

Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
 Data File : BF098597.D  
 Acq On : 18 Sep 2017 12:55  
 Operator : SJ/JU  
 Sample : I5229-11  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 UT5400S21

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-BF091117.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         | 2.963       | 146           | 149         | 164          | rBV      | 90959          | 204124        | 4.39%           | 0.441%        |
| 2         | 4.122       | 340           | 346         | 354          | rBV2     | 30549          | 49611         | 1.07%           | 0.107%        |
| 3         | 4.822       | 461           | 465         | 476          | rBV      | 257373         | 402262        | 8.65%           | 0.870%        |
| 4         | 5.246       | 533           | 537         | 559          | rBV      | 3468215        | 3707719       | 79.72%          | 8.018%        |
| 5         | 6.293       | 710           | 715         | 718          | rBV      | 3451361        | 3830612       | 82.36%          | 8.284%        |
| 6         | 6.410       | 730           | 735         | 738          | rBV      | 4348256        | 3944665       | 84.82%          | 8.530%        |
| 7         | 6.634       | 769           | 773         | 776          | rBV      | 896047         | 813947        | 17.50%          | 1.760%        |
| 8         | 6.787       | 795           | 799         | 803          | rBV      | 3005736        | 2774082       | 59.65%          | 5.999%        |
| 9         | 6.828       | 804           | 806         | 812          | rVB      | 41913          | 48200         | 1.04%           | 0.104%        |
| 10        | 7.204       | 865           | 870         | 873          | rBV      | 2477642        | 2579235       | 55.46%          | 5.578%        |
| 11        | 7.334       | 886           | 892         | 898          | rVB      | 58829          | 70802         | 1.52%           | 0.153%        |
| 12        | 7.828       | 971           | 976         | 982          | rBV      | 90930          | 89229         | 1.92%           | 0.193%        |
| 13        | 7.916       | 987           | 991         | 994          | rBV      | 1264309        | 1083899       | 23.31%          | 2.344%        |
| 14        | 8.992       | 1168          | 1174        | 1177         | rBV      | 4382284        | 4650904       | 100.00%         | 10.058%       |
| 15        | 9.392       | 1237          | 1242        | 1245         | rBV      | 866604         | 714593        | 15.36%          | 1.545%        |
| 16        | 9.663       | 1280          | 1288        | 1292         | rBV      | 1362394        | 1338342       | 28.78%          | 2.894%        |
| 17        | 10.098      | 1359          | 1362        | 1366         | rVB      | 76850          | 68649         | 1.48%           | 0.148%        |
| 18        | 10.457      | 1417          | 1423        | 1427         | rBV      | 2677823        | 2883943       | 62.01%          | 6.236%        |
| 19        | 10.575      | 1440          | 1443        | 1447         | rBV      | 108164         | 108549        | 2.33%           | 0.235%        |
| 20        | 11.016      | 1515          | 1518        | 1521         | rBV2     | 63043          | 59782         | 1.29%           | 0.129%        |
| 21        | 11.145      | 1536          | 1540        | 1544         | rBV      | 1485470        | 1413372       | 30.39%          | 3.056%        |
| 22        | 11.180      | 1544          | 1546        | 1548         | rVB      | 67193          | 49638         | 1.07%           | 0.107%        |
| 23        | 11.375      | 1573          | 1579        | 1585         | rBV4     | 81245          | 112086        | 2.41%           | 0.242%        |
| 24        | 11.545      | 1604          | 1608        | 1612         | rVB      | 76780          | 69773         | 1.50%           | 0.151%        |
| 25        | 11.692      | 1628          | 1633        | 1639         | rBV2     | 288546         | 334106        | 7.18%           | 0.723%        |
| 26        | 11.851      | 1656          | 1660        | 1666         | rVB4     | 36186          | 52612         | 1.13%           | 0.114%        |
| 27        | 12.251      | 1723          | 1728        | 1732         | rVB4     | 66875          | 81438         | 1.75%           | 0.176%        |
| 28        | 12.357      | 1740          | 1746        | 1749         | rBV4     | 34810          | 63238         | 1.36%           | 0.137%        |
| 29        | 12.469      | 1760          | 1765        | 1769         | rBV      | 74503          | 87467         | 1.88%           | 0.189%        |
| 30        | 12.733      | 1805          | 1810        | 1813         | rBV      | 4084806        | 4147544       | 89.18%          | 8.969%        |
| 31        | 12.939      | 1840          | 1845        | 1847         | rBV4     | 49572          | 60173         | 1.29%           | 0.130%        |
| 32        | 13.627      | 1958          | 1962        | 1969         | rVB      | 377989         | 442431        | 9.51%           | 0.957%        |
| 33        | 13.780      | 1984          | 1988        | 1994         | rVB      | 1148473        | 983013        | 21.14%          | 2.126%        |
| 34        | 13.874      | 1998          | 2004        | 2009         | rBV10    | 31266          | 84706         | 1.82%           | 0.183%        |

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ALS Vial : 3 Sample Multiplier: 1

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BNA\_F  
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-BF091117.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |       |         |         |        |        |
|----|--------|------|------|------|-------|---------|---------|--------|--------|
| 35 | 13.945 | 2012 | 2016 | 2023 | rVB3  | 46417   | 72297   | 1.55%  | 0.156% |
| 36 | 14.069 | 2034 | 2037 | 2042 | rVB2  | 138162  | 124587  | 2.68%  | 0.269% |
| 37 | 14.257 | 2064 | 2069 | 2075 | rBV   | 693741  | 826377  | 17.77% | 1.787% |
| 38 | 14.527 | 2112 | 2115 | 2124 | rBV2  | 292520  | 410456  | 8.83%  | 0.888% |
| 39 | 14.610 | 2126 | 2129 | 2133 | rVV   | 180667  | 176573  | 3.80%  | 0.382% |
| 40 | 14.674 | 2137 | 2140 | 2144 | rVB   | 308721  | 300343  | 6.46%  | 0.649% |
| 41 | 14.851 | 2166 | 2170 | 2180 | rBV   | 1920319 | 2400156 | 51.61% | 5.190% |
| 42 | 15.174 | 2220 | 2225 | 2231 | rBV   | 658397  | 801247  | 17.23% | 1.733% |
| 43 | 15.368 | 2254 | 2258 | 2263 | rBV   | 407895  | 504850  | 10.85% | 1.092% |
| 44 | 15.580 | 2288 | 2294 | 2298 | rBV   | 500387  | 700810  | 15.07% | 1.515% |
| 45 | 15.621 | 2298 | 2301 | 2308 | rVB   | 84693   | 141070  | 3.03%  | 0.305% |
| 46 | 16.280 | 2407 | 2413 | 2423 | rBV2  | 303436  | 521955  | 11.22% | 1.129% |
| 47 | 16.486 | 2442 | 2448 | 2452 | rBV8  | 29200   | 64929   | 1.40%  | 0.140% |
| 48 | 16.545 | 2453 | 2458 | 2464 | rVB2  | 61847   | 120957  | 2.60%  | 0.262% |
| 49 | 16.621 | 2465 | 2471 | 2479 | rBV5  | 79865   | 172339  | 3.71%  | 0.373% |
| 50 | 16.974 | 2524 | 2531 | 2541 | rBV4  | 177134  | 398265  | 8.56%  | 0.861% |
| 51 | 17.162 | 2558 | 2563 | 2569 | rVB6  | 50213   | 91392   | 1.97%  | 0.198% |
| 52 | 17.680 | 2645 | 2651 | 2666 | rBV6  | 100162  | 328944  | 7.07%  | 0.711% |
| 53 | 17.815 | 2668 | 2674 | 2682 | rBV4  | 125340  | 324172  | 6.97%  | 0.701% |
| 54 | 18.268 | 2744 | 2751 | 2765 | rVB9  | 82916   | 281111  | 6.04%  | 0.608% |
| 55 | 18.804 | 2838 | 2842 | 2852 | rVB10 | 30972   | 75447   | 1.62%  | 0.163% |

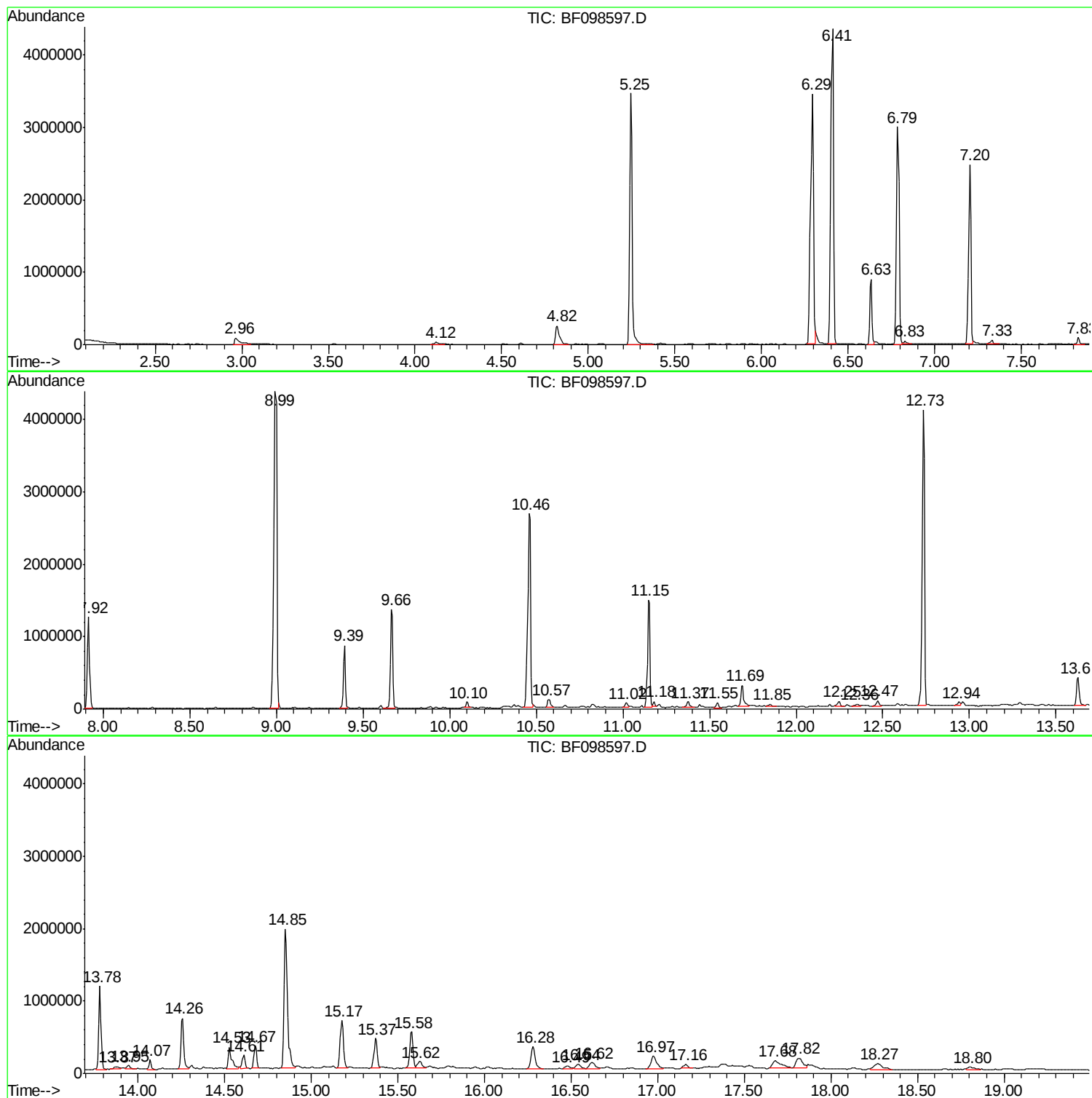
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

