

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072518\  
 Data File : BF107654.D  
 Acq On : 25 Jul 2018 13:59  
 Operator : JU/SJ  
 Sample : J4096-10  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 DW-12

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:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF072018.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|--------|----------|------------|----------|-----------|-------|-------------|------------|--------------|------------|
| 1      | 5.213    | 484        | 489      | 500       | rBV   | 565305      | 858072     | 16.07%       | 1.729%     |
| 2      | 5.601    | 551        | 555      | 594       | rBV   | 3542466     | 5340191    | 100.00%      | 10.757%    |
| 3      | 6.601    | 720        | 725      | 744       | rBV   | 3456198     | 5169062    | 96.80%       | 10.413%    |
| 4      | 6.742    | 744        | 749      | 763       | rVV   | 4271821     | 5189684    | 97.18%       | 10.454%    |
| 5      | 6.966    | 783        | 787      | 803       | rBV   | 1304252     | 1614635    | 30.24%       | 3.253%     |
| 6      | 7.119    | 809        | 813      | 829       | rBV   | 3497547     | 4006499    | 75.03%       | 8.071%     |
| 7      | 7.530    | 878        | 883      | 907       | rBV   | 2620369     | 3488315    | 65.32%       | 7.027%     |
| 8      | 8.248    | 1001       | 1005     | 1027      | rBV   | 1950583     | 2139460    | 40.06%       | 4.310%     |
| 9      | 9.324    | 1180       | 1188     | 1202      | rBV   | 4635712     | 5147562    | 96.39%       | 10.369%    |
| 10     | 9.713    | 1250       | 1254     | 1260      | rBV   | 428180      | 400437     | 7.50%        | 0.807%     |
| 11     | 10.007   | 1300       | 1304     | 1313      | rBV2  | 2170877     | 2067514    | 38.72%       | 4.165%     |
| 12     | 10.801   | 1435       | 1439     | 1451      | rBV   | 2871584     | 3231772    | 60.52%       | 6.510%     |
| 13     | 10.889   | 1452       | 1454     | 1460      | rVB5  | 39179       | 64586      | 1.21%        | 0.130%     |
| 14     | 11.501   | 1554       | 1558     | 1570      | rBV   | 1885075     | 2102710    | 39.38%       | 4.236%     |
| 15     | 12.007   | 1641       | 1644     | 1655      | rBV3  | 227950      | 301271     | 5.64%        | 0.607%     |
| 16     | 12.718   | 1762       | 1765     | 1769      | rBV   | 216703      | 217523     | 4.07%        | 0.438%     |
| 17     | 12.889   | 1791       | 1794     | 1799      | rVB   | 121243      | 107684     | 2.02%        | 0.217%     |
