

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\  
 Data File : BF096348.D  
 Acq On : 30 Jun 2017 20:48  
 Operator : SJ/MA  
 Sample : I3959-07 5X  
 Misc :  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 BU-03-062717-C

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-BF062717.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         | 4.940       | 481           | 485         | 491          | rBV      | 103190         | 101126        | 5.41%           | 0.655%        |
| 2         | 5.363       | 553           | 557         | 561          | rVB      | 847521         | 720089        | 38.49%          | 4.663%        |
| 3         | 6.381       | 726           | 730         | 736          | rVB      | 967269         | 752652        | 40.23%          | 4.874%        |
| 4         | 6.522       | 750           | 754         | 758          | rBV      | 898986         | 735750        | 39.33%          | 4.764%        |
| 5         | 6.757       | 790           | 794         | 798          | rBV      | 1130149        | 950087        | 50.79%          | 6.152%        |
| 6         | 6.916       | 817           | 821         | 824          | rBV      | 582741         | 517184        | 27.65%          | 3.349%        |
| 7         | 7.310       | 884           | 888         | 891          | rBV      | 517233         | 420906        | 22.50%          | 2.726%        |
| 8         | 7.733       | 956           | 960         | 963          | rBV      | 29364          | 28797         | 1.54%           | 0.186%        |
| 9         | 8.039       | 1007          | 1012        | 1016         | rBV      | 1511853        | 1291848       | 69.06%          | 8.365%        |
| 10        | 9.116       | 1190          | 1195        | 1198         | rBV      | 914548         | 712969        | 38.11%          | 4.617%        |
| 11        | 9.210       | 1207          | 1211        | 1214         | rBV3     | 22745          | 22426         | 1.20%           | 0.145%        |
| 12        | 9.380       | 1236          | 1240        | 1245         | rBV      | 26249          | 27259         | 1.46%           | 0.177%        |
| 13        | 9.451       | 1248          | 1252        | 1255         | rBV3     | 17668          | 22393         | 1.20%           | 0.145%        |
| 14        | 9.510       | 1259          | 1262        | 1264         | rBV      | 111322         | 98380         | 5.26%           | 0.637%        |
| 15        | 9.792       | 1305          | 1310        | 1314         | rBV2     | 1297941        | 1152732       | 61.62%          | 7.465%        |
| 16        | 9.822       | 1314          | 1315        | 1318         | rVB      | 28446          | 22302         | 1.19%           | 0.144%        |
| 17        | 9.998       | 1341          | 1345        | 1347         | rVB      | 31270          | 26716         | 1.43%           | 0.173%        |
| 18        | 10.239      | 1383          | 1386        | 1388         | rVB      | 30151          | 23825         | 1.27%           | 0.154%        |
| 19        | 10.574      | 1439          | 1443        | 1447         | rVB      | 414268         | 335116        | 17.91%          | 2.170%        |
| 20        | 10.710      | 1463          | 1466        | 1468         | rBV2     | 33086          | 32131         | 1.72%           | 0.208%        |
| 21        | 11.157      | 1539          | 1542        | 1546         | rBV2     | 24590          | 26833         | 1.43%           | 0.174%        |
| 22        | 11.274      | 1558          | 1562        | 1564         | rBV      | 952302         | 852524        | 45.57%          | 5.521%        |
| 23        | 11.292      | 1564          | 1565        | 1568         | rVV      | 100786         | 75818         | 4.05%           | 0.491%        |
| 24        | 11.345      | 1572          | 1574        | 1577         | rVB      | 27282          | 21561         | 1.15%           | 0.140%        |
| 25        | 11.680      | 1627          | 1631        | 1634         | rVB      | 558969         | 494906        | 26.46%          | 3.205%        |
| 26        | 11.804      | 1649          | 1652        | 1656         | rBV2     | 92724          | 84131         | 4.50%           | 0.545%        |
| 27        | 11.880      | 1663          | 1665        | 1668         | rBV      | 24534          | 23260         | 1.24%           | 0.151%        |
| 28        | 12.363      | 1743          | 1747        | 1749         | rBV      | 2097815        | 1870697       | 100.00%         | 12.114%       |
| 29        | 12.380      | 1749          | 1750        | 1757         | rVB      | 1228486        | 1094060       | 58.48%          | 7.085%        |
| 30        | 12.468      | 1762          | 1765        | 1771         | rBV2     | 317324         | 415577        | 22.22%          | 2.691%        |
| 31        | 12.592      | 1783          | 1786        | 1791         | rVB5     | 31155          | 34069         | 1.82%           | 0.221%        |
| 32        | 12.704      | 1801          | 1805        | 1809         | rVB      | 143225         | 155746        | 8.33%           | 1.009%        |
| 33        | 12.851      | 1827          | 1830        | 1834         | rBV      | 498569         | 479877        | 25.65%          | 3.107%        |
| 34        | 13.039      | 1859          | 1862        | 1864         | rBV3     | 19733          | 20782         | 1.11%           | 0.135%        |