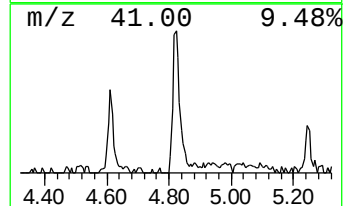
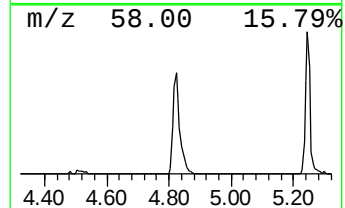
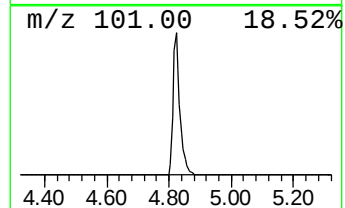
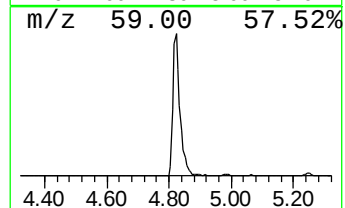
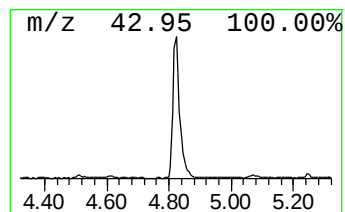
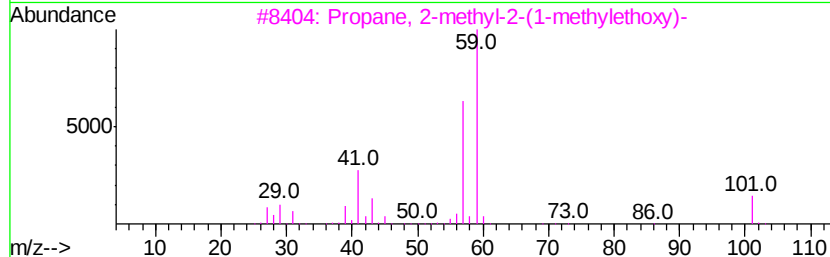
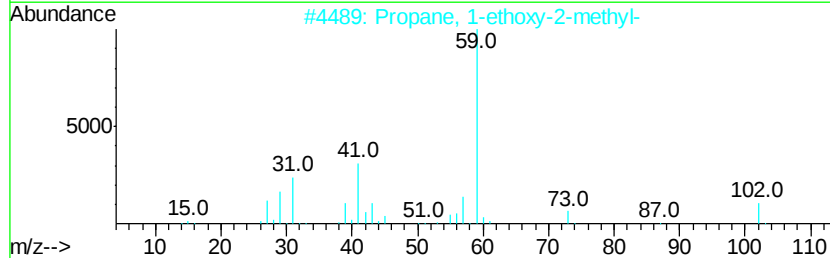
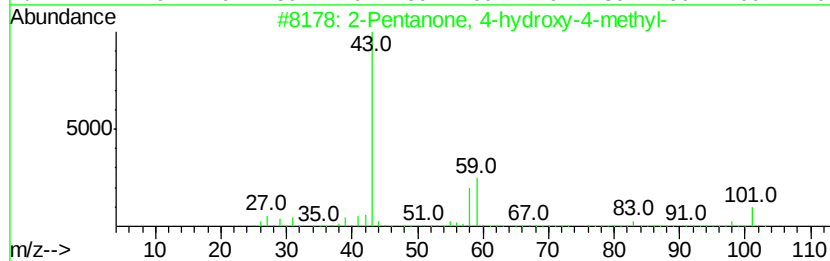
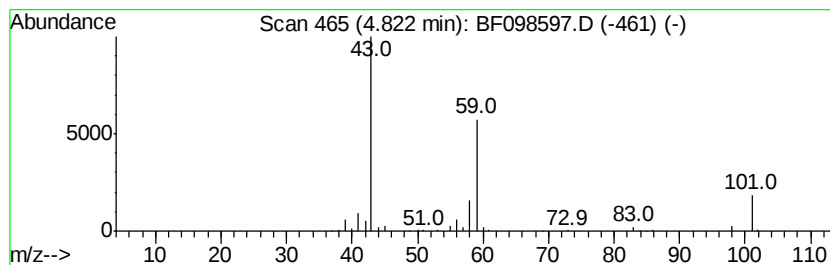
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.82 | 9.88 ng | 402262 | 1,4-Dichlorobenzene-d4 | 6.63 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2 | 000123-42-2 | 64   |
| 2    |    |   | Propane, 1-ethoxy-2-methyl-          | 102 | C6H14O  | 000627-02-1 | 43   |
| 3    |    |   | Propane, 2-methyl-2-(1-methylethyl)- | 116 | C7H16O  | 017348-59-3 | 33   |
| 4    |    |   | Acetone                              | 58  | C3H6O   | 000067-64-1 | 12   |
| 5    |    |   | Guanidine                            | 59  | CH5N3   | 000113-00-8 | 9    |



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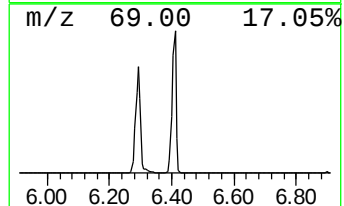
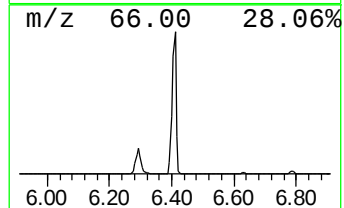
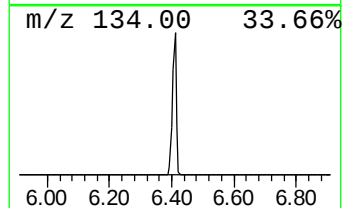
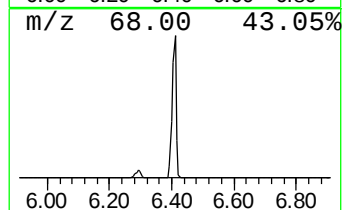
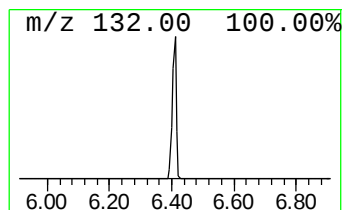
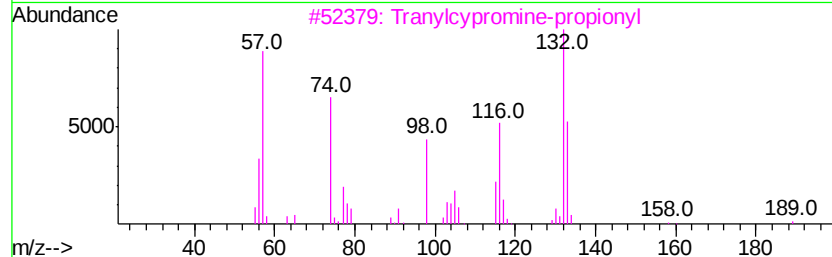
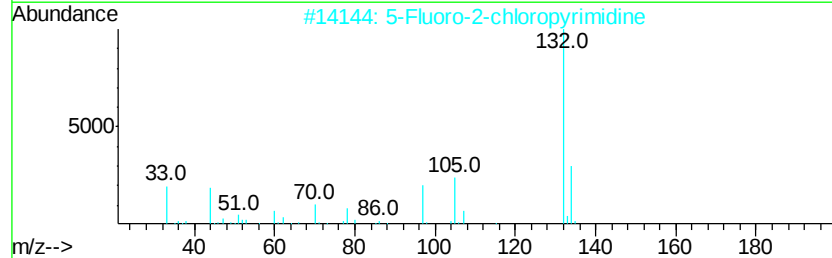
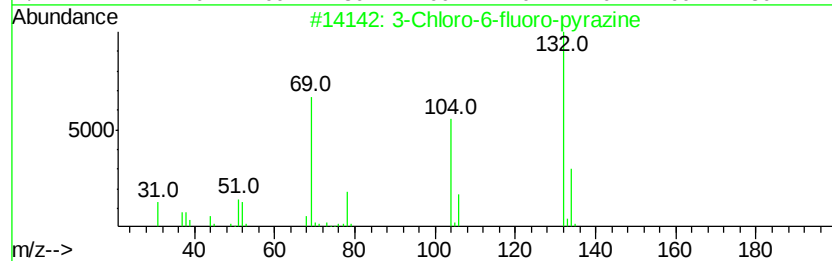
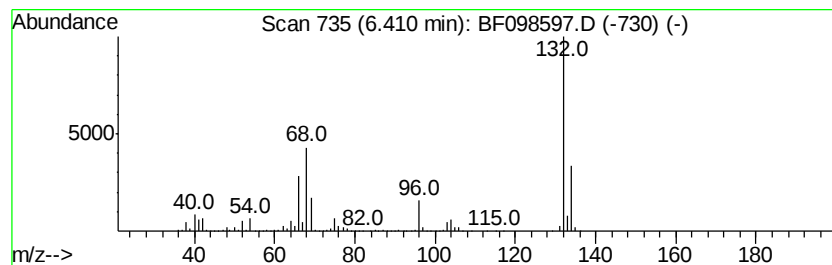
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 unknown6.41 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.41 | 96.93 ng | 3944670 | 1,4-Dichlorobenzene-d4 | 6.63 |

| 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  | 16   |
| 3    |    | Tranvlcyproline-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | 4-Chloro-2-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-00-5  | 9    |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

