

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF081917\  
 Data File : BF097875.D  
 Acq On : 19 Aug 2017 13:35  
 Operator : SJ/JU  
 Sample : I4846-09  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PI-3(3)

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         | 2.122       | 4             | 6           | 23           | rVB3     | 57301          | 146658        | 2.95%           | 0.353%        |
| 2         | 4.963       | 485           | 489         | 499          | rVB      | 553319         | 881438        | 17.71%          | 2.120%        |
| 3         | 5.375       | 553           | 559         | 562          | rBV      | 3469824        | 4143664       | 83.26%          | 9.967%        |
| 4         | 6.398       | 721           | 733         | 736          | rBV      | 3445650        | 4557440       | 91.57%          | 10.963%       |
| 5         | 6.534       | 750           | 756         | 759          | rBV      | 3769741        | 4133428       | 83.05%          | 9.943%        |
| 6         | 6.757       | 791           | 794         | 798          | rBV      | 1025921        | 913447        | 18.35%          | 2.197%        |
| 7         | 6.916       | 816           | 821         | 825          | rBV      | 3124601        | 3189745       | 64.09%          | 7.673%        |
| 8         | 7.328       | 885           | 891         | 894          | rBV      | 2610351        | 2876129       | 57.79%          | 6.918%        |
| 9         | 7.410       | 900           | 905         | 909          | rVB      | 51095          | 63665         | 1.28%           | 0.153%        |
| 10        | 8.039       | 1004          | 1012        | 1016         | rBV      | 1304113        | 1276579       | 25.65%          | 3.071%        |
| 11        | 9.122       | 1190          | 1196        | 1199         | rBV      | 4471422        | 4976809       | 100.00%         | 11.971%       |
| 12        | 9.198       | 1204          | 1209        | 1214         | rBV4     | 54102          | 87432         | 1.76%           | 0.210%        |
| 13        | 9.510       | 1258          | 1262        | 1266         | rBV      | 752451         | 678183        | 13.63%          | 1.631%        |
| 14        | 9.792       | 1305          | 1310        | 1314         | rBV2     | 1546949        | 1464319       | 29.42%          | 3.522%        |
| 15        | 10.233      | 1382          | 1385        | 1387         | rVB      | 67792          | 51361         | 1.03%           | 0.124%        |
| 16        | 10.586      | 1439          | 1445        | 1448         | rBV      | 2647912        | 3001114       | 60.30%          | 7.219%        |
| 17        | 10.704      | 1462          | 1465        | 1474         | rBV      | 131116         | 234577        | 4.71%           | 0.564%        |
| 18        | 11.151      | 1539          | 1541        | 1543         | rBV      | 89300          | 63151         | 1.27%           | 0.152%        |
| 19        | 11.274      | 1558          | 1562        | 1569         | rBV      | 1629022        | 1522923       | 30.60%          | 3.663%        |
| 20        | 11.451      | 1590          | 1592        | 1596         | rVB3     | 97635          | 82137         | 1.65%           | 0.198%        |
| 21        | 12.868      | 1828          | 1833        | 1836         | rBV      | 3671980        | 4556239       | 91.55%          | 10.960%       |
| 22        | 13.757      | 1981          | 1984        | 1991         | rVB      | 324205         | 344786        | 6.93%           | 0.829%        |
| 23        | 13.910      | 2005          | 2010        | 2013         | rBV      | 1191908        | 1182620       | 23.76%          | 2.845%        |
| 24        | 14.392      | 2089          | 2092        | 2095         | rVB2     | 58491          | 53637         | 1.08%           | 0.129%        |
| 25        | 14.757      | 2151          | 2154        | 2158         | rVB      | 89270          | 87835         | 1.76%           | 0.211%        |
| 26        | 15.010      | 2194          | 2197        | 2200         | rBV      | 58823          | 65314         | 1.31%           | 0.157%        |
| 27        | 15.327      | 2246          | 2251        | 2256         | rBV      | 655258         | 774574        | 15.56%          | 1.863%        |
| 28        | 15.374      | 2256          | 2259        | 2264         | rVB2     | 46866          | 56742         | 1.14%           | 0.136%        |
| 29        | 15.786      | 2326          | 2329        | 2334         | rVB2     | 40466          | 53450         | 1.07%           | 0.129%        |
| 30        | 16.268      | 2407          | 2411        | 2418         | rVB5     | 31208          | 52776         | 1.06%           | 0.127%        |

