

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\  
 Data File : BF106603.D  
 Acq On : 20 Jun 2018 00:43  
 Operator : JU/SJ  
 Sample : J3554-09  
 Misc :  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 A-8(3.0)

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:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF061918.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         | 5.207       | 484           | 488         | 503          | rVB      | 193144         | 251471        | 10.26%          | 1.153%        |
| 2         | 5.607       | 553           | 556         | 561          | rBV      | 2371910        | 2340761       | 95.47%          | 10.731%       |
| 3         | 6.607       | 721           | 726         | 729          | rBV      | 2328090        | 2368922       | 96.62%          | 10.860%       |
| 4         | 6.743       | 744           | 749         | 752          | rBV      | 2429618        | 2413743       | 98.45%          | 11.065%       |
| 5         | 6.960       | 783           | 786         | 790          | rVB      | 769778         | 606074        | 24.72%          | 2.778%        |
| 6         | 7.119       | 809           | 813         | 816          | rBV      | 2183588        | 1990644       | 81.19%          | 9.126%        |
| 7         | 7.525       | 877           | 882         | 885          | rBV      | 1514740        | 1640429       | 66.91%          | 7.520%        |
| 8         | 8.242       | 1000          | 1004        | 1008         | rBV      | 845031         | 705101        | 28.76%          | 3.232%        |