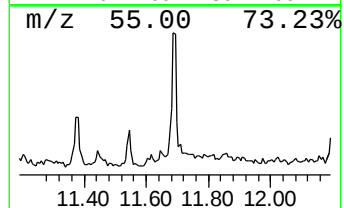
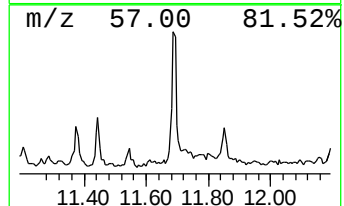
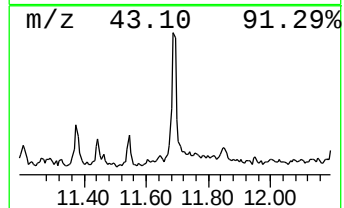
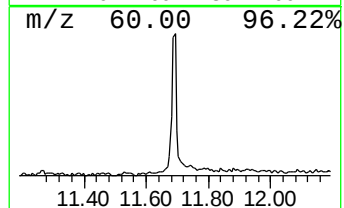
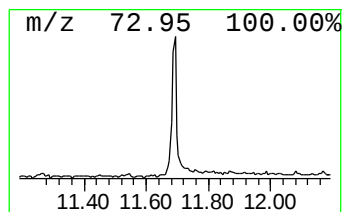
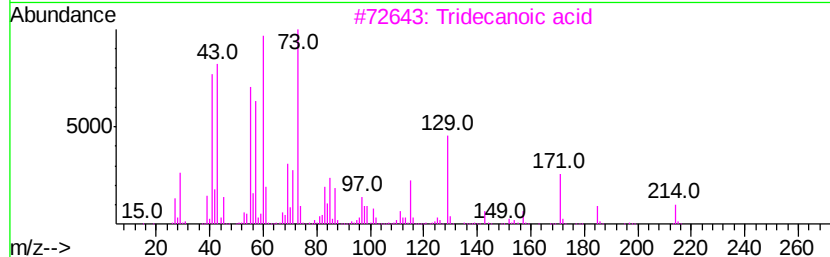
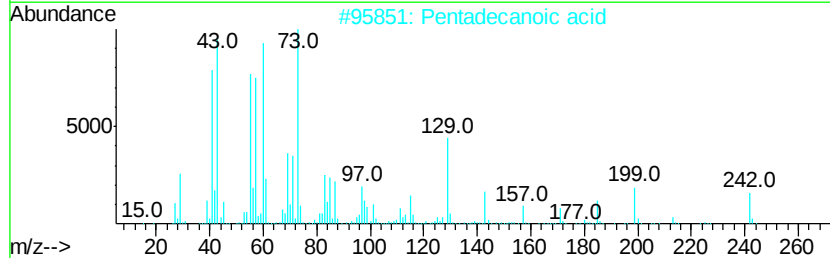
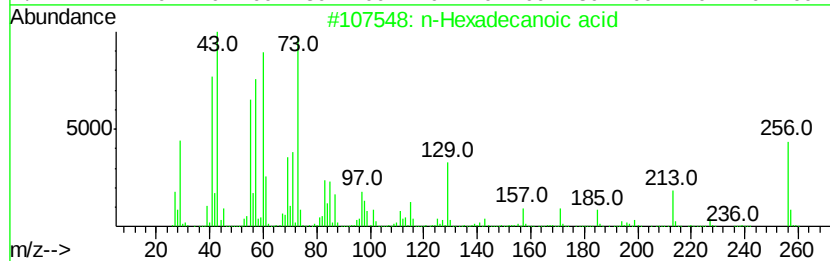
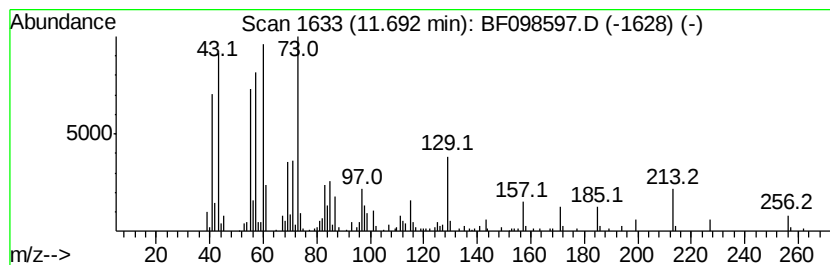
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 n-Hexadecanoic acid Concentration Rank 17

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.69 | 4.73 ng | 334106 | Phenanthrene-d10 | 11.15 |

| Hit# of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|---------|---|---------------------|-----|----------|-------------|------|
| 1       |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2       |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 91   |
| 3       |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 89   |
| 4       |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |
| 5       |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 62   |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

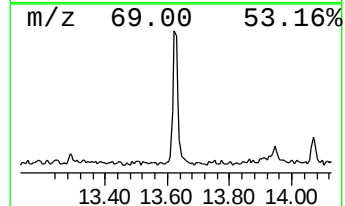
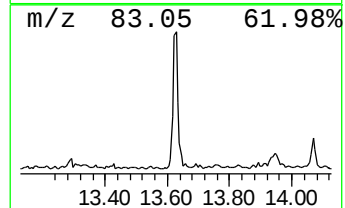
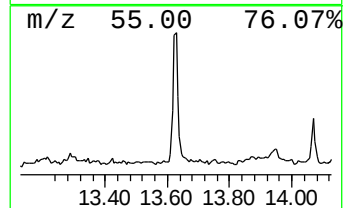
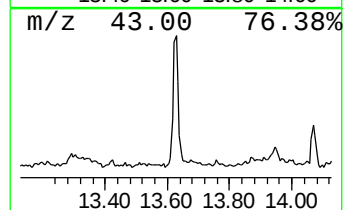
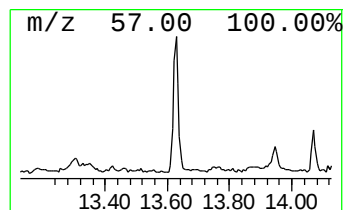
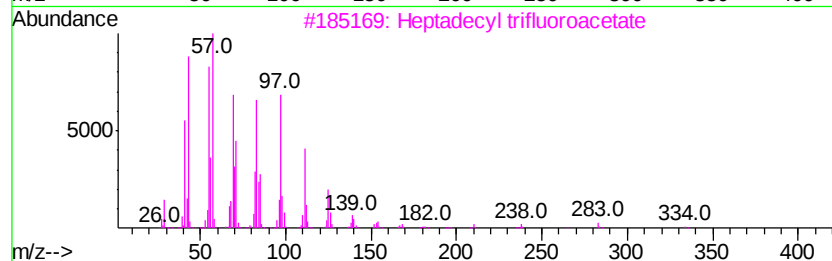
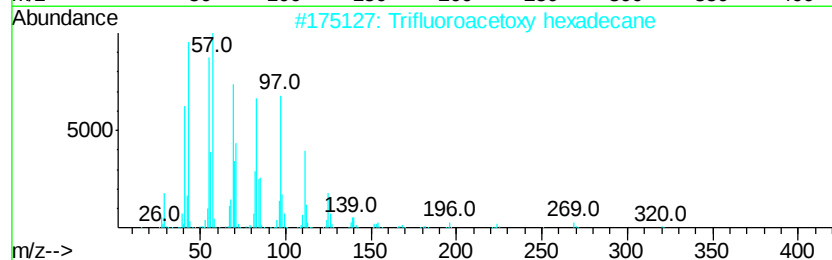
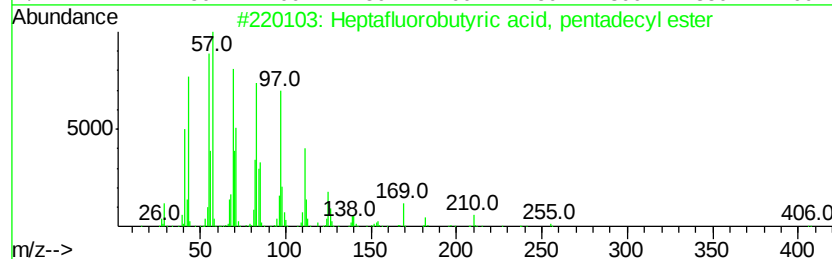
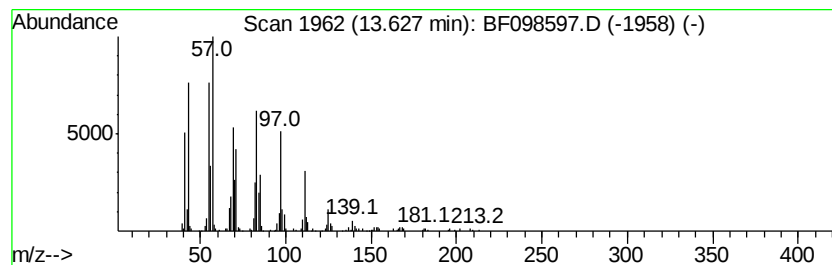
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TIC Integration Parameters: LSCINT.P

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Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 11

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.63 | 9.00 ng | 442431 | Chrysene-d12     | 13.78 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5  | 91   |
| 2    |    | Trifluoroacetoxy hexadecane         | 338 | C18H33F3O2 | 006222-03-3  | 91   |
| 3    |    | Heptadecyl trifluoroacetate         | 352 | C19H35F3O2 | 1000351-87-0 | 91   |
| 4    |    | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1  | 91   |
| 5    |    | Octadecyl trifluoroacetate          | 366 | C20H37F3O2 | 079392-43-1  | 91   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

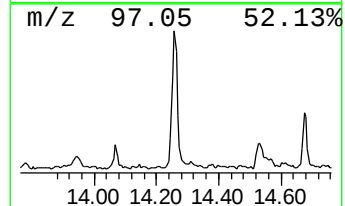
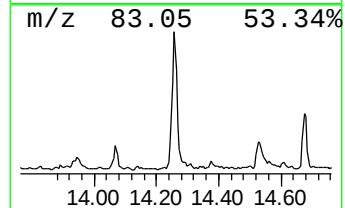
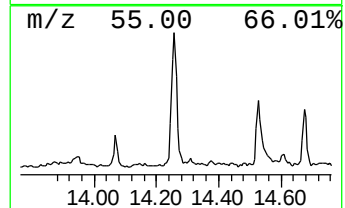
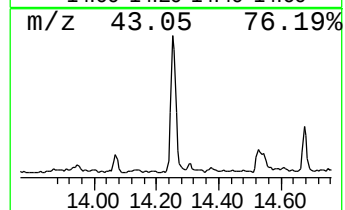
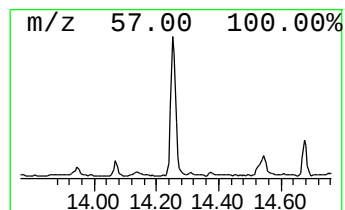
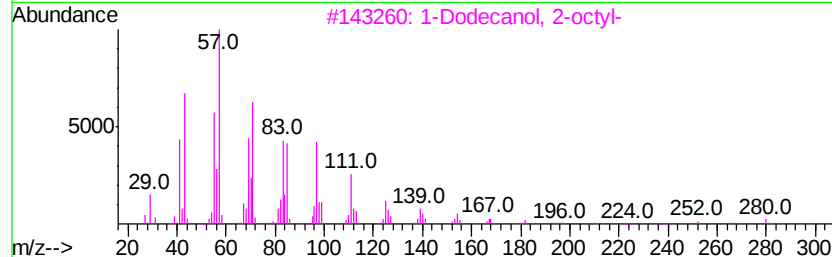
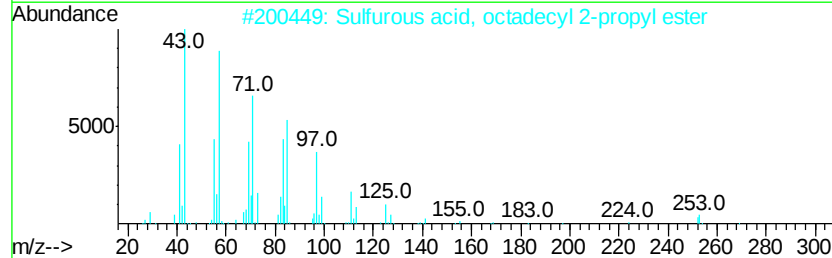
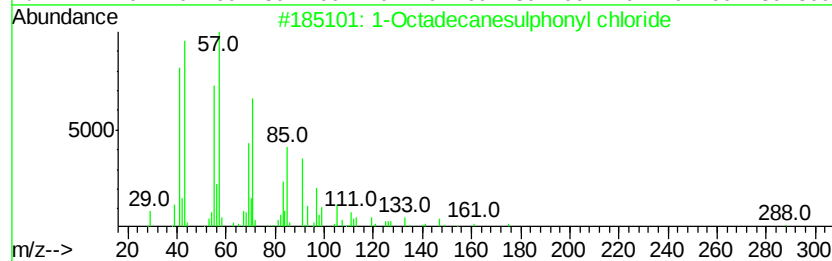
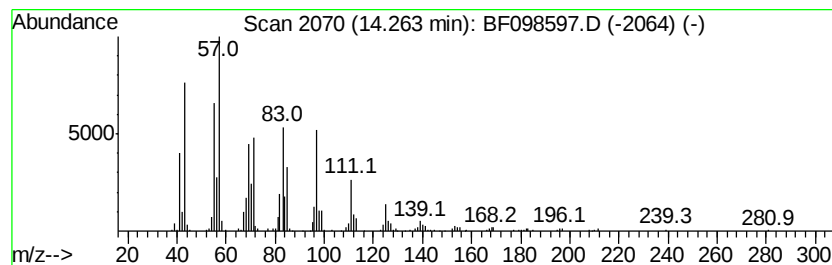
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 7 1-Octadecanesulphonyl chloride Concentration Rank 5

