

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF101315\  
 Data File : BF082246.D  
 Acq On : 13 Oct 2015 6:30  
 Operator : UM/IZ  
 Sample : G3990-24  
 Misc :  
 ALS Vial : 28 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 MW35

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 1 % 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-BF101015.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         | 4.994       | 248           | 250         | 260          | rVB      | 300298         | 420004        | 16.77%          | 2.446%        |
| 2         | 5.428       | 285           | 288         | 290          | rBV      | 786388         | 888450        | 35.47%          | 5.175%        |
| 3         | 5.829       | 321           | 323         | 328          | rVB      | 32441          | 30532         | 1.22%           | 0.178%        |
| 4         | 6.469       | 376           | 379         | 381          | rBV      | 449459         | 537546        | 21.46%          | 3.131%        |
| 5         | 6.594       | 388           | 390         | 393          | rBV      | 1412466        | 1546890       | 61.75%          | 9.010%        |
| 6         | 6.834       | 409           | 411         | 413          | rBV      | 295705         | 328598        | 13.12%          | 1.914%        |
| 7         | 6.983       | 422           | 424         | 427          | rBV      | 1343754        | 1544551       | 61.66%          | 8.996%        |
| 8         | 7.406       | 458           | 461         | 463          | rBV      | 1149699        | 1259679       | 50.29%          | 7.337%        |
| 9         | 7.520       | 469           | 471         | 475          | rVB      | 25673          | 26227         | 1.05%           | 0.153%        |
| 10        | 7.806       | 494           | 496         | 498          | rVB      | 28857          | 30001         | 1.20%           | 0.175%        |
| 11        | 8.114       | 521           | 523         | 531          | rBV      | 443070         | 508136        | 20.29%          | 2.960%        |
| 12        | 8.320       | 538           | 541         | 543          | rBV      | 22774          | 30013         | 1.20%           | 0.175%        |
| 13        | 8.572       | 558           | 563         | 564          | rBV2     | 17549          | 25208         | 1.01%           | 0.147%        |
| 14        | 8.675       | 571           | 572         | 574          | rVB      | 49361          | 43255         | 1.73%           | 0.252%        |
| 15        | 8.835       | 583           | 586         | 590          | rVB4     | 15861          | 32122         | 1.28%           | 0.187%        |
| 16        | 9.040       | 600           | 604         | 605          | rBV3     | 37180          | 68758         | 2.74%           | 0.400%        |
| 17        | 9.063       | 605           | 606         | 608          | rVV      | 35224          | 36618         | 1.46%           | 0.213%        |
| 18        | 9.097       | 608           | 609         | 613          | rVB4     | 29912          | 28244         | 1.13%           | 0.165%        |
| 19        | 9.200       | 615           | 618         | 620          | rBV      | 2633041        | 2504965       | 100.00%         | 14.591%       |
| 20        | 9.337       | 627           | 630         | 632          | rVB3     | 16008          | 29806         | 1.19%           | 0.174%        |
| 21        | 9.406       | 634           | 636         | 639          | rVB3     | 15149          | 26405         | 1.05%           | 0.154%        |
| 22        | 9.463       | 639           | 641         | 642          | rBV2     | 29088          | 31520         | 1.26%           | 0.184%        |
| 23        | 9.566       | 645           | 650         | 651          | rVV4     | 24159          | 60323         | 2.41%           | 0.351%        |
| 24        | 9.589       | 651           | 652         | 655          | rVV2     | 34599          | 58845         | 2.35%           | 0.343%        |
| 25        | 9.646       | 655           | 657         | 662          | rVB3     | 43166          | 100875        | 4.03%           | 0.588%        |
| 26        | 9.875       | 673           | 677         | 679          | rBV      | 690566         | 660198        | 26.36%          | 3.845%        |
| 27        | 9.909       | 679           | 680         | 682          | rVB      | 61706          | 48636         | 1.94%           | 0.283%        |
| 28        | 10.035      | 689           | 691         | 693          | rBV2     | 18858          | 25764         | 1.03%           | 0.150%        |
| 29        | 10.080      | 693           | 695         | 699          | rVB3     | 17840          | 41175         | 1.64%           | 0.240%        |
| 30        | 10.412      | 723           | 724         | 726          | rVB      | 43661          | 35025         | 1.40%           | 0.204%        |
| 31        | 10.503      | 726           | 732         | 733          | rBV2     | 60502          | 126594        | 5.05%           | 0.737%        |
| 32        | 10.572      | 736           | 738         | 743          | rVB3     | 23909          | 56696         | 2.26%           | 0.330%        |
| 33        | 10.663      | 743           | 746         | 749          | rBV2     | 1261891        | 1512763       | 60.39%          | 8.811%        |
| 34        | 10.766      | 752           | 755         | 756          | rBV3     | 14048          | 28274         | 1.13%           | 0.165%        |

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Misc :  
ALS Vial : 28 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW35

