

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF070217\  
 Data File : BF096415.D  
 Acq On : 2 Jul 2017 14:49  
 Operator : SJ/MA  
 Sample : I3950-10  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 B5-6-8

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-BF070117.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         | 4.934       | 479           | 484         | 492          | rBV      | 451903         | 595791        | 17.32%          | 2.329%        |
| 2         | 5.351       | 550           | 555         | 558          | rBV      | 3415819        | 3438925       | 100.00%         | 13.442%       |
| 3         | 6.375       | 723           | 729         | 733          | rBV      | 2662448        | 3080657       | 89.58%          | 12.042%       |
| 4         | 6.504       | 746           | 751         | 754          | rBV      | 3154108        | 2970617       | 86.38%          | 11.612%       |
| 5         | 6.734       | 786           | 790         | 793          | rBV      | 1111147        | 884950        | 25.73%          | 3.459%        |
| 6         | 6.892       | 812           | 817         | 820          | rBV      | 2287330        | 2027815       | 58.97%          | 7.926%        |
| 7         | 7.292       | 879           | 885         | 888          | rBV      | 1827949        | 1818091       | 52.87%          | 7.107%        |
| 8         | 8.016       | 1003          | 1008        | 1011         | rBV      | 1449132        | 1151935       | 33.50%          | 4.503%        |
| 9         | 9.092       | 1186          | 1191        | 1194         | rBV      | 2784422        | 2324605       | 67.60%          | 9.086%        |
| 10        | 9.480       | 1254          | 1257        | 1260         | rBV      | 446392         | 379684        | 11.04%          | 1.484%        |
| 11        | 9.710       | 1293          | 1296        | 1301         | rVB      | 60160          | 54753         | 1.59%           | 0.214%        |
| 12        | 9.769       | 1301          | 1306        | 1309         | rBV      | 1127906        | 1069719       | 31.11%          | 4.181%        |
| 13        | 10.210      | 1378          | 1381        | 1384         | rVB      | 92065          | 69905         | 2.03%           | 0.273%        |
| 14        | 10.433      | 1412          | 1419        | 1425         | rBV2     | 23659          | 46472         | 1.35%           | 0.182%        |
| 15        | 10.551      | 1434          | 1439        | 1442         | rBV      | 1511846        | 1347653       | 39.19%          | 5.268%        |
| 16        | 10.680      | 1458          | 1461        | 1468         | rBV      | 77145          | 88295         | 2.57%           | 0.345%        |
