

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051115\  
 Data File : BF079131.D  
 Acq On : 11 May 2015 22:33  
 Operator : TP/IZ  
 Sample : G2176-10  
 Misc :  
 ALS Vial : 23 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PS-29(15-20)

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-BF043015.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         | 1.450       | 20            | 23          | 26           | rVB      | 5128988        | 5823678       | 100.00%         | 22.402%       |
| 2         | 1.575       | 31            | 34          | 39           | rVB      | 249708         | 493979        | 8.48%           | 1.900%        |
| 3         | 1.735       | 47            | 48          | 57           | rVV2     | 377943         | 778657        | 13.37%          | 2.995%        |
| 4         | 1.861       | 57            | 59          | 91           | rVB      | 2097759        | 3763814       | 64.63%          | 14.479%       |
| 5         | 5.096       | 340           | 342         | 347          | rVB      | 71959          | 104155        | 1.79%           | 0.401%        |
| 6         | 5.599       | 383           | 386         | 389          | rBV      | 1549009        | 1516722       | 26.04%          | 5.834%        |
| 7         | 6.856       | 494           | 496         | 499          | rBV      | 1197193        | 1554317       | 26.69%          | 5.979%        |
| 8         | 7.004       | 507           | 509         | 512          | rBV      | 1174362        | 1616067       | 27.75%          | 6.217%        |
| 9         | 7.302       | 532           | 535         | 537          | rBV      | 248034         | 305938        | 5.25%           | 1.177%        |
| 10        | 7.484       | 549           | 551         | 553          | rBV      | 1369237        | 1229279       | 21.11%          | 4.729%        |
| 11        | 7.987       | 593           | 595         | 597          | rBV      | 1119904        | 953893        | 16.38%          | 3.669%        |
| 12        | 8.867       | 670           | 672         | 675          | rBV      | 358881         | 426621        | 7.33%           | 1.641%        |
| 13        | 10.216      | 788           | 790         | 793          | rBV      | 1825452        | 1793503       | 30.80%          | 6.899%        |
| 14        | 10.719      | 833           | 834         | 837          | rVB      | 67581          | 72033         | 1.24%           | 0.277%        |
| 15        | 11.051      | 861           | 863         | 865          | rBV      | 500948         | 480741        | 8.25%           | 1.849%        |
| 16        | 12.033      | 946           | 949         | 951          | rBV      | 1059187        | 1213524       | 20.84%          | 4.668%        |
| 17        | 12.891      | 1022          | 1024        | 1027         | rBV      | 496577         | 493122        | 8.47%           | 1.897%        |
| 18        | 14.891      | 1196          | 1199        | 1202         | rBV      | 2022054        | 1999176       | 34.33%          | 7.690%        |
| 19        | 16.068      | 1300          | 1302        | 1310         | rVB      | 45902          | 69400         | 1.19%           | 0.267%        |
| 20        | 16.182      | 1310          | 1312        | 1314         | rBV      | 494505         | 566746        | 9.73%           | 2.180%        |
| 21        | 16.823      | 1365          | 1368        | 1371         | rBV      | 83503          | 136216        | 2.34%           | 0.524%        |
| 22        | 17.908      | 1460          | 1463        | 1466         | rBV      | 430610         | 604257        | 10.38%          | 2.324%        |

