

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051217\  
 Data File : BF095110.D  
 Acq On : 12 May 2017 14:12  
 Operator : SJ/MA  
 Sample : I3100-07  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 MW-1-051017

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-BF050217.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         | 4.984       | 514           | 518         | 533          | rBV      | 62119          | 132086        | 4.42%           | 0.585%        |
| 2         | 5.648       | 627           | 631         | 658          | rBV      | 319725         | 847003        | 28.33%          | 3.751%        |
| 3         | 7.260       | 902           | 905         | 918          | rBV      | 157643         | 445855        | 14.92%          | 1.975%        |
| 4         | 7.360       | 918           | 922         | 941          | rVB      | 1221571        | 2040440       | 68.26%          | 9.036%        |
| 5         | 7.695       | 975           | 979         | 994          | rVB      | 433146         | 519964        | 17.39%          | 2.303%        |
| 6         | 7.930       | 1015          | 1019        | 1034         | rBV      | 1504681        | 1896920       | 63.46%          | 8.401%        |
| 7         | 8.601       | 1128          | 1133        | 1154         | rBV      | 1088750        | 1506686       | 50.40%          | 6.672%        |
| 8         | 9.719       | 1319          | 1323        | 1340         | rVB      | 460117         | 657667        | 22.00%          | 2.913%        |
| 9         | 11.495      | 1619          | 1625        | 1640         | rVB      | 2315156        | 2841063       | 95.04%          | 12.582%       |
| 10        | 12.195      | 1739          | 1744        | 1750         | rBV      | 73917          | 96904         | 3.24%           | 0.429%        |
| 11        | 12.548      | 1799          | 1804        | 1812         | rBV2     | 560245         | 798147        | 26.70%          | 3.535%        |
| 12        | 13.071      | 1890          | 1893        | 1899         | rBV4     | 28928          | 38291         | 1.28%           | 0.170%        |
| 13        | 13.848      | 2019          | 2025        | 2039         | rBV      | 1196375        | 1810258       | 60.56%          | 8.017%        |
| 14        | 14.159      | 2073          | 2078        | 2084         | rBV4     | 18753          | 32801         | 1.10%           | 0.145%        |
| 15        | 14.601      | 2147          | 2153        | 2163         | rBV7     | 24129          | 42576         | 1.42%           | 0.189%        |
| 16        | 14.948      | 2208          | 2212        | 2225         | rBV      | 554862         | 790745        | 26.45%          | 3.502%        |
| 17        | 15.930      | 2372          | 2379        | 2391         | rBV      | 634510         | 903649        | 30.23%          | 4.002%        |
| 18        | 16.871      | 2535          | 2539        | 2541         | rBV      | 80796          | 112834        | 3.77%           | 0.500%        |
| 19        | 16.895      | 2541          | 2543        | 2552         | rVB      | 90374          | 149006        | 4.98%           | 0.660%        |
| 20        | 17.030      | 2557          | 2566        | 2580         | rVV      | 1406102        | 2442477       | 81.71%          | 10.817%       |
| 21        | 17.283      | 2603          | 2609        | 2612         | rBV      | 2390589        | 2989276       | 100.00%         | 13.238%       |
| 22        | 17.953      | 2720          | 2723        | 2732         | rBV5     | 47934          | 72421         | 2.42%           | 0.321%        |
| 23        | 18.624      | 2833          | 2837        | 2849         | rBV      | 554369         | 763644        | 25.55%          | 3.382%        |
| 24        | 20.294      | 3115          | 3121        | 3131         | rBV      | 347892         | 554977        | 18.57%          | 2.458%        |
| 25        | 22.865      | 3550          | 3558        | 3570         | rVB3     | 24404          | 94926         | 3.18%           | 0.420%        |