| 17        | 11.127      | 1534          | 1537        | 1540         | rBV2     | 47491          | 41860         | 1.22%           | 0.164%        |
| 18        | 11.245      | 1553          | 1557        | 1560         | rBV      | 1025071        | 835961        | 24.31%          | 3.268%        |
| 19        | 11.780      | 1644          | 1648        | 1651         | rBV2     | 77724          | 74256         | 2.16%           | 0.290%        |
| 20        | 12.451      | 1759          | 1762        | 1765         | rBV      | 55320          | 45691         | 1.33%           | 0.179%        |
| 21        | 12.680      | 1794          | 1801        | 1803         | rBV2     | 46475          | 61267         | 1.78%           | 0.239%        |
| 22        | 12.827      | 1822          | 1826        | 1830         | rBV      | 1669551        | 1451587       | 42.21%          | 5.674%        |
| 23        | 13.310      | 1904          | 1908        | 1916         | rVB2     | 74063          | 88614         | 2.58%           | 0.346%        |
| 24        | 13.733      | 1976          | 1980        | 1988         | rVB      | 199388         | 218389        | 6.35%           | 0.854%        |
| 25        | 13.874      | 1999          | 2004        | 2007         | rBV      | 811983         | 798147        | 23.21%          | 3.120%        |
| 26        | 15.286      | 2239          | 2244        | 2248         | rBV      | 500669         | 575219        | 16.73%          | 2.248%        |