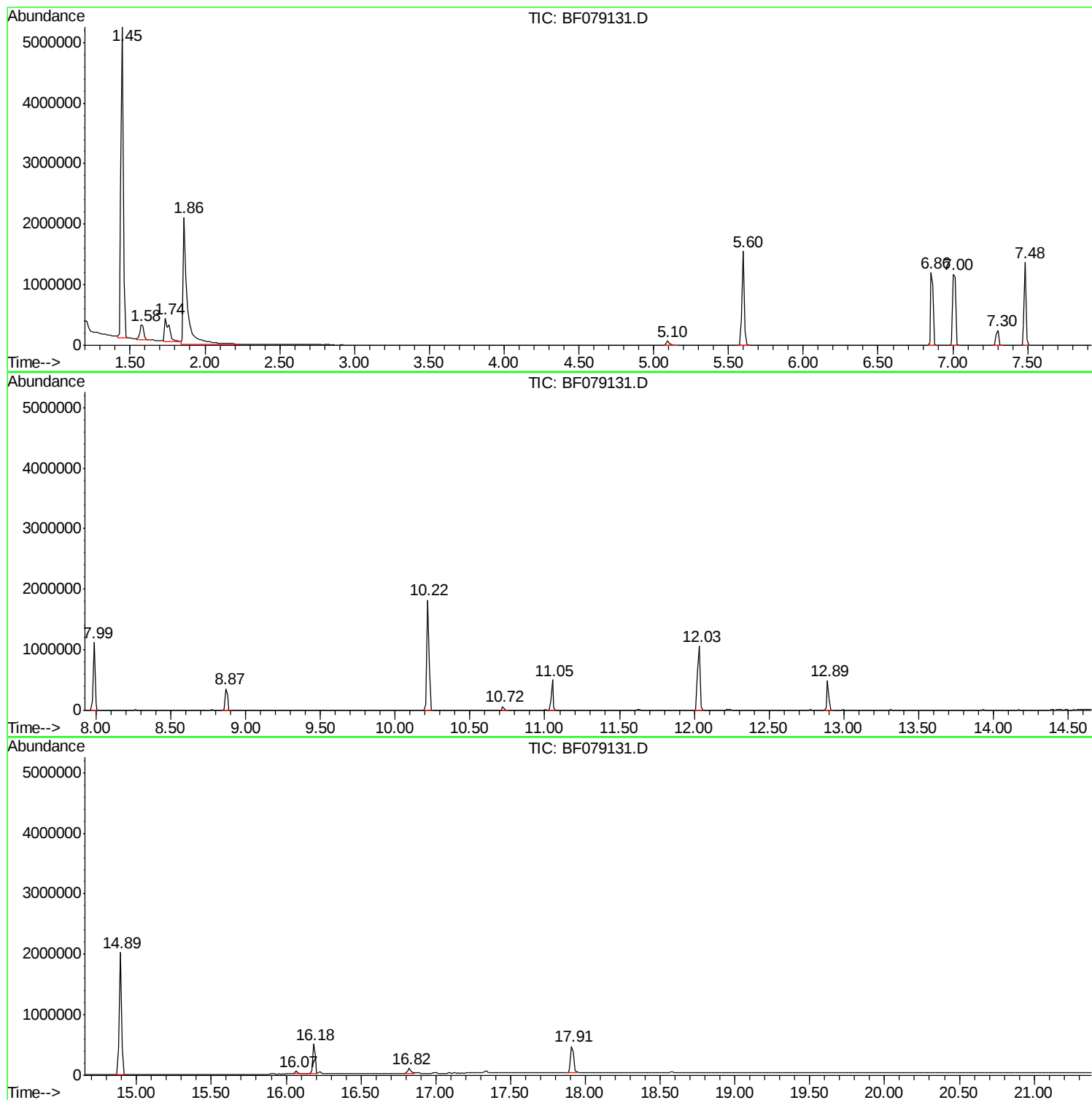
Sum of corrected areas: 25995838

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051115\  
Data File : BF079131.D  
Acq On : 11 May 2015 22:33  
Operator : TP/IZ  
Sample : G2176-10  
Misc :  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PS-29(15-20)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF043015.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\BF051115\  
Data File : BF079131.D  
Acq On : 11 May 2015 22:33  
Operator : TP/IZ  
Sample : G2176-10  
Misc :  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PS-29(15-20)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF043015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

