | 2557 | 2562 | 2567 | rVB2  | 21311  | 38011  | 1.15%  | 0.120% |
| 45 | 17.856 | 2675 | 2681 | 2688 | rVB6  | 35037  | 83390  | 2.53%  | 0.262% |
| 46 | 19.297 | 2918 | 2926 | 2935 | rVB10 | 26974  | 83827  | 2.55%  | 0.264% |

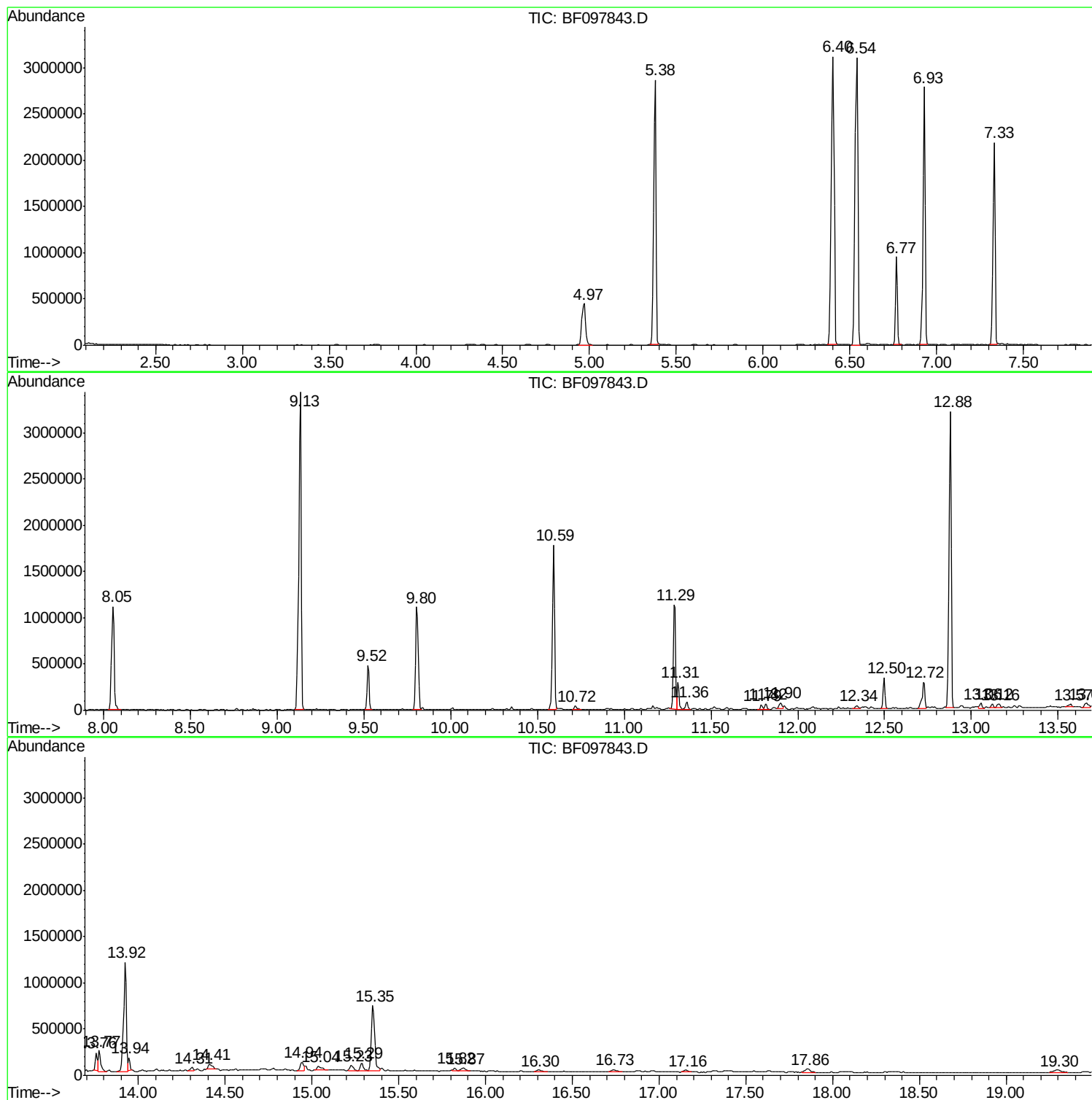
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ClientSampleId :  
EP-12

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.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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Instrument :  
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

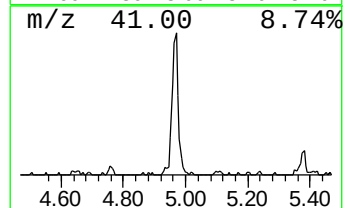
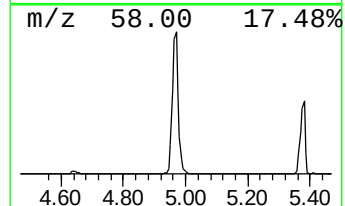
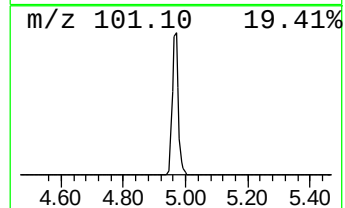
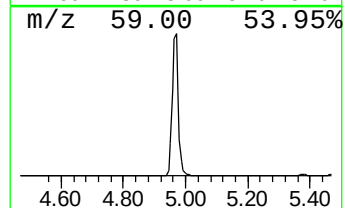
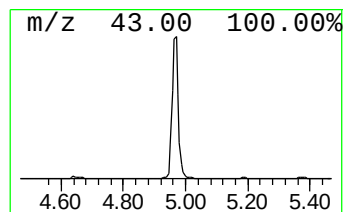