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ALS Vial : 25 Sample Multiplier: 1

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ClientSampleId :  
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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-BF062717.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 35 | 13.104 | 1870 | 1873 | 1877 | rBV3 | 34695  | 42323  | 2.26%  | 0.274% |
| 36 | 13.192 | 1886 | 1888 | 1891 | rVB3 | 24720  | 23320  | 1.25%  | 0.151% |
| 37 | 13.304 | 1903 | 1907 | 1908 | rBV3 | 25592  | 34012  | 1.82%  | 0.220% |
| 38 | 13.615 | 1958 | 1960 | 1963 | rVB2 | 50170  | 40181  | 2.15%  | 0.260% |
| 39 | 13.757 | 1982 | 1984 | 1990 | rVB3 | 54695  | 54309  | 2.90%  | 0.352% |
| 40 | 13.904 | 2004 | 2009 | 2012 | rBV  | 964079 | 954260 | 51.01% | 6.179% |
| 41 | 13.927 | 2012 | 2013 | 2015 | rVB  | 54262  | 26611  | 1.42%  | 0.172% |
| 42 | 15.321 | 2246 | 2250 | 2254 | rBV2 | 529630 | 623079 | 33.31% | 4.035% |

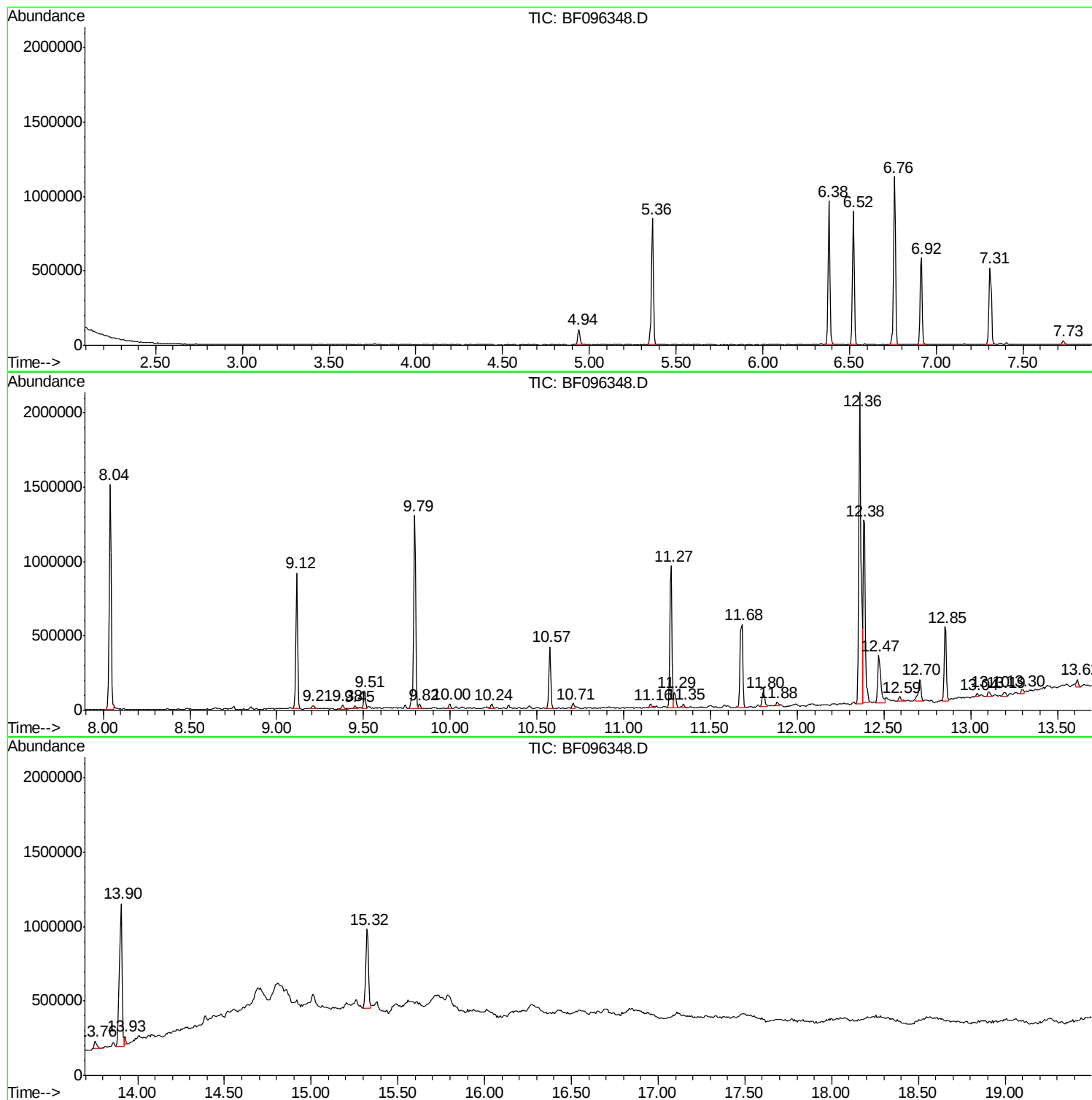
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF062717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