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 14.26 | 16.81 ng | 826377 | Chrysene-d12     | 13.78 |

| Hit# of | 5 | Tentative ID                          | MW  | MolForm     | CAS#         | Qual |
|---------|---|---------------------------------------|-----|-------------|--------------|------|
| 1       |   | 1-Octadecanesulphonyl chloride        | 352 | C18H37ClO2S | 1000342-70-4 | 91   |
| 2       |   | Sulfurous acid, octadecyl 2-propyl... | 376 | C21H44O3S   | 1000309-12-7 | 90   |
| 3       |   | 1-Dodecanol, 2-octyl-                 | 298 | C20H42O     | 005333-42-6  | 83   |
| 4       |   | Hexacosane                            | 366 | C26H54      | 000630-01-3  | 68   |
| 5       |   | Heneicosane                           | 296 | C21H44      | 000629-94-7  | 68   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

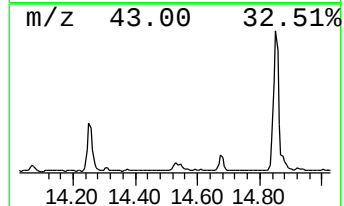
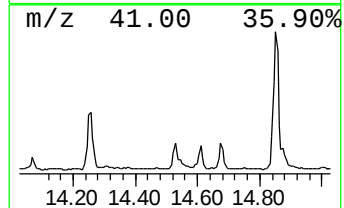
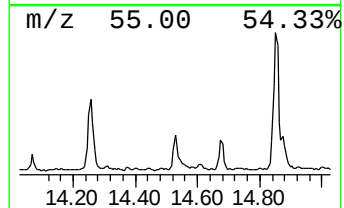
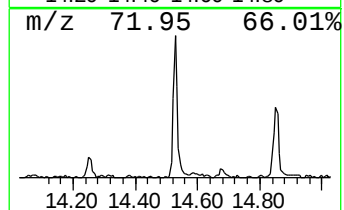
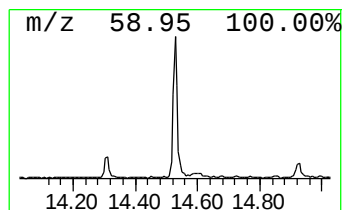
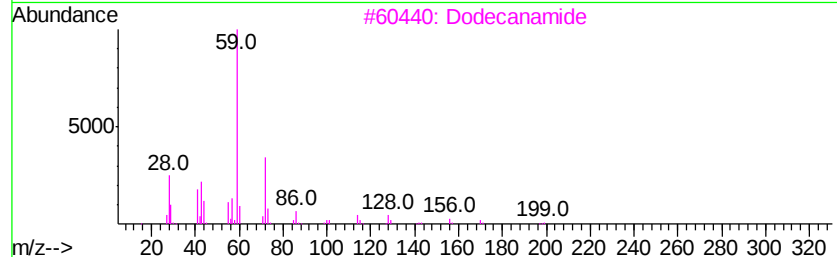
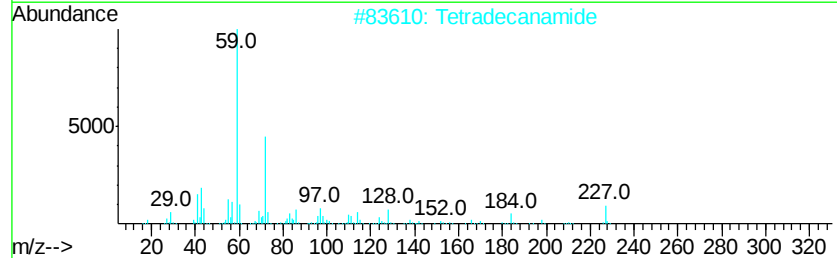
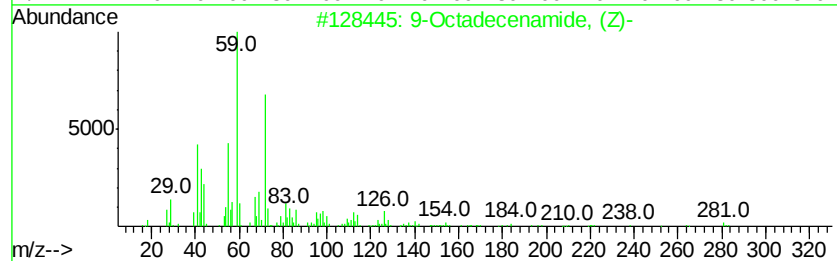
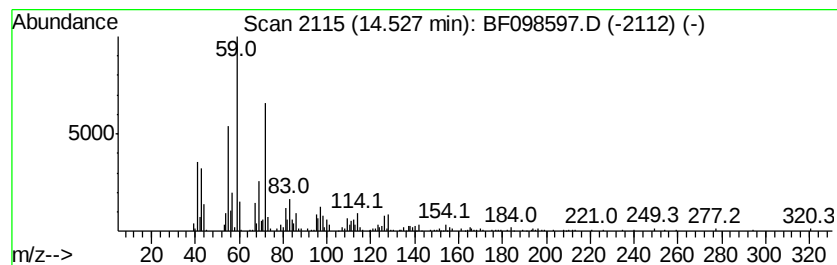
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 8

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 14.53 | 10.25 ng | 410456 | Perylene-d12     | 15.17 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|-------------------------------------|-----|------------|-------------|------|
| 1    | 5  | 9-Octadecenamide, (Z)-              | 281 | C18H35NO   | 000301-02-0 | 86   |
| 2    |    | Tetradecanamide                     | 227 | C14H29NO   | 000638-58-4 | 83   |
| 3    |    | Dodecanamide                        | 199 | C12H25NO   | 001120-16-7 | 68   |
| 4    |    | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FN03 | 061338-98-5 | 59   |
| 5    |    | Octadecanamide                      | 283 | C18H37NO   | 000124-26-5 | 59   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

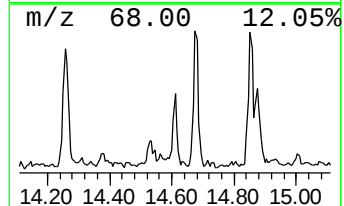
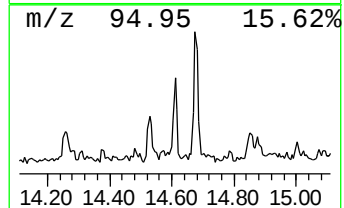
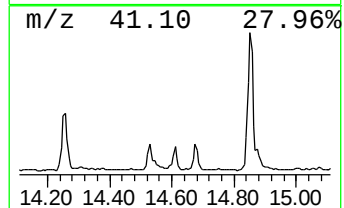
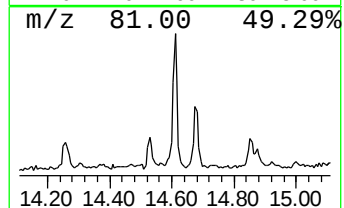
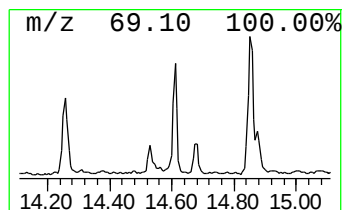
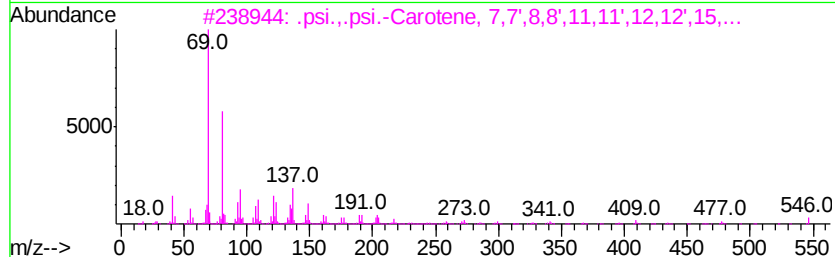
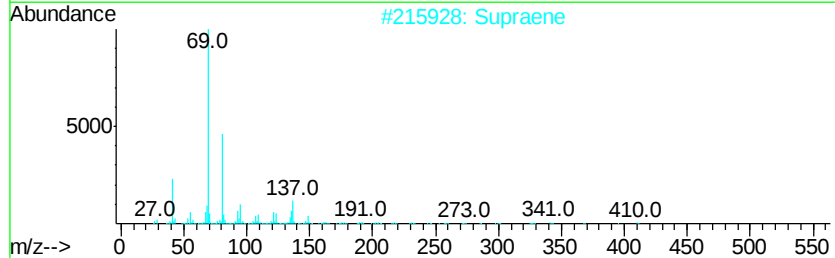
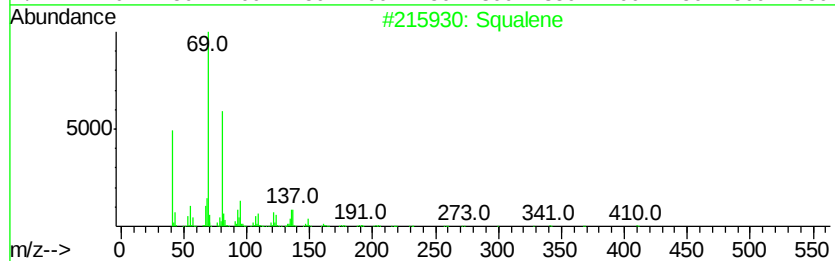
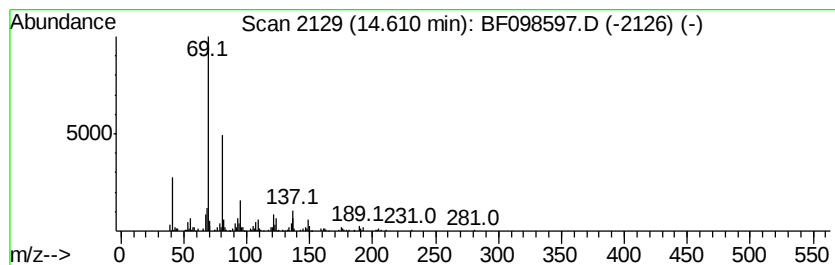
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 9 Squalene Concentration Rank 18

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.61 | 4.41 ng | 176573 | Perylene-d12     | 15.17 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | Squalene                            | 410 | C30H50     | 000111-02-4  | 91   |
| 2    |    | Supraene                            | 410 | C30H50     | 007683-64-9  | 83   |
| 3    |    | .psi.,.psi.-Carotene, 7,7',8,8',... | 547 | C40H66     | 000502-62-5  | 78   |
| 4    |    | (.+/-)-Lavandulol, pentafluorop...  | 300 | C13H17F5O2 | 1000352-63-1 | 72   |
| 5    |    | 1,5,9-Decatriene, 2,3,5,8-tetram... | 192 | C14H24     | 230646-72-7  | 72   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