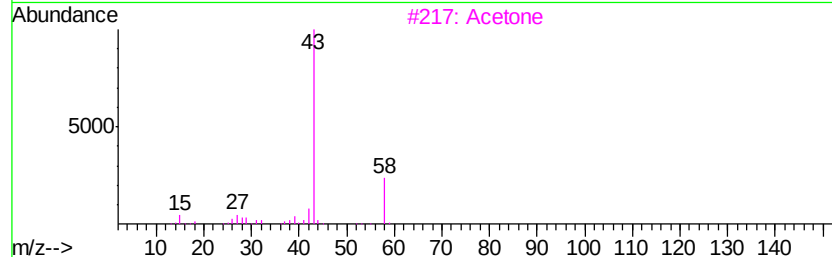
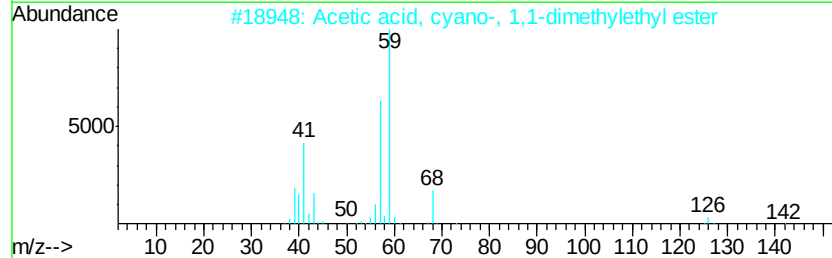
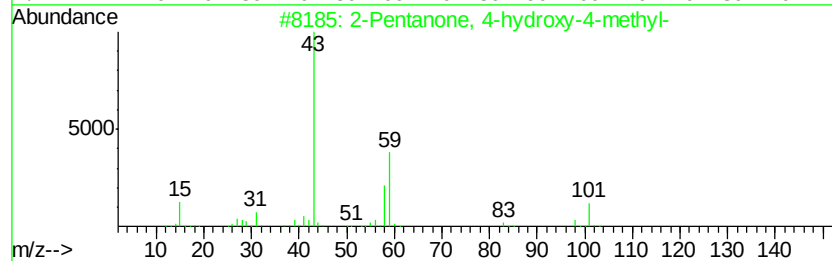
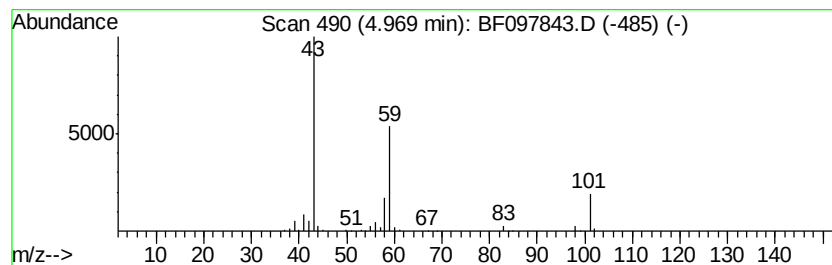
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.97 | 15.93 ng | 604258 | 1,4-Dichlorobenzene-d4 | 6.77 |

| 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, cyano-, 1,1-dimethyl... | 141          | C7H11NO2 | 001116-98-9 | 17   |      |
| 3       | Acetone                              | 58           | C3H6O    | 000067-64-1 | 14   |      |
| 4       | 2,3-Butanedione, monooxime           | 101          | C4H7NO2  | 000057-71-6 | 12   |      |
| 5       | 5-Hexen-2-one                        | 98           | C6H10O   | 000109-49-9 | 9    |      |



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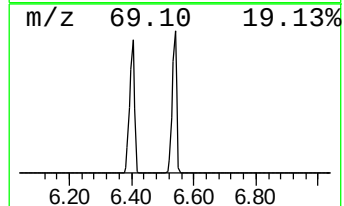