| 9         | 9.319       | 1182          | 1187        | 1190         | rBV      | 2734111        | 2451765       | 100.00%         | 11.239%       |
| 10        | 9.707       | 1250          | 1253        | 1258         | rBV      | 298362         | 248025        | 10.12%          | 1.137%        |
| 11        | 9.913       | 1285          | 1288        | 1293         | rBV      | 39574          | 37090         | 1.51%           | 0.170%        |
| 12        | 10.001      | 1299          | 1303        | 1307         | rBV      | 728367         | 651120        | 26.56%          | 2.985%        |
| 13        | 10.131      | 1322          | 1325        | 1331         | rBV      | 127692         | 117547        | 4.79%           | 0.539%        |
| 14        | 10.419      | 1371          | 1374        | 1376         | rVB      | 55311          | 45284         | 1.85%           | 0.208%        |
| 15        | 10.507      | 1386          | 1389        | 1394         | rBV      | 104416         | 79900         | 3.26%           | 0.366%        |
| 16        | 10.795      | 1434          | 1438        | 1442         | rBV      | 1368494        | 1247949       | 50.90%          | 5.721%        |
| 17        | 10.889      | 1451          | 1454        | 1459         | rBV      | 52421          | 47129         | 1.92%           | 0.216%        |
| 18        | 11.495      | 1553          | 1557        | 1560         | rBV      | 650572         | 550971        | 22.47%          | 2.526%        |