| 18     | 12.948   | 1799       | 1804     | 1810      | rBV   | 180169      | 286405     | 5.36%        | 0.577%     |
| 19     | 13.083   | 1823       | 1827     | 1838      | rBV   | 3291647     | 3611700    | 67.63%       | 7.275%     |
| 20     | 13.595   | 1911       | 1914     | 1918      | rVB2  | 102747      | 98546      | 1.85%        | 0.199%     |
| 21     | 13.636   | 1918       | 1921     | 1923      | rBV2  | 71185       | 65162      | 1.22%        | 0.131%     |
| 22     | 13.971   | 1974       | 1978     | 1985      | rBV3  | 187642      | 254620     | 4.77%        | 0.513%     |
| 23     | 14.107   | 1998       | 2001     | 2004      | rBV   | 103049      | 91885      | 1.72%        | 0.185%     |
| 24     | 14.154   | 2004       | 2009     | 2020      | rVV   | 1338160     | 1690877    | 31.66%       | 3.406%     |
| 25     | 14.283   | 2029       | 2031     | 2034      | rBV   | 75921       | 65166      | 1.22%        | 0.131%     |
| 26     | 14.589   | 2081       | 2083     | 2091      | rVB   | 103431      | 105923     | 1.98%        | 0.213%     |
| 27     | 14.912   | 2135       | 2138     | 2140      | rVB   | 72933       | 75599      | 1.42%        | 0.152%     |
| 28     | 15.224   | 2188       | 2191     | 2195      | rBV   | 101472      | 164974     | 3.09%        | 0.332%     |