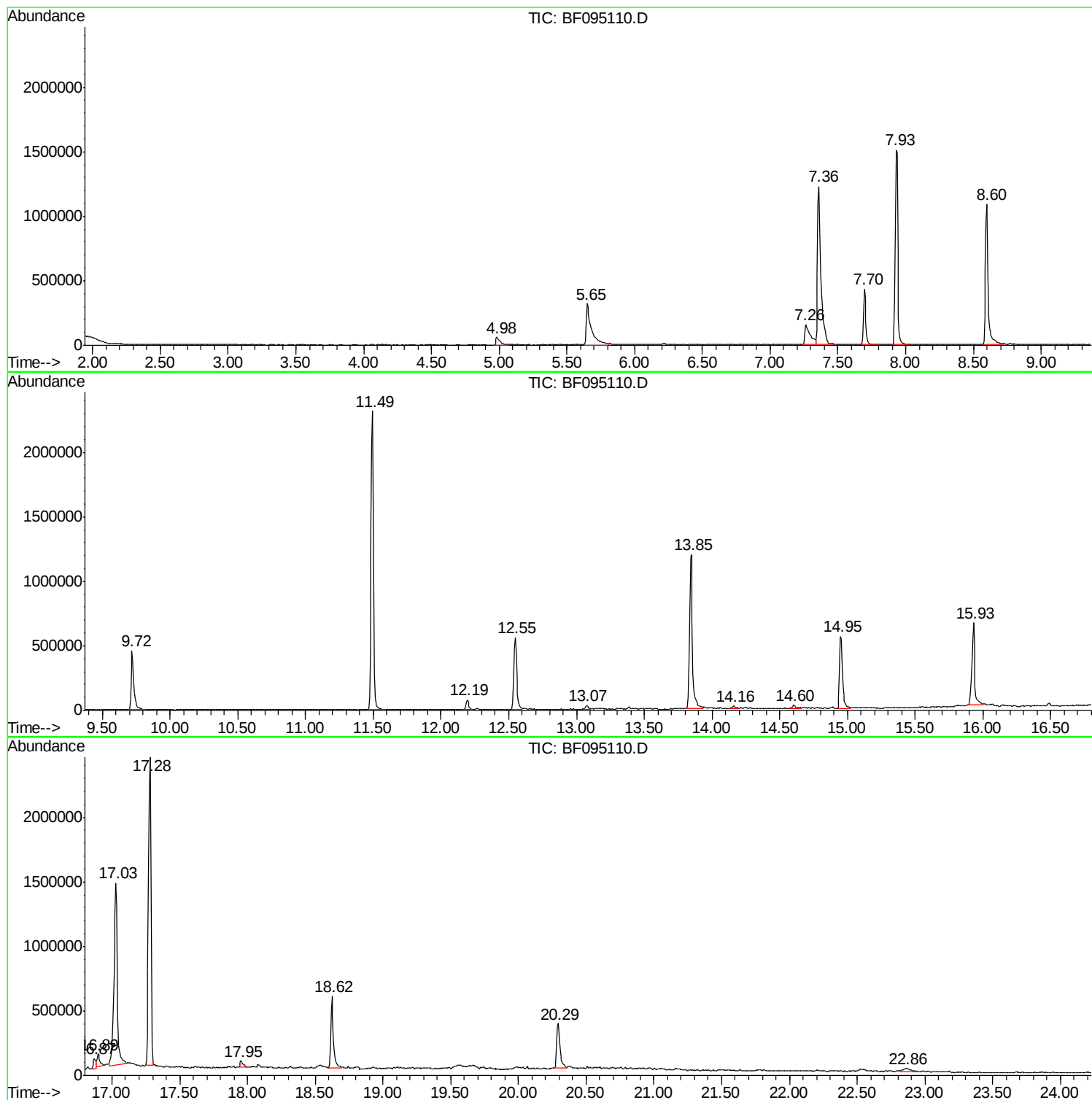
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF050217.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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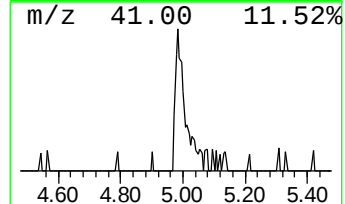
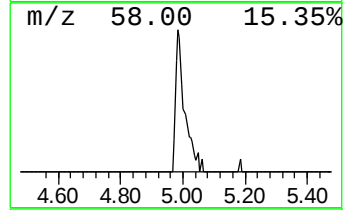
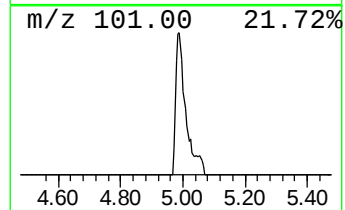
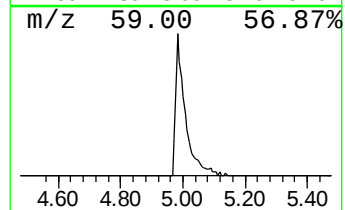
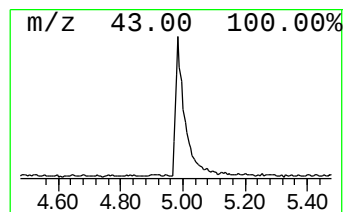
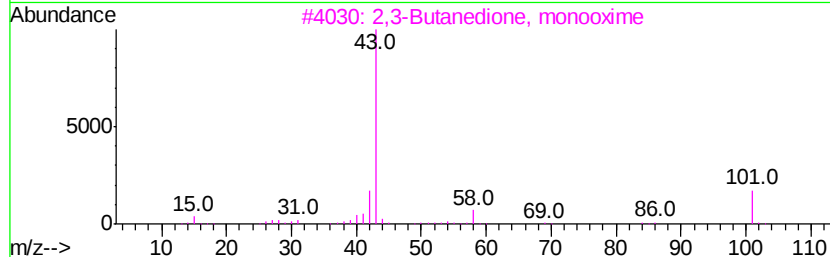
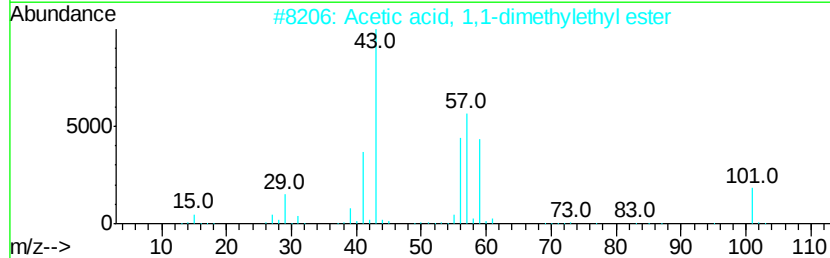
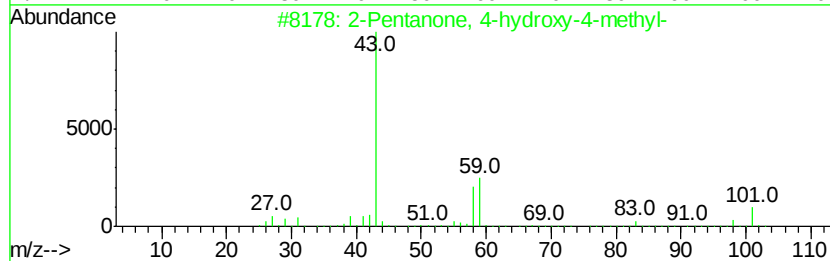
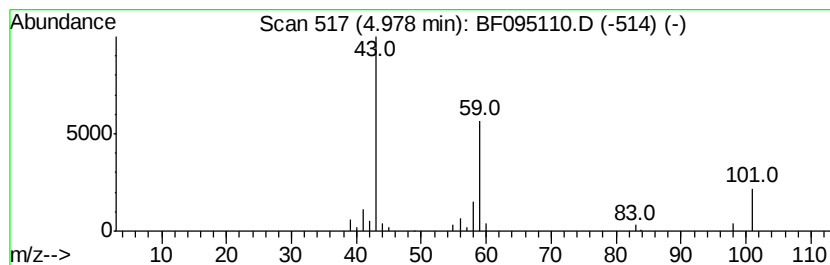
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 5