| 19        | 11.519      | 1560          | 1561        | 1566         | rVB      | 63511          | 35848         | 1.46%           | 0.164%        |
| 20        | 12.713      | 1760          | 1764        | 1768         | rVB      | 103834         | 86309         | 3.52%           | 0.396%        |
| 21        | 12.942      | 1800          | 1803        | 1805         | rBV      | 93539          | 68773         | 2.81%           | 0.315%        |
| 22        | 13.083      | 1822          | 1827        | 1830         | rBV      | 2200003        | 2001123       | 81.62%          | 9.174%        |
| 23        | 13.272      | 1852          | 1859        | 1861         | rBV      | 21294          | 26665         | 1.09%           | 0.122%        |
| 24        | 13.960      | 1972          | 1976        | 1986         | rBV3     | 182466         | 208355        | 8.50%           | 0.955%        |
| 25        | 14.148      | 2003          | 2008        | 2011         | rBV      | 761472         | 763076        | 31.12%          | 3.498%        |
| 26        | 14.171      | 2011          | 2012        | 2017         | rVB      | 60117          | 41123         | 1.68%           | 0.189%        |
| 27        | 14.607      | 2083          | 2086        | 2090         | rBV3     | 31364          | 40599         | 1.66%           | 0.186%        |
| 28        | 15.224      | 2188          | 2191        | 2195         | rBV2     | 34772          | 55003         | 2.24%           | 0.252%        |