| 27        | 17.056      | 2542          | 2545        | 2548         | rBV5     | 28744          | 42208         | 1.23%           | 0.165%        |

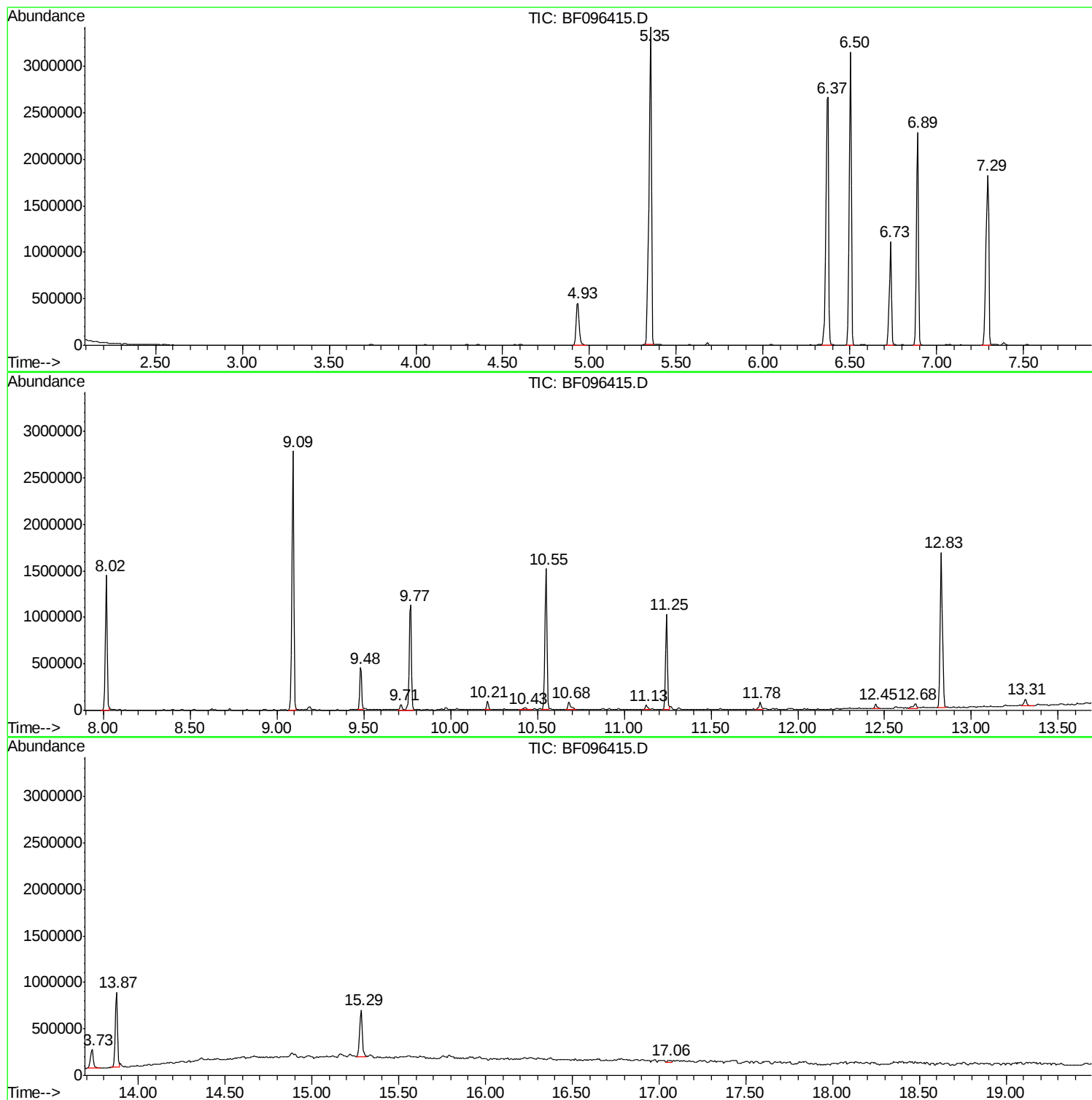
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B5-6-8

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.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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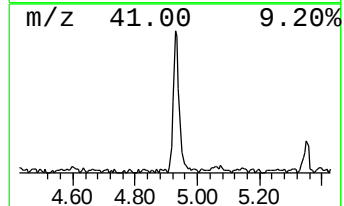
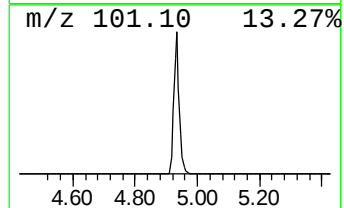
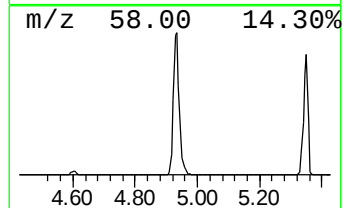
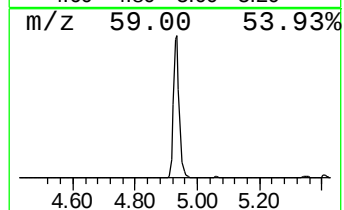
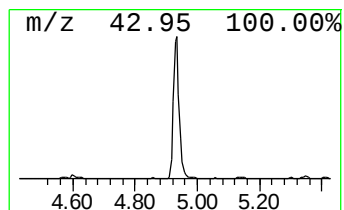
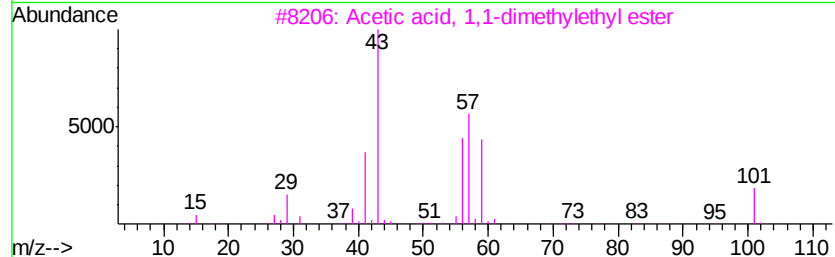
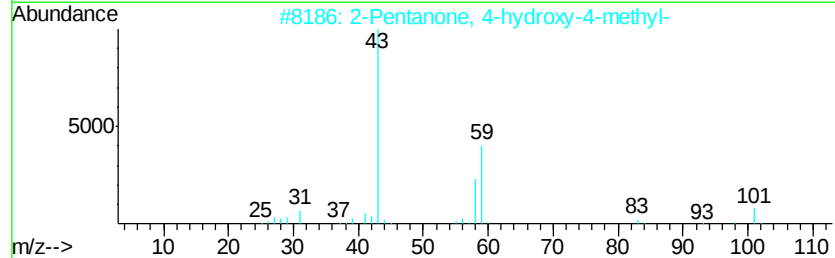
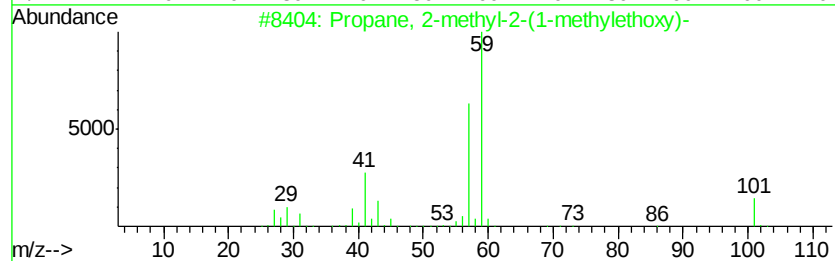
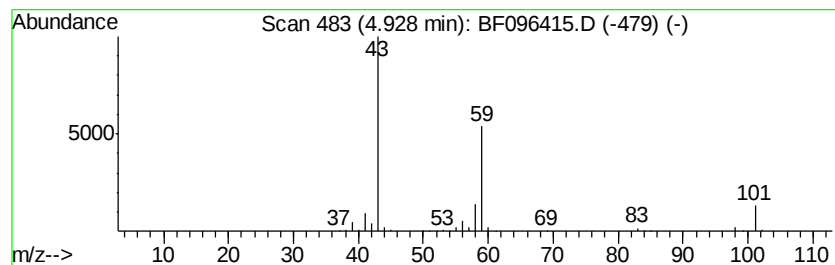
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.93 | 13.47 ng | 595791 | 1,4-Dichlorobenzene-d4 | 6.73 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 53   |
| 2    |    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 50   |
| 3    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 38   |
| 4    |    | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 28   |
| 5    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |



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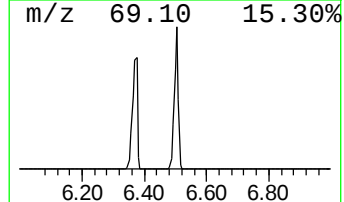