Integration Parameters: rteint.p  
Integrator: RTE  
Smoothing : OFF Filtering: 5  
Sampling : 1 Min Area: 1 % 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-BF101015.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |         |        |         |
|----|--------|------|------|------|------|---------|---------|--------|---------|
| 35 | 10.960 | 770  | 772  | 774  | rBV2 | 25906   | 30969   | 1.24%  | 0.180%  |
| 36 | 11.029 | 774  | 778  | 779  | rVV4 | 17966   | 46745   | 1.87%  | 0.272%  |
| 37 | 11.098 | 782  | 784  | 788  | rVB2 | 18237   | 42581   | 1.70%  | 0.248%  |
| 38 | 11.361 | 804  | 807  | 815  | rVB  | 626656  | 622171  | 24.84% | 3.624%  |
| 39 | 11.886 | 851  | 853  | 856  | rBV3 | 41239   | 50209   | 2.00%  | 0.292%  |
| 40 | 12.138 | 871  | 875  | 880  | rVB5 | 14803   | 35575   | 1.42%  | 0.207%  |
| 41 | 12.949 | 943  | 946  | 949  | rBV  | 2380839 | 2479432 | 98.98% | 14.442% |
| 42 | 13.841 | 1022 | 1024 | 1028 | rBV2 | 29487   | 36202   | 1.45%  | 0.211%  |
| 43 | 14.001 | 1035 | 1038 | 1044 | rBV  | 616120  | 622109  | 24.84% | 3.624%  |
| 44 | 15.441 | 1161 | 1164 | 1171 | rBV  | 295042  | 469733  | 18.75% | 2.736%  |

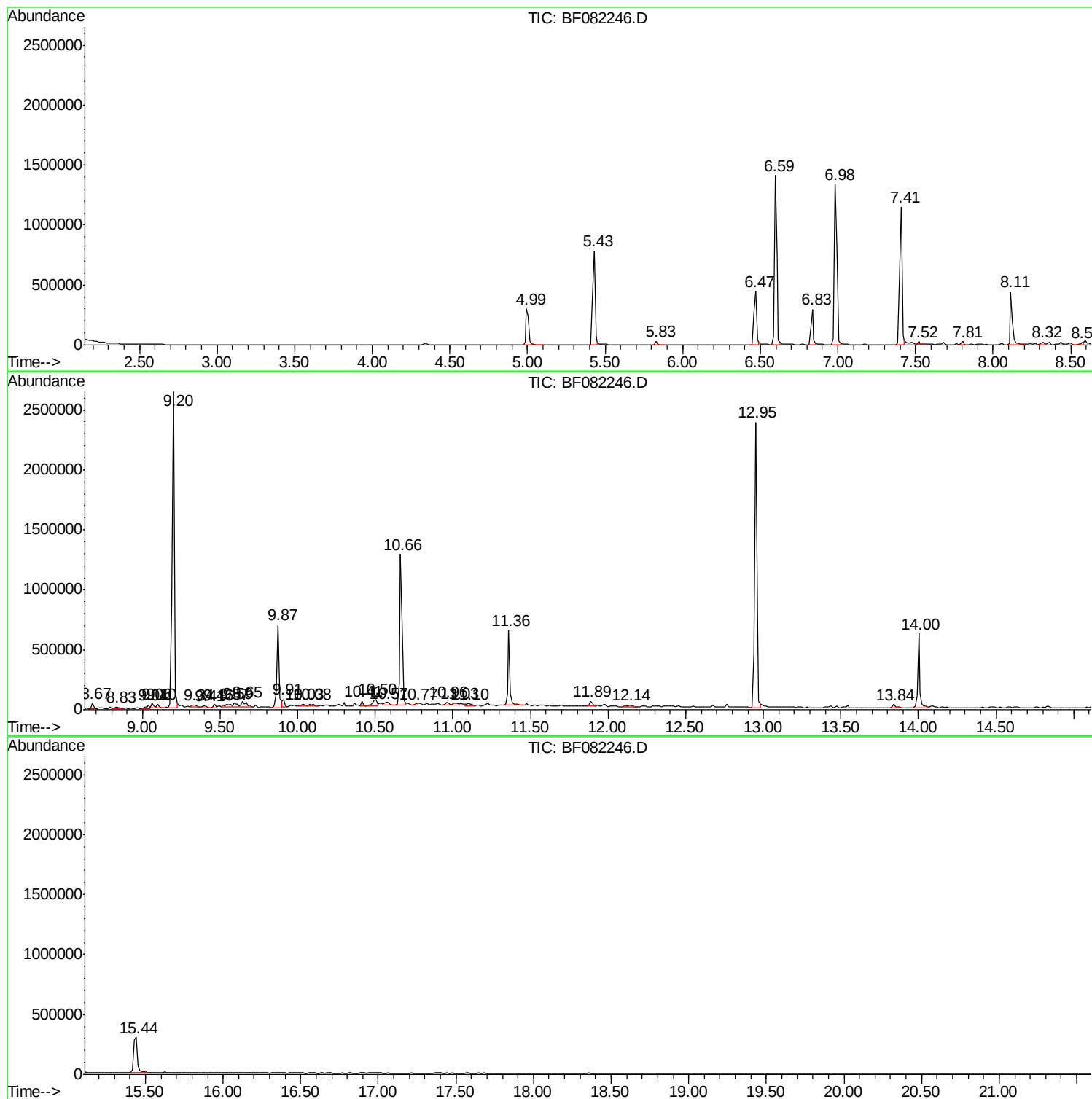
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Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF101315\  
Data File : BF082246.D  
Acq On : 13 Oct 2015 6:30  
Operator : UM/IZ  
Sample : G3990-24  
Misc :  
ALS Vial : 28 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW35

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF101015.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\BF101315\  
Data File : BF082246.D  
Acq On : 13 Oct 2015 6:30  
Operator : UM/IZ  
Sample : G3990-24  
Misc :  
ALS Vial : 28 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW35