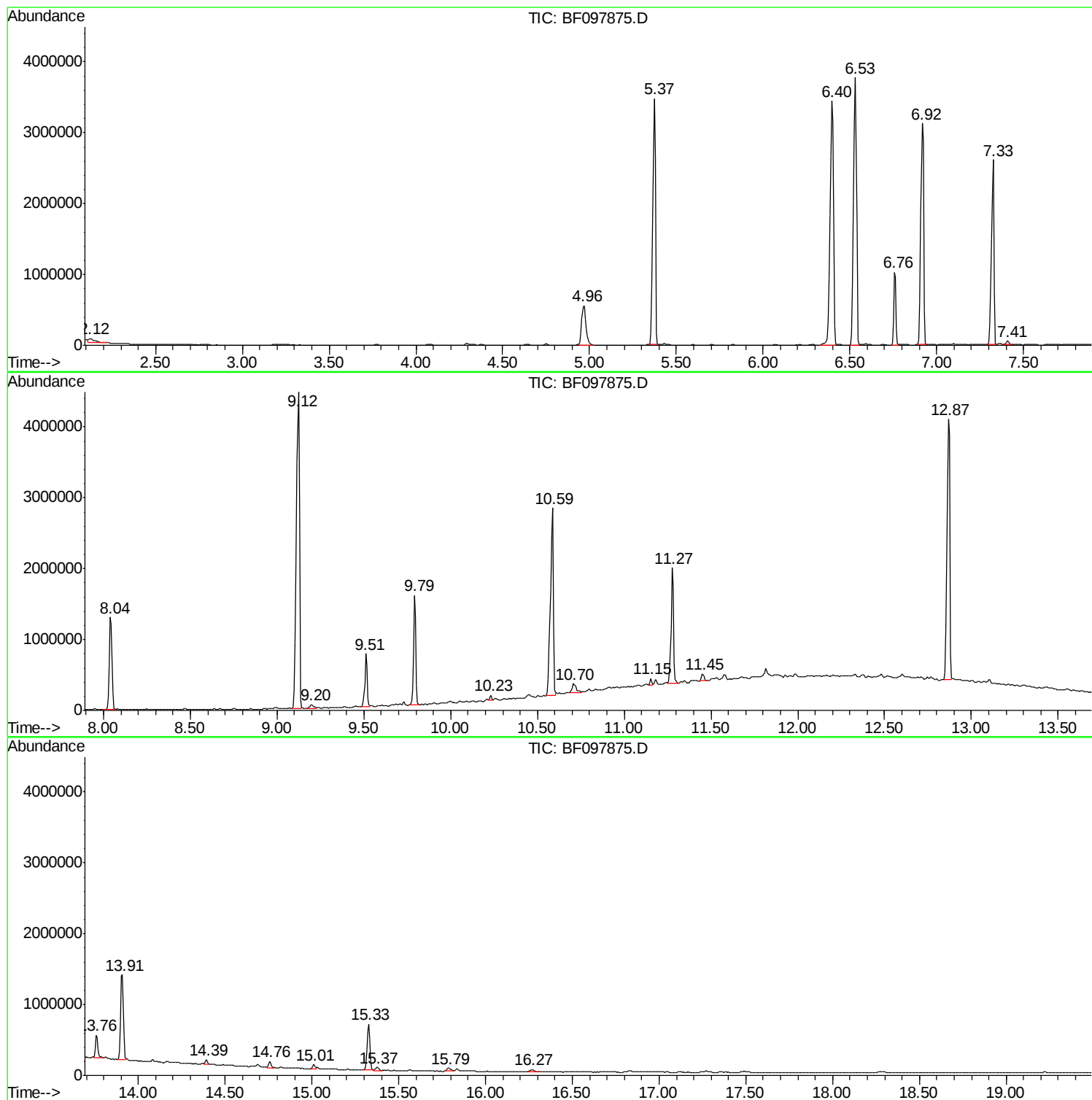
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PI-3(3)