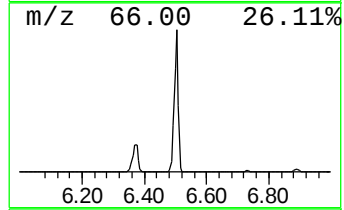
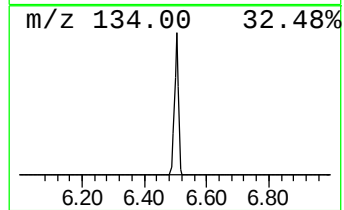
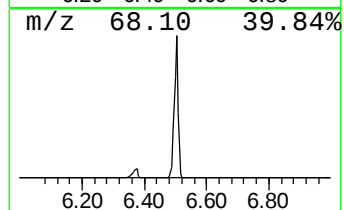
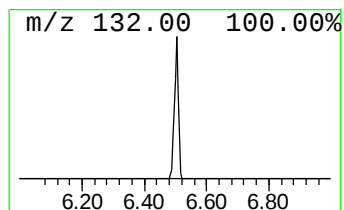
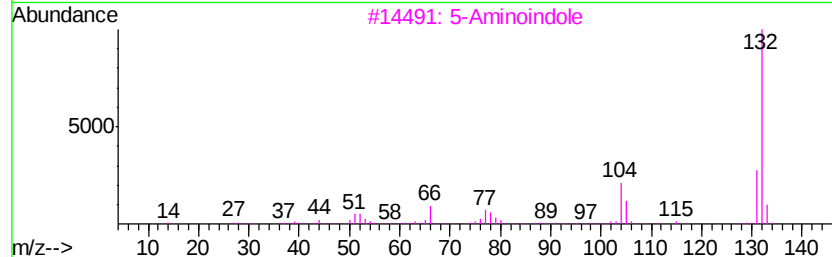
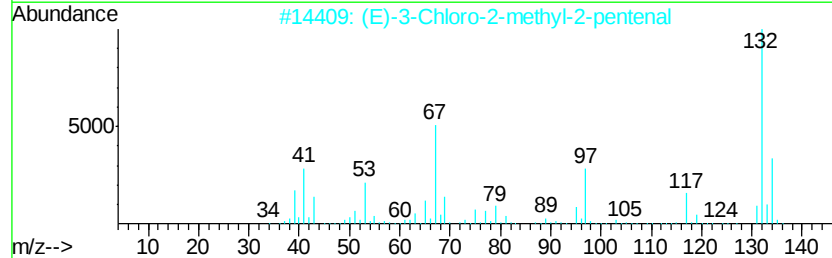
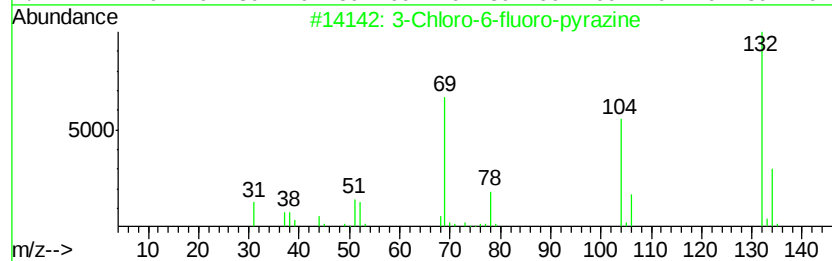
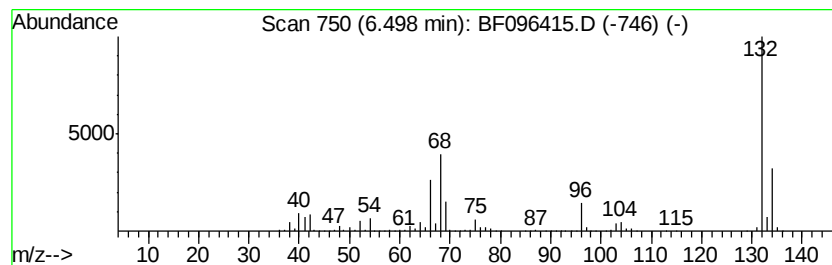
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.50 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.50 | 67.14 ng | 2970620 | 1,4-Dichlorobenzene-d4 | 6.73 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 12   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | 1,3,5-Trifluorobenzene           | 132 | C6H3F3    | 000372-38-3  | 9    |



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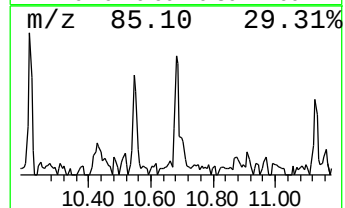
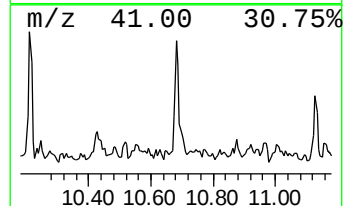
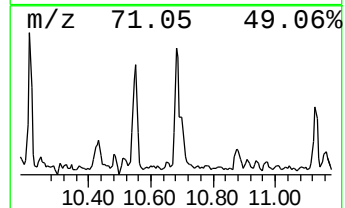
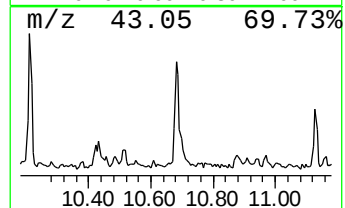
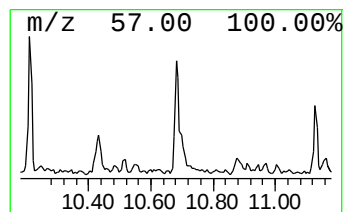
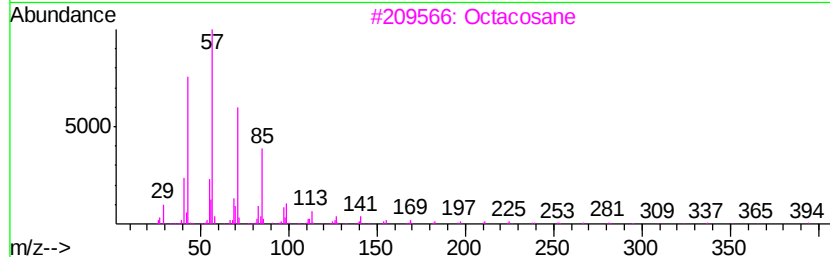
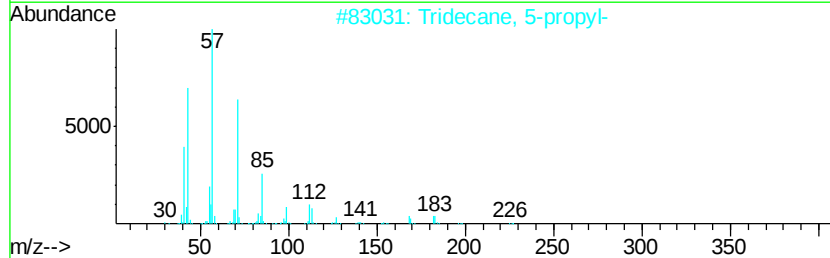
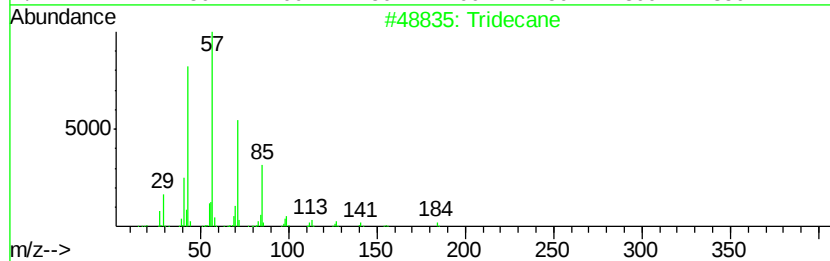
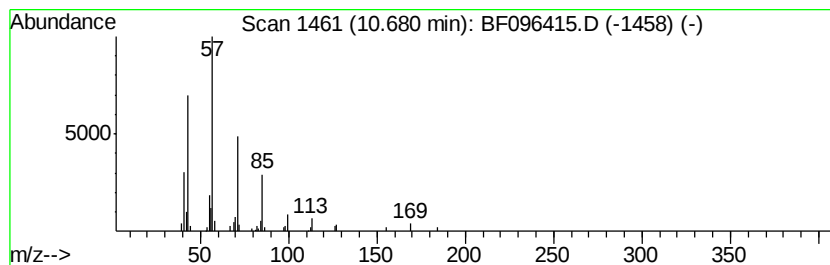
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ClientSampleId :  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Tridecane Concentration Rank 6

| R.T.      | EstConc              | Area  | Relative to ISTD |             | R.T.  |
|-----------|----------------------|-------|------------------|-------------|-------|