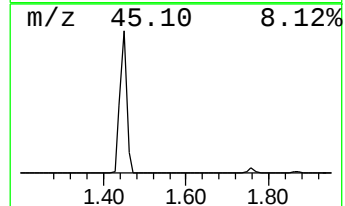
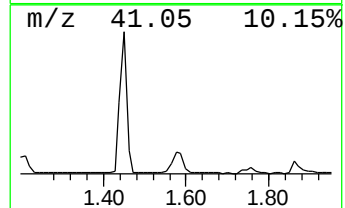
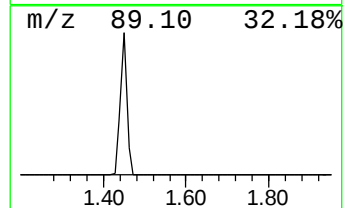
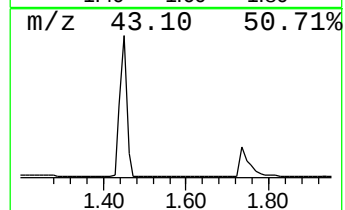
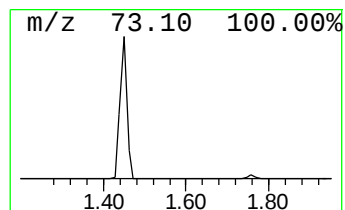
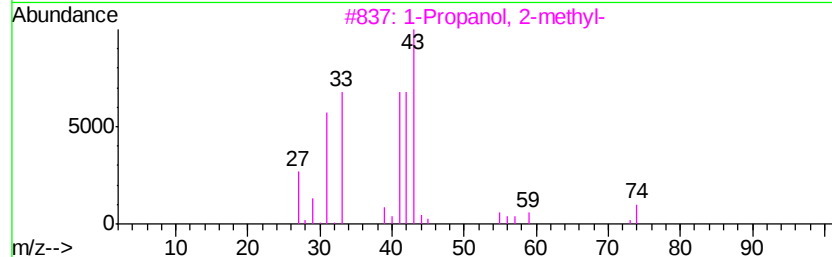
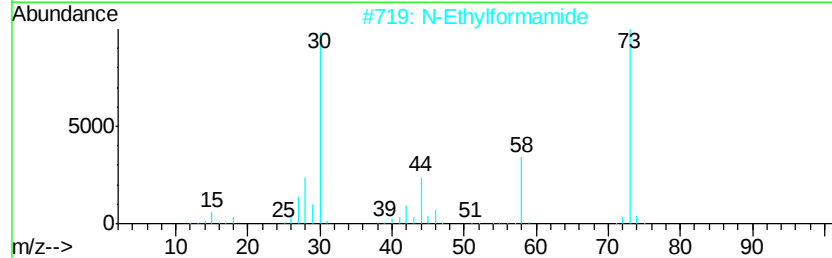
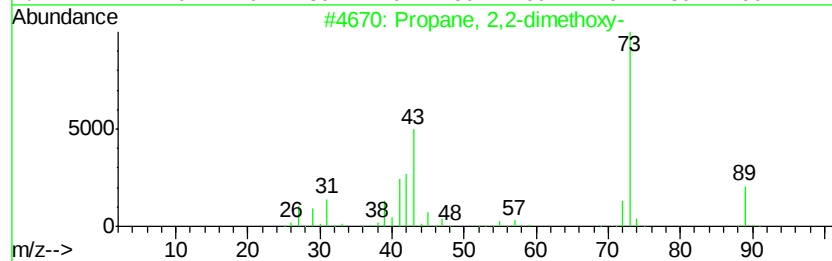
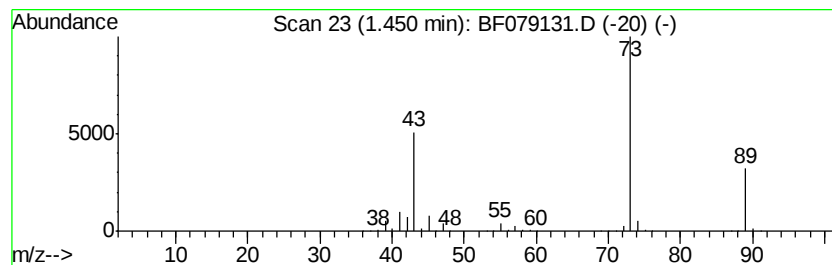
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 unknown1.45 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 1.45 | 380.71 ng | 5823680 | 1,4-Dichlorobenzene-d4 | 7.30 |

| Hit# | of | Tentative ID                 | MW  | MolForm | CAS#        | Qual |
|------|----|------------------------------|-----|---------|-------------|------|
| 1    | 5  | Propane, 2,2-dimethoxy-      | 104 | C5H12O2 | 000077-76-9 | 38   |
| 2    |    | N-Ethylformamide             | 73  | C3H7NO  | 000627-45-2 | 9    |
| 3    |    | 1-Propanol, 2-methyl-        | 74  | C4H10O  | 000078-83-1 | 9    |
| 4    |    | 1,3-Diaminoquanidine         | 89  | CH7N5   | 004364-78-7 | 9    |
| 5    |    | Propane, 2-methoxy-2-methyl- | 88  | C5H12O  | 001634-04-4 | 9    |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF051115\  
Data File : BF079131.D  
Acq On : 11 May 2015 22:33  
Operator : TP/IZ  
Sample : G2176-10  
Misc :  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PS-29(15-20)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF043015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