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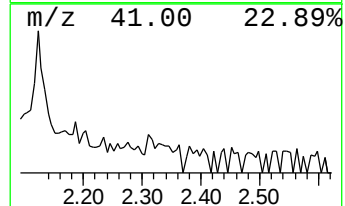
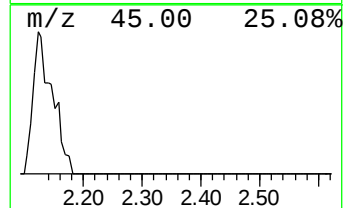
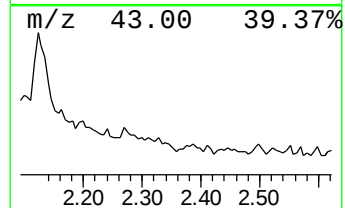
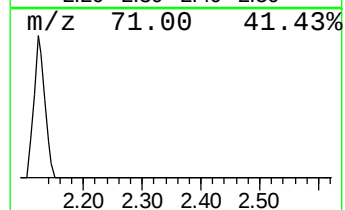
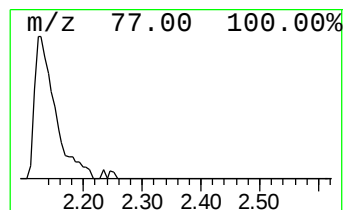
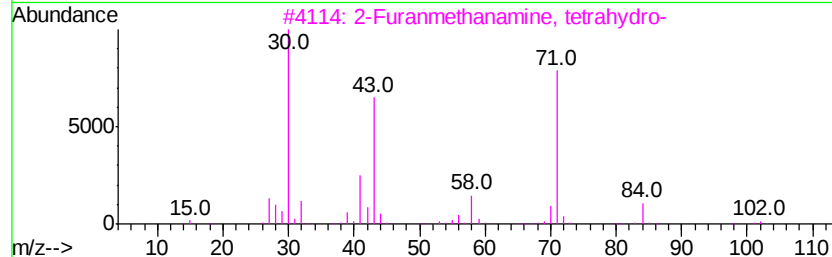
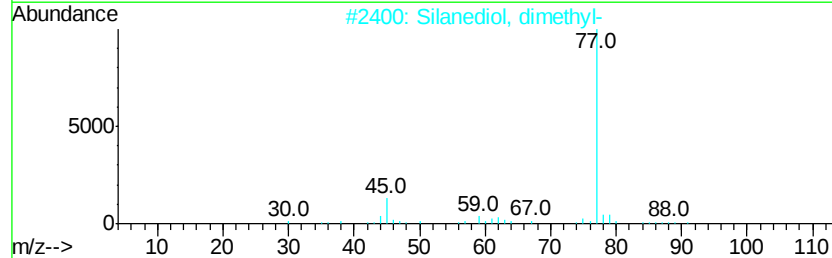
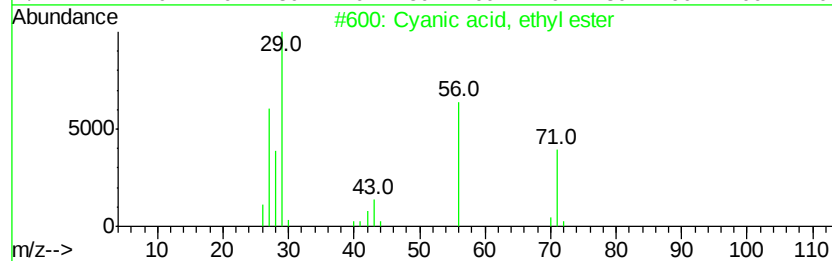
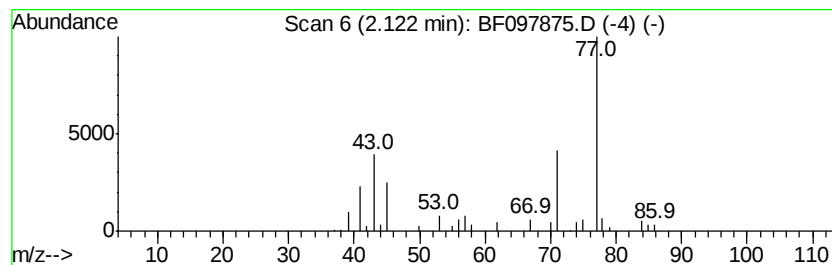
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown2.12 Concentration Rank 5

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 2.12 | 3.21 ng | 146658 | 1,4-Dichlorobenzene-d4 | 6.76 |