| 10.68     | 2.11 ng              | 88295 | Phenanthrene-d10 |             | 11.24 |
| Hit# of 5 | Tentative ID         | MW    | MolForm          | CAS#        | Qual  |
| 1         | Tridecane            | 184   | C13H28           | 000629-50-5 | 93    |
| 2         | Tridecane, 5-propyl- | 226   | C16H34           | 055045-11-9 | 90    |
| 3         | Octacosane           | 394   | C28H58           | 000630-02-4 | 90    |
| 4         | Hexadecane           | 226   | C16H34           | 000544-76-3 | 86    |
| 5         | Pentadecane          | 212   | C15H32           | 000629-62-9 | 86    |



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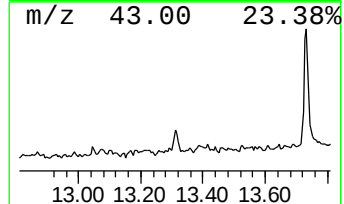
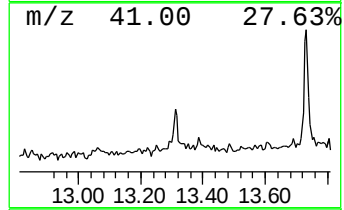
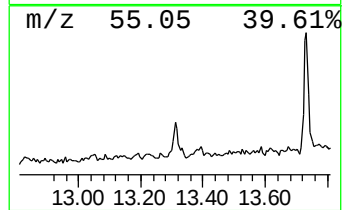
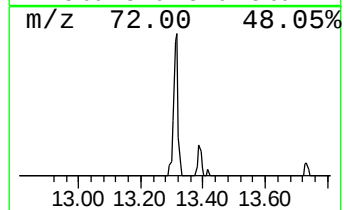
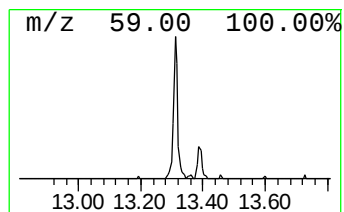
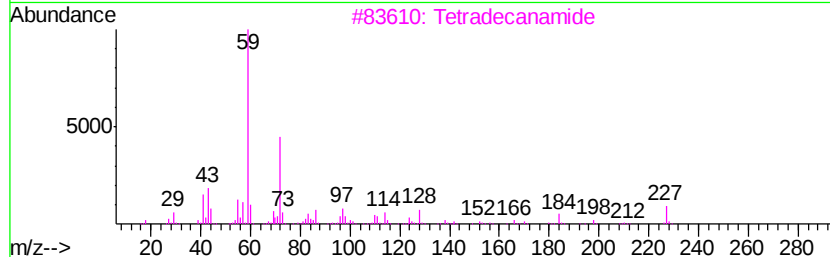
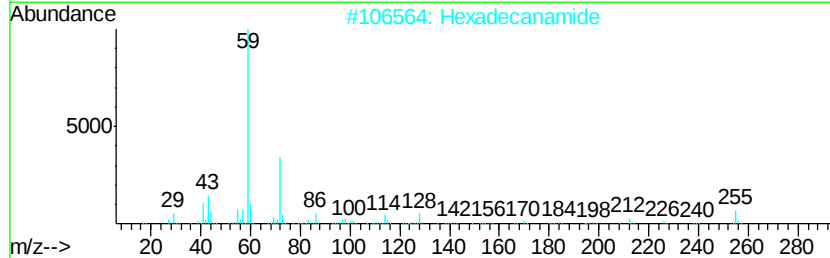
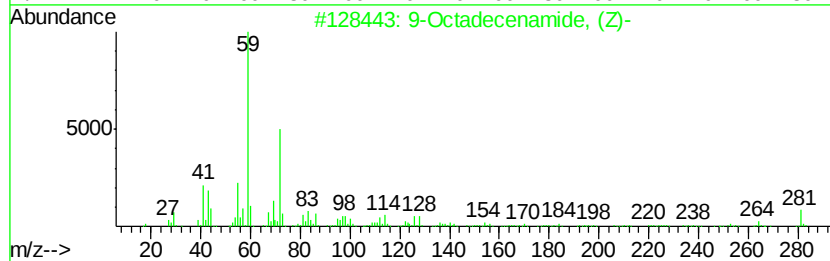
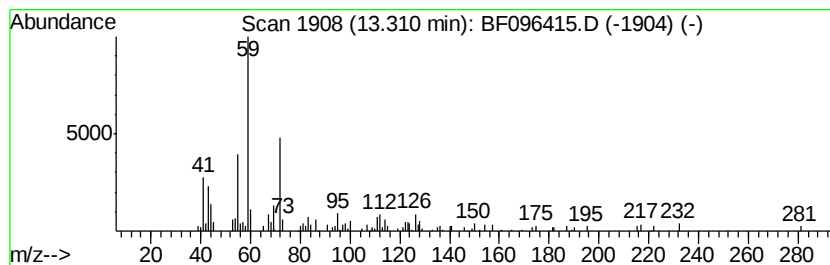
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\*\*\*\*\*  
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

| R.T.      | EstConc                    | Area  | Relative to ISTD |              | R.T.  |
|-----------|----------------------------|-------|------------------|--------------|-------|