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

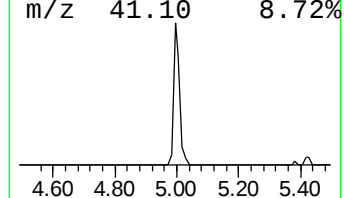
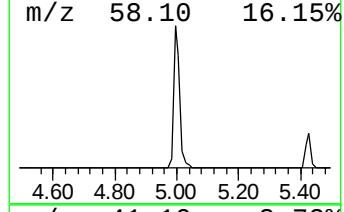
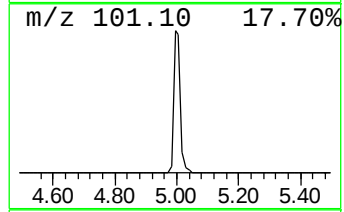
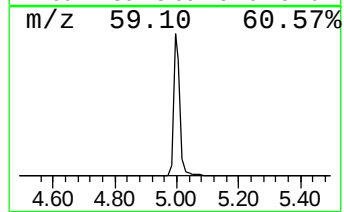
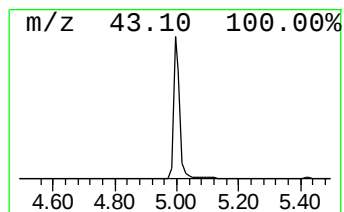
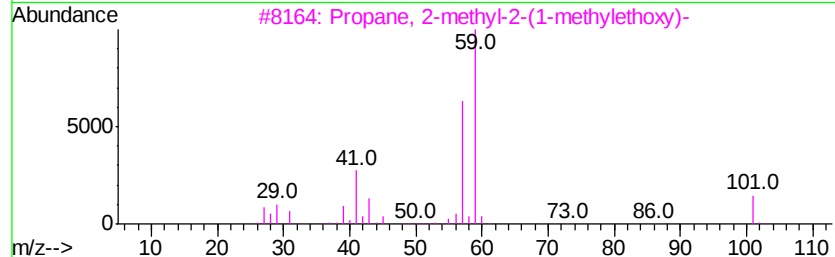
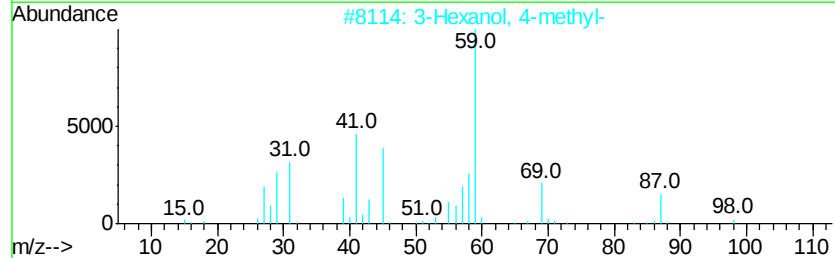
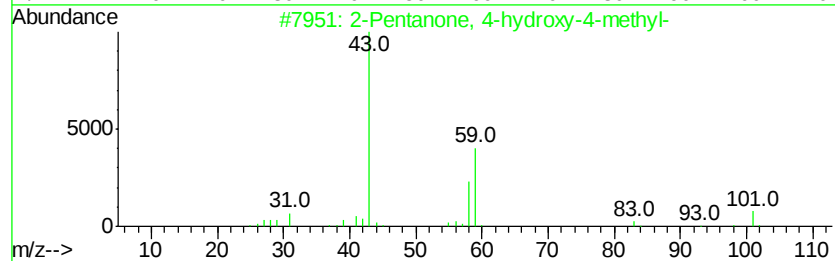
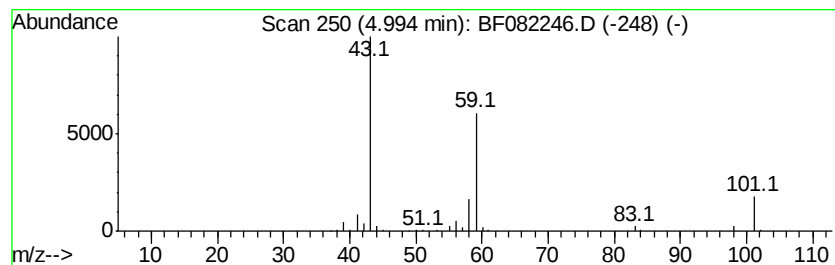
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|--------|------------------------|------|
| 4.99 | 25.56 ng | 420004 | 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 | 64   |      |
| 2       | 3-Hexanol, 4-methyl-                  | 116          | C7H16O   | 000615-29-2 | 33   |      |
| 3       | Propane, 2-methyl-2-(1-methylethoxy)- | 116          | C7H16O   | 017348-59-3 | 33   |      |
| 4       | 2-Hexanol, 2-methyl-                  | 116          | C7H16O   | 000625-23-0 | 28   |      |
| 5       | Acetic acid, cyano-, 1,1-dimethyl-    | 141          | C7H11NO2 | 001116-98-9 | 23   |      |



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Misc :  
ALS Vial : 28 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
MW35

