

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121616\  
 Data File : BF091677.D  
 Acq On : 16 Dec 2016 17:20  
 Operator : UM/SJ  
 Sample : PB95306BL  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB95306BL

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-BF120916.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         | 4.281       | 189           | 192         | 196          | rBV      | 162754         | 240064        | 3.23%           | 0.399%        |
| 2         | 4.956       | 247           | 251         | 260          | rBV      | 1411513        | 2247541       | 30.20%          | 3.736%        |
| 3         | 5.379       | 285           | 288         | 291          | rBV      | 5086262        | 5702127       | 76.61%          | 9.479%        |
| 4         | 6.419       | 375           | 379         | 381          | rBV      | 5494586        | 6313533       | 84.82%          | 10.495%       |
| 5         | 6.544       | 387           | 390         | 392          | rBV      | 6281289        | 6477895       | 87.03%          | 10.769%       |
| 6         | 6.773       | 408           | 410         | 412          | rBV      | 1682734        | 1486194       | 19.97%          | 2.471%        |
| 7         | 6.933       | 421           | 424         | 426          | rBV      | 4473943        | 5131872       | 68.95%          | 8.531%        |
| 8         | 7.333       | 456           | 459         | 462          | rBV      | 3071277        | 3596410       | 48.32%          | 5.979%        |
| 9         | 8.053       | 519           | 522         | 525          | rBV      | 1795595        | 1894401       | 25.45%          | 3.149%        |
| 10        | 9.139       | 613           | 617         | 619          | rBV      | 6206286        | 7075951       | 95.07%          | 11.763%       |
| 11        | 9.813       | 673           | 676         | 678          | rBV      | 1800211        | 2200122       | 29.56%          | 3.657%        |
| 12        | 10.602      | 741           | 745         | 747          | rBV      | 3094074        | 4238305       | 56.94%          | 7.046%        |
| 13        | 11.288      | 802           | 805         | 807          | rBV      | 2372212        | 2068088       | 27.79%          | 3.438%        |
| 14        | 12.876      | 941           | 944         | 947          | rBV      | 6307467        | 7443056       | 100.00%         | 12.373%       |
| 15        | 13.916      | 1032          | 1035        | 1038         | rBV      | 2429934        | 2203596       | 29.61%          | 3.663%        |
| 16        | 15.322      | 1155          | 1158        | 1160         | rBV      | 1509485        | 1836200       | 24.67%          | 3.052%        |