| 13.31     | 2.22 ng                    | 88614 | Chrysene-d12     |              | 13.87 |
| Hit# of 5 | Tentative ID               | MW    | MolForm          | CAS#         | Qual  |
| 1         | 9-Octadecenamide, (Z)-     | 281   | C18H35NO         | 000301-02-0  | 87    |
| 2         | Hexadecanamide             | 255   | C16H33NO         | 000629-54-9  | 72    |
| 3         | Tetradecanamide            | 227   | C14H29NO         | 000638-58-4  | 56    |
| 4         | Dodecanamide               | 199   | C12H25NO         | 001120-16-7  | 53    |
| 5         | Pentadecanamide, 15-bromo- | 319   | C15H30BrNO       | 1000163-86-1 | 53    |



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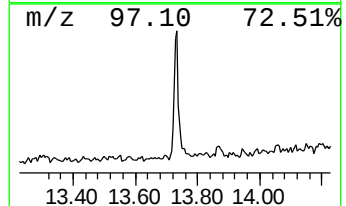
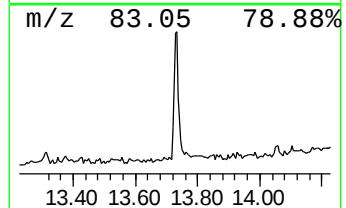
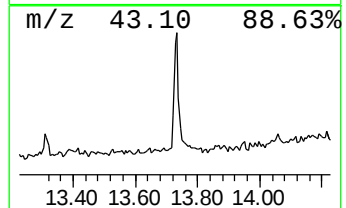
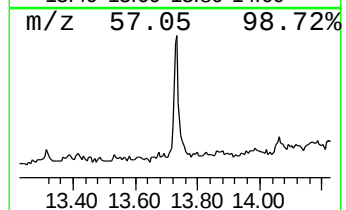
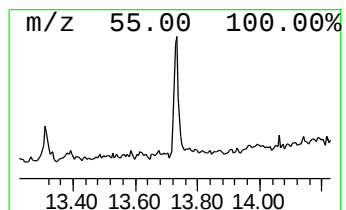
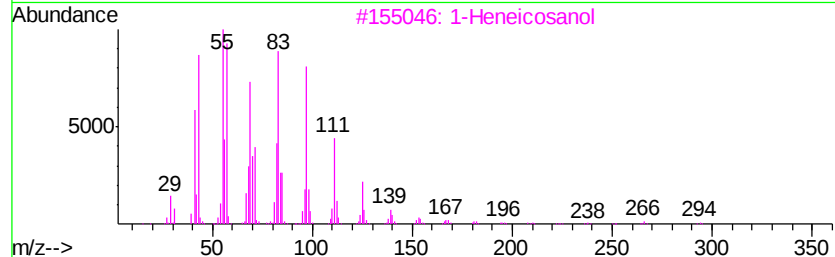
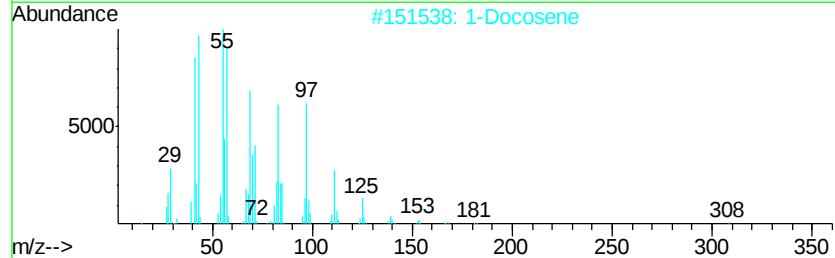
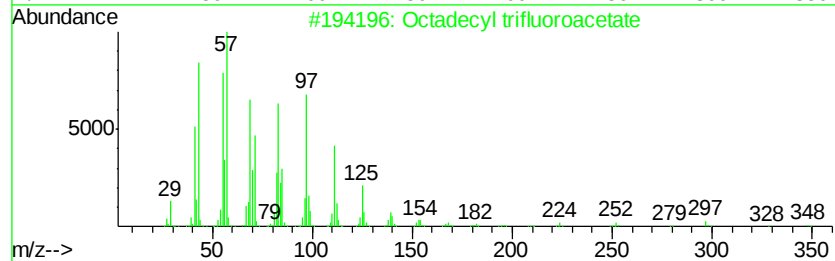
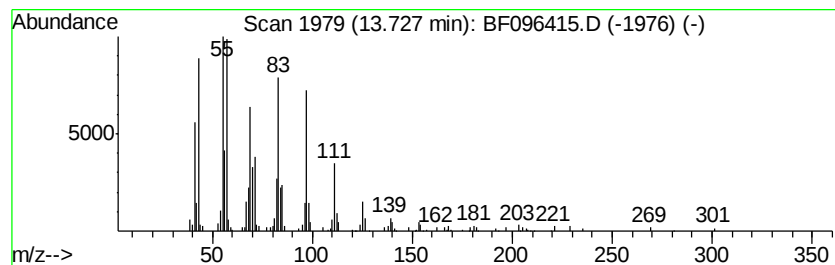
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TIC Integration Parameters: LSCINT.P

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Peak Number 6 Octadecyl trifluoroacetate Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.73 | 5.47 ng | 218389 | Chrysene-d12     | 13.87 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|-------------------------------------|-----|-------------|-------------|------|