| 29     | 15.265   | 2196       | 2198     | 2203      | rVB   | 156846      | 168143     | 3.15%        | 0.339%     |
| 30     | 15.683   | 2264       | 2269     | 2284      | rVB2  | 915568      | 1516300    | 28.39%       | 3.054%     |

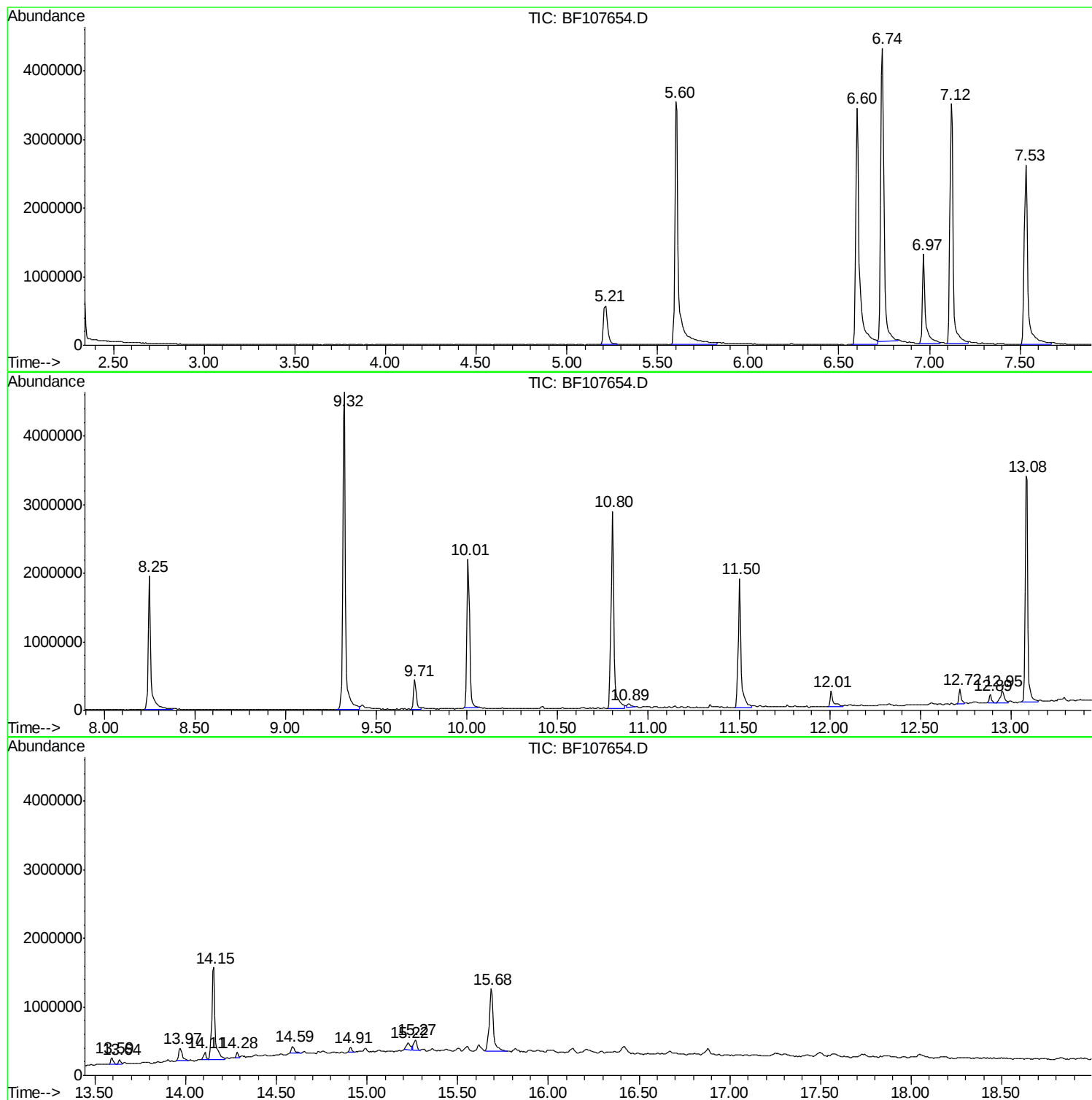
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ALS Vial : 7 Sample Multiplier: 1

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BNA\_F  
ClientSampled :  
DW-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF072018.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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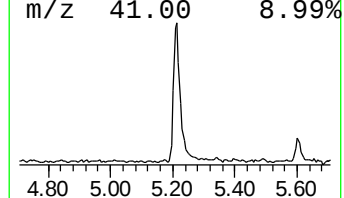
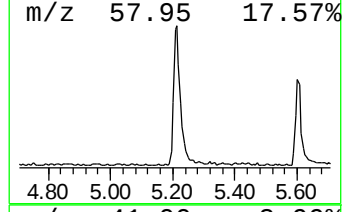
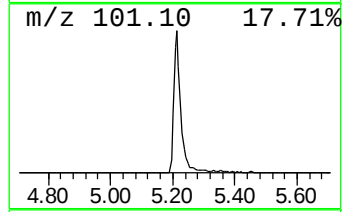
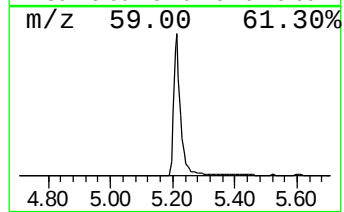
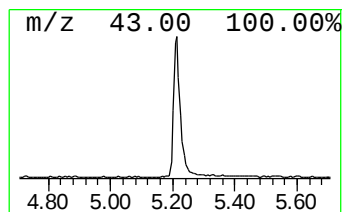
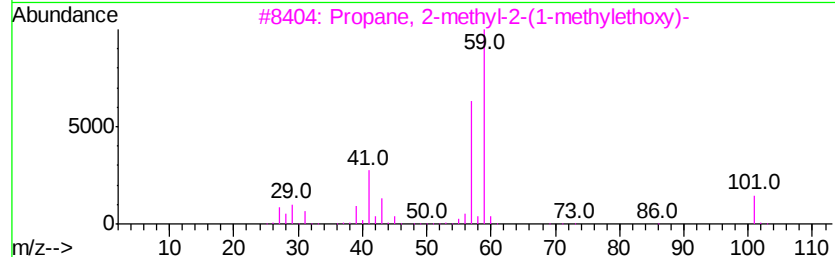
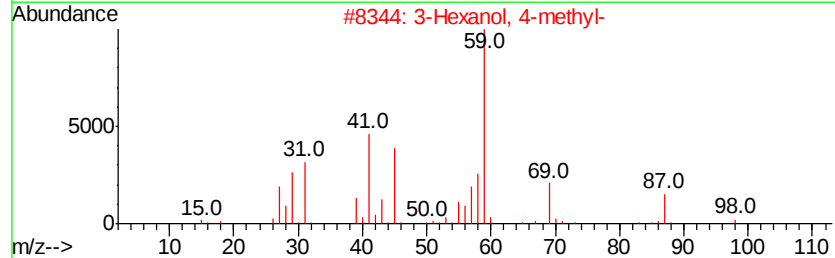
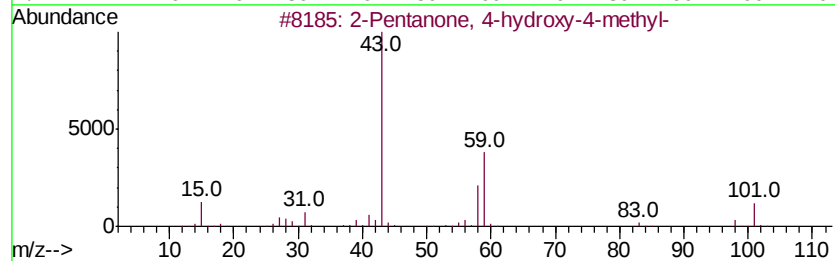
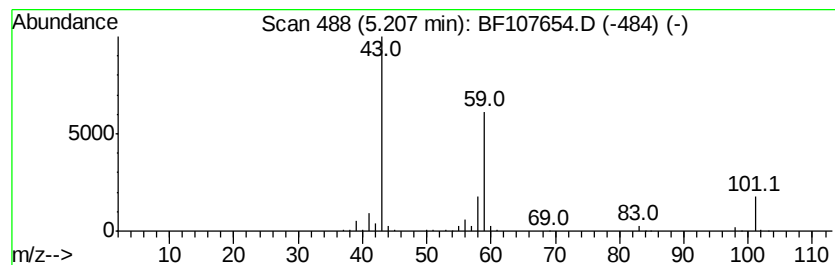
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.21 | 10.63 ng | 858072 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# | of | 5 | Tentative ID                          | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-      | 116 | C6H12O2  | 000123-42-2 | 53   |
| 2    |    |   | 3-Hexanol, 4-methyl-                  | 116 | C7H16O   | 000615-29-2 | 28   |