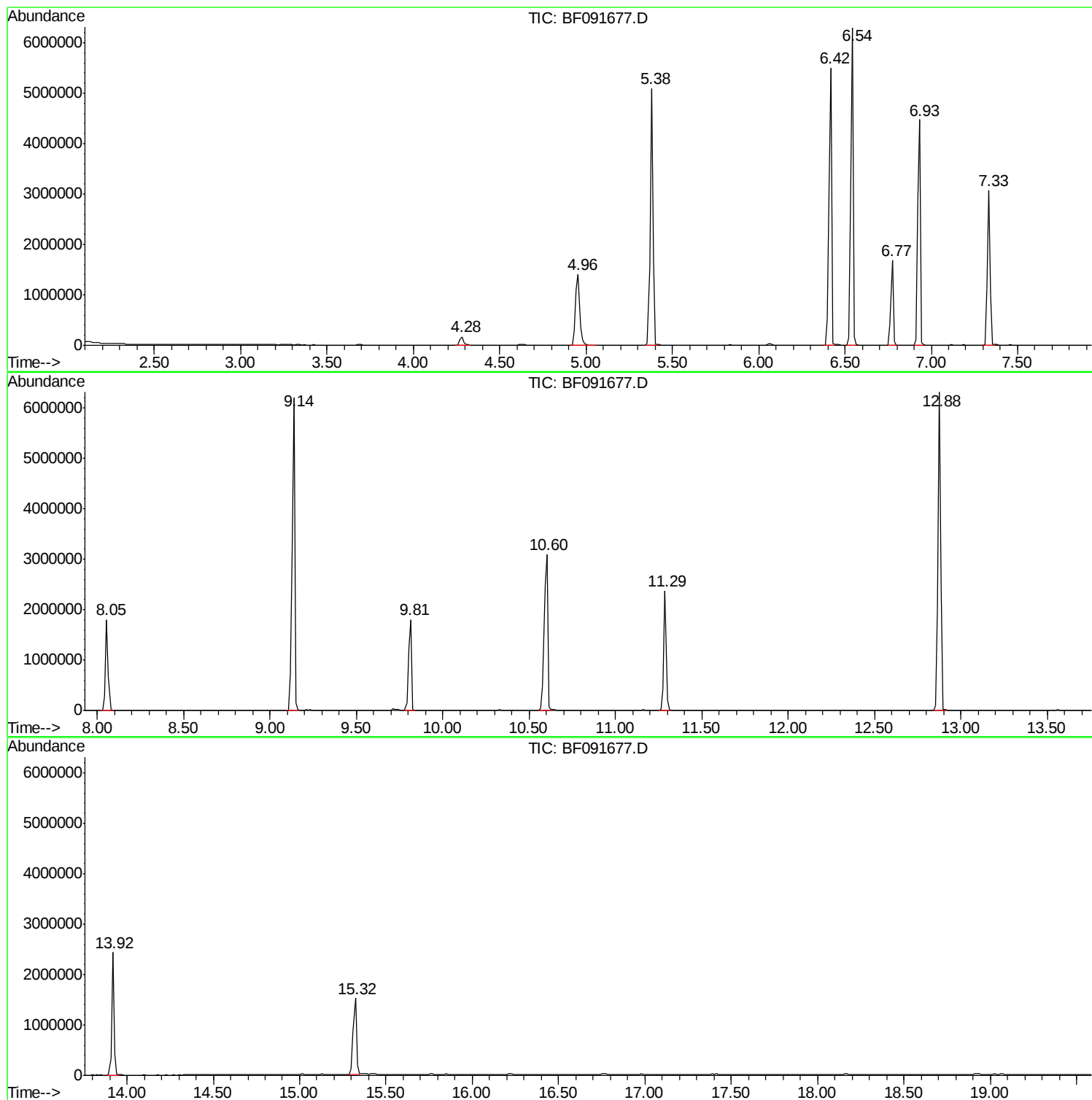
Sum of corrected areas: 60155355

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121616\  
Data File : BF091677.D  
Acq On : 16 Dec 2016 17:20  
Operator : UM/SJ  
Sample : PB95306BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB95306BL

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF120916.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121616\  
Data File : BF091677.D  
Acq On : 16 Dec 2016 17:20  
Operator : UM/SJ  
Sample : PB95306BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB95306BL