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.98 | 5.08 ng | 132086 | 1,4-Dichlorobenzene-d4 | 7.70 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 56   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39   |
| 3    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 38   |
| 4    |    |   | Butyl aldoxime, 3-methyl-, syn-     | 101 | C5H11NO | 005780-40-5 | 25   |
| 5    |    |   | (+)-4-Amino-4,5-dihydro-2(3H)-f...  | 101 | C4H7NO2 | 016504-58-8 | 9    |



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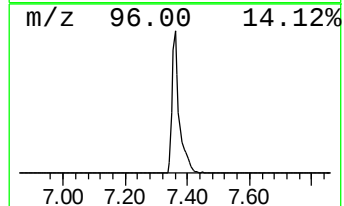
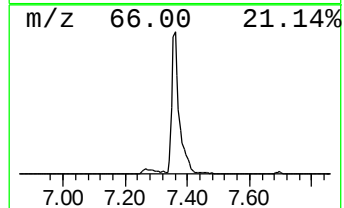
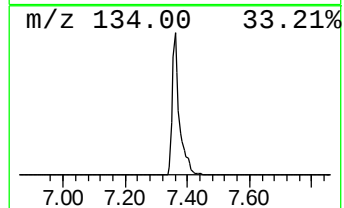
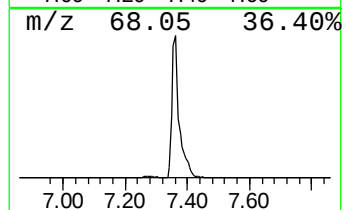
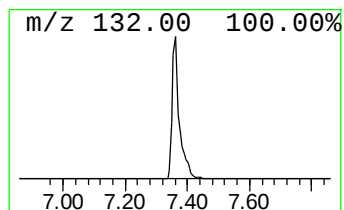
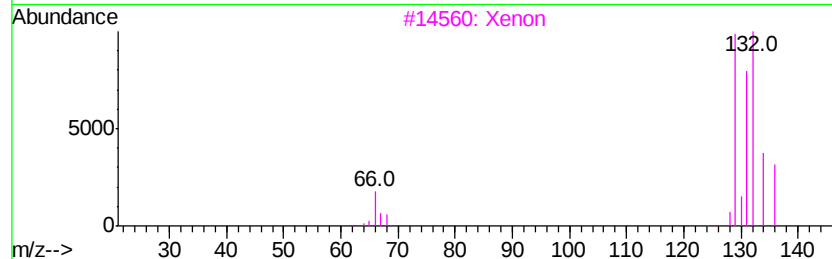
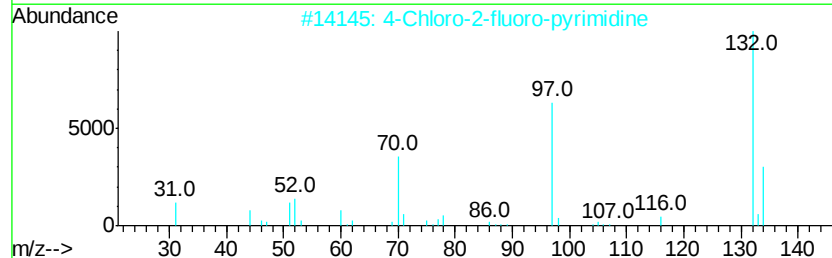
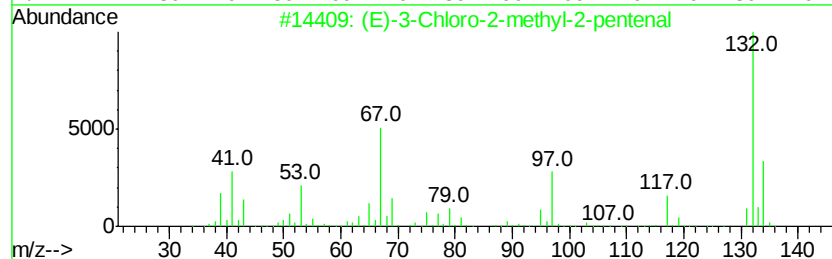
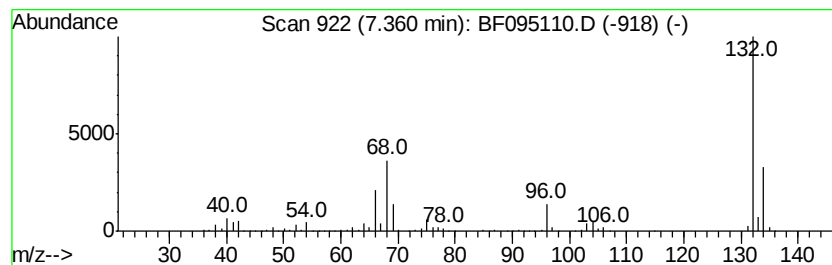
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown7.36 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.36 | 78.48 ng | 2040440 | 1,4-Dichlorobenzene-d4 | 7.70 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|-------------------------------------|-----|-----------|-------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3 | 35   |
| 2    |    | 4-Chloro-2-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-00-5 | 9    |
| 3    |    | Xenon                               | 132 | Xe        | 007440-63-3 | 9    |
| 4    |    | 1H-Benzimidazole, 2-methyl-         | 132 | C8H8N2    | 000615-15-6 | 9    |
| 5    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6 | 9    |