| 29        | 15.548      | 2244          | 2246        | 2252         | rVB      | 23650          | 28729         | 1.17%           | 0.132%        |
| 30        | 15.613      | 2254          | 2257        | 2263         | rVV      | 30638          | 36735         | 1.50%           | 0.168%        |
| 31        | 15.683      | 2264          | 2269        | 2280         | rVB      | 422333         | 563912        | 23.00%          | 2.585%        |
| 32        | 16.142      | 2344          | 2347        | 2352         | rVB4     | 18013          | 27550         | 1.12%           | 0.126%        |
| 33        | 17.412      | 2560          | 2563        | 2571         | rVB10    | 17933          | 36153         | 1.47%           | 0.166%        |

## LSC Area Percent Report

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Instrument :  
BNA\_F  
ClientSampleId :  
A-8(3.0)

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:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF061918.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

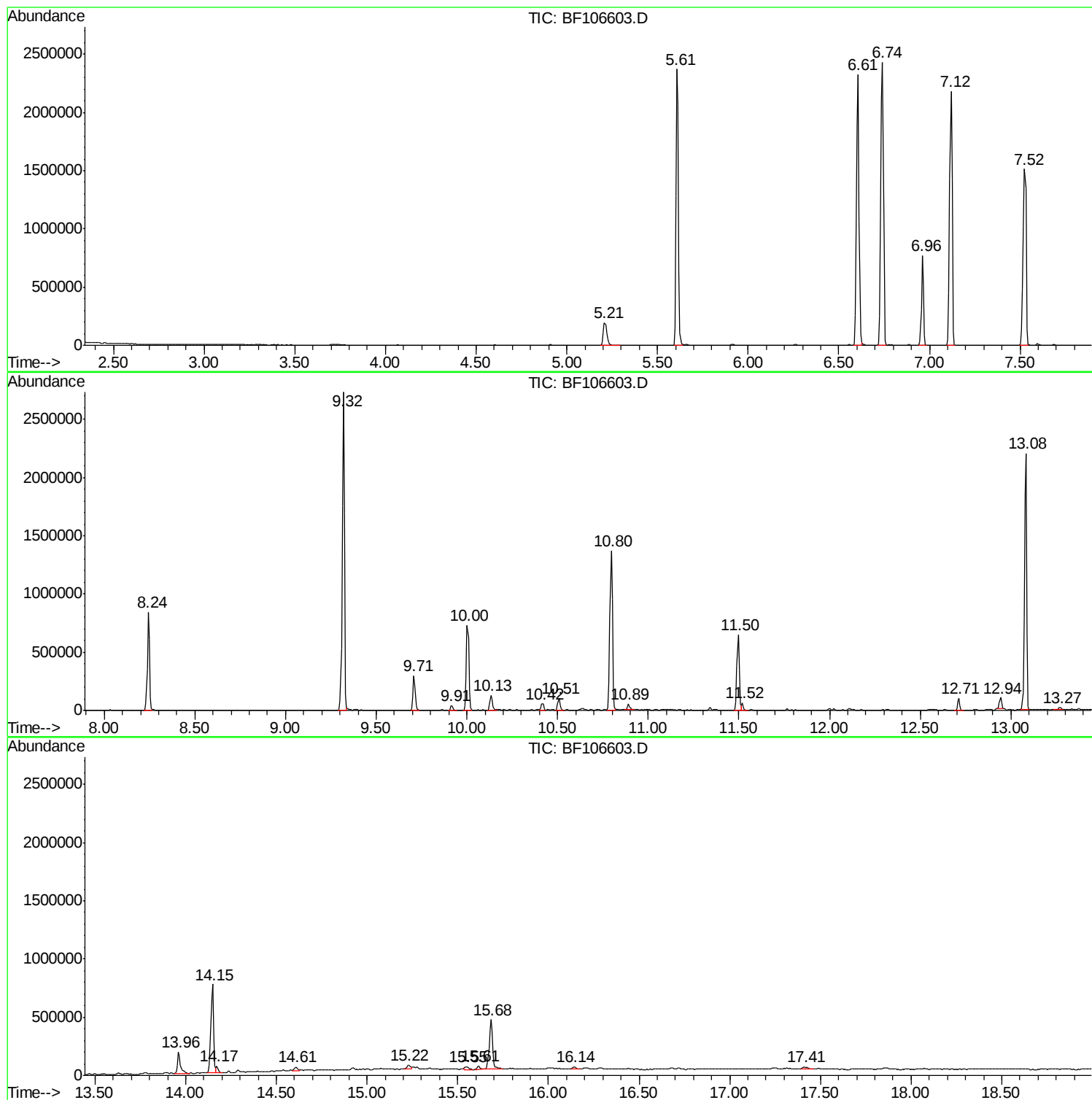
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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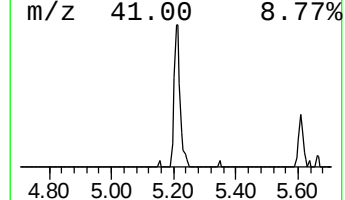
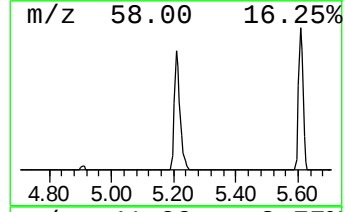
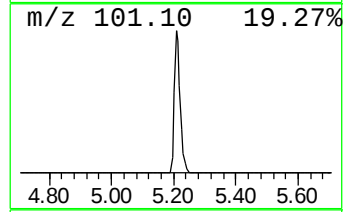
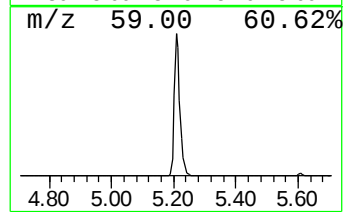
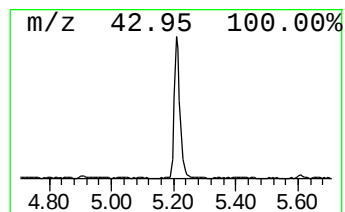
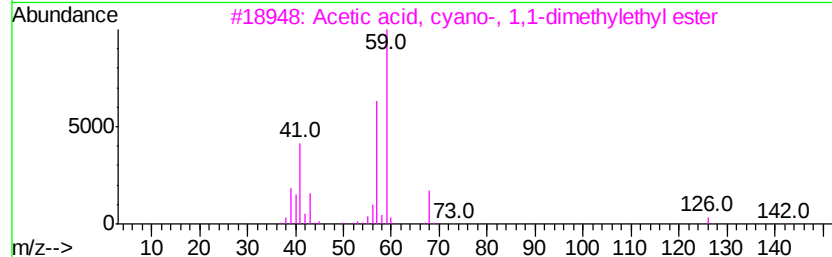
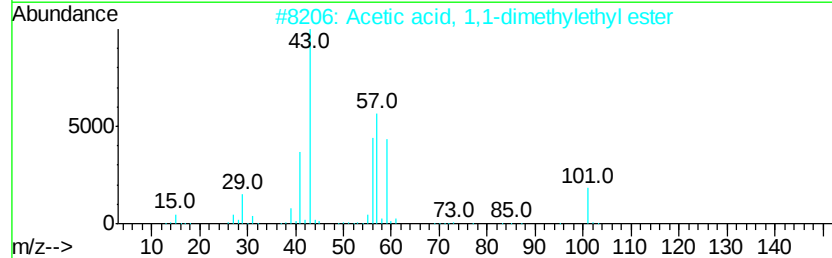