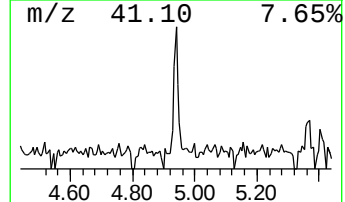
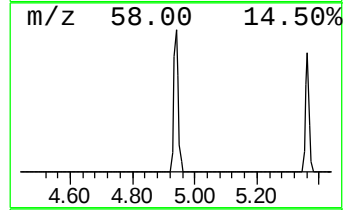
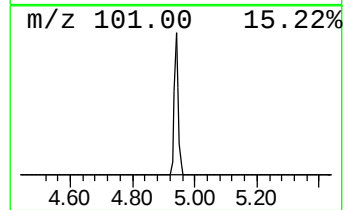
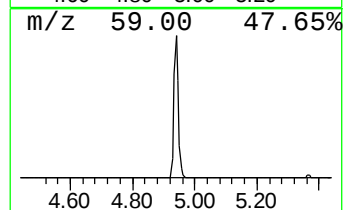
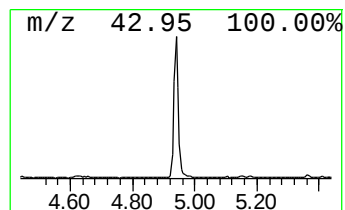
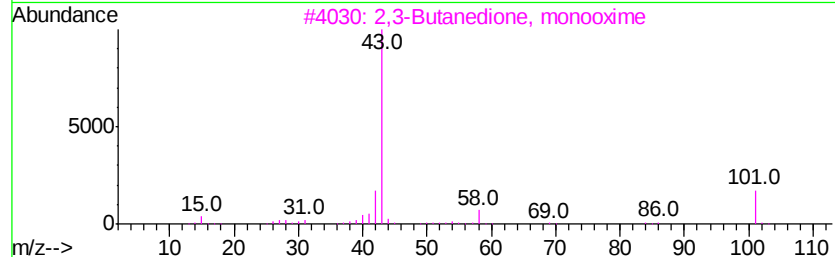
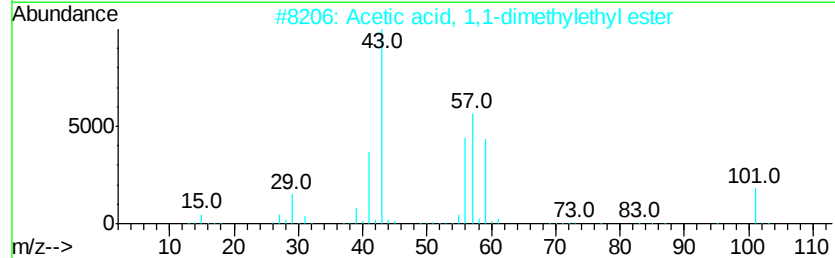
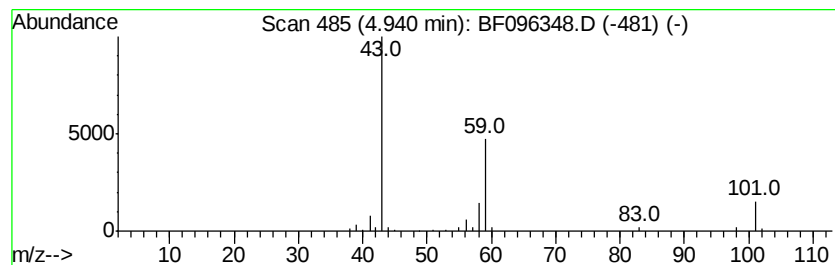
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.94 | 2.13 ng | 101126 | 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    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 38   |
| 3    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 16   |
| 4    |    | Diacetamide                         | 101 | C4H7NO2 | 000625-77-4 | 7    |
| 5    |    | (+)-4-Amino-4,5-dihydro-2(3H)-f...  | 101 | C4H7NO2 | 016504-58-8 | 7    |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