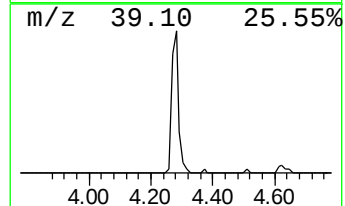
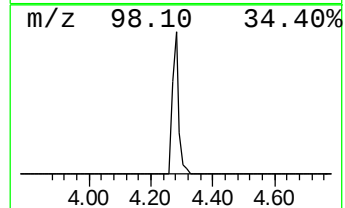
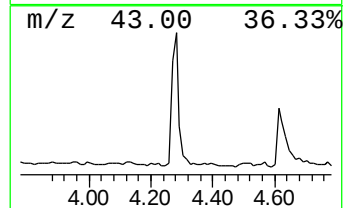
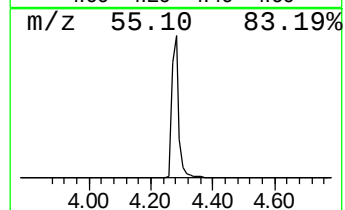
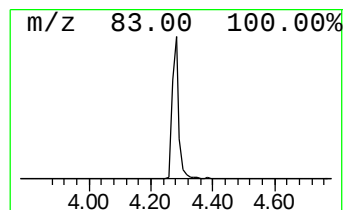
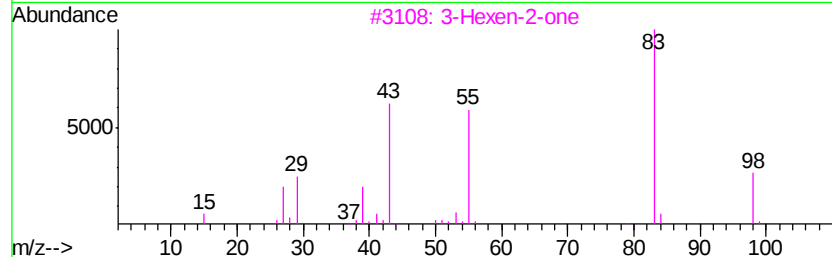
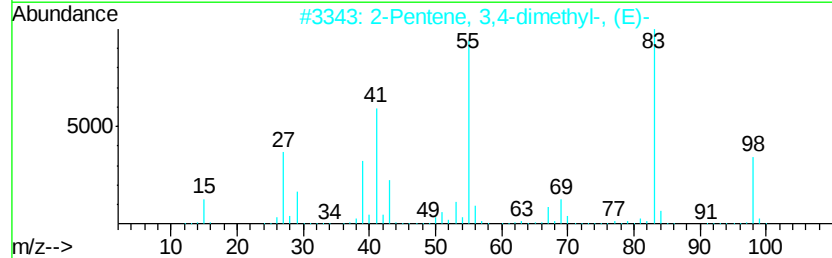
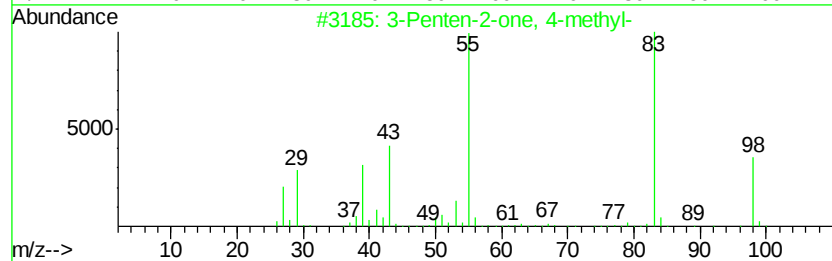
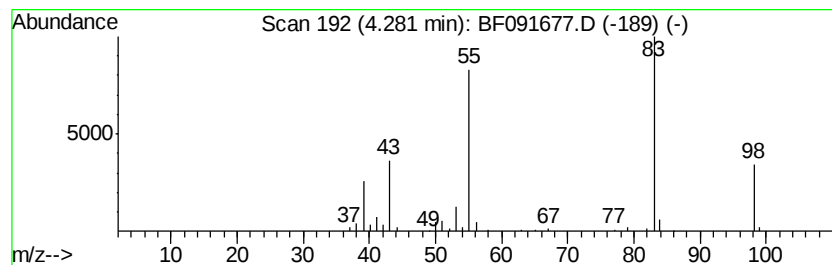
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF120916.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.28 | 3.23 ng | 240064 | 1,4-Dichlorobenzene-d4 | 6.77 |

| Hit# | of | 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|----|---------|-------------|------|
| 1    |    |   | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 94   |
| 2    |    |   | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 90   |
| 3    |    |   | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 90   |
| 4    |    |   | 2-Pentene, 2,4-dimethyl-       | 98 | C7H14   | 000625-65-0 | 87   |
| 5    |    |   | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14   | 000690-08-4 | 86   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\  
Data File : BF091677.D  
Acq On : 16 Dec 2016 17:20  
Operator : UM/SJ  
Sample : PB95306BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB95306BL