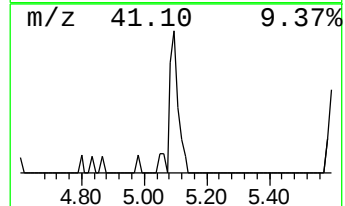
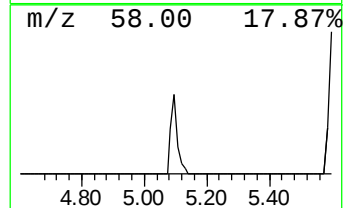
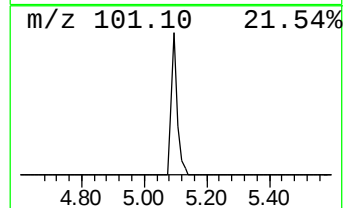
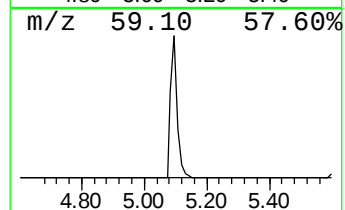
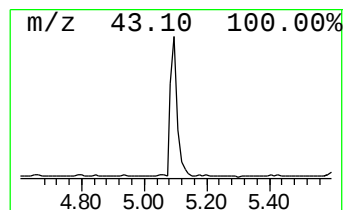
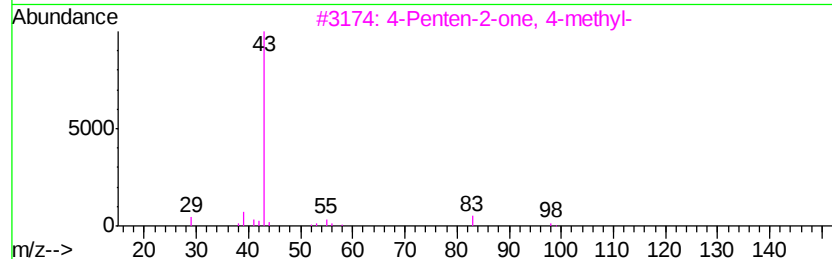
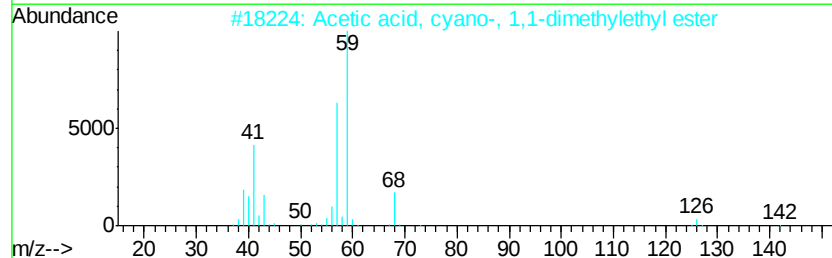
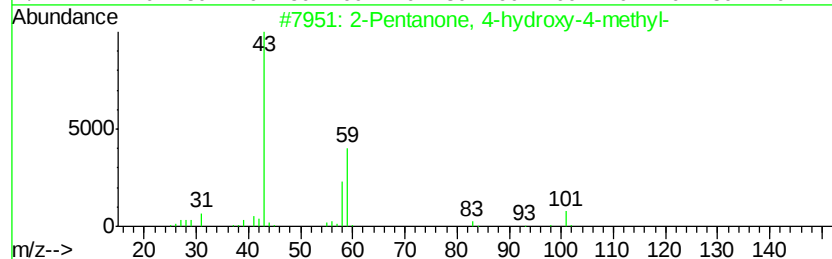
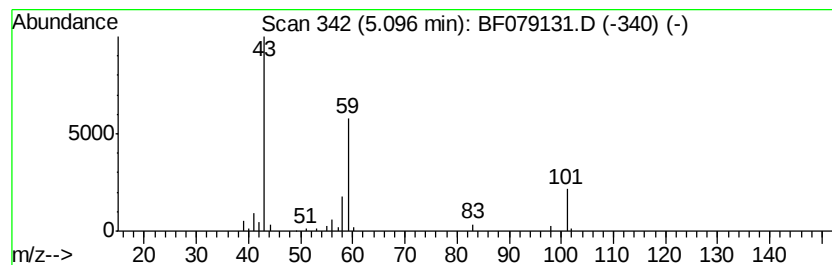
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.10 | 6.81 ng | 104155 | 1,4-Dichlorobenzene-d4 | 7.30 |