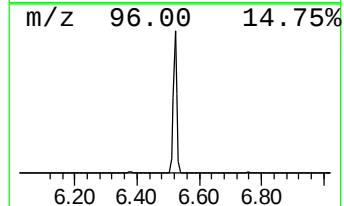
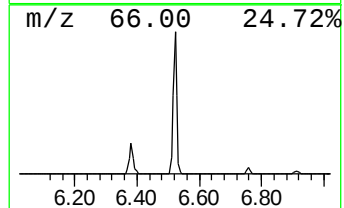
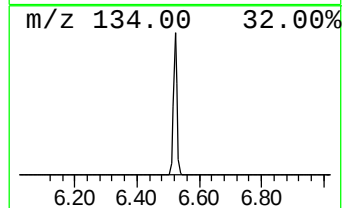
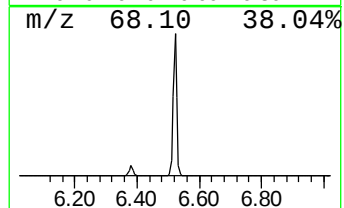
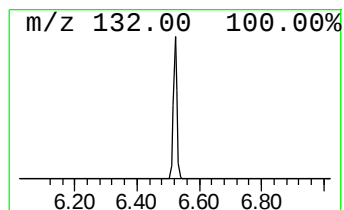
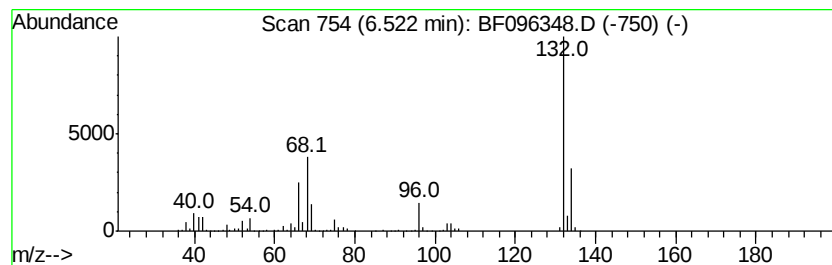
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.52 Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 6.52 | 15.49 ng | 735750 | 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 | 35   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 25   |
| 3    |    | Tranvlcypropine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 4    |    | Amphetaminil                     | 250 | C17H18N2  | 017590-01-1  | 12   |
| 5    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