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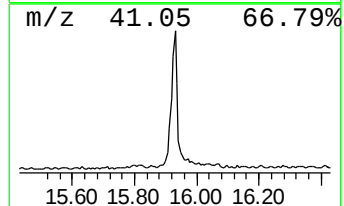
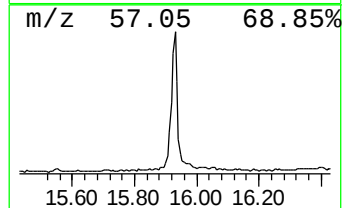
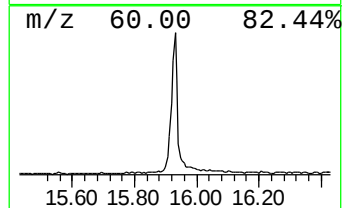
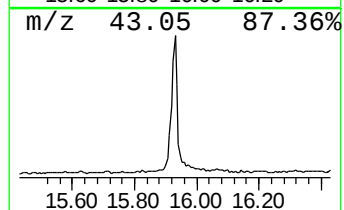
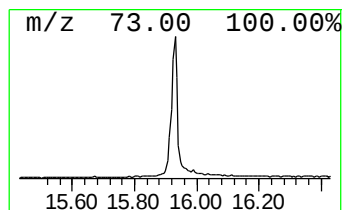
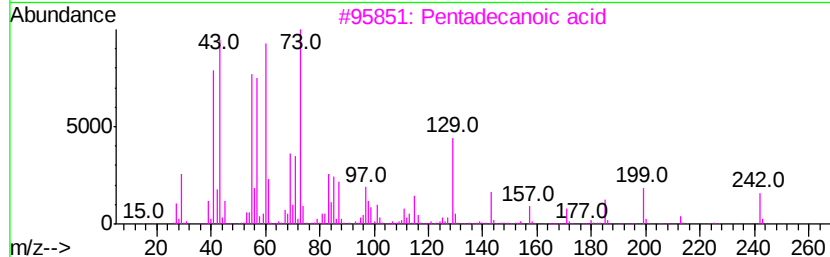
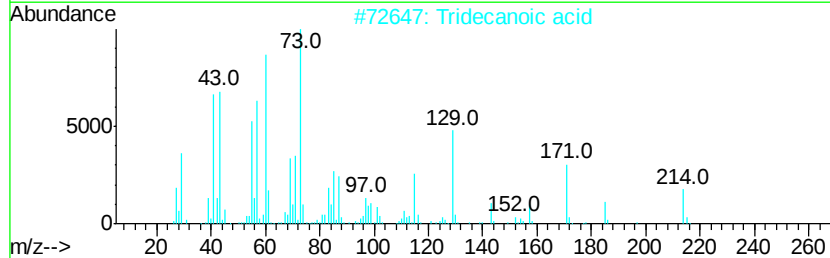
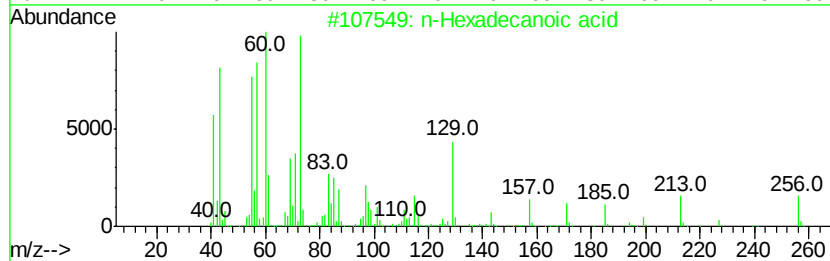
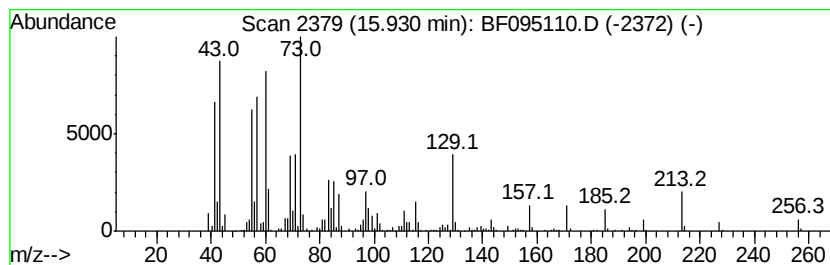
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 15.93 | 22.86 ng | 903649 | Phenanthrene-d10 | 14.95 |

| Hit# of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|---------|---|---------------------|-----|----------|-------------|------|
| 1       |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2       |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 94   |
| 3       |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4       |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 81   |
| 5       |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 62   |



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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW-1-051017