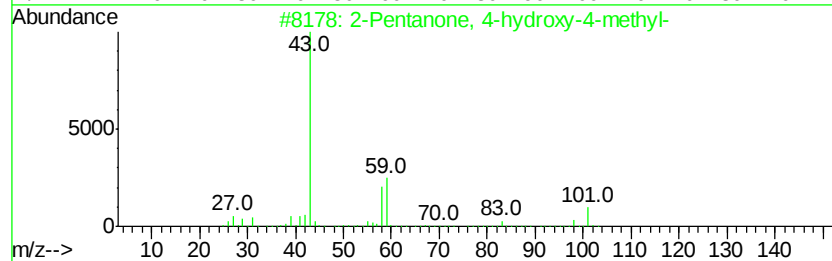
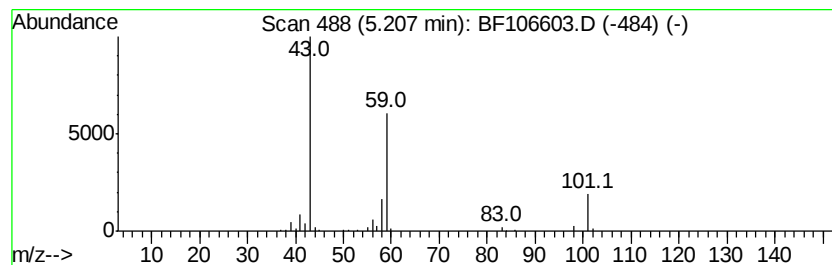
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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. |
|------|---------|--------|------------------------|------|
| 5.21 | 8.30 ng | 251471 | 1,4-Dichlorobenzene-d4 | 6.96 |

| 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 | 39   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 4    |    |   | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |
| 5    |    |   | 3-Hydroxy-3-methyl-2-butanone       | 102 | C5H10O2  | 000115-22-0 | 9    |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

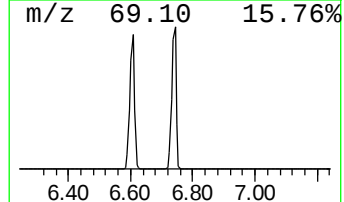
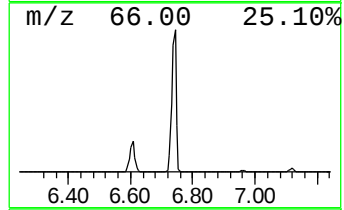
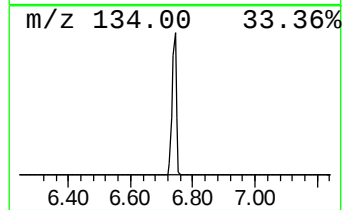
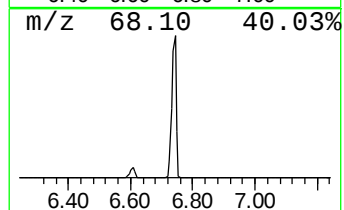
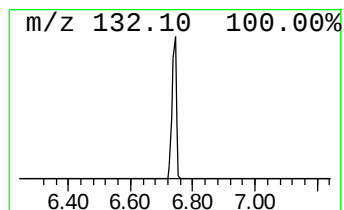
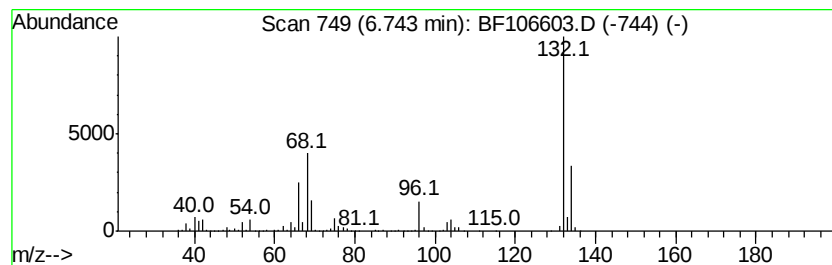
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.74 | 79.65 ng | 2413740 | 1,4-Dichlorobenzene-d4 | 6.96 |

| 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  | 17   |
| 3    |    | Tranvlcypropine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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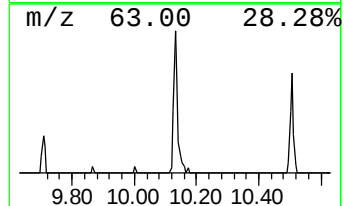
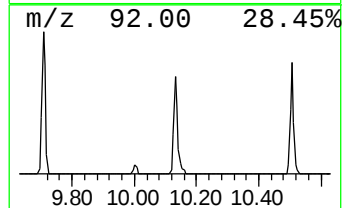
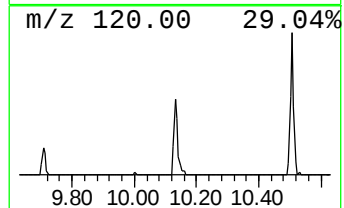
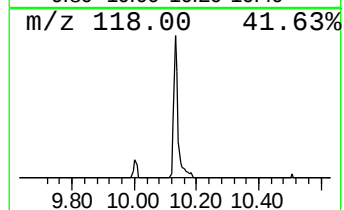
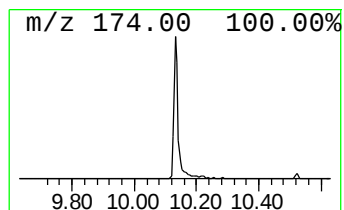
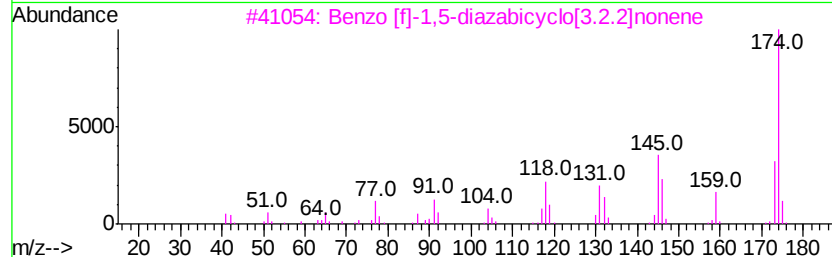
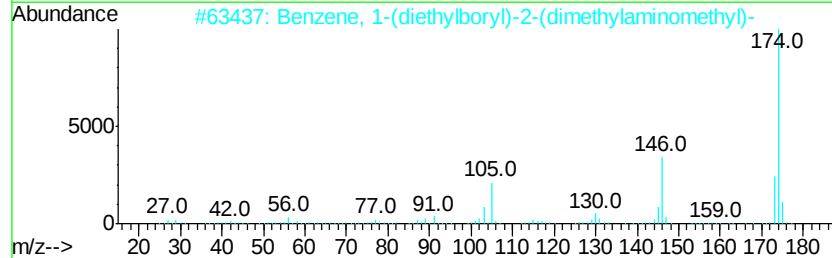
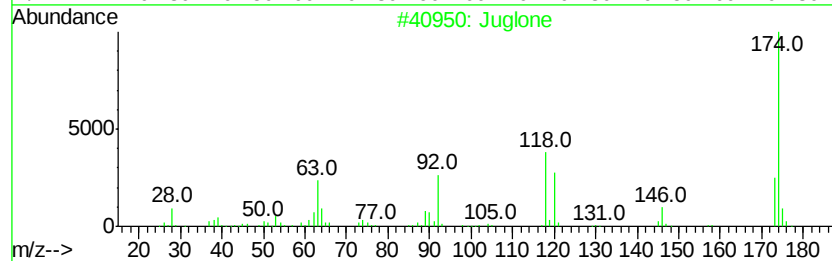