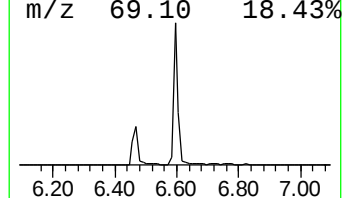
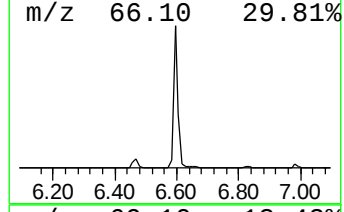
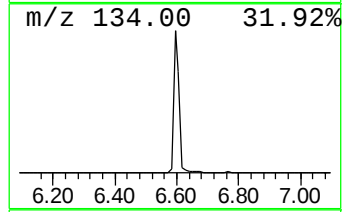
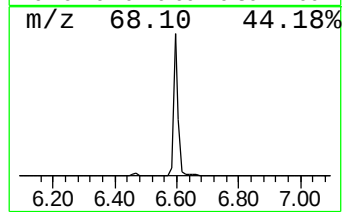
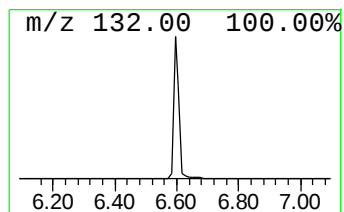
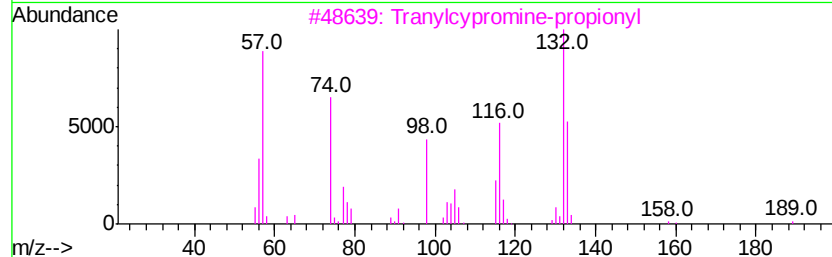
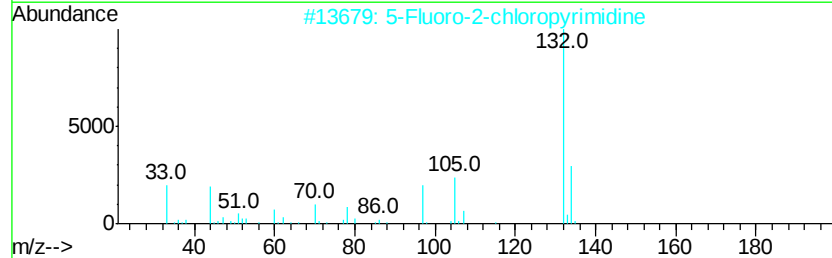
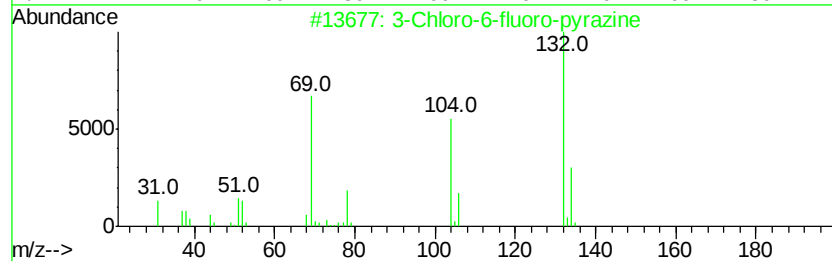
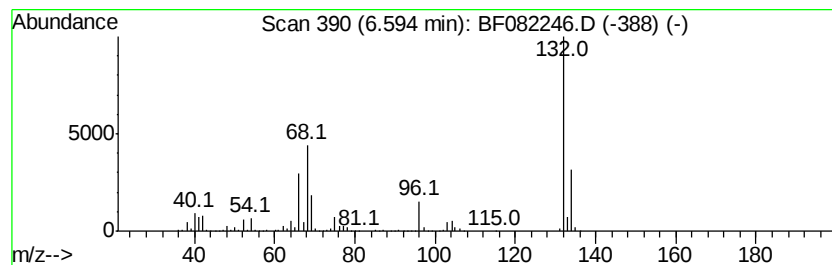
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.59 | 94.15 ng | 1546890 | 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 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 3    |    | Tranvlcypramine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2  | 029490-19-5  | 9    |



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Instrument :  
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ClientSampleId :  
MW35

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF101015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