| Hit# of | 5 | Tentative ID                    | MW  | MolForm  | CAS#        | Qual |
|---------|---|---------------------------------|-----|----------|-------------|------|
| 1       |   | Cyanoic acid, ethyl ester       | 71  | C3H5NO   | 000627-48-5 | 4    |
| 2       |   | Silanediol, dimethyl-           | 92  | C2H8O2Si | 001066-42-8 | 4    |
| 3       |   | 2-Furanmethanamine, tetrahydro- | 101 | C5H11NO  | 004795-29-3 | 4    |
| 4       |   | (Aminomethyl)cyclopropane       | 71  | C4H9N    | 002516-47-4 | 3    |
| 5       |   | Mercaptamine                    | 77  | C2H7NS   | 000060-23-1 | 2    |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M  
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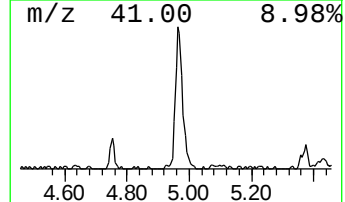
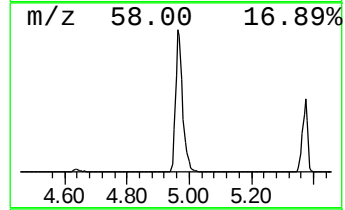
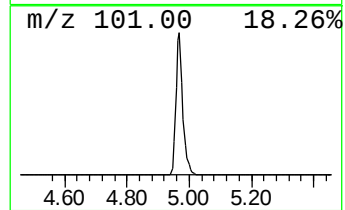
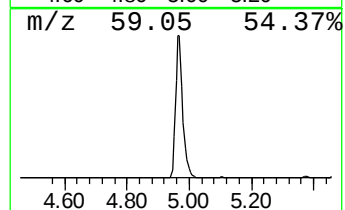
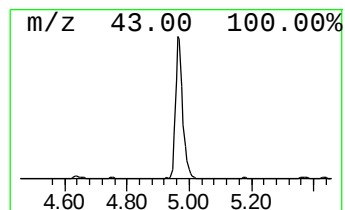
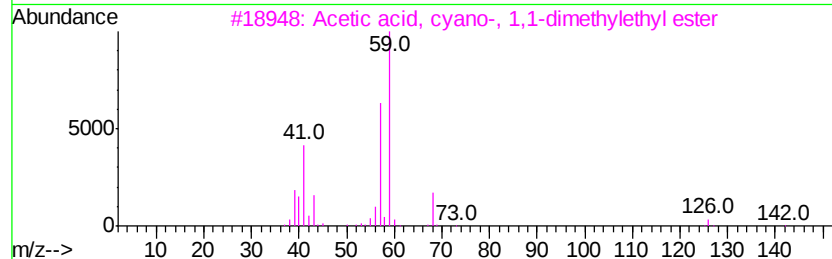
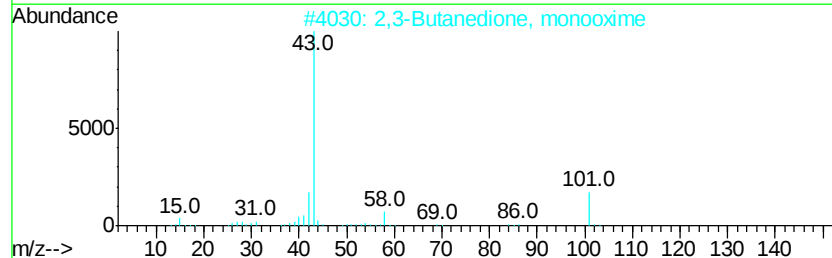
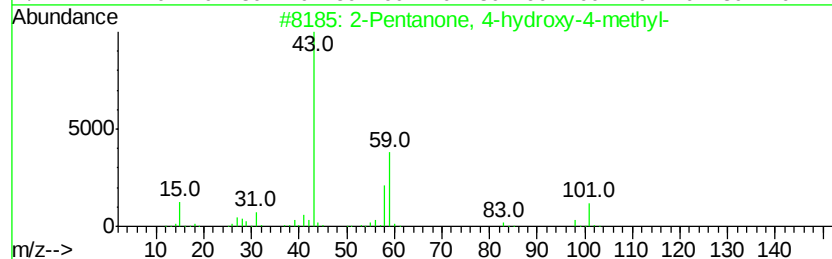
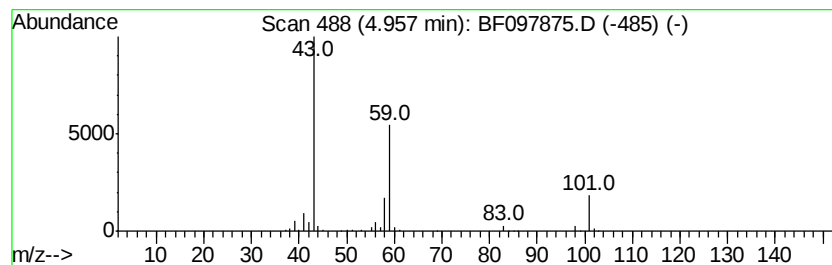
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.96 | 19.30 ng | 881438 | 1,4-Dichlorobenzene-d4 | 6.76 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 25   |
| 3    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 17   |
| 4    |    | 5-Hexen-2-one                        | 98  | C6H10O   | 000109-49-9 | 9    |
| 5    |    | Morpholine, 4-methyl-                | 101 | C5H11NO  | 000109-02-4 | 9    |