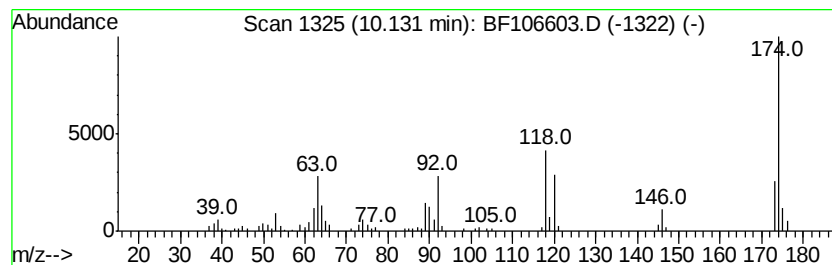
Instrument :  
BNA\_F  
ClientSampleId :  
A-8(3.0)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.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 4 Juglone Concentration Rank 5

| R.T.    | EstConc                             | Area         | Relative to ISTD | R.T.            |
|---------|-------------------------------------|--------------|------------------|-----------------|
| 10.13   | 3.61 ng                             | 117547       | Acenaphthene-d10 | 10.00           |
| Hit# of | 5                                   | Tentative ID | MW MolForm       | CAS# Qual       |
| 1       | Juglone                             |              | 174 C10H6O3      | 000481-39-0 98  |
| 2       | Benzene, 1-(diethylboryl)-2-(dim... |              | 203 C13H22BN     | 1000162-42-1 35 |
| 3       | Benzo [f]1,5-diazabicyclo[3.2.2...  |              | 174 C11H14N2     | 007092-76-4 32  |
| 4       | 2-Cyanomethyl-1,3-benzothiazole     |              | 174 C9H6N2S      | 056278-50-3 32  |
| 5       | Benzene, 1,3-diisocyanato-2-methyl- |              | 174 C9H6N2O2     | 000091-08-7 27  |



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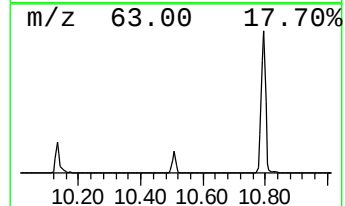
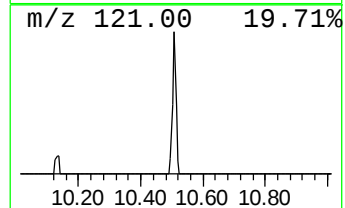
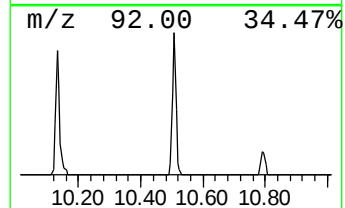
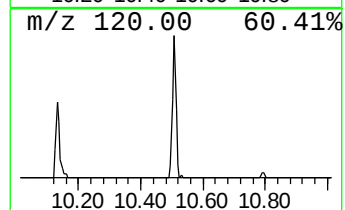
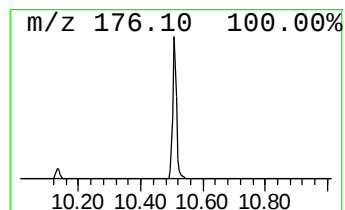
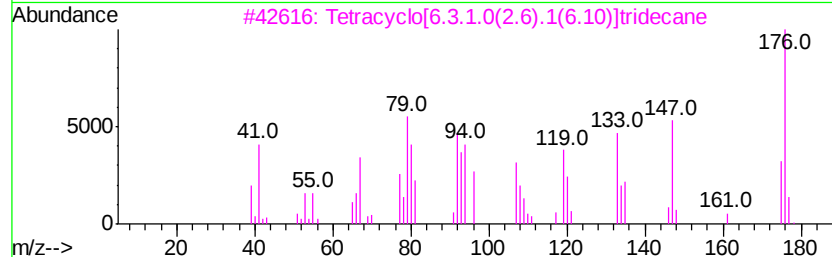
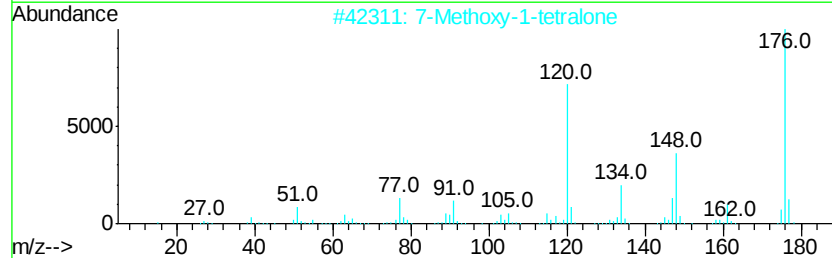