| Hit# | of                                   | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|--------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2      | 000123-42-2 | 42      |      |      |
| 2    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2     | 001116-98-9 | 17      |      |      |
| 3    | 4-Penten-2-one, 4-methyl-            | 98  | C6H10O       | 003744-02-3 | 9       |      |      |
| 4    | Morpholine, 4-methyl-                | 101 | C5H11NO      | 000109-02-4 | 9       |      |      |
| 5    | (+)-4-Amino-4,5-dihydro-2(3H)-f...   | 101 | C4H7NO2      | 016504-58-8 | 9       |      |      |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051115\  
Data File : BF079131.D  
Acq On : 11 May 2015 22:33  
Operator : TP/IZ  
Sample : G2176-10  
Misc :  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PS-29(15-20)

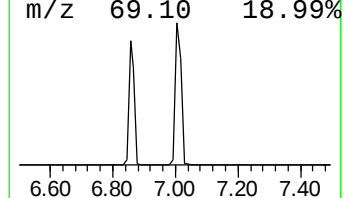
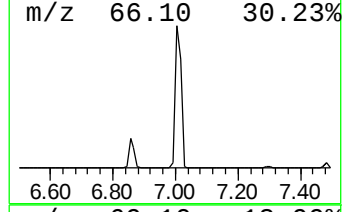
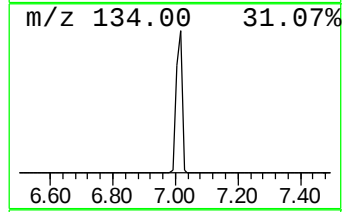
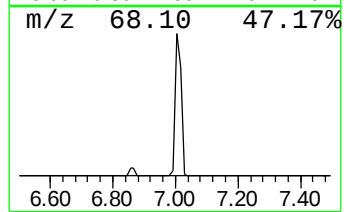
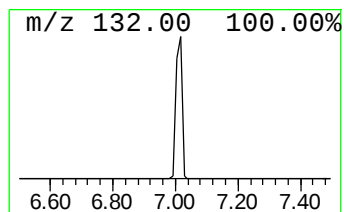
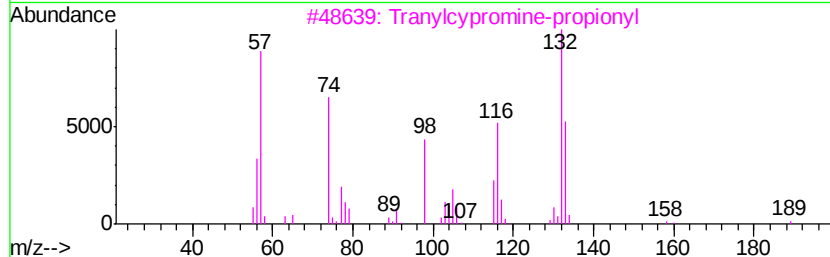
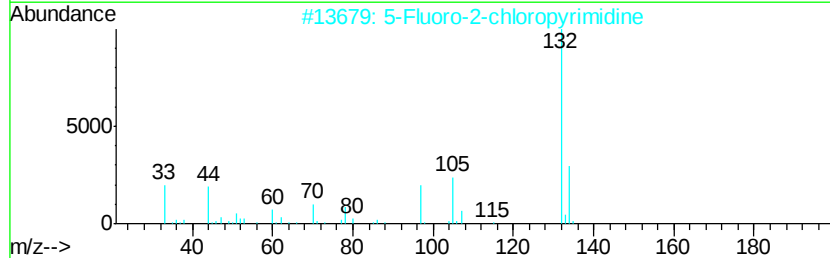
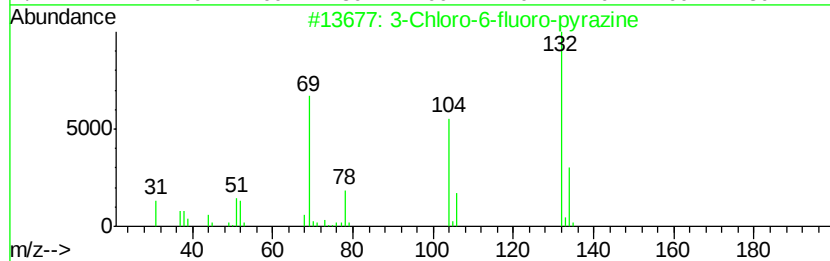
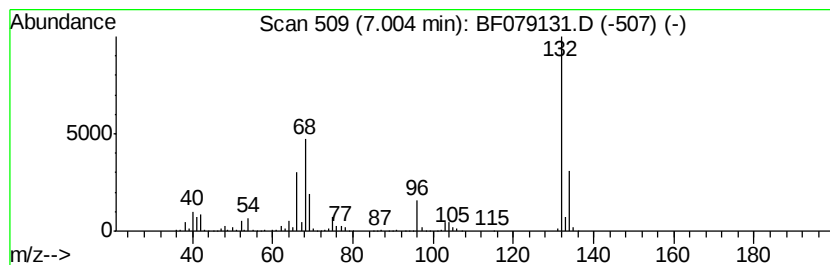
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF043015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 unknown7.00 Concentration Rank 3