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M  
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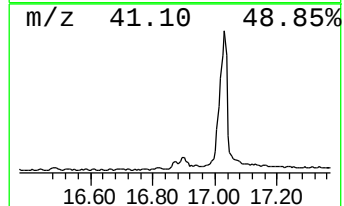
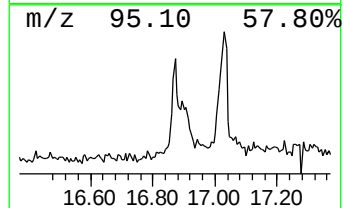
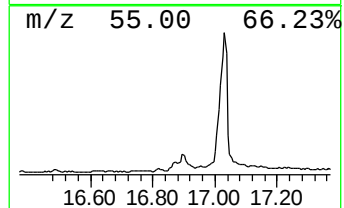
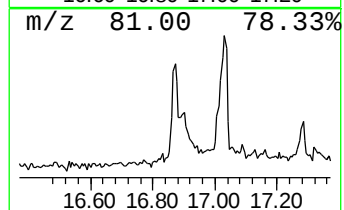
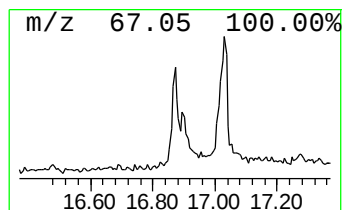
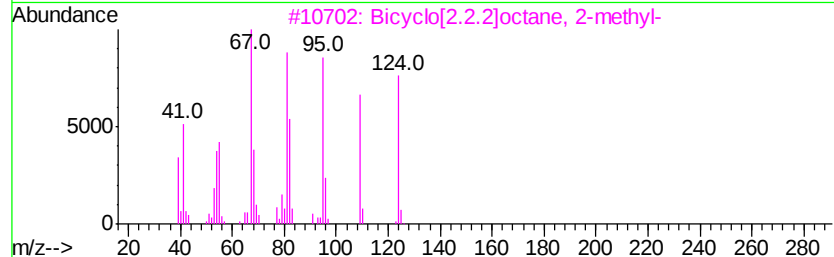
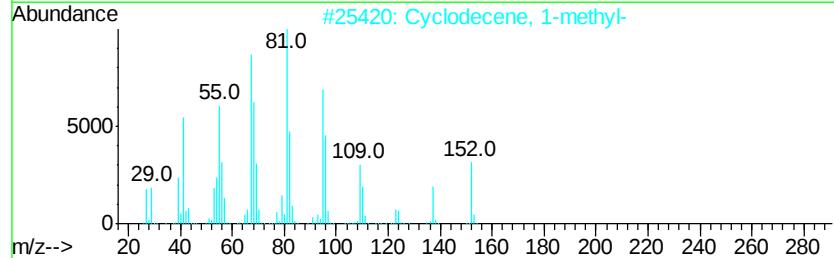
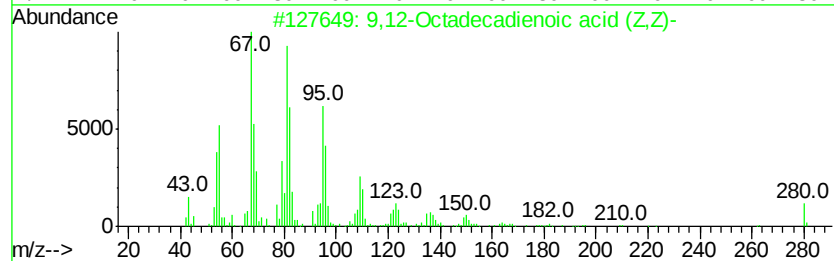
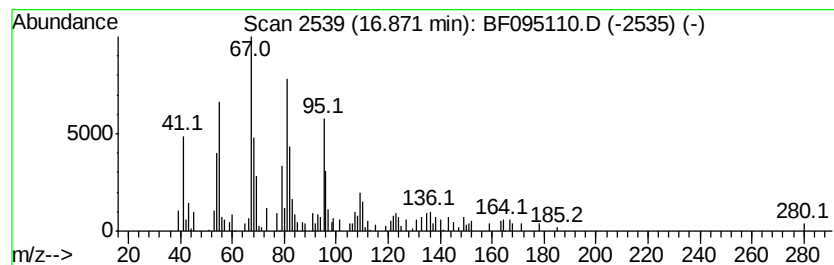
TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 8

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 16.87 | 2.96 ng | 112834 | Chrysene-d12     | 18.62 |

| Hit# | of | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|------|----|----------------------------------|-----|----------|-------------|------|
| 1    | 5  | 9,12-Octadecadienoic acid (Z,Z)- | 280 | C18H32O2 | 000060-33-3 | 96   |
| 2    |    | Cyclodecene, 1-methyl-           | 152 | C11H20   | 066633-38-3 | 87   |
| 3    |    | Bicyclo[2.2.2]octane, 2-methyl-  | 124 | C9H16    | 000766-53-0 | 83   |
| 4    |    | 1,9-Cyclohexadecadiene           | 220 | C16H28   | 004277-06-9 | 80   |
| 5    |    | 3,4-Octadiene, 7-methyl-         | 124 | C9H16    | 037050-05-8 | 76   |