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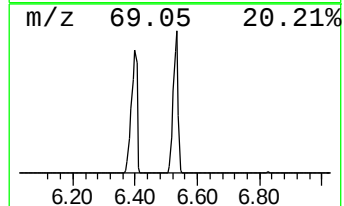
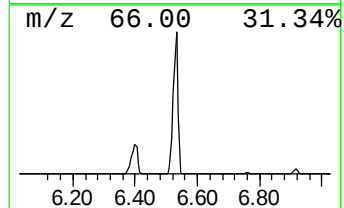
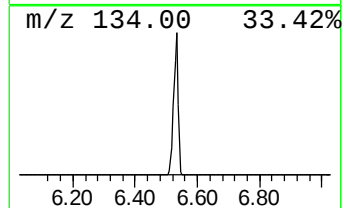
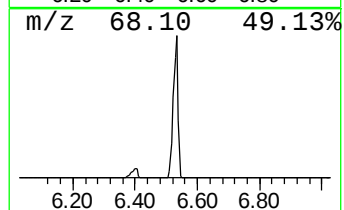
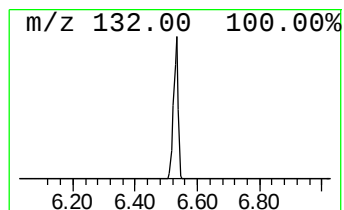
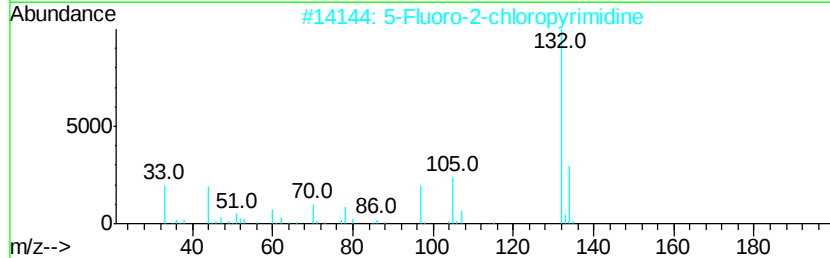
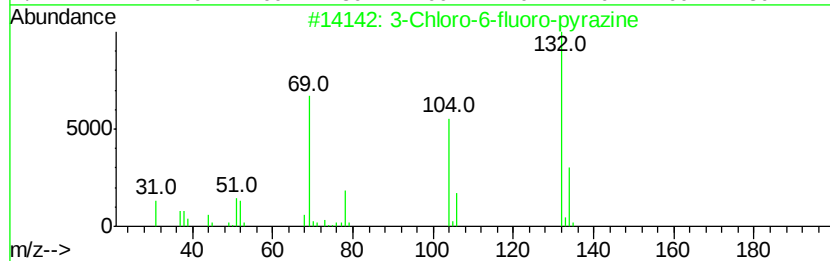
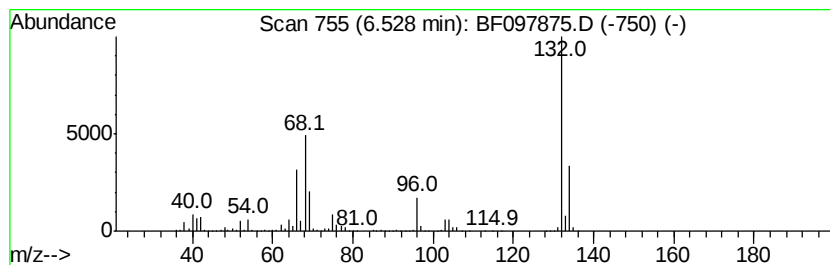
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 unknown6.53 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.53 | 90.50 ng | 4133430 | 1,4-Dichlorobenzene-d4 | 6.76 |

| 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    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 9    |