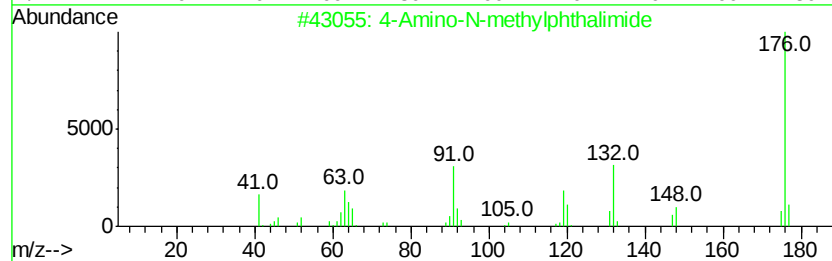
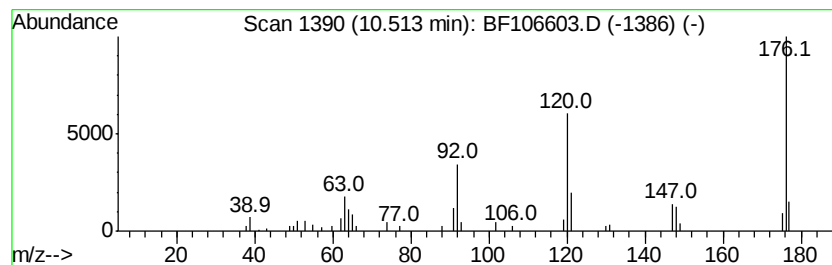
Instrument :  
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 4-Amino-N-methylphthalimide Concentration Rank 6

| R.T.    | EstConc | Area                                 | Relative to ISTD | R.T.            |
|---------|---------|--------------------------------------|------------------|-----------------|
| 10.51   | 2.45 ng | 79900                                | Acenaphthene-d10 | 10.00           |
| Hit# of | 5       | Tentative ID                         | MW MolForm       | CAS# Qual       |
| 1       |         | 4-Amino-N-methylphthalimide          | 176 C9H8N2O2     | 002257-85-4 52  |
| 2       |         | 7-Methoxy-1-tetralone                | 176 C11H12O2     | 006836-19-7 50  |
| 3       |         | Tetracyclo[6.3.1.0(2.6).1(6.10)]...  | 176 C13H20       | 1000215-30-3 46 |
| 4       |         | 2-Propenal, 3-(1,3-benzodioxol-5-... | 176 C10H8O3      | 014756-00-4 43  |
| 5       |         | 5,6-Dimethylpyridine-3,4-dicarbo...  | 176 C9H8N2O2     | 090417-36-0 43  |



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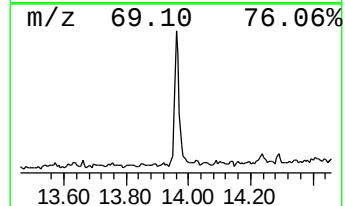
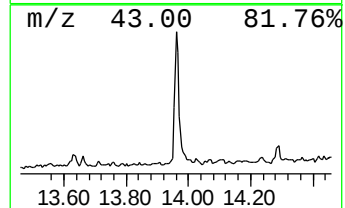
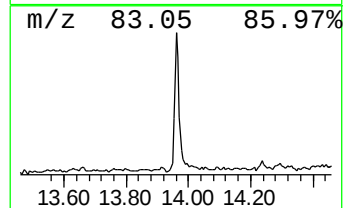
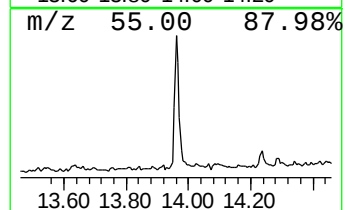
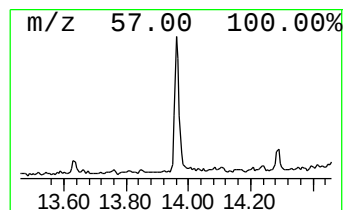
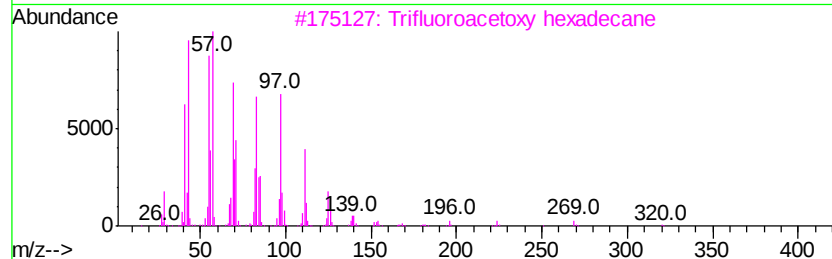
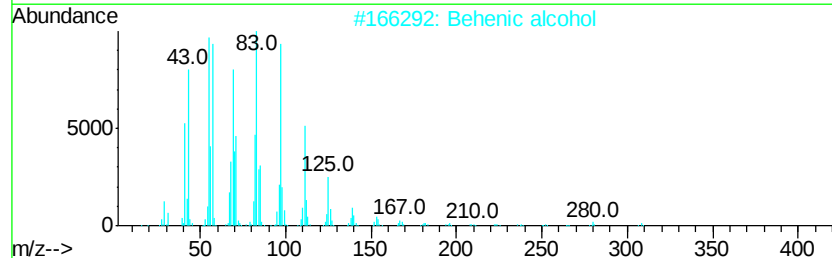
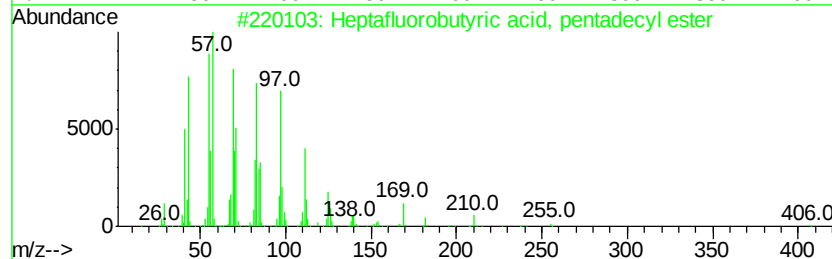
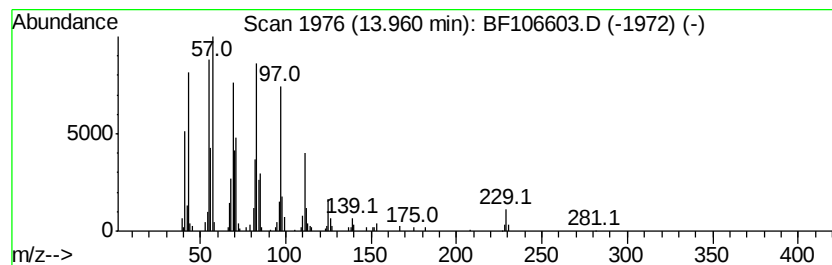