| 1    | 5  | Octadecyl trifluoroacetate          | 366 | C20H37F3O2  | 079392-43-1 | 94   |
| 2    |    | 1-Docosene                          | 308 | C22H44      | 001599-67-3 | 91   |
| 3    |    | 1-Heneicosanol                      | 312 | C21H44O     | 015594-90-8 | 91   |
| 4    |    | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91   |
| 5    |    | Octacosanol                         | 410 | C28H58O     | 000557-61-9 | 91   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF070217\  
Data File : BF096415.D  
Acq On : 2 Jul 2017 14:49  
Operator : SJ/MA  
Sample : I3950-10  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
B5-6-8

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.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 |
| Propane, 2-methyl... | 4.93  | 13.5    | ng    | 595791   | 1                     | 6.73  | 884950 | 20.0 |
| unknown6.50          | 6.50  | 67.1    | ng    | 2970620  | 1                     | 6.73  | 884950 | 20.0 |
| Tridecane            | 10.68 | 2.1     | ng    | 88295    | 4                     | 11.24 | 835961 | 20.0 |
| 9-Octadecenamide,... | 13.31 | 2.2     | ng    | 88614    | 5                     | 13.87 | 798147 | 20.0 |
| Octadecyl trifluo... | 13.73 | 5.5     | ng    | 218389   | 5                     | 13.87 | 798147 | 20.0 |