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

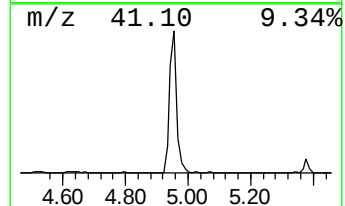
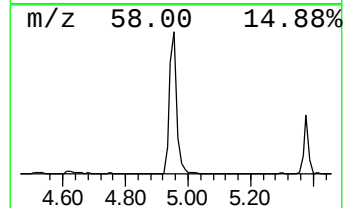
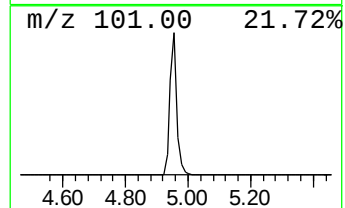
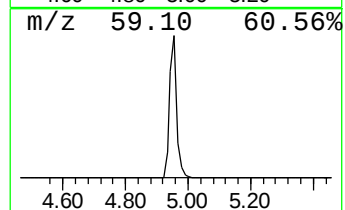
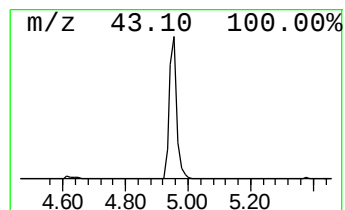
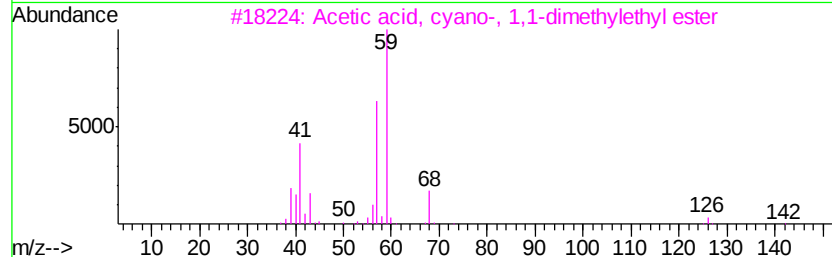
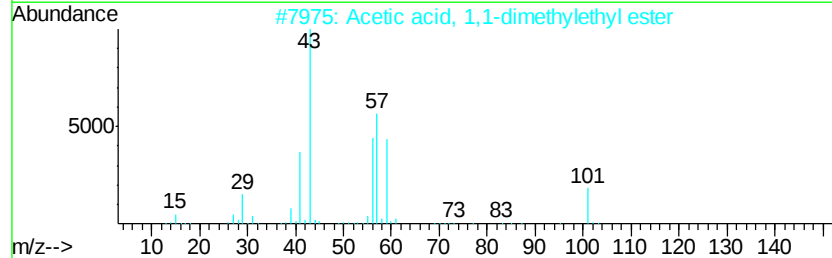
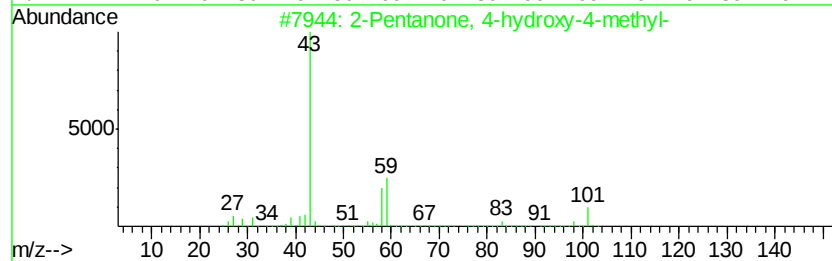
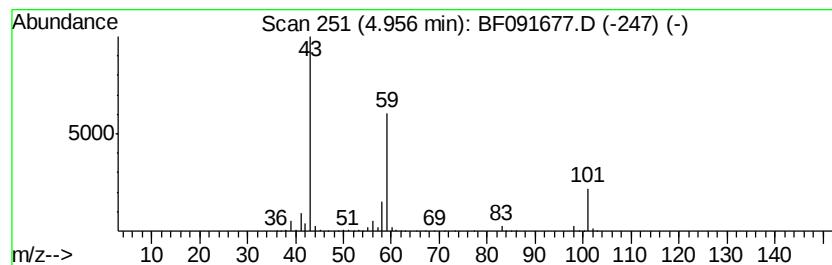
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 4.96 | 30.25 ng | 2247540 | 1,4-Dichlorobenzene-d4 | 6.77 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 64   |
| 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    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 17   |
| 5    |    | 5-Hexen-2-one                       | 98  | C6H10O   | 000109-49-9 | 9    |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121616\  
Data File : BF091677.D  
Acq On : 16 Dec 2016 17:20  
Operator : UM/SJ  
Sample : PB95306BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB95306BL