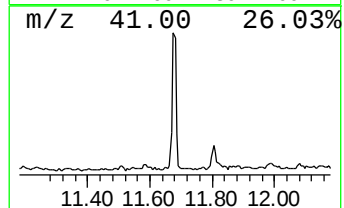
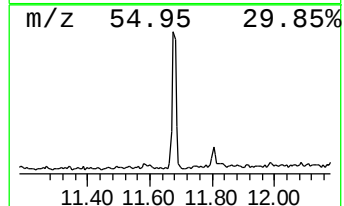
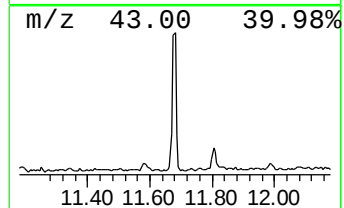
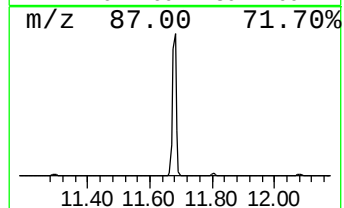
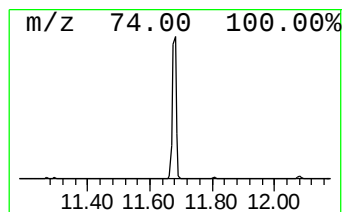
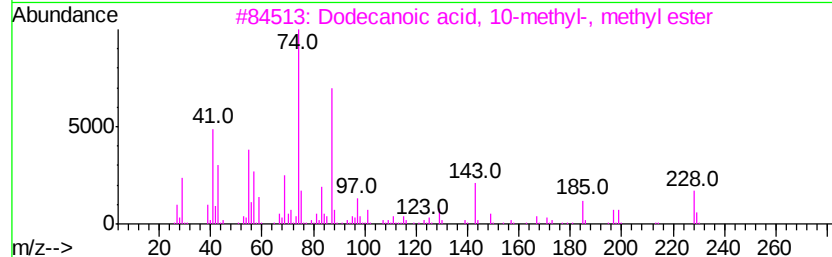
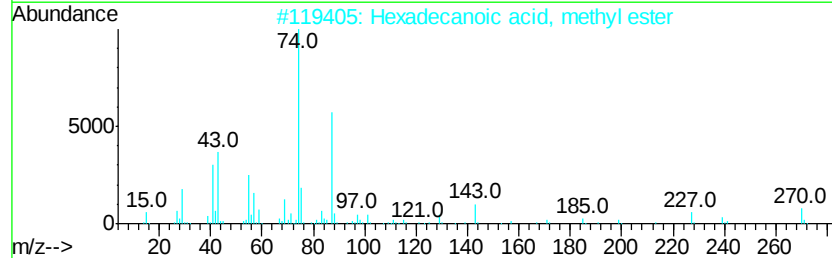
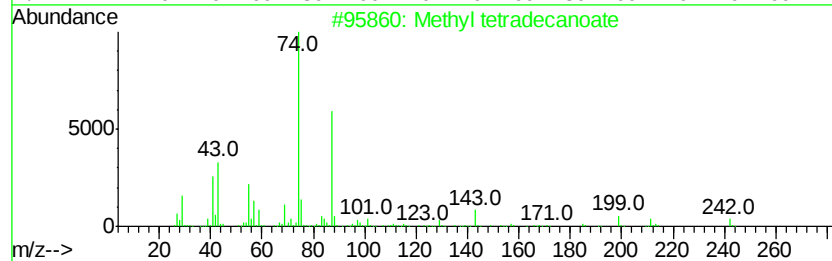
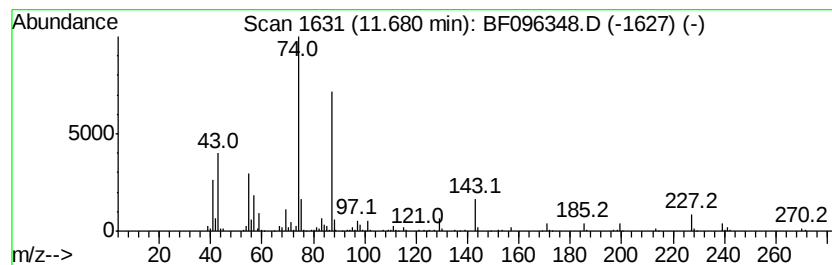
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 Methyl tetradecanoate Concentration Rank 4