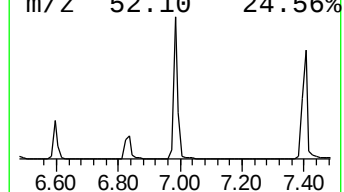
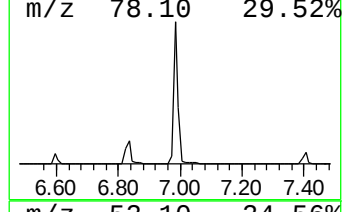
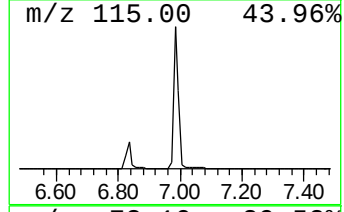
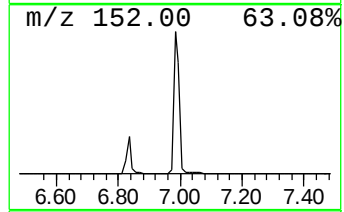
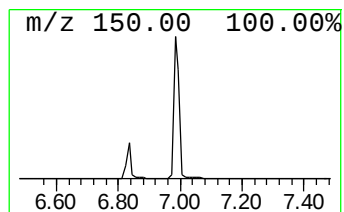
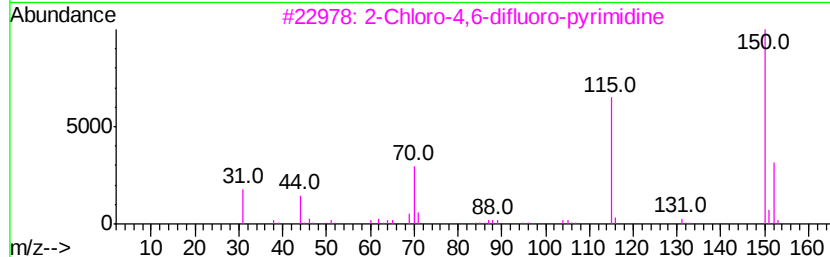
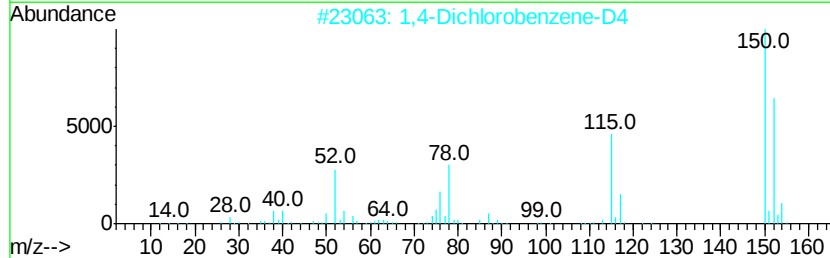
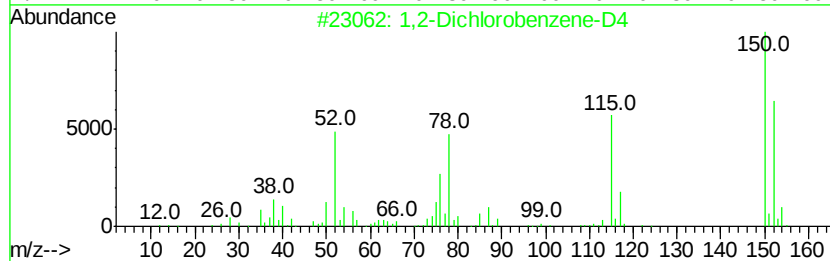
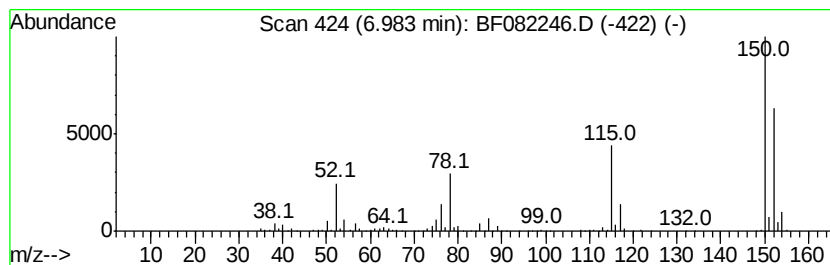
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 1,2-Dichlorobenzene-D4 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.98 | 94.01 ng | 1544550 | 1,4-Dichlorobenzene-d4 | 6.83 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#        | Qual |
|------|----|----------------------------------|-----|-----------|-------------|------|
| 1    | 5  | 1,2-Dichlorobenzene-D4           | 150 | C6D4Cl2   | 002199-69-1 | 94   |
| 2    |    | 1,4-Dichlorobenzene-D4           | 150 | C6D4Cl2   | 003855-82-1 | 94   |
| 3    |    | 2-Chloro-4,6-difluoro-pyrimidine | 150 | C4HClF2N2 | 038953-30-9 | 35   |
| 4    |    | 2-Bromo-3'-nitroacetophenone     | 243 | C8H6BrNO3 | 002227-64-7 | 14   |
| 5    |    | 2-Bromo-2'-nitroacetophenone     | 243 | C8H6BrNO3 | 006851-99-6 | 10   |