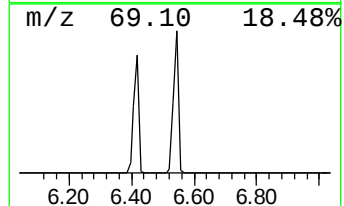
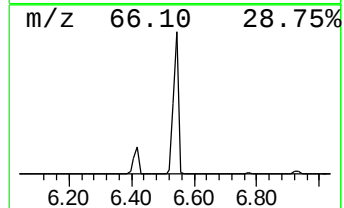
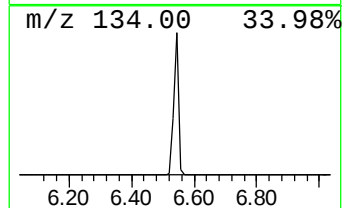
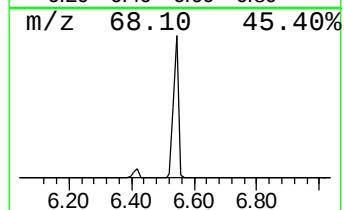
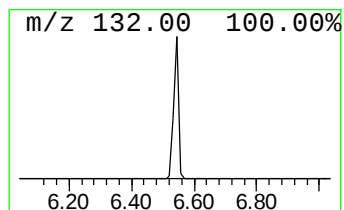
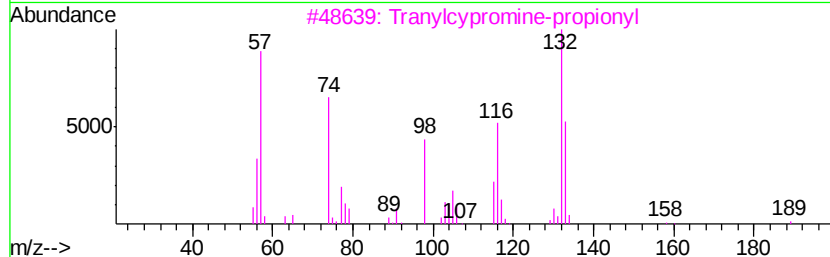
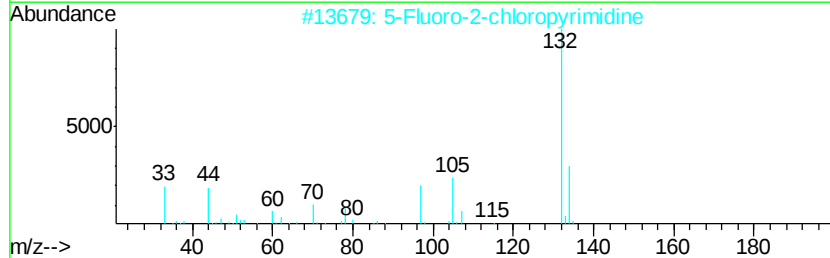
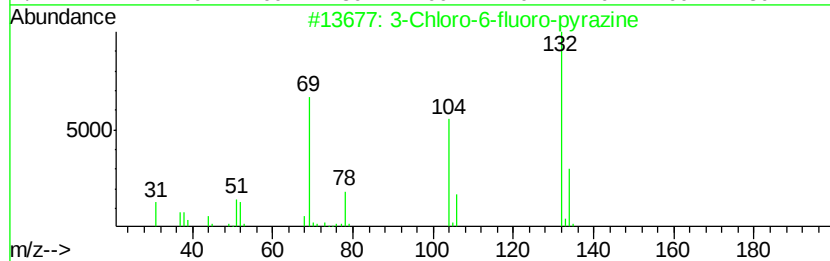
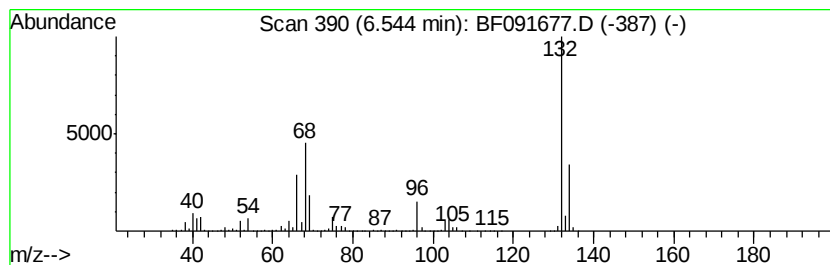
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 unknown6.54 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.54 | 87.17 ng | 6477900 | 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 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 16   |
| 3    |    | Tranvlcypropine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | Benzene, 1,3,5-trifluoro-           | 132 | C6H3F3    | 000372-38-3  | 9    |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121616\  
Data File : BF091677.D  
Acq On : 16 Dec 2016 17:20  
Operator : UM/SJ  
Sample : PB95306BL  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB95306BL

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF120916.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |         |      |
|----------------------|------|---------|-------|----------|-----------------------|------|---------|------|
|                      |      |         |       |          | #                     | RT   | Resp    | Conc |
| 3-Penten-2-one, 4... | 4.28 | 3.2     | ng    | 240064   | 1                     | 6.77 | 1486190 | 20.0 |
| 2-Pentanone, 4-hy... | 4.96 | 30.3    | ng    | 2247540  | 1                     | 6.77 | 1486190 | 20.0 |
| unknown6.54          | 6.54 | 87.2    | ng    | 6477900  | 1                     | 6.77 | 1486190 | 20.0 |