| 3    |    |   | Propane, 2-methyl-2-(1-methylethoxy)- | 116 | C7H16O   | 017348-59-3 | 28   |
| 4    |    |   | Acetic acid, cyano-, 1,1-dimethyl-    | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 5    |    |   | 2,3-Butanedione, monooxime            | 101 | C4H7NO2  | 000057-71-6 | 9    |



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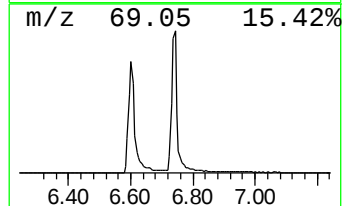
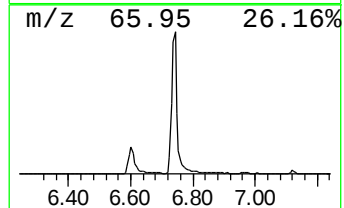
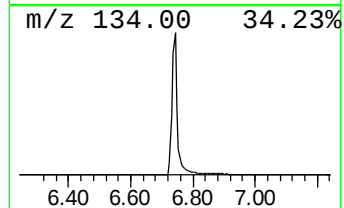
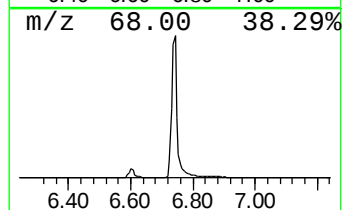
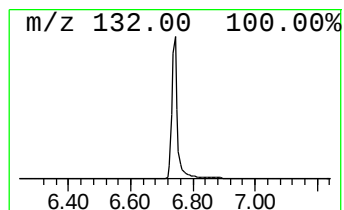
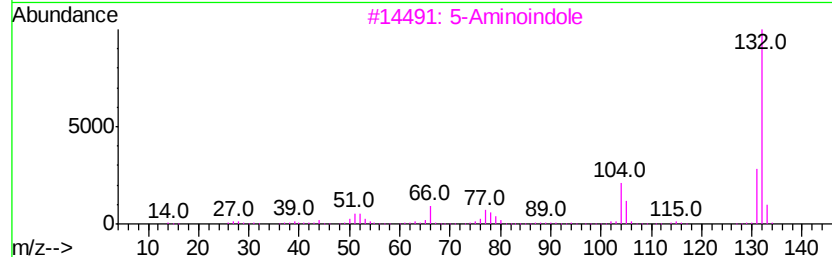
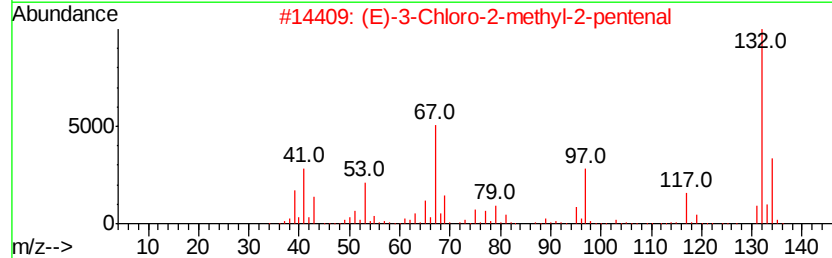
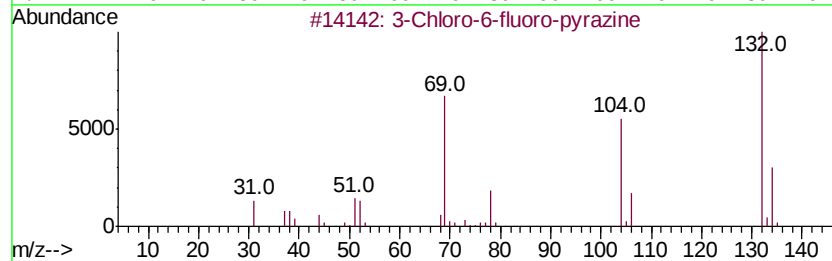
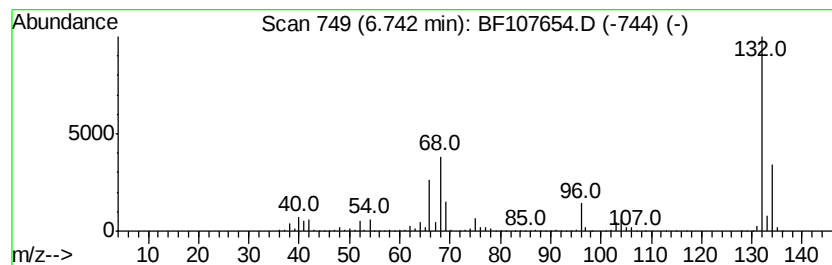
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.74 | 64.28 ng | 5189680 | 1,4-Dichlorobenzene-d4 | 6.97 |

| 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  | 16   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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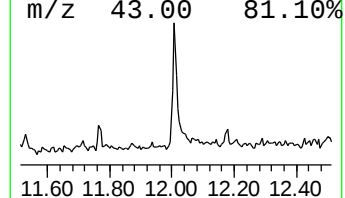
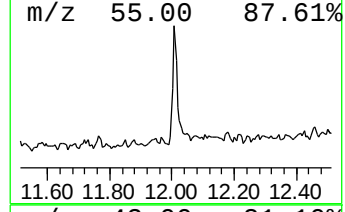
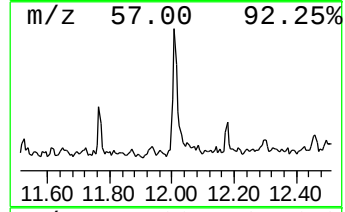
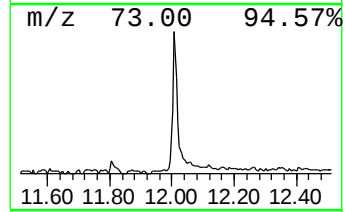
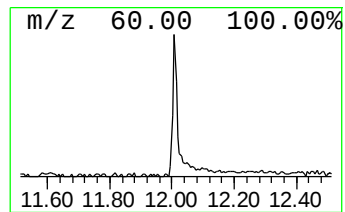
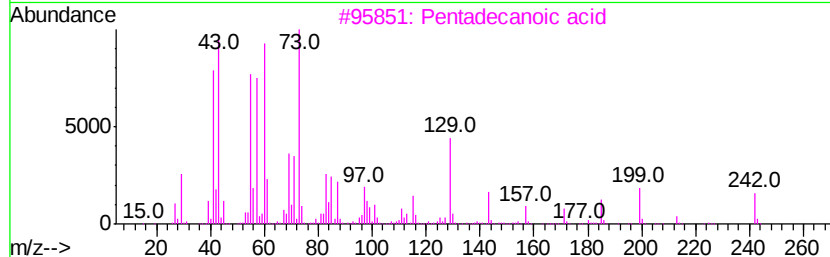