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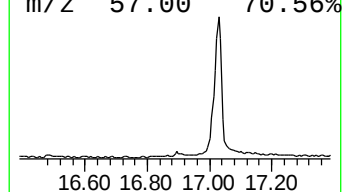
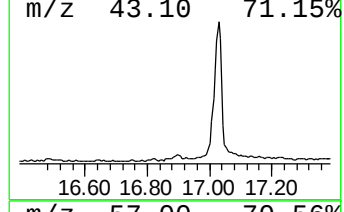
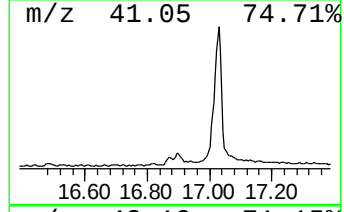
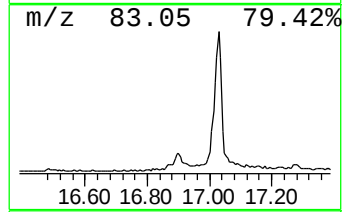
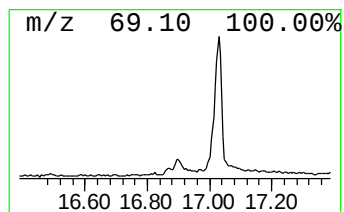
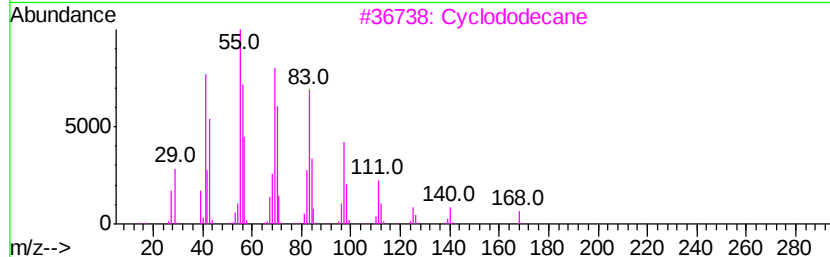
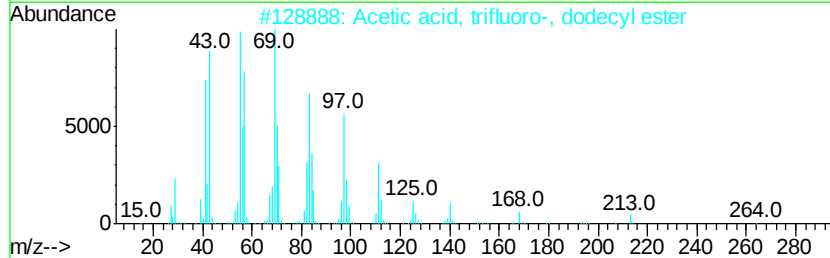
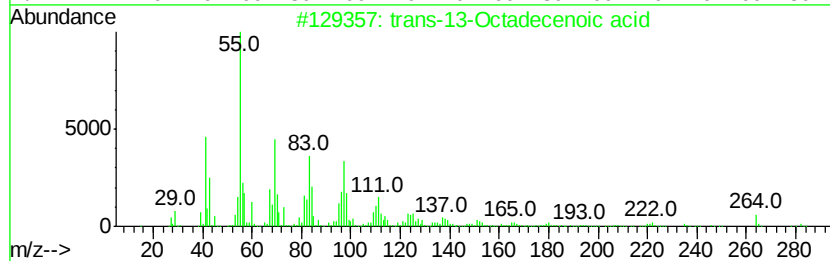
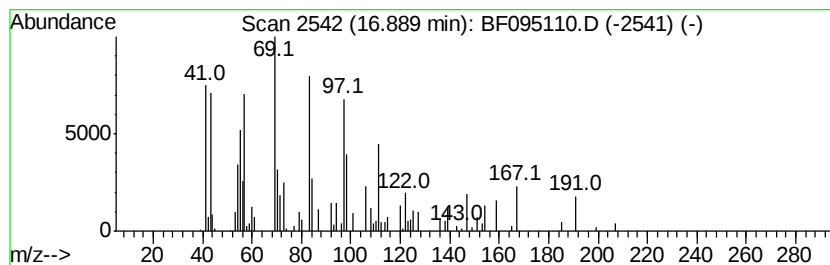
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Peak Number 6 trans-13-Octadecenoic acid Concentration Rank 6

| R.T.    | EstConc                             | Area         | Relative to ISTD | R.T.        |      |      |
|---------|-------------------------------------|--------------|------------------|-------------|------|------|
| 16.89   | 3.90 ng                             | 149006       | Chrysene-d12     | 18.62       |      |      |
| Hit# of | 5                                   | Tentative ID | MW               | MolForm     | CAS# | Qual |
| 1       | trans-13-Octadecenoic acid          | 282          | C18H34O2         | 000693-71-0 | 64   |      |
| 2       | Acetic acid, trifluoro-, dodecyl... | 282          | C14H25F3O2       | 006222-00-0 | 58   |      |
| 3       | Cyclododecane                       | 168          | C12H24           | 000294-62-2 | 47   |      |
| 4       | 2-Butenedioic acid (Z)-, monodod... | 284          | C16H28O4         | 002424-61-5 | 43   |      |
| 5       | Tetradecyl trifluoroacetate         | 310          | C16H29F3O2       | 006222-02-2 | 43   |      |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF051217\  
Data File : BF095110.D  
Acq On : 12 May 2017 14:12  
Operator : SJ/MA  
Sample : I3100-07  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