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 7.00 | 105.65 ng | 1616070 | 1,4-Dichlorobenzene-d4 | 7.30 |

| 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    |    | Tranvlcypropine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 10   |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051115\  
Data File : BF079131.D  
Acq On : 11 May 2015 22:33  
Operator : TP/IZ  
Sample : G2176-10  
Misc :  
ALS Vial : 23 Sample Multiplier: 1

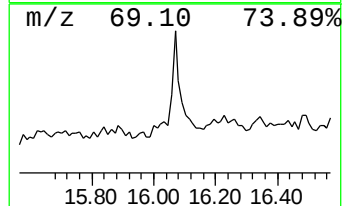
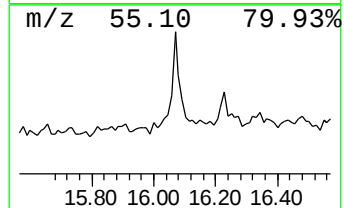
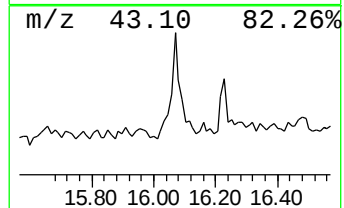
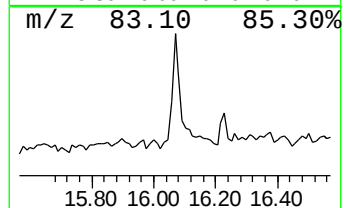
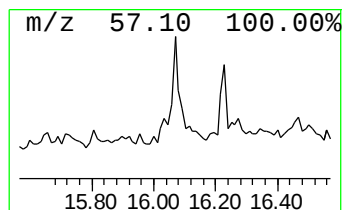
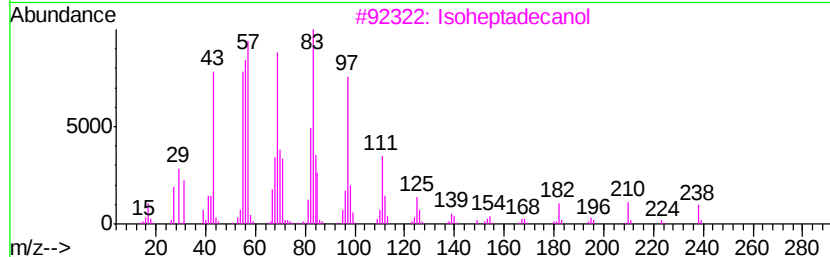
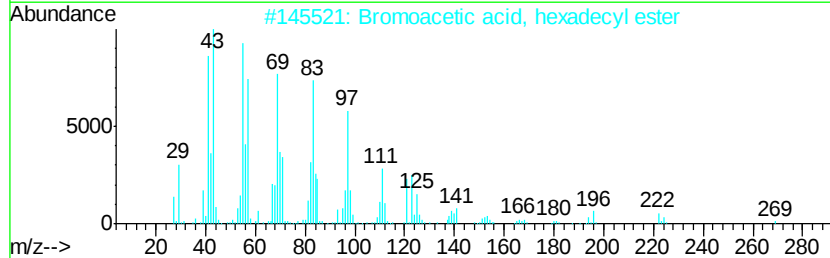
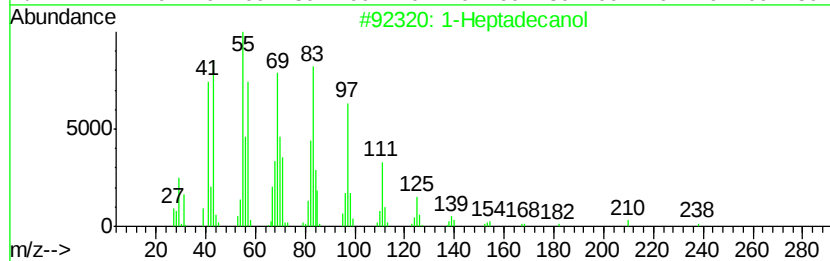
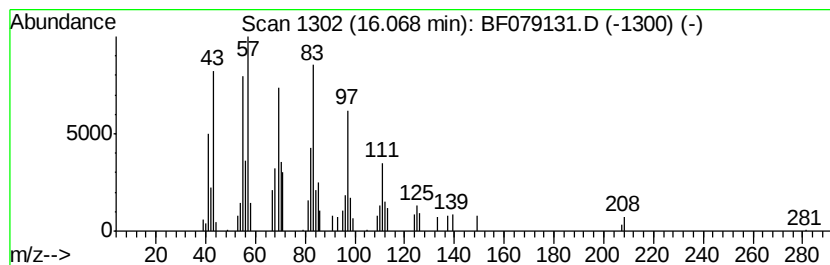
Instrument :  
BNA\_F  
ClientSampleId :  
PS-29(15-20)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF043015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 8 1-Heptadecanol Concentration Rank 9