| 5    |    | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2  | 029490-19-5  | 9    |



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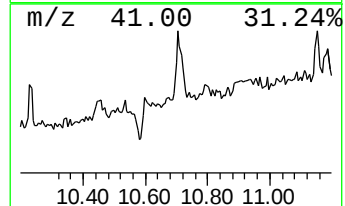
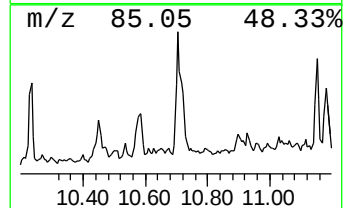
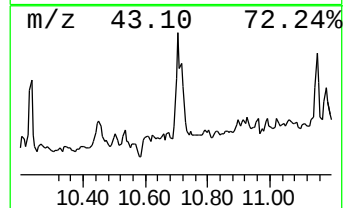
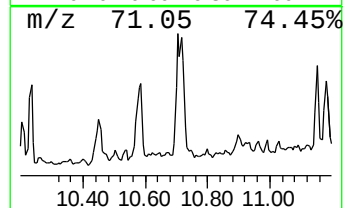
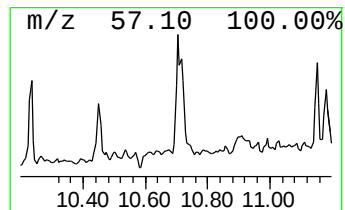
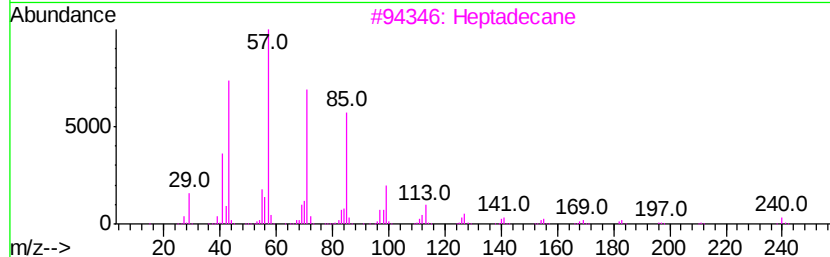
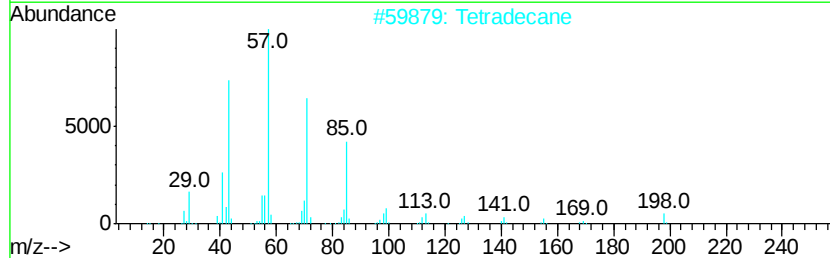
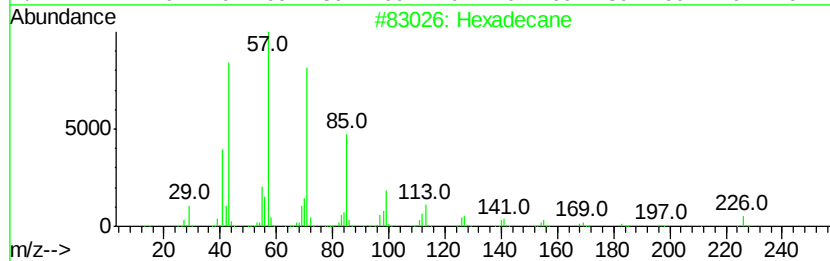
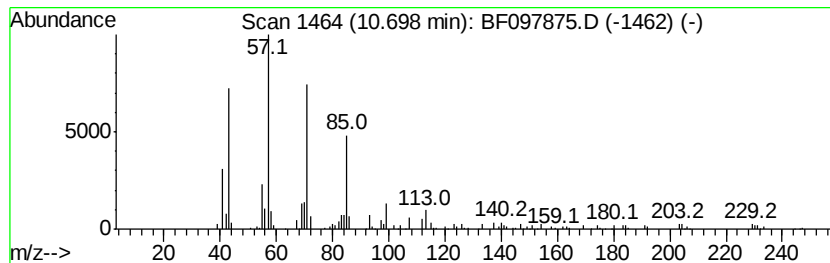
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Peak Number 5 Hexadecane Concentration Rank 6