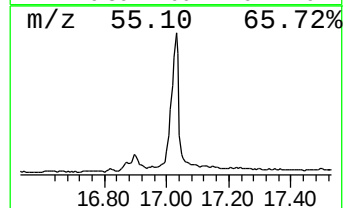
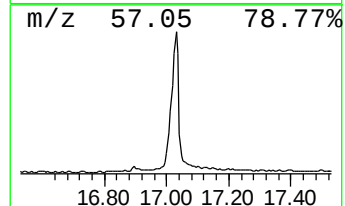
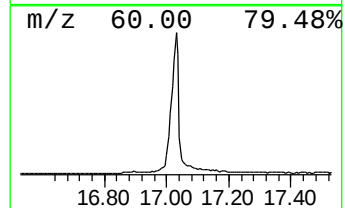
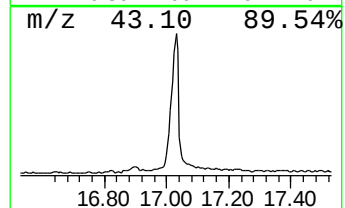
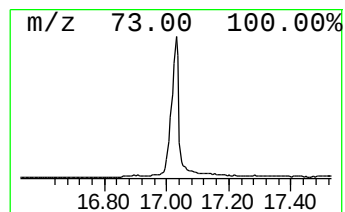
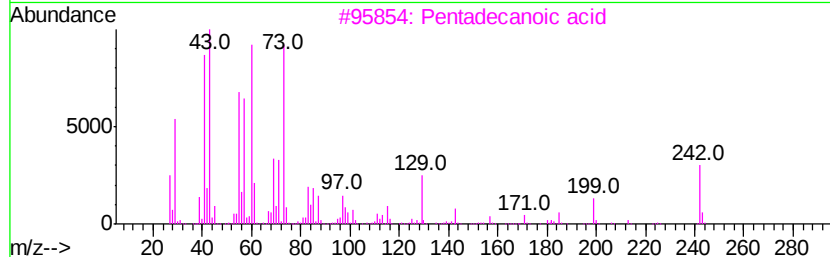
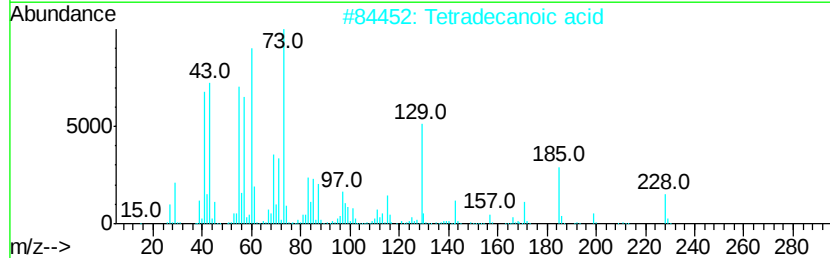
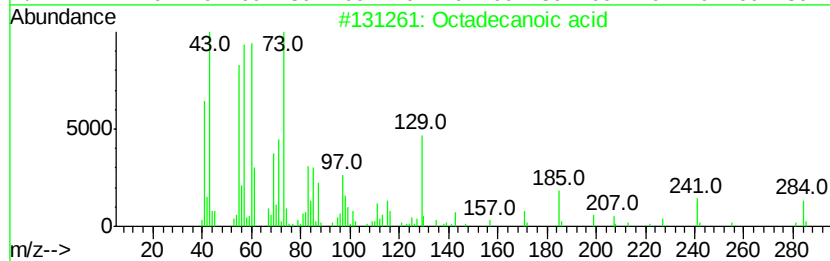
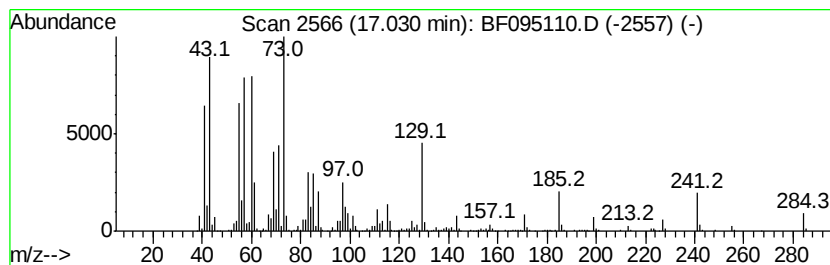
Instrument :  
BNA\_F  
ClientSampleId :  
MW-1-051017

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF050217.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 Octadecanoic acid Concentration Rank 3

| R.T.      | EstConc                             | Area    | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|---------|------------------|--------------|------|
| 17.03     | 63.97 ng                            | 2442480 | Chrysene-d12     | 18.62        |      |
| Hit# of 5 | Tentative ID                        | MW      | MolForm          | CAS#         | Qual |
| 1         | Octadecanoic acid                   | 284     | C18H36O2         | 000057-11-4  | 99   |
| 2         | Tetradecanoic acid                  | 228     | C14H28O2         | 000544-63-8  | 90   |
| 3         | Pentadecanoic acid                  | 242     | C15H30O2         | 001002-84-2  | 72   |
| 4         | n-Decanoic acid                     | 172     | C10H20O2         | 000334-48-5  | 62   |
| 5         | Oxalic acid, propyl tetradecyl e... | 328     | C19H36O4         | 1000309-26-7 | 20   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051217\  
Data File : BF095110.D  
Acq On : 12 May 2017 14:12  
Operator : SJ/MA  
Sample : I3100-07  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW-1-051017