| R.T.      | EstConc                            | Area  | Relative to ISTD | R.T.        |      |
|-----------|------------------------------------|-------|------------------|-------------|------|
| 16.07     | 2.45 ng                            | 69400 | Chrysene-d12     | 16.18       |      |
| Hit# of 5 | Tentative ID                       | MW    | MolForm          | CAS#        | Qual |
| 1         | 1-Heptadecanol                     | 256   | C17H36O          | 001454-85-9 | 90   |
| 2         | Bromoacetic acid, hexadecyl ester  | 362   | C18H35BrO2       | 005454-48-8 | 90   |
| 3         | Isoheptadecanol                    | 256   | C17H36O          | 057289-07-3 | 87   |
| 4         | Bromoacetic acid, pentadecyl ester | 348   | C17H33BrO2       | 131143-01-6 | 83   |
| 5         | 1-Nonadecanol                      | 284   | C19H40O          | 001454-84-8 | 81   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051115\  
Data File : BF079131.D  
Acq On : 11 May 2015 22:33  
Operator : TP/IZ  
Sample : G2176-10  
Misc :  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PS-29(15-20)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF043015.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

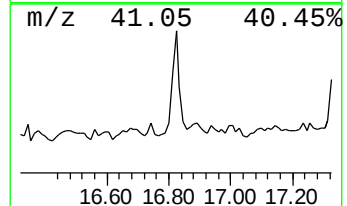
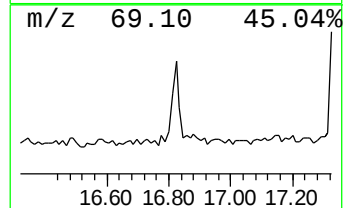
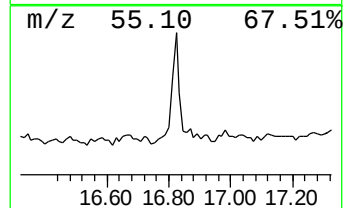
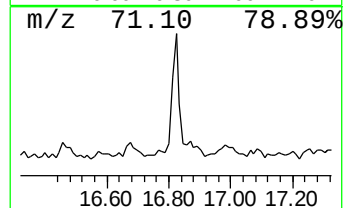
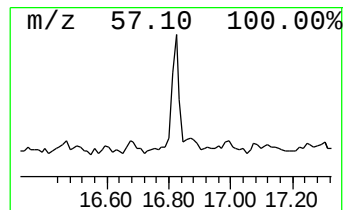
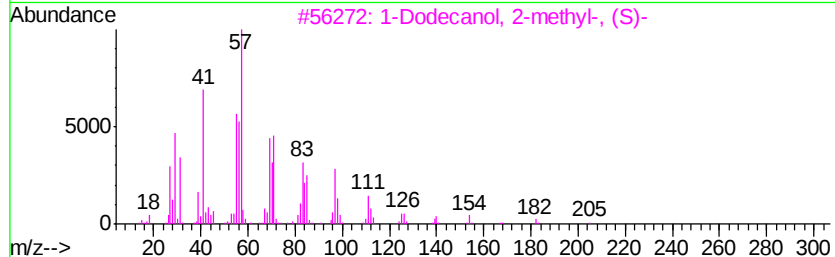
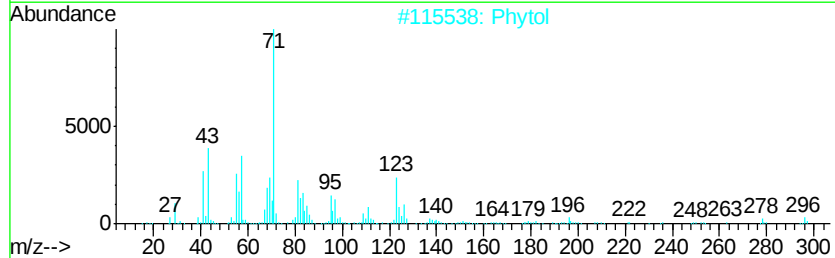
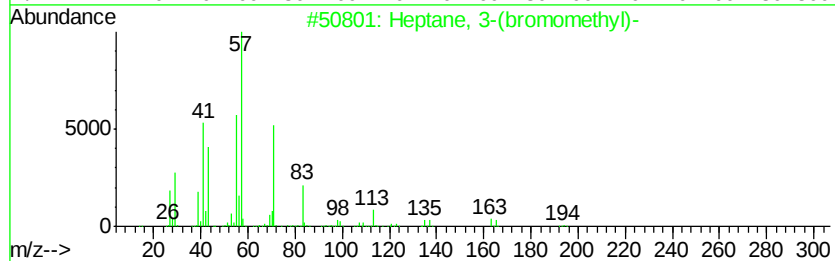
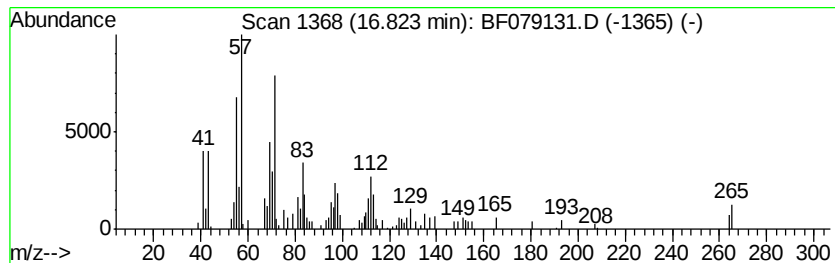
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 9 unknown16.82 Concentration Rank 8