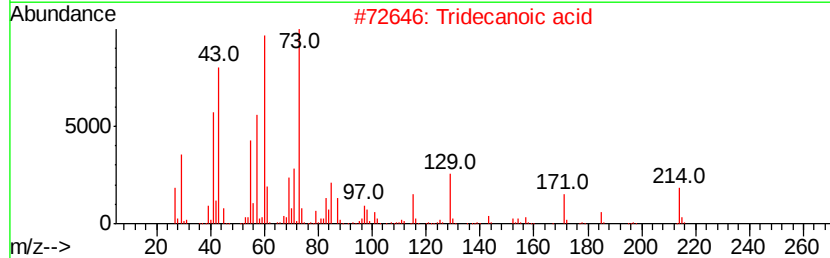
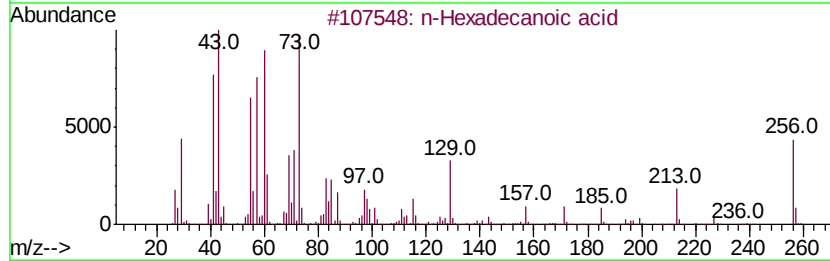
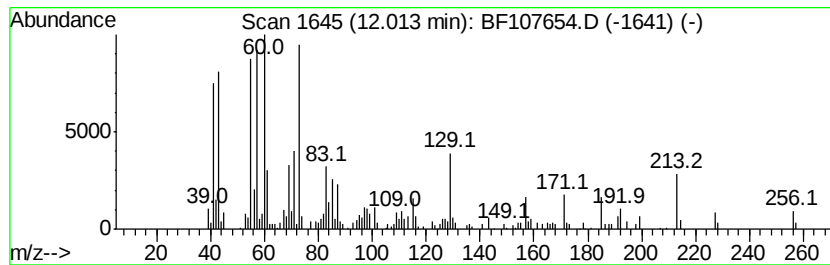
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.      | EstConc             | Area   | Relative to ISTD |             | R.T.  |
|-----------|---------------------|--------|------------------|-------------|-------|
| 12.01     | 2.87 ng             | 301271 | Phenanthrene-d10 |             | 11.50 |
| Hit# of 5 | Tentative ID        | MW     | MolForm          | CAS#        | Qual  |
| 1         | n-Hexadecanoic acid | 256    | C16H32O2         | 000057-10-3 | 90    |
| 2         | Tridecanoic acid    | 214    | C13H26O2         | 000638-53-9 | 74    |
| 3         | Pentadecanoic acid  | 242    | C15H30O2         | 001002-84-2 | 68    |
| 4         | Tetradecanoic acid  | 228    | C14H28O2         | 000544-63-8 | 64    |
| 5         | Dodecanoic acid     | 200    | C12H24O2         | 000143-07-7 | 64    |



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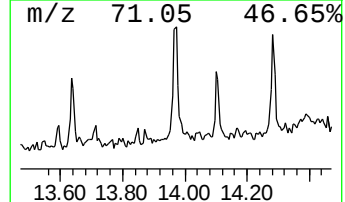
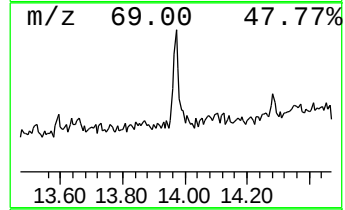
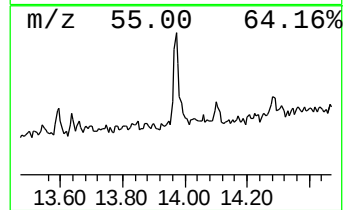
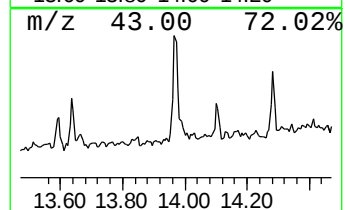
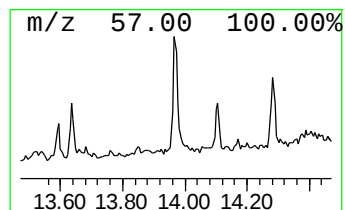
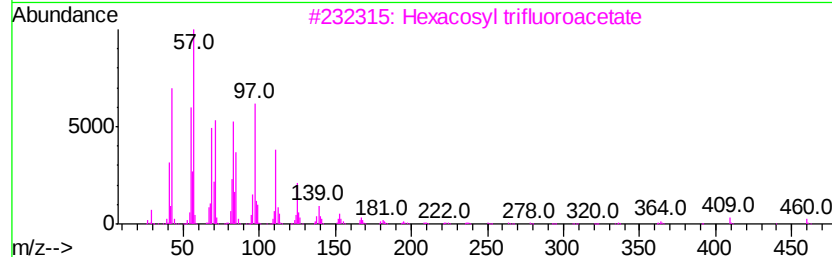
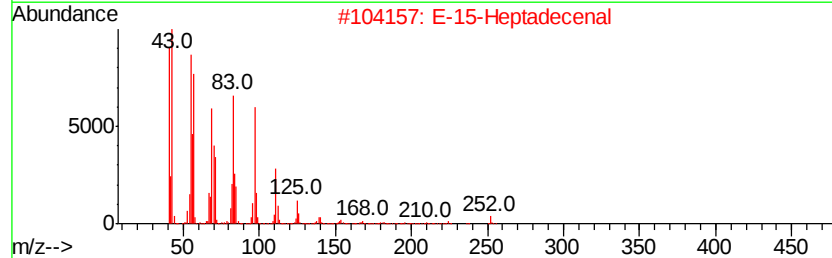
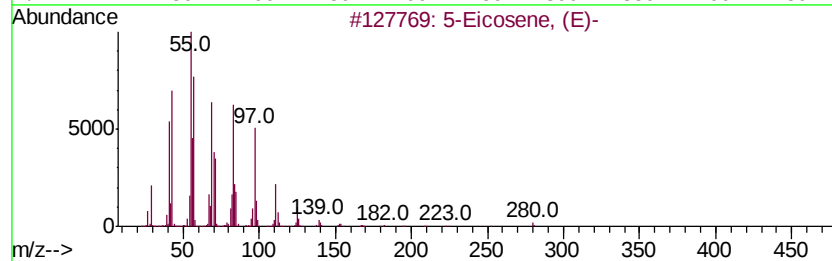