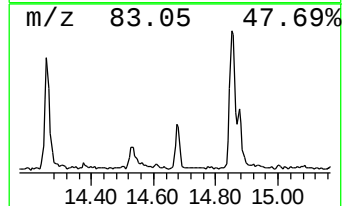
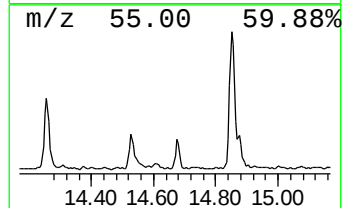
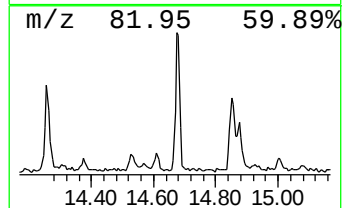
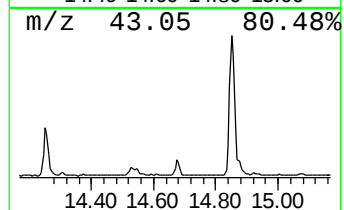
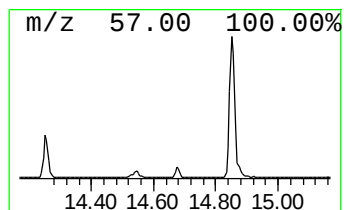
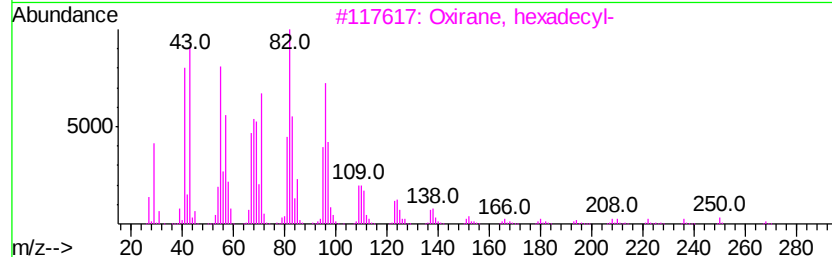
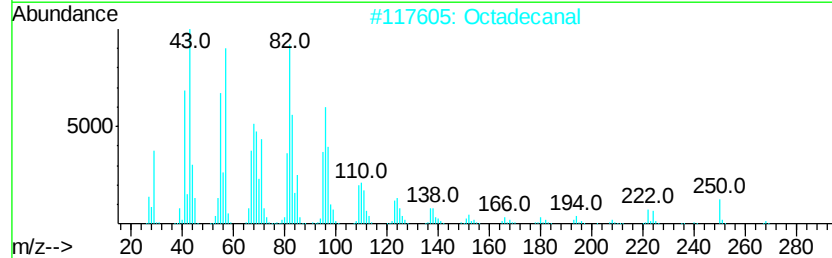
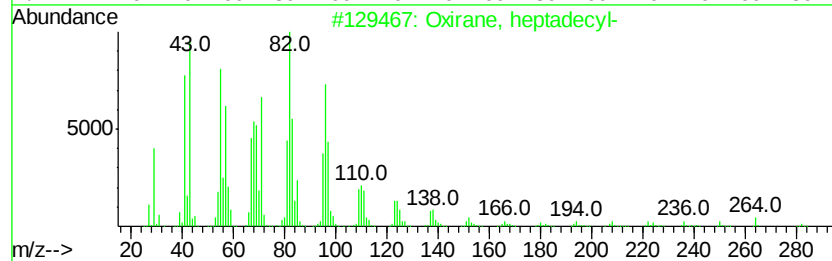
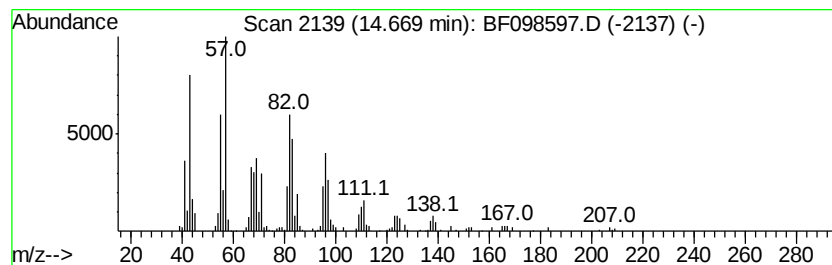
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 10 Oxirane, heptadecyl- Concentration Rank 14

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.67 | 7.50 ng | 300343 | Perylene-d12     | 15.17 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------|-----|---------|-------------|------|
| 1    |    |   | Oxirane, heptadecyl- | 282 | C19H38O | 067860-04-2 | 91   |
| 2    |    |   | Octadecanal          | 268 | C18H36O | 000638-66-4 | 91   |
| 3    |    |   | Oxirane, hexadecyl-  | 268 | C18H36O | 007390-81-0 | 91   |
| 4    |    |   | Cycloheptadecanol    | 254 | C17H34O | 004429-77-0 | 76   |
| 5    |    |   | 1,19-Eicosadiene     | 278 | C20H38  | 014811-95-1 | 76   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

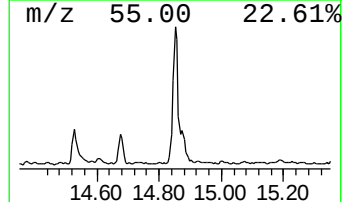
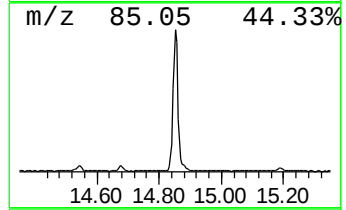
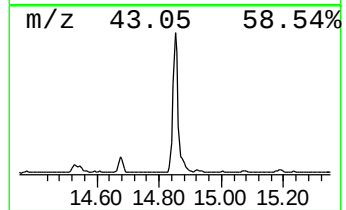
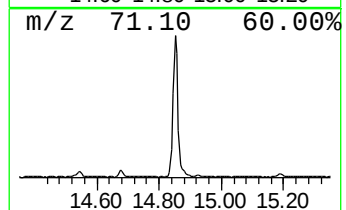
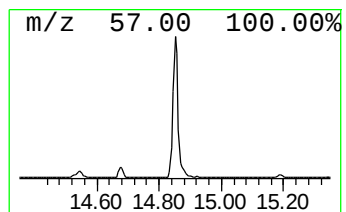
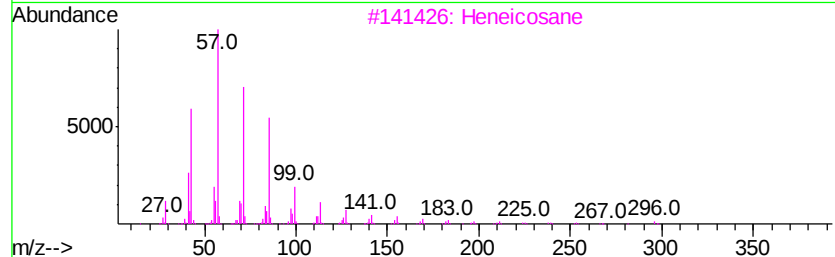
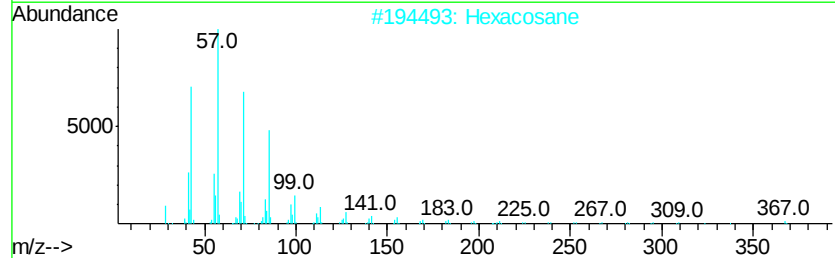
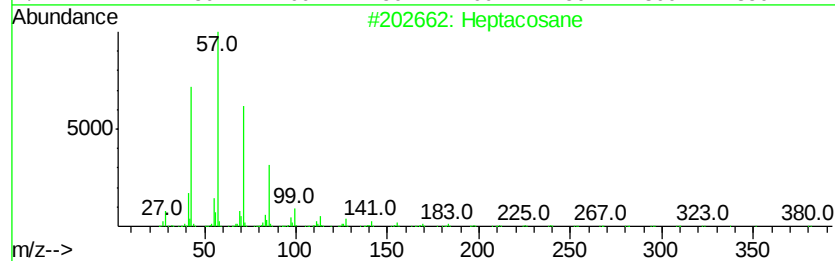
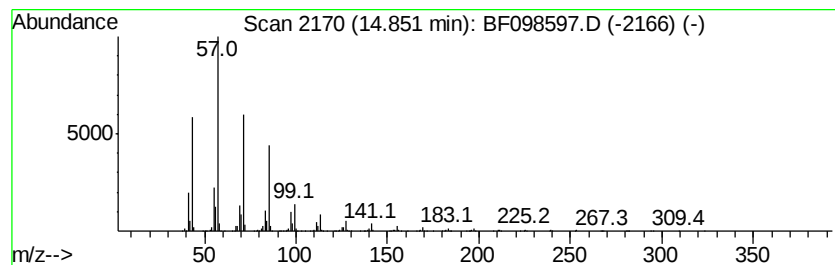
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 11 Heptacosane Concentration Rank 3

| R.T.  | EstConc  | Area    | Relative to ISTD | R.T.  |
|-------|----------|---------|------------------|-------|
| 14.85 | 59.91 ng | 2400160 | Perylene-d12     | 15.17 |

| Hit# | of | Tentative ID       | MW  | MolForm | CAS#         | Qual |
|------|----|--------------------|-----|---------|--------------|------|
| 1    | 5  | Heptacosane        | 380 | C27H56  | 000593-49-7  | 91   |
| 2    |    | Hexacosane         | 366 | C26H54  | 000630-01-3  | 91   |
| 3    |    | Heneicosane        | 296 | C21H44  | 000629-94-7  | 91   |
| 4    |    | Octacosane         | 394 | C28H58  | 000630-02-4  | 91   |
| 5    |    | 2-methyloctacosane | 408 | C29H60  | 1000376-72-8 | 90   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