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 16.82 | 4.81 ng | 136216 | Chrysene-d12     | 16.18 |

| Hit# | of | Tentative ID                     | MW  | MolForm    | CAS#        | Qual |
|------|----|----------------------------------|-----|------------|-------------|------|
| 1    | 5  | Heptane, 3-(bromomethyl)-        | 192 | C8H17Br    | 018908-66-2 | 38   |
| 2    |    | Phytol                           | 296 | C20H40O    | 000150-86-7 | 38   |
| 3    |    | 1-Dodecanol, 2-methyl-, (S)-     | 200 | C13H28O    | 057289-26-6 | 35   |
| 4    |    | 3-Trifluoroacetoxy-6-ethyldecane | 282 | C14H25F3O2 | 116436-59-0 | 27   |
| 5    |    | 2-Methyl-1-undecanol             | 186 | C12H26O    | 010522-26-6 | 22   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF051115\  
Data File : BF079131.D  
Acq On : 11 May 2015 22:33  
Operator : TP/IZ  
Sample : G2176-10  
Misc :  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PS-29(15-20)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF043015.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 |
| unknown1.45          | 1.45  | 380.7   | ng    | 5823680  | 1                     | 7.30  | 305938 | 20.0 |
| 2-Pentanone, 4-hy... | 5.10  | 6.8     | ng    | 104155   | 1                     | 7.30  | 305938 | 20.0 |
| unknown7.00          | 7.00  | 105.7   | ng    | 1616070  | 1                     | 7.30  | 305938 | 20.0 |
| 1-Heptadecanol       | 16.07 | 2.5     | ng    | 69400    | 5                     | 16.18 | 566746 | 20.0 |
| unknown16.82         | 16.82 | 4.8     | ng    | 136216   | 5                     | 16.18 | 566746 | 20.0 |