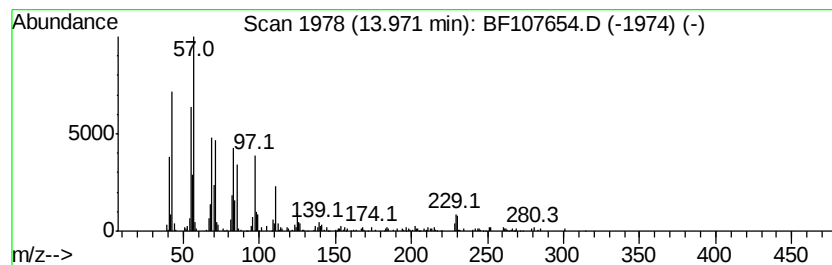
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.97 | 3.01 ng | 254620 | Chrysene-d12     | 14.15 |

| Hit# of | 5 | Tentative ID                  | MW  | MolForm    | CAS#         | Qual |
|---------|---|-------------------------------|-----|------------|--------------|------|
| 1       |   | 5-Eicosene, (E)-              | 280 | C20H40     | 074685-30-6  | 96   |
| 2       |   | E-15-Heptadecenal             | 252 | C17H32O    | 1000130-97-9 | 93   |
| 3       |   | Hexacosyl trifluoroacetate    | 478 | C28H53F3O2 | 1000351-75-0 | 91   |
| 4       |   | Ethanol, 2-(tetradecyloxy)-   | 258 | C16H34O2   | 002136-70-1  | 91   |
| 5       |   | Triacetyl heptafluorobutyrate | 634 | C34H61F7O2 | 1000351-83-2 | 91   |



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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... | 5.21  | 10.6    | ng    | 858072   | 1                     | 6.97  | 1614640 | 20.0 |
| unknown6.74          | 6.74  | 64.3    | ng    | 5189680  | 1                     | 6.97  | 1614640 | 20.0 |
| n-Hexadecanoic acid  | 12.01 | 2.9     | ng    | 301271   | 4                     | 11.50 | 2102710 | 20.0 |
| 5-Eicosene, (E)-     | 13.97 | 3.0     | ng    | 254620   | 5                     | 14.15 | 1690880 | 20.0 |