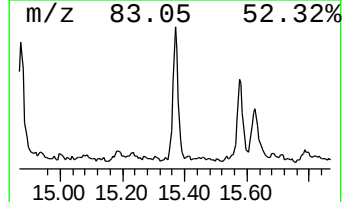
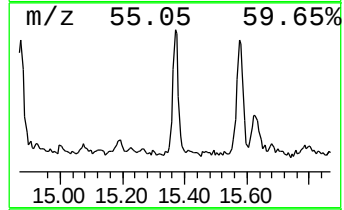
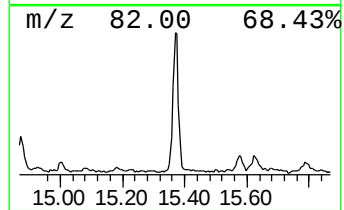
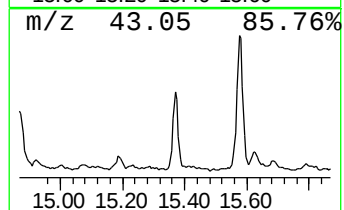
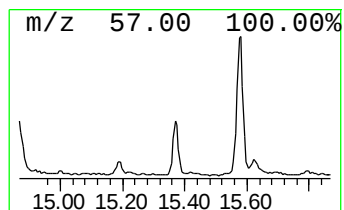
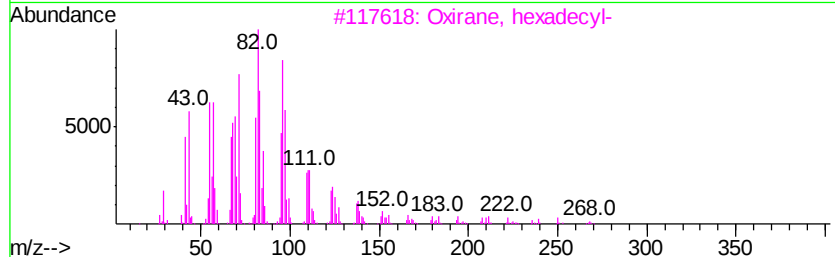
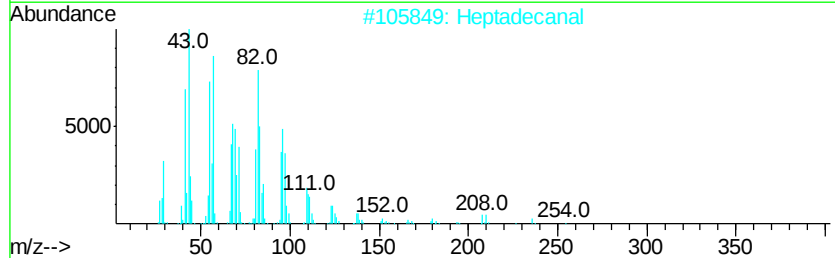
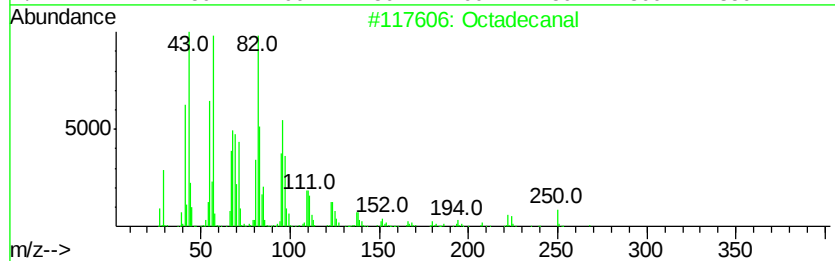
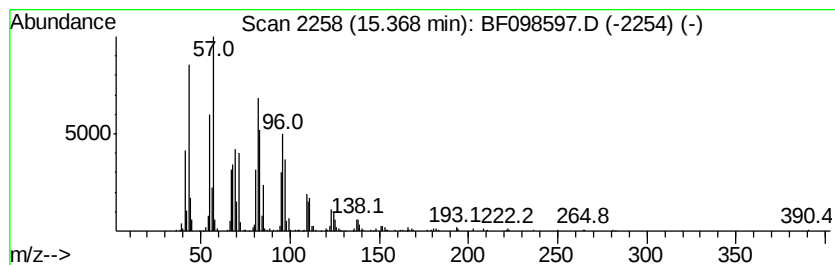
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 12 Octadecanal Concentration Rank 7

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 15.37 | 12.60 ng | 504850 | Perylene-d12     | 15.17 |

| Hit# of 5 | Tentative ID              | MW  | MolForm  | CAS#         | Qual |
|-----------|---------------------------|-----|----------|--------------|------|
| 1         | Octadecanal               | 268 | C18H36O  | 000638-66-4  | 91   |
| 2         | Heptadecanal              | 254 | C17H34O  | 1000376-70-0 | 90   |
| 3         | Oxirane, hexadecyl-       | 268 | C18H36O  | 007390-81-0  | 90   |
| 4         | (Z)-14-Tricosenyl formate | 366 | C24H46O2 | 077899-10-6  | 89   |
| 5         | Oxirane, heptadecyl-      | 282 | C19H38O  | 067860-04-2  | 83   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

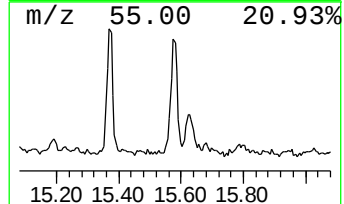
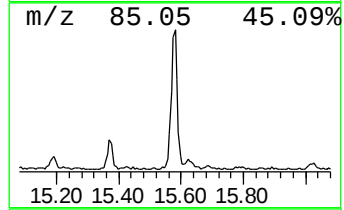
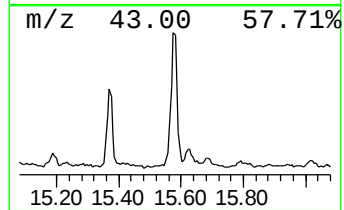
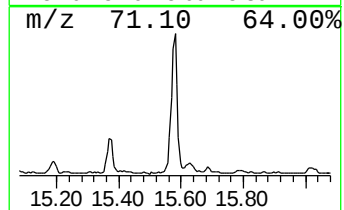
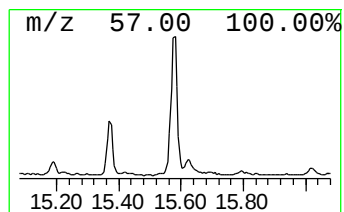
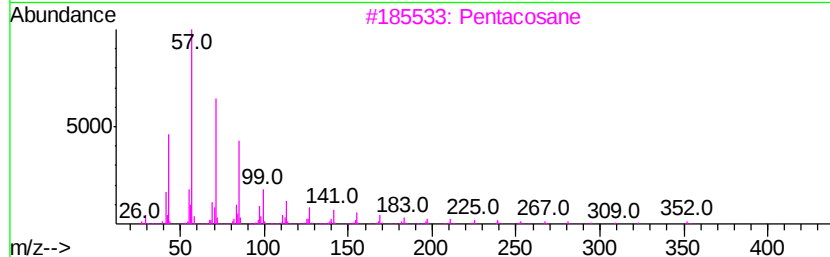
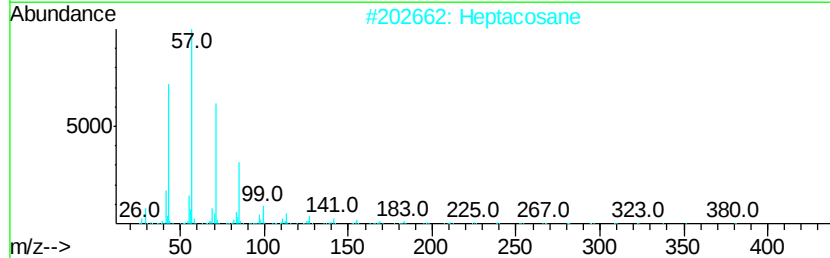
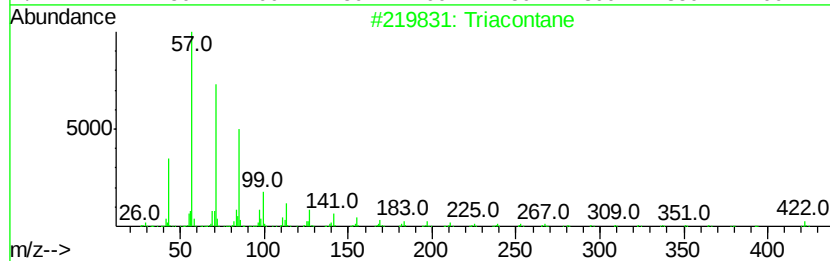
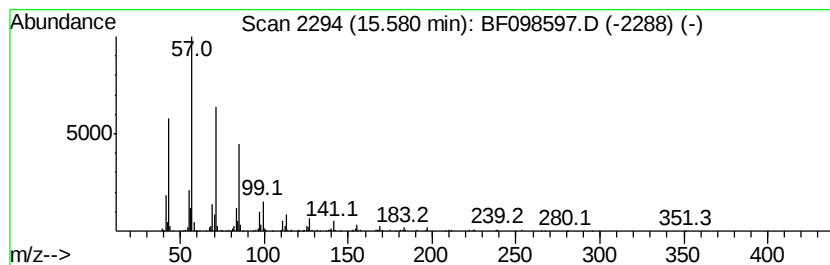
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TIC Integration Parameters: LSCINT.P

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Peak Number 13 Triacontane Concentration Rank 4

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 15.58 | 17.49 ng | 700810 | Perylene-d12     | 15.17 |

| Hit# | of | Tentative ID        | MW  | MolForm | CAS#        | Qual |
|------|----|---------------------|-----|---------|-------------|------|
| 1    | 5  | Triacontane         | 422 | C30H62  | 000638-68-6 | 91   |
| 2    |    | Heptacosane         | 380 | C27H56  | 000593-49-7 | 91   |
| 3    |    | Pentacosane         | 352 | C25H52  | 000629-99-2 | 91   |
| 4    |    | Docosane, 11-butyl- | 366 | C26H54  | 013475-76-8 | 91   |
| 5    |    | Heneicosane         | 296 | C21H44  | 000629-94-7 | 90   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
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Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

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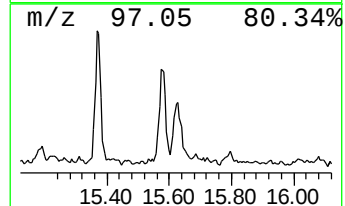
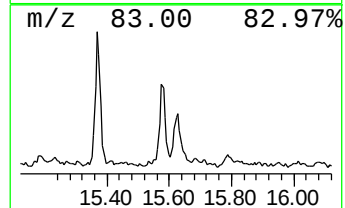
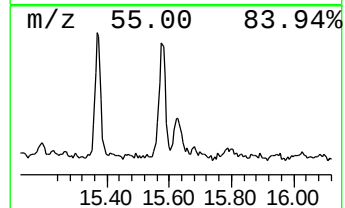
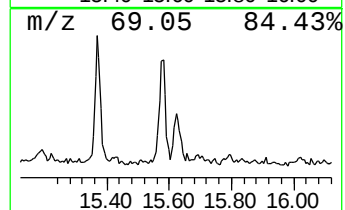
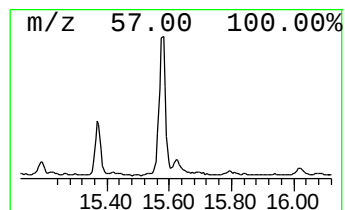
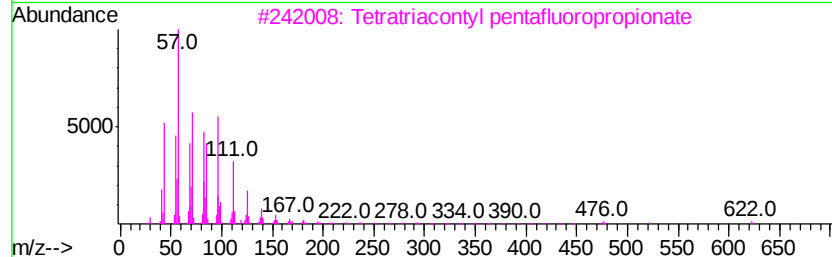
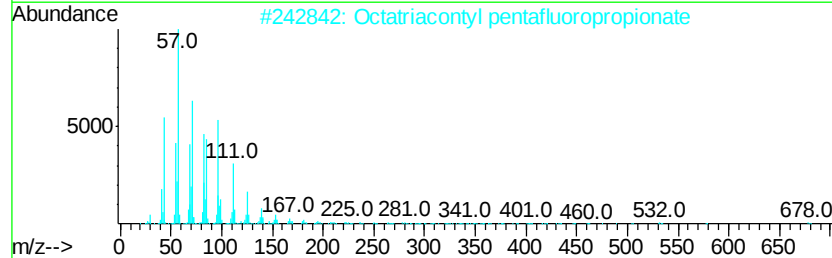
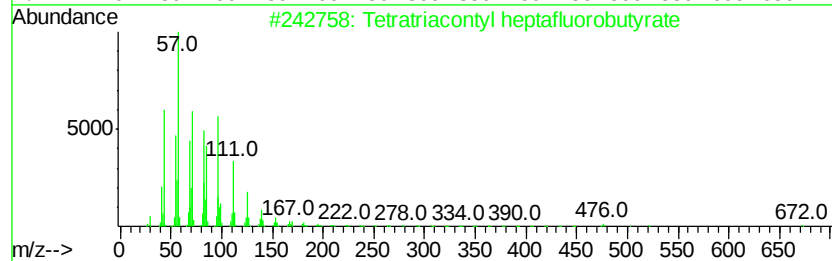
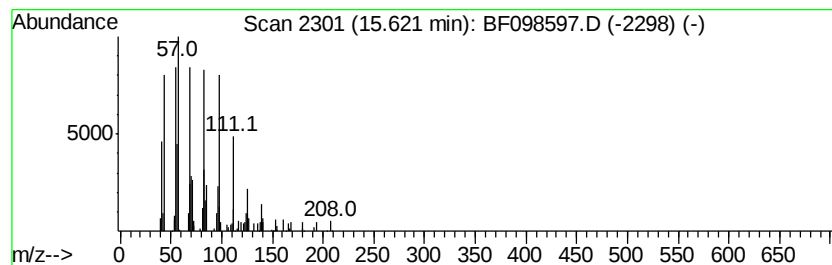
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TIC Integration Parameters: LSCINT.P