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MW35

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

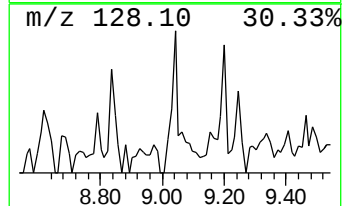
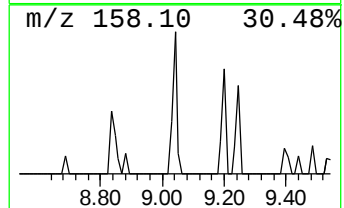
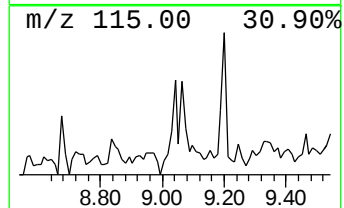
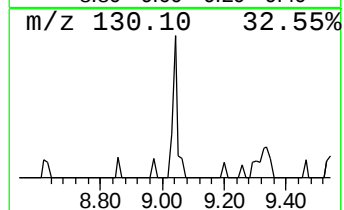
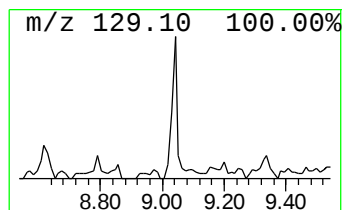
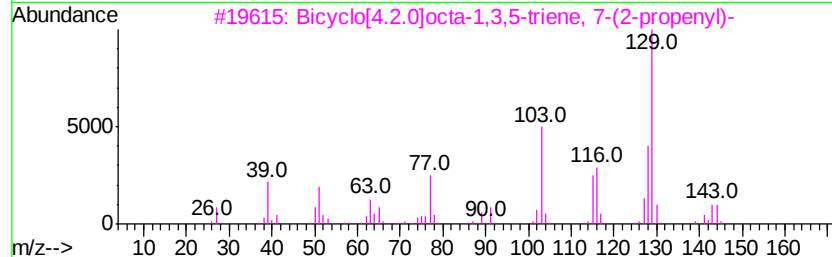
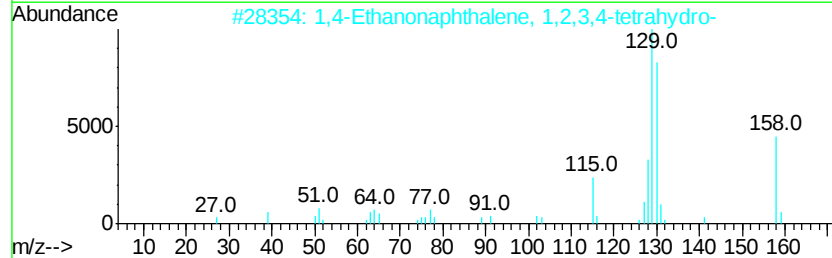
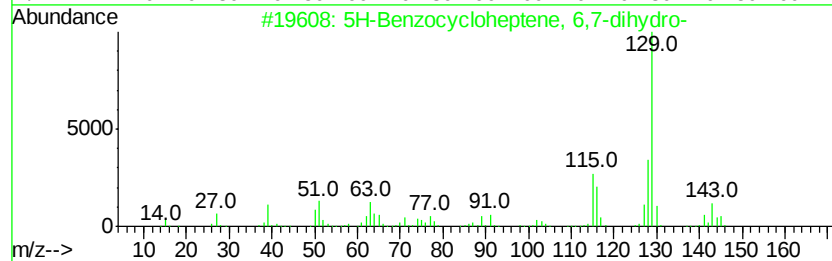
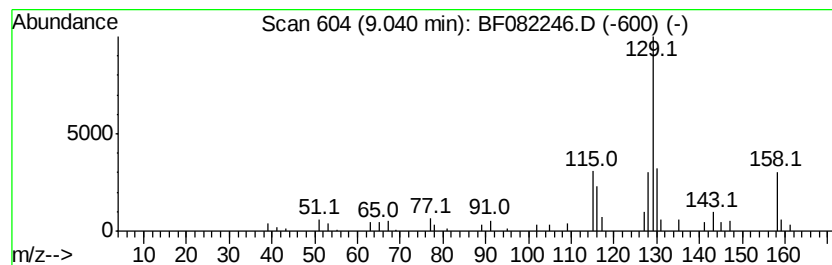
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 5H-Benzocycloheptene, 6,7-d... Concentration Rank 6

| R.T. | EstConc | Area  | Relative to ISTD | R.T. |
|------|---------|-------|------------------|------|
| 9.04 | 2.08 ng | 68758 | Acenaphthene-d10 | 9.87 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 5H-Benzocycloheptene, 6,7-dihydro-  | 144 | C11H12  | 007125-62-4 | 59   |
| 2    |    | 1,4-Ethanonaphthalene, 1,2,3,4-t... | 158 | C12H14  | 004175-52-4 | 59   |
| 3    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 144 | C11H12  | 071721-26-1 | 42   |
| 4    |    | Cyclohexene, 1-phenyl-              | 158 | C12H14  | 000771-98-2 | 38   |
| 5    |    | Benzene, 2-cyclohexen-1-yl-         | 158 | C12H14  | 015232-96-9 | 35   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101315\  
Data File : BF082246.D  
Acq On : 13 Oct 2015 6:30  
Operator : UM/IZ  
Sample : G3990-24  
Misc :  
ALS Vial : 28 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW35