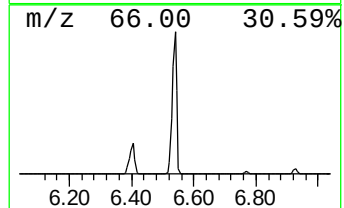
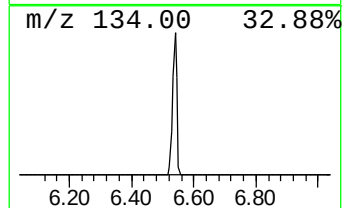
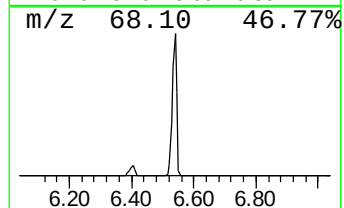
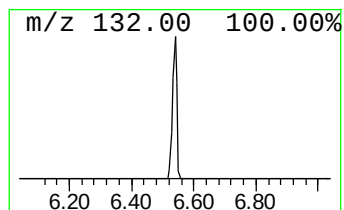
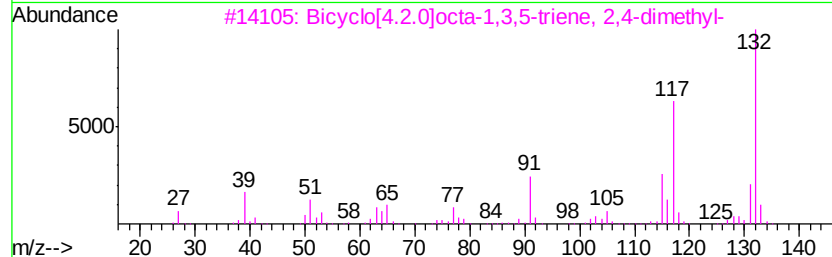
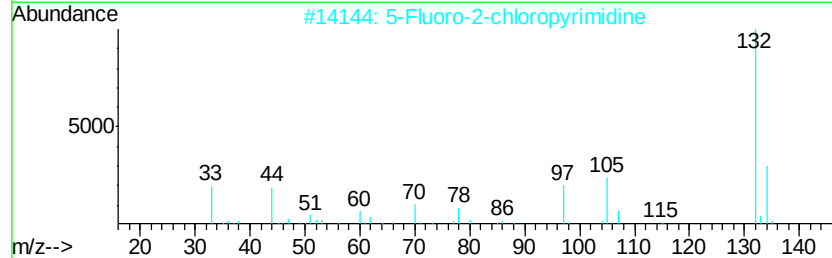
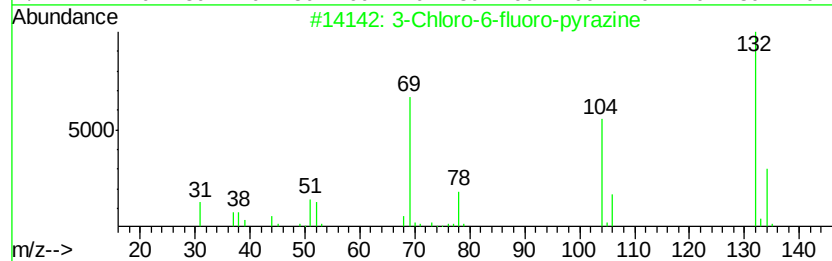
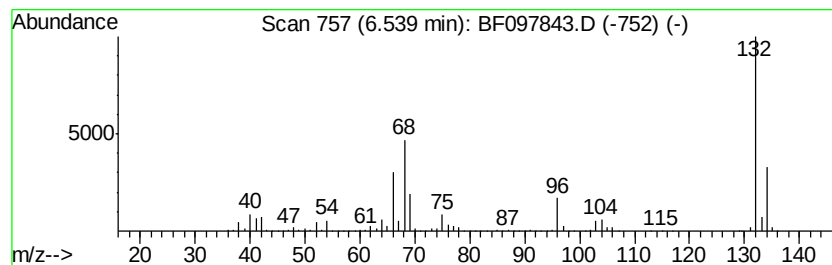
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown6.54 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.54 | 82.17 ng | 3117520 | 1,4-Dichlorobenzene-d4 | 6.77 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 16   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 3    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 4    |    | (5-Methyl-2-pyridyl)acetonitrile    | 132 | C8H8N2    | 1000241-93-9 | 9    |