| R.T.      | EstConc            | Area   | Relative to ISTD | R.T.        |      |
|-----------|--------------------|--------|------------------|-------------|------|
| 10.70     | 3.08 ng            | 234577 | Phenanthrene-d10 | 11.27       |      |
| Hit# of 5 | Tentative ID       | MW     | MolForm          | CAS#        | Qual |
| 1         | Hexadecane         | 226    | C16H34           | 000544-76-3 | 90   |
| 2         | Tetradecane        | 198    | C14H30           | 000629-59-4 | 90   |
| 3         | Heptadecane        | 240    | C17H36           | 000629-78-7 | 90   |
| 4         | Tridecane, 1-iodo- | 310    | C13H27I          | 035599-77-0 | 87   |
| 5         | Eicosane           | 282    | C20H42           | 000112-95-8 | 80   |



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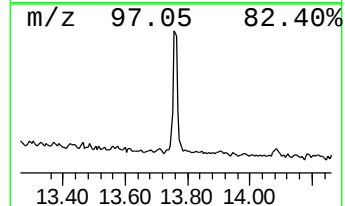
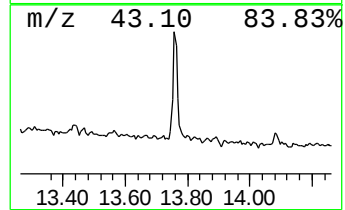
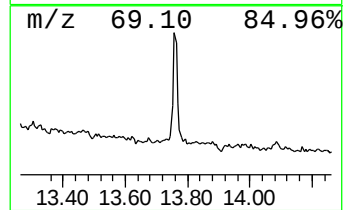
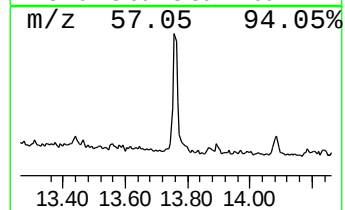
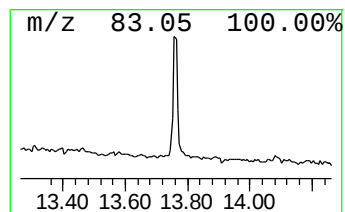
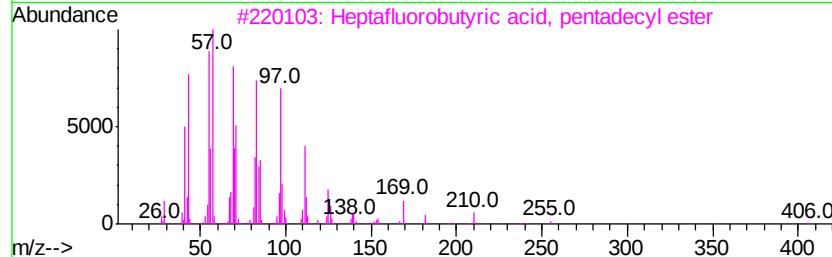
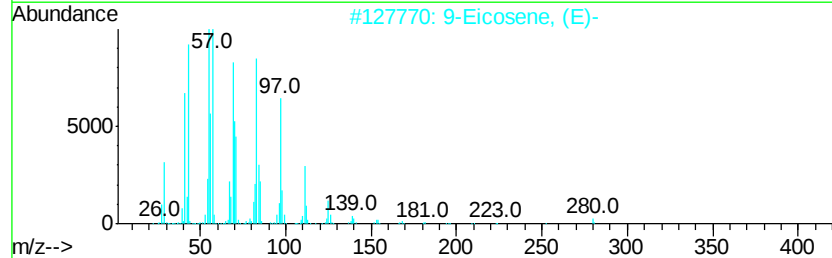
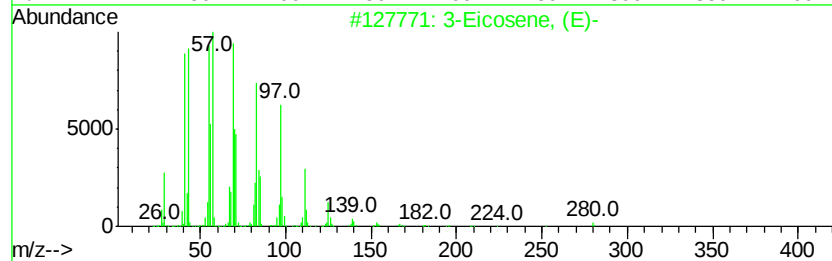
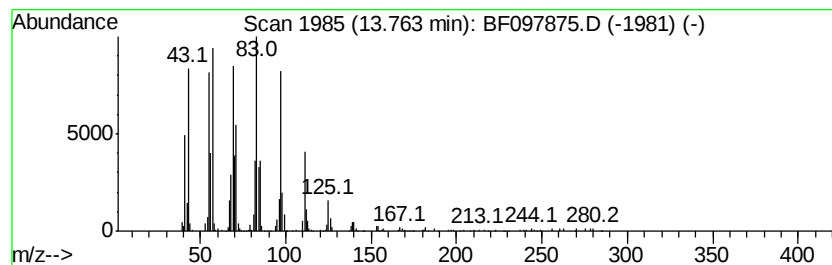
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TIC Integration Parameters: LSCINT.P

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Peak Number 6 3-Eicosene, (E)- Concentration Rank 4

| R.T.    | EstConc                             | Area           | Relative to ISTD | R.T.      |
|---------|-------------------------------------|----------------|------------------|-----------|
| 13.76   | 5.83 ng                             | 344786         | Chrysene-d12     | 13.91     |
| Hit# of | 5                                   | Tentative ID   | MW MolForm       | CAS# Qual |
| 1       | 3-Eicosene, (E)-                    | 280 C20H40     | 074685-33-9      | 99        |
| 2       | 9-Eicosene, (E)-                    | 280 C20H40     | 074685-29-3      | 93        |
| 3       | Heptafluorobutyric acid, pentade... | 424 C19H31F7O2 | 959261-23-5      | 93        |
| 4       | n-Tetracosanol-1                    | 354 C24H50O    | 000506-51-4      | 91        |
| 5       | 1-Heneicosanol                      | 312 C21H44O    | 015594-90-8      | 91        |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF081917\  
Data File : BF097875.D  
Acq On : 19 Aug 2017 13:35  
Operator : SJ/JU  
Sample : I4846-09  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PI-3(3)