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

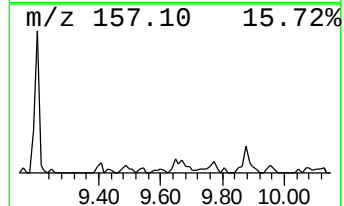
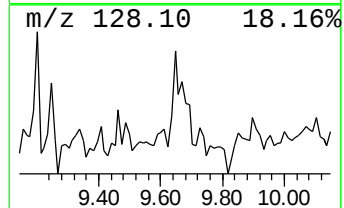
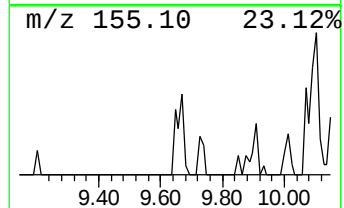
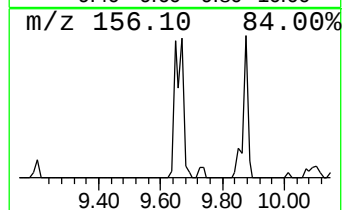
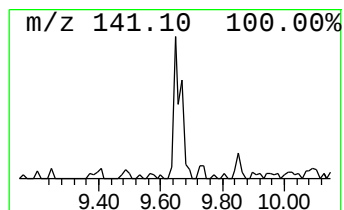
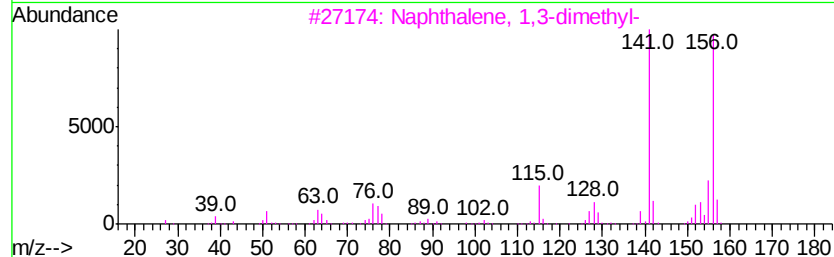
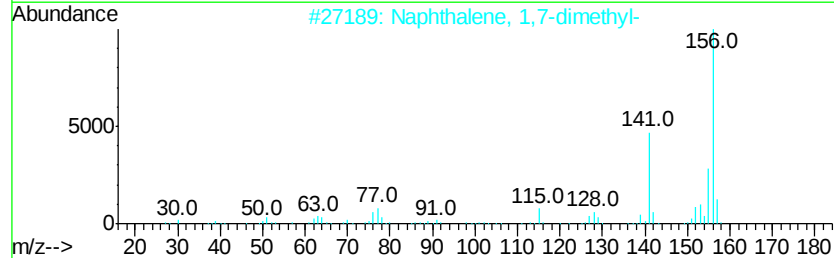
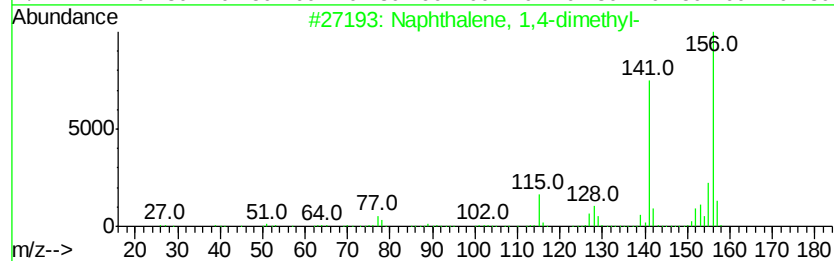
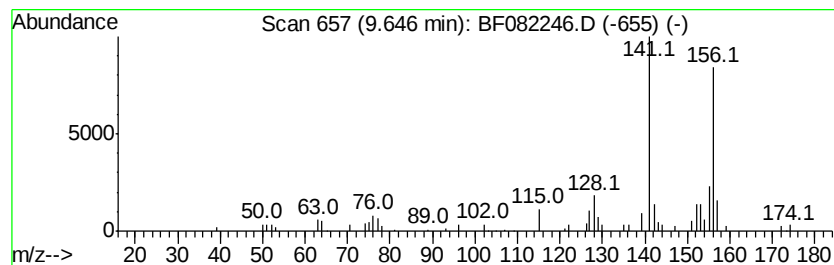
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Naphthalene, 1,4-dimethyl- Concentration Rank 5

| R.T. | EstConc | Area   | Relative to ISTD | R.T. |
|------|---------|--------|------------------|------|
| 9.65 | 3.06 ng | 100875 | Acenaphthene-d10 | 9.87 |

| Hit# | of | Tentative ID               | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------------|-----|---------|-------------|------|
| 1    | 5  | Naphthalene, 1,4-dimethyl- | 156 | C12H12  | 000571-58-4 | 96   |
| 2    |    | Naphthalene, 1,7-dimethyl- | 156 | C12H12  | 000575-37-1 | 96   |
| 3    |    | Naphthalene, 1,3-dimethyl- | 156 | C12H12  | 000575-41-7 | 94   |
| 4    |    | Naphthalene, 2,3-dimethyl- | 156 | C12H12  | 000581-40-8 | 94   |
| 5    |    | Naphthalene, 1,6-dimethyl- | 156 | C12H12  | 000575-43-9 | 94   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF101315\  
Data File : BF082246.D  
Acq On : 13 Oct 2015 6:30  
Operator : UM/IZ  
Sample : G3990-24  
Misc :  
ALS Vial : 28 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW35

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF101015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