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 11.68 | 11.61 ng | 494906 | Phenanthrene-d10 | 11.27 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|---------|---|-------------------------------------|-----|----------|-------------|------|
| 1       |   | Methyl tetradecanoate               | 242 | C15H30O2 | 000124-10-7 | 93   |
| 2       |   | Hexadecanoic acid, methyl ester     | 270 | C17H34O2 | 000112-39-0 | 91   |
| 3       |   | Dodecanoic acid, 10-methyl-, met... | 228 | C14H28O2 | 005129-65-7 | 87   |
| 4       |   | Pentadecanoic acid, 14-methyl-, ... | 270 | C17H34O2 | 005129-60-2 | 87   |
| 5       |   | Pentadecanoic acid, methyl ester    | 256 | C16H32O2 | 007132-64-1 | 86   |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

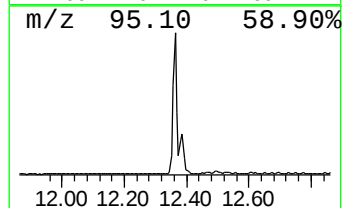
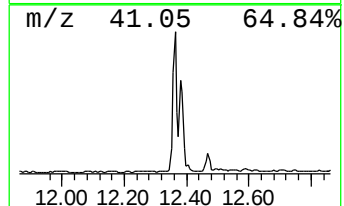
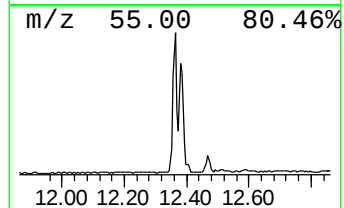
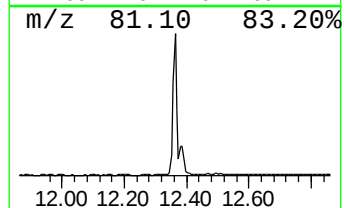
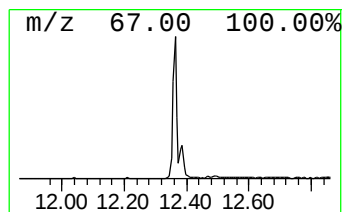
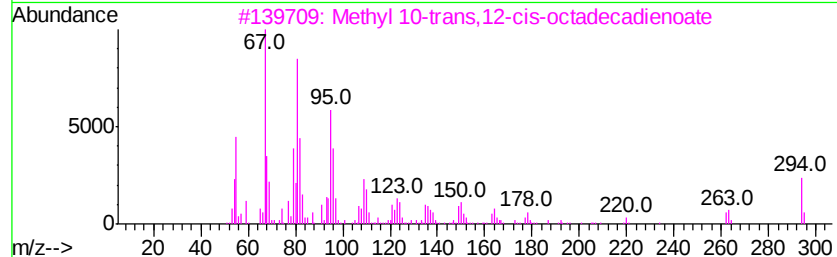
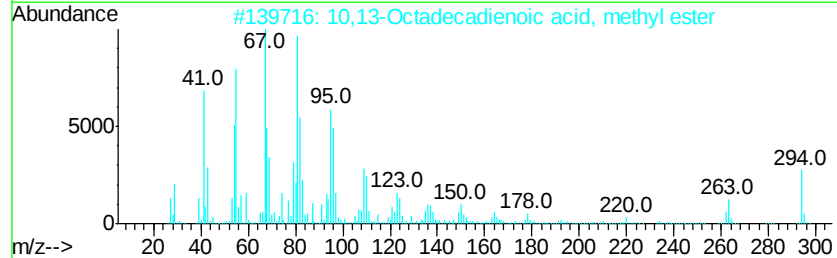
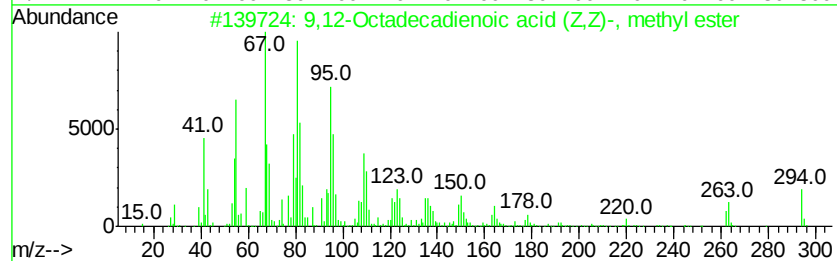
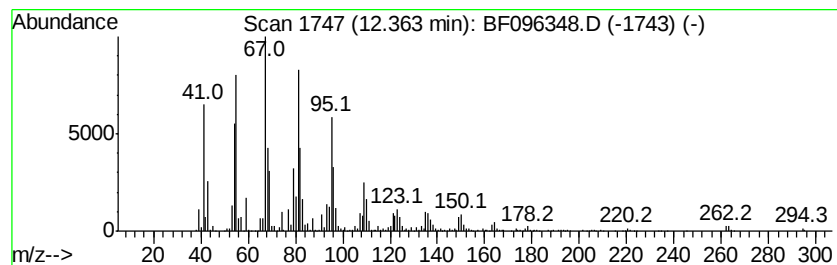
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 1