| 5    |    | 1-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-59-9  | 9    |



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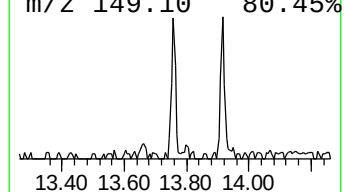
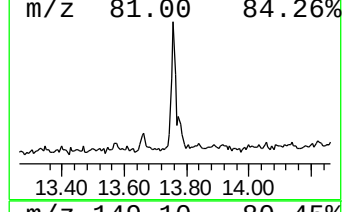
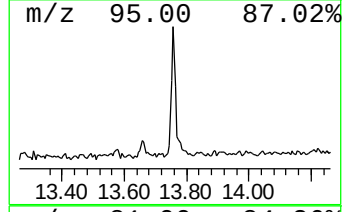
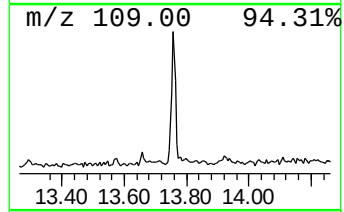
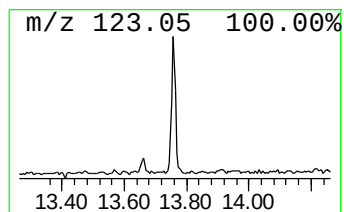
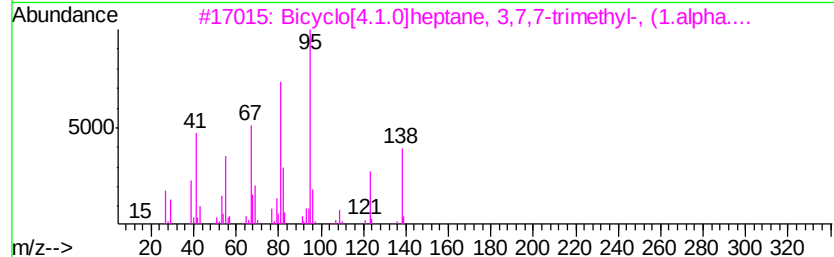
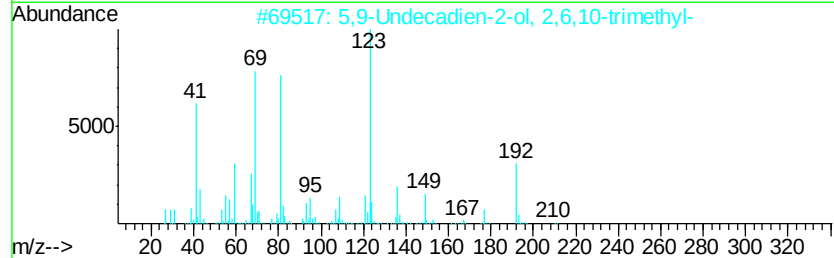
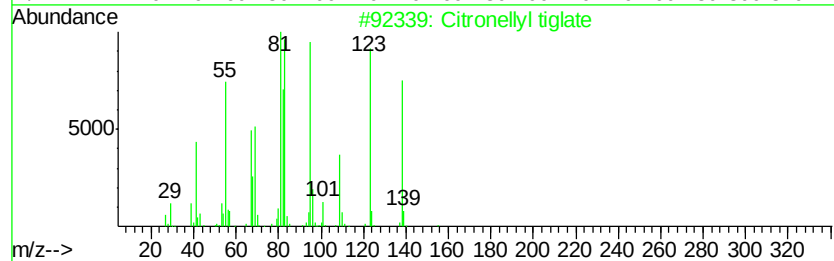
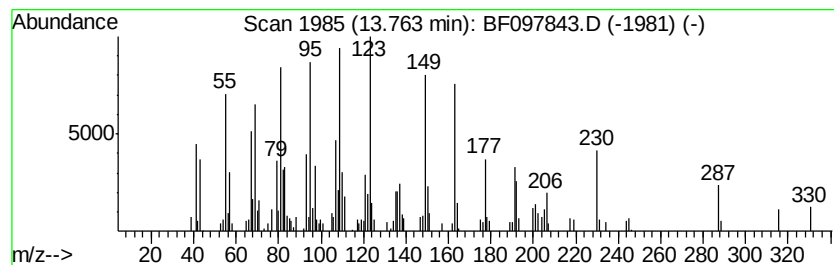
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 unknown13.76 Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.76 | 2.98 ng | 190445 | Chrysene-d12     | 13.92 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Citronellvl tiglate                 | 238 | C15H26O2 | 024717-85-9 | 43   |
| 2    |    | 5,9-Undecadien-2-ol, 2,6,10-trim... | 210 | C14H26O  | 021980-62-1 | 35   |
| 3    |    | Bicyclo[4.1.0]heptane, 3,7,7-tri... | 138 | C10H18   | 018968-23-5 | 30   |
| 4    |    | Cyclopentene, 1,3-dimethyl-2-(1-... | 138 | C10H18   | 061142-32-3 | 27   |
| 5    |    | (2Z,4E)-3,7,11-Trimethyl-2,4,10-... | 206 | C15H26   | 172549-29-0 | 27   |



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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 |
| 2-Pentanone, 4-hy... | 4.97  | 15.9    | ng    | 604258   | 1                     | 6.77  | 758832  | 20.0 |
| unknown6.54          | 6.54  | 82.2    | ng    | 3117520  | 1                     | 6.77  | 758832  | 20.0 |
| unknown13.76         | 13.76 | 3.0     | ng    | 190445   | 5                     | 13.92 | 1279680 | 20.0 |