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Peak Number 14 Tetratriacontyl heptafluoro... Concentration Rank 20

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.62 | 3.52 ng | 141070 | Perylene-d12     | 15.17 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Tetratriacontyl heptafluorobutyrate | 691 | C38H69F7O2 | 1000351-84-1 | 64   |
| 2    |    |   | Octatriacontyl pentafluoropropio... | 697 | C41H77F5O2 | 1000351-89-1 | 64   |
| 3    |    |   | Tetratriacontyl pentafluoropropi... | 641 | C37H69F5O2 | 1000351-81-5 | 64   |
| 4    |    |   | Octacosyl trifluoroacetate          | 506 | C30H57F3O2 | 1000351-74-9 | 62   |
| 5    |    |   | Docosyl pentafluoropropionate       | 472 | C25H45F5O2 | 1000351-80-9 | 62   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

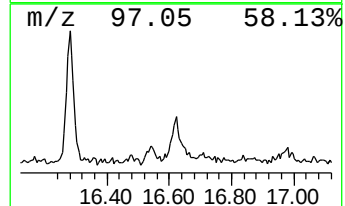
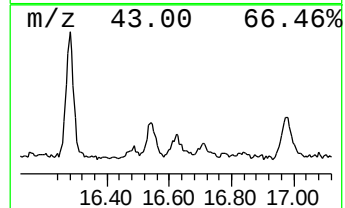
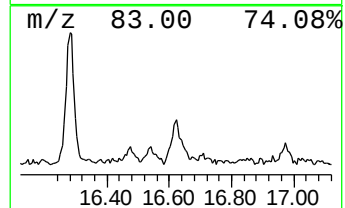
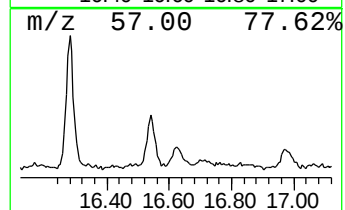
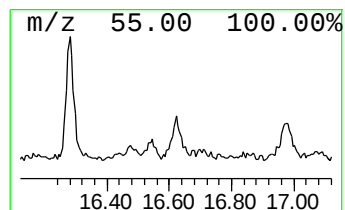
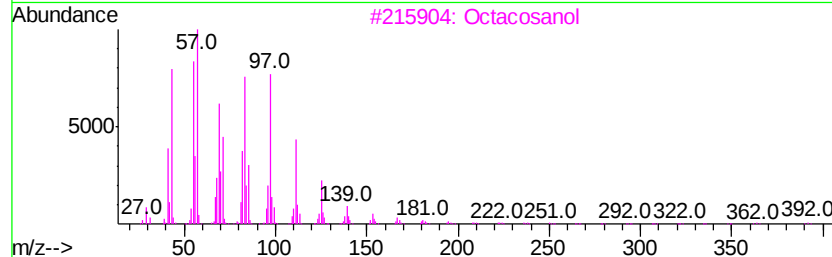
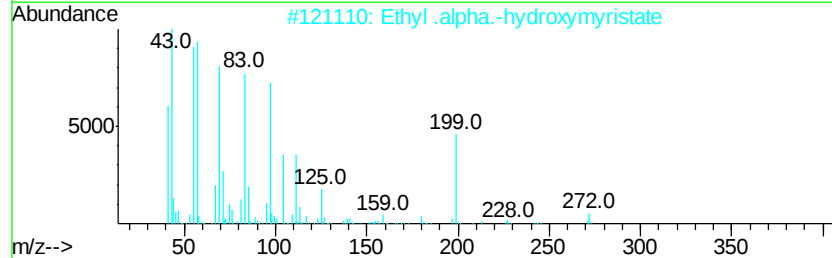
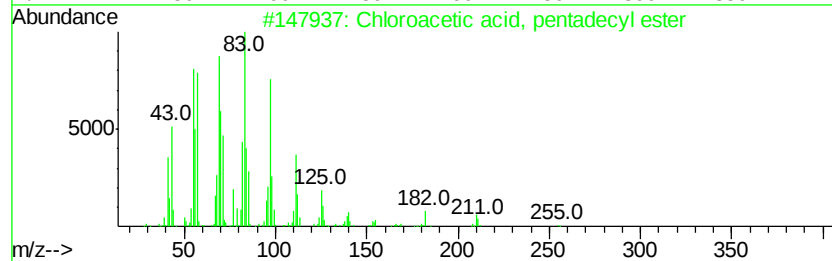
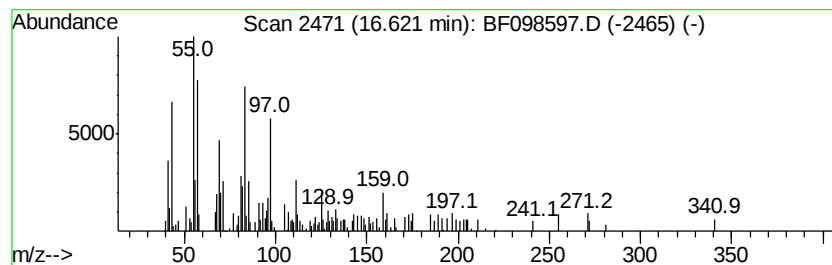
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 16 Chloroacetic acid, pentadec... Concentration Rank 19

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 16.62 | 4.30 ng | 172339 | Perylene-d12     | 15.17 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | Chloroacetic acid, pentadecyl ester | 304 | C17H33ClO2 | 070301-47-2  | 53   |
| 2    |    | Ethyl .alpha.-hydroxymyristate      | 272 | C16H32O3   | 129086-73-3  | 49   |
| 3    |    | Octacosanol                         | 410 | C28H58O    | 000557-61-9  | 47   |
| 4    |    | Docosyl pentafluoropropionate       | 472 | C25H45F5O2 | 1000351-80-9 | 47   |
| 5    |    | n-Tetracosanol-1                    | 354 | C24H50O    | 000506-51-4  | 43   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

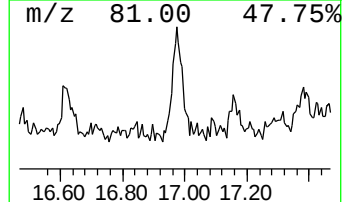
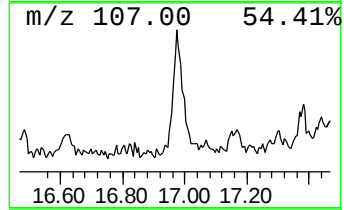
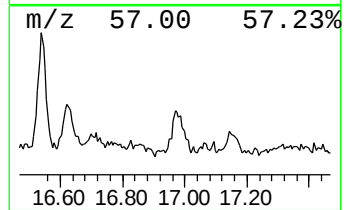
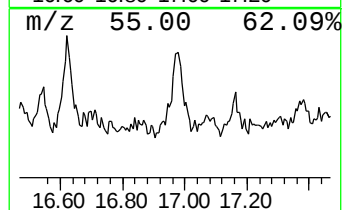
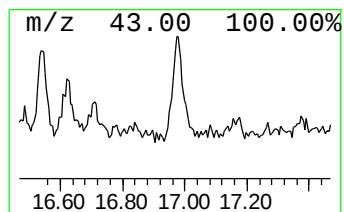
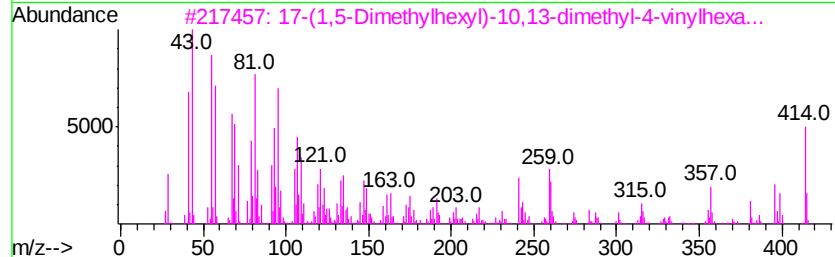
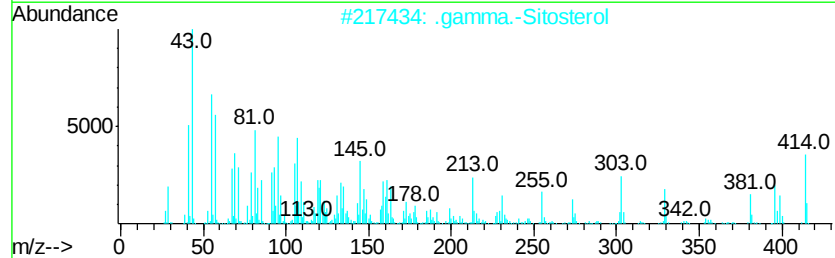
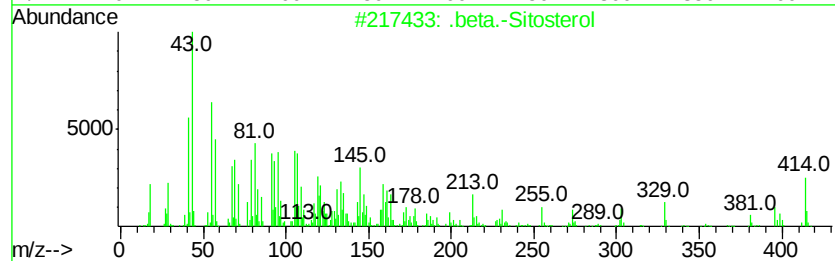
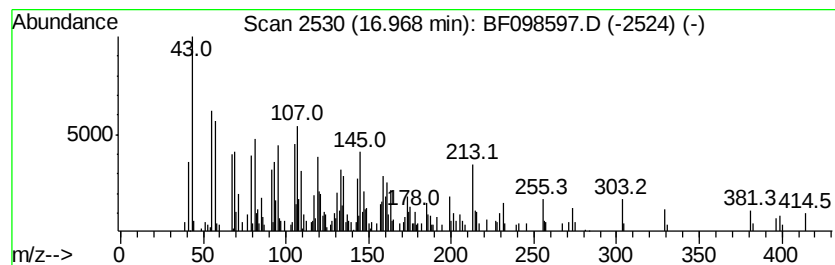
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 17 .beta.-Sitosterol Concentration Rank 9