| R.T.  | EstConc  | Area    | Relative to ISTD | R.T.  |
|-------|----------|---------|------------------|-------|
| 12.36 | 43.89 ng | 1870700 | Phenanthrene-d10 | 11.27 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|---------|---|-------------------------------------|-----|----------|--------------|------|
| 1       |   | 9,12-Octadecadienoic acid (Z,Z)-... | 294 | C19H34O2 | 000112-63-0  | 99   |
| 2       |   | 10,13-Octadecadienoic acid, meth... | 294 | C19H34O2 | 056554-62-2  | 99   |
| 3       |   | Methyl 10-trans,12-cis-octadecad... | 294 | C19H34O2 | 1000336-44-2 | 99   |
| 4       |   | 8,11-Octadecadienoic acid, methy... | 294 | C19H34O2 | 056599-58-7  | 99   |
| 5       |   | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4  | 99   |



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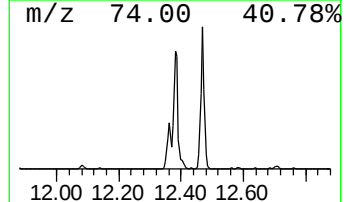
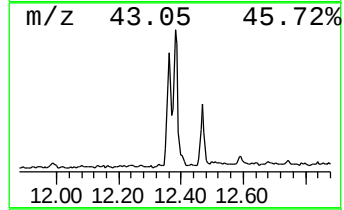
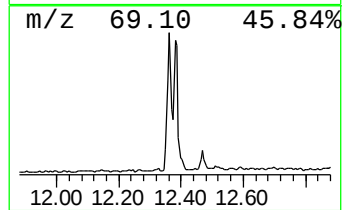
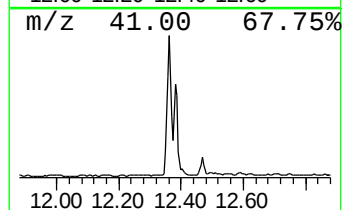
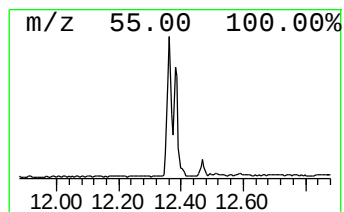
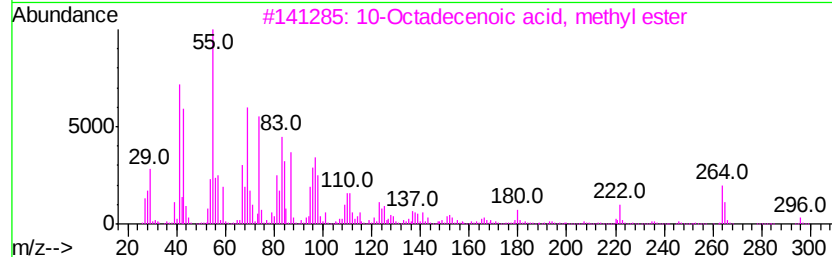
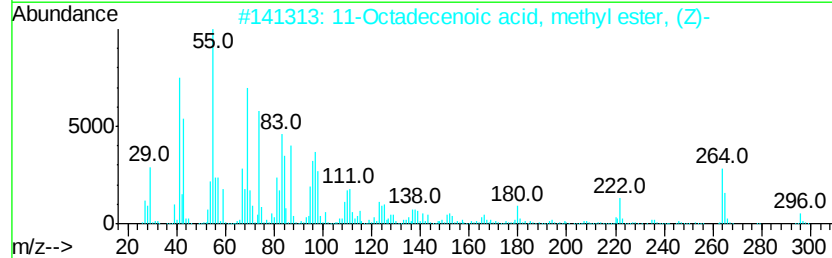
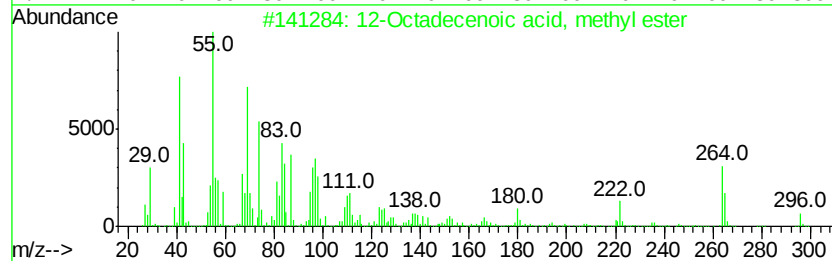
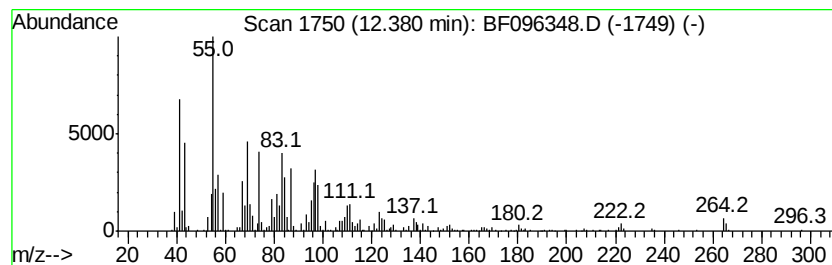
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 12-Octadecenoic acid, methyl... Concentration Rank 2