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.96 | 5.46 ng | 208355 | Chrysene-d12     | 14.15 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|-------------------------------------|-----|-------------|-------------|------|
| 1    | 5  | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2  | 959261-23-5 | 94   |
| 2    |    | Behenic alcohol                     | 326 | C22H46O     | 000661-19-8 | 94   |
| 3    |    | Trifluoroacetoxv hexadecane         | 338 | C18H33F3O2  | 006222-03-3 | 94   |
| 4    |    | 1-Heneicosanol                      | 312 | C21H44O     | 015594-90-8 | 94   |
| 5    |    | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF061918\  
Data File : BF106603.D  
Acq On : 20 Jun 2018 00:43  
Operator : JU/SJ  
Sample : J3554-09  
Misc :  
ALS Vial : 24 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
A-8(3.0)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF061918.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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... | 5.21  | 8.3     | ng    | 251471   | 1                     | 6.96  | 606074 | 20.0 |
| unknown6.74          | 6.74  | 79.7    | ng    | 2413740  | 1                     | 6.96  | 606074 | 20.0 |
| Juglone              | 10.13 | 3.6     | ng    | 117547   | 3                     | 10.00 | 651120 | 20.0 |
| 4-Amino-N-methylp... | 10.51 | 2.5     | ng    | 79900    | 3                     | 10.00 | 651120 | 20.0 |
| Heptafluorobutyri... | 13.96 | 5.5     | ng    | 208355   | 5                     | 14.15 | 763076 | 20.0 |