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 16.97 | 9.94 ng | 398265 | Perylene-d12     | 15.17 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | .beta.-Sitosterol                   | 414 | C29H50O  | 000083-46-5  | 97   |
| 2    |    | .gamma.-Sitosterol                  | 414 | C29H50O  | 000083-47-6  | 91   |
| 3    |    | 17-(1,5-Dimethylhexyl)-10,13-dim... | 414 | C29H50O  | 1000210-86-9 | 38   |
| 4    |    | Kauren-18-ol, acetate, (4.beta.)-   | 330 | C22H34O2 | 072150-74-4  | 25   |
| 5    |    | Stigmastan-3,5-diene                | 396 | C29H48   | 1000214-16-4 | 25   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleID :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

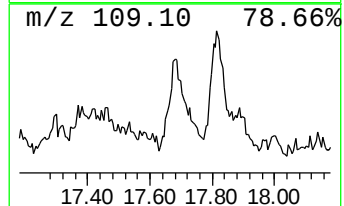
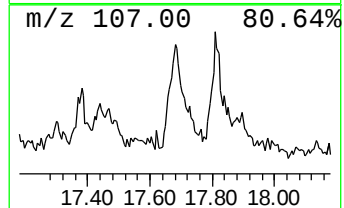
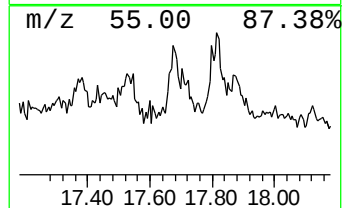
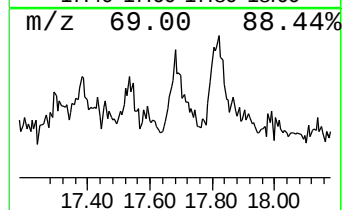
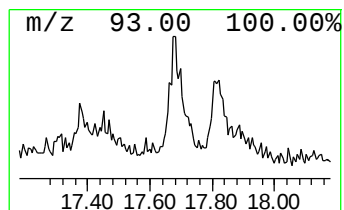
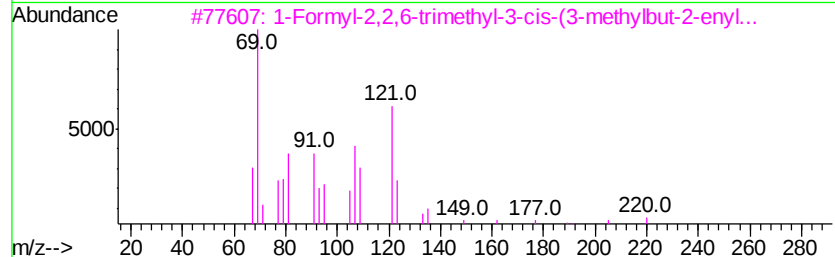
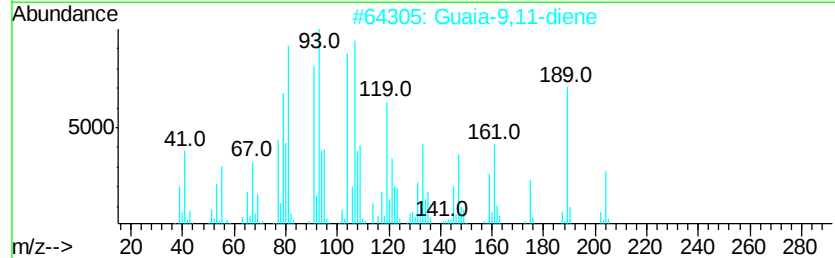
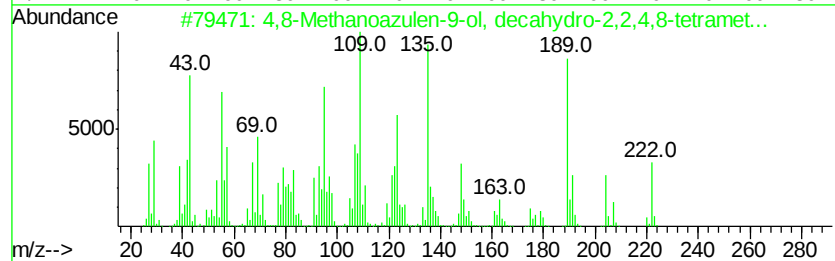
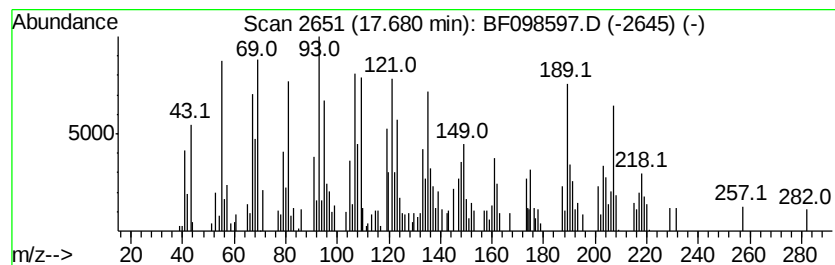
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TIC Integration Parameters: LSCINT.P

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Peak Number 18 4,8-Methanoazulen-9-ol, dec... Concentration Rank 12

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 17.68 | 8.21 ng | 328944 | Perylene-d12     | 15.17 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|-------------------------------------|-----|---------|--------------|------|
| 1    | 5  | 4,8-Methanoazulen-9-ol, decahydr... | 222 | C15H26O | 004586-22-5  | 50   |
| 2    |    | Guaia-9,11-diene                    | 204 | C15H24  | 1000374-19-8 | 42   |
| 3    |    | 1-Formyl-2,2,6-trimethyl-3-cis-(... | 220 | C15H24O | 1000144-10-1 | 38   |
| 4    |    | Naphthalene, 1,2,3,4,4a,5,6,8a-o... | 204 | C15H24  | 000473-13-2  | 30   |
| 5    |    | Cyclopropa[d]naphthalen-2(4aH)-o... | 204 | C14H20O | 004677-90-1  | 30   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

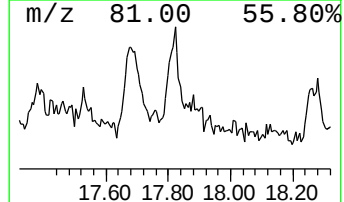
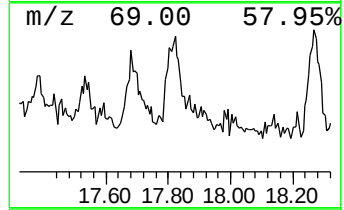
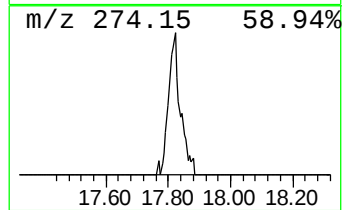
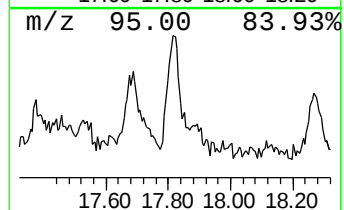
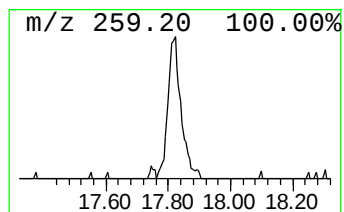
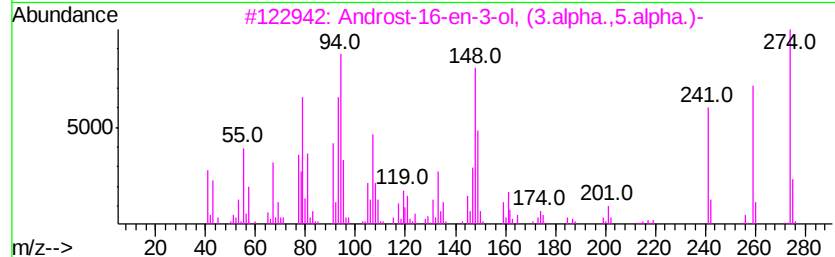
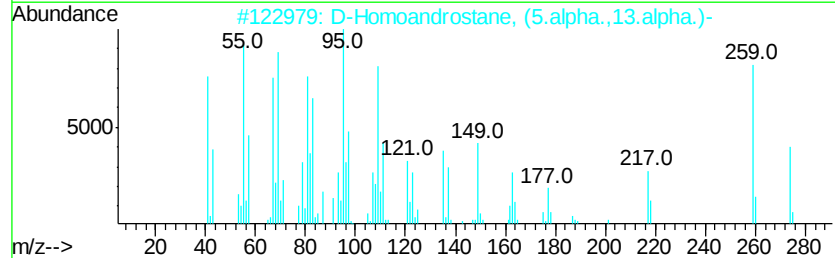
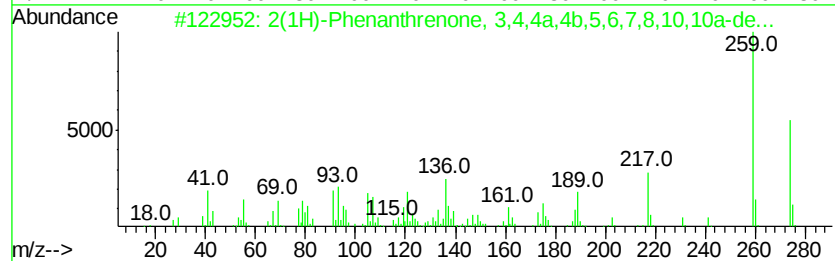
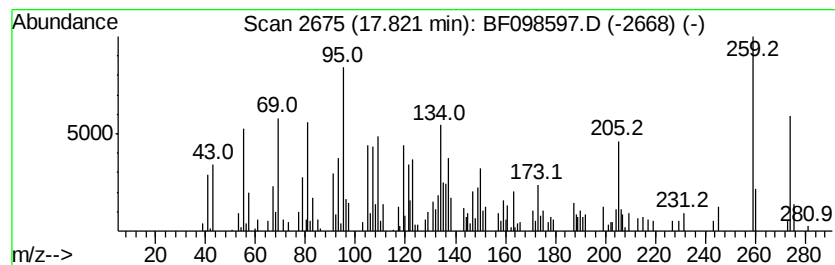
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 19 unknown17.82 Concentration Rank 13

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 17.82 | 8.09 ng | 324172 | Perylene-d12     | 15.17 |

| Hit# | of | Tentative ID                         | MW  | MolForm | CAS#         | Qual |
|------|----|--------------------------------------|-----|---------|--------------|------|
| 1    | 5  | 2(1H)-Phenanthrenone, 3,4,4a,4b,...  | 274 | C19H300 | 007715-44-8  | 38   |
| 2    |    | D-Homoandrostande, (5.alpha.,13.a... | 274 | C20H34  | 054482-31-4  | 38   |
| 3    |    | Androst-16-en-3-ol, (3.alpha.,5....  | 274 | C19H300 | 001153-51-1  | 25   |
| 4    |    | Bicyclo[2.2.1]heptane, 2,2,3-tri...  | 138 | C10H18  | 020536-40-7  | 25   |
| 5    |    | Androst-7-en-3-ol                    | 274 | C19H300 | 1000148-48-7 | 25   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF091817\  
Data File : BF098597.D  
Acq On : 18 Sep 2017 12:55  
Operator : SJ/JU  
Sample : I5229-11  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
UT5400S21

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

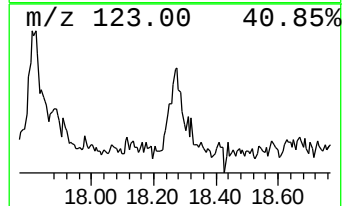