| R.T.  | EstConc  | Area    | Relative to ISTD | R.T.  |
|-------|----------|---------|------------------|-------|
| 12.38 | 25.67 ng | 1094060 | Phenanthrene-d10 | 11.27 |

| Hit# | of | Tentative ID                          | MW  | MolForm  | CAS#         | Qual |
|------|----|---------------------------------------|-----|----------|--------------|------|
| 1    | 5  | 12-Octadecenoic acid, methyl ester    | 296 | C19H36O2 | 056554-46-2  | 99   |
| 2    |    | 11-Octadecenoic acid, methyl ester... | 296 | C19H36O2 | 001937-63-9  | 99   |
| 3    |    | 10-Octadecenoic acid, methyl ester    | 296 | C19H36O2 | 013481-95-3  | 99   |
| 4    |    | 9-Octadecenoic acid, methyl ester...  | 296 | C19H36O2 | 001937-62-8  | 98   |
| 5    |    | cis-13-Octadecenoic acid, methyl...   | 296 | C19H36O2 | 1000333-58-3 | 96   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF063017\  
Data File : BF096348.D  
Acq On : 30 Jun 2017 20:48  
Operator : SJ/MA  
Sample : I3959-07 5X  
Misc :  
ALS Vial : 25 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BU-03-062717-C

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF062717.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... | 4.94  | 2.1     | ng    | 101126   | 1                     | 6.76  | 950087 | 20.0 |
| unknown6.52          | 6.52  | 15.5    | ng    | 735750   | 1                     | 6.76  | 950087 | 20.0 |
| Methyl tetradecan... | 11.68 | 11.6    | ng    | 494906   | 4                     | 11.27 | 852524 | 20.0 |
| 9,12-Octadecadien... | 12.36 | 43.9    | ng    | 1870700  | 4                     | 11.27 | 852524 | 20.0 |
| 12-Octadecenoic a... | 12.38 | 25.7    | ng    | 1094060  | 4                     | 11.27 | 852524 | 20.0 |