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

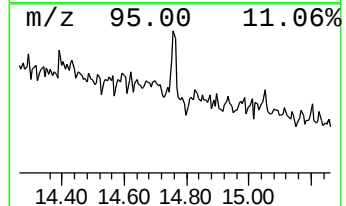
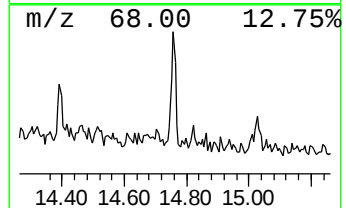
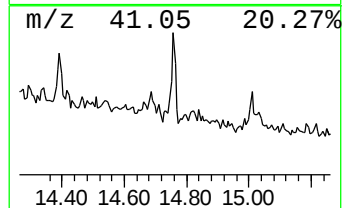
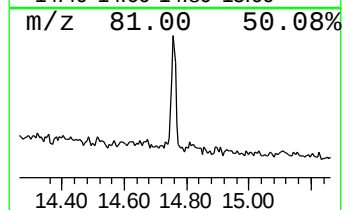
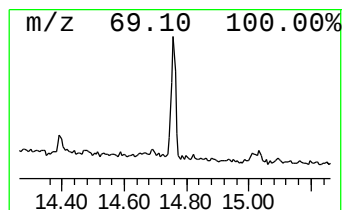
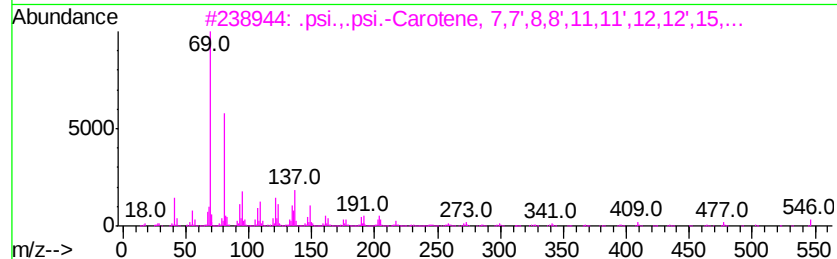
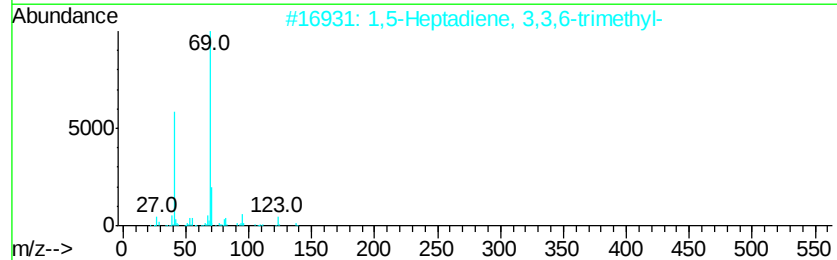
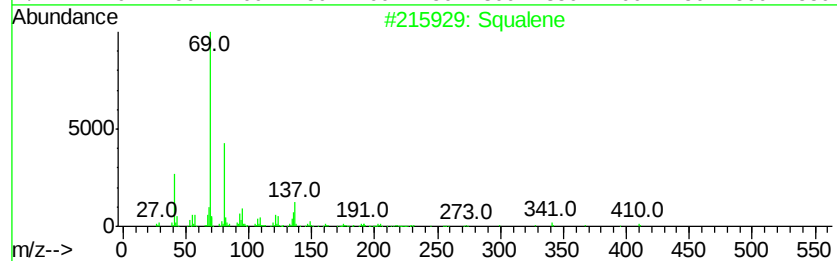
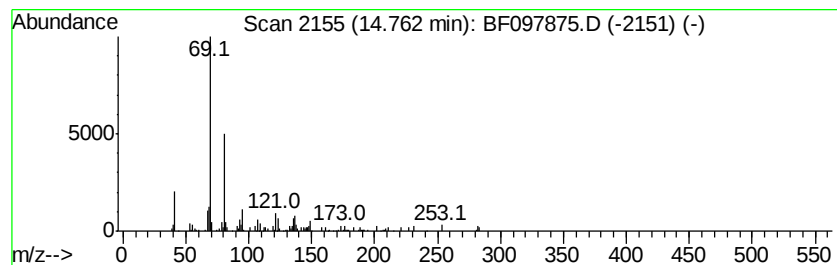
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Squalene Concentration Rank 7

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 14.76 | 2.27 ng | 87835 | Perylene-d12     | 15.33 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Squalene                            | 410 | C30H50  | 000111-02-4 | 80   |
| 2    |    | 1,5-Heptadiene, 3,3,6-trimethyl-    | 138 | C10H18  | 035387-63-4 | 64   |
| 3    |    | .psi.,.psi.-Carotene, 7,7',8,8',... | 547 | C40H66  | 000502-62-5 | 56   |
| 4    |    | 1,5-Heptadiene, 2,6-dimethyl-       | 124 | C9H16   | 006709-39-3 | 50   |
| 5    |    | 2,6-Octadiene, 4,5-dimethyl-        | 138 | C10H18  | 018476-57-8 | 50   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF081917\  
Data File : BF097875.D  
Acq On : 19 Aug 2017 13:35  
Operator : SJ/JU  
Sample : I4846-09  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PI-3(3)

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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| unknown2.12          | 2.12  | 3.2     | ng    | 146658   | 1                     | 6.76  | 913447  | 20.0 |
| 2-Pentanone, 4-hy... | 4.96  | 19.3    | ng    | 881438   | 1                     | 6.76  | 913447  | 20.0 |
| unknown6.53          | 6.53  | 90.5    | ng    | 4133430  | 1                     | 6.76  | 913447  | 20.0 |
| Hexadecane           | 10.70 | 3.1     | ng    | 234577   | 4                     | 11.27 | 1522920 | 20.0 |
| 3-Eicosene, (E)-     | 13.76 | 5.8     | ng    | 344786   | 5                     | 13.91 | 1182620 | 20.0 |
| Squalene             | 14.76 | 2.3     | ng    | 87835    | 6                     | 15.33 | 774574  | 20.0 |