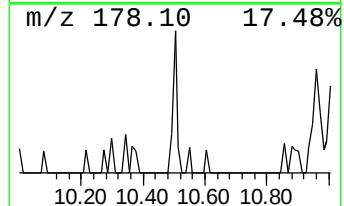
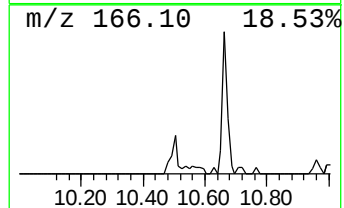
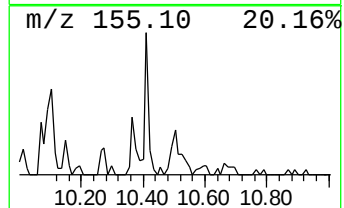
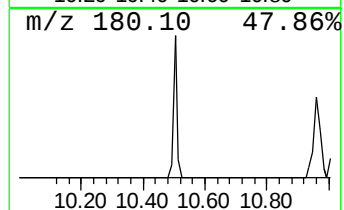
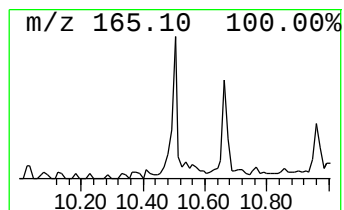
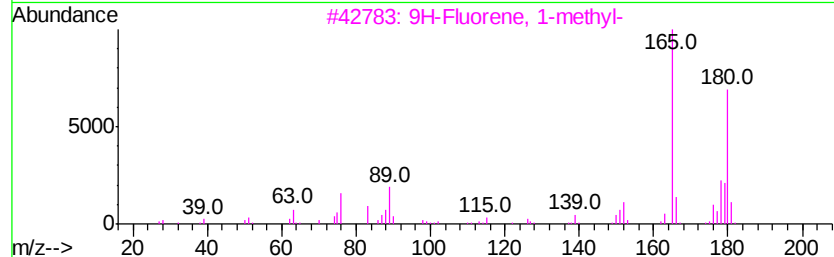
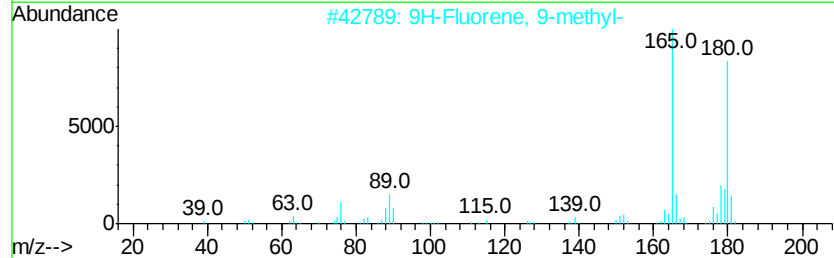
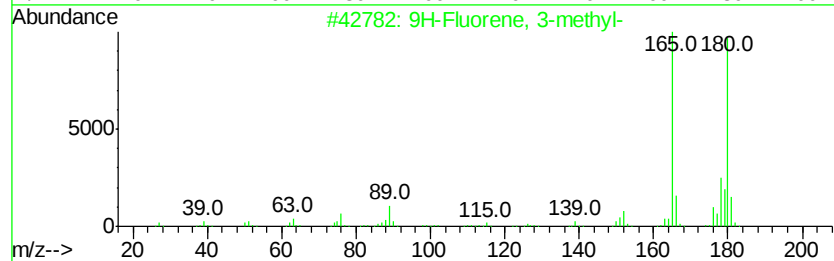
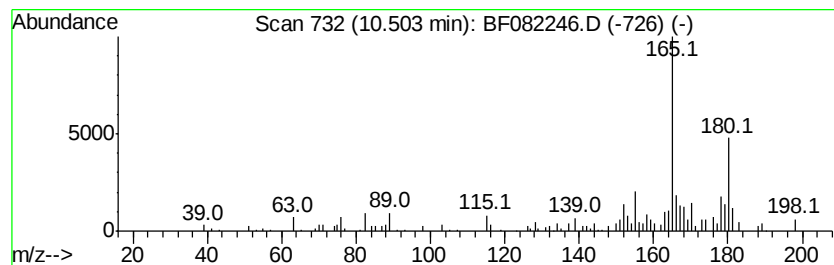
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 9H-Fluorene, 3-methyl- Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T. |
|-------|---------|--------|------------------|------|
| 10.50 | 3.84 ng | 126594 | Acenaphthene-d10 | 9.87 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 9H-Fluorene, 3-methyl-              | 180 | C14H12  | 002523-39-9 | 70   |
| 2    |    |   | 9H-Fluorene, 9-methyl-              | 180 | C14H12  | 002523-37-7 | 64   |
| 3    |    |   | 9H-Fluorene, 1-methyl-              | 180 | C14H12  | 001730-37-6 | 64   |
| 4    |    |   | 9H-Fluorene, 2-methyl-              | 180 | C14H12  | 001430-97-3 | 64   |
| 5    |    |   | Benzenethiol, 4-(1,1-dimethyleth... | 180 | C11H16S | 015570-10-2 | 64   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF101315\  
Data File : BF082246.D  
Acq On : 13 Oct 2015 6:30  
Operator : UM/IZ  
Sample : G3990-24  
Misc :  
ALS Vial : 28 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW35

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF101015.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 |
| 2-Pentanone, 4-hy... | 4.99  | 25.6    | ng    | 420004   | 1                     | 6.83 | 328598 | 20.0 |
| 3-Chloro-6-fluoro... | 6.59  | 94.2    | ng    | 1546890  | 1                     | 6.83 | 328598 | 20.0 |
| 1,2-Dichlorobenze... | 6.98  | 94.0    | ng    | 1544550  | 1                     | 6.83 | 328598 | 20.0 |
| 5H-Benzocyclohept... | 9.04  | 2.1     | ng    | 68758    | 3                     | 9.87 | 660198 | 20.0 |
| Naphthalene, 1,4-... | 9.65  | 3.1     | ng    | 100875   | 3                     | 9.87 | 660198 | 20.0 |
| 9H-Fluorene, 3-me... | 10.50 | 3.8     | ng    | 126594   | 3                     | 9.87 | 660198 | 20.0 |