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

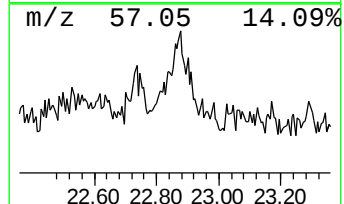
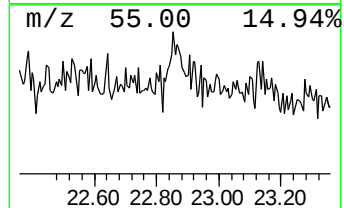
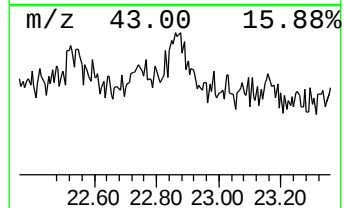
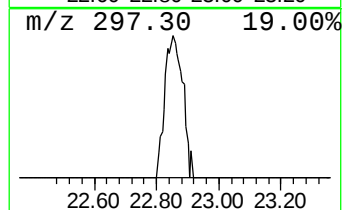
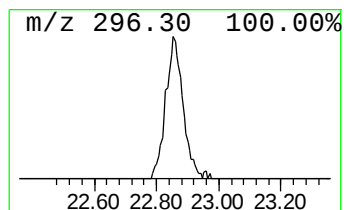
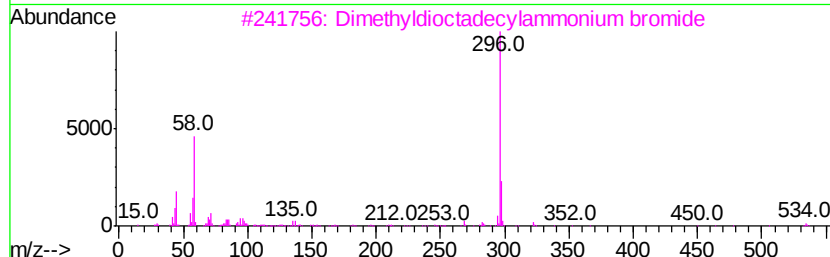
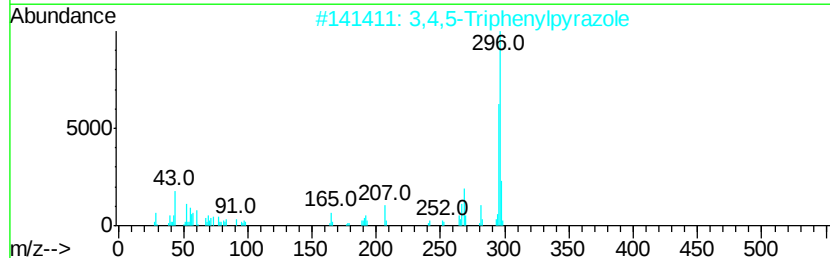
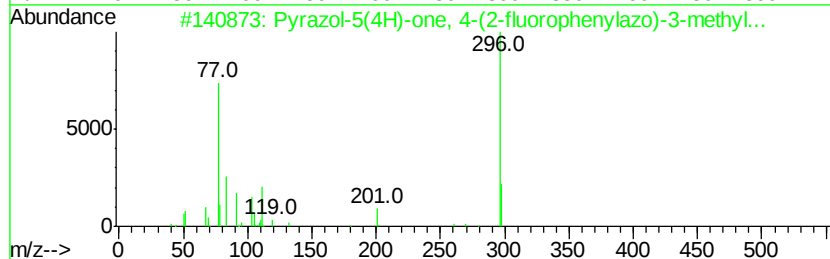
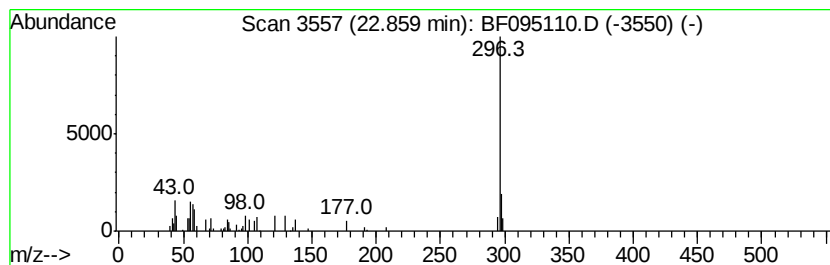
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 Pyrazol-5(4H)-one, 4-(2-flu... Concentration Rank 7

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 22.86 | 3.42 ng | 94926 | Perylene-d12     | 20.29 |

| Hit# | of | Tentative ID                                         | MW  | MolForm    | CAS#         | Qual |
|------|----|------------------------------------------------------|-----|------------|--------------|------|
| 1    | 5  | Pyrazol-5(4H)-one, 4-(2-fluorophenylazo)-3-methyl... | 296 | C16H13FN4O | 125910-81-8  | 50   |
| 2    |    | 3,4,5-Triphenylpyrazole                              | 296 | C21H16N2   | 018076-30-7  | 50   |
| 3    |    | Dimethyldioctadecylammonium bromide                  | 630 | C38H80BrN  | 003700-67-2  | 45   |
| 4    |    | 3-Methoxy-D-homoestra-1,3,5(10),...                  | 296 | C20H24O2   | 1000215-85-6 | 9    |
| 5    |    | 2-(2-Quinoly1)(1,2,4)triazolo(1,...                  | 296 | C19H12N4   | 1000241-15-8 | 9    |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF051217\  
Data File : BF095110.D  
Acq On : 12 May 2017 14:12  
Operator : SJ/MA  
Sample : I3100-07  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW-1-051017

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF050217.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... | 4.98  | 5.1 ng  |       | 132086   | 1                     | 7.70  | 519964 | 20.0 |
| unknown7.36          | 7.36  | 78.5 ng |       | 2040440  | 1                     | 7.70  | 519964 | 20.0 |
| n-Hexadecanoic acid  | 15.93 | 22.9 ng |       | 903649   | 4                     | 14.95 | 790745 | 20.0 |
| 9,12-Octadecadien... | 16.87 | 3.0 ng  |       | 112834   | 5                     | 18.62 | 763644 | 20.0 |
| trans-13-Octadece... | 16.89 | 3.9 ng  |       | 149006   | 5                     | 18.62 | 763644 | 20.0 |
| Octadecanoic acid    | 17.03 | 64.0 ng |       | 2442480  | 5                     | 18.62 | 763644 | 20.0 |
| Pyrazol-5(4H)-one... | 22.86 | 3.4 ng  |       | 94926    | 6                     | 20.29 | 554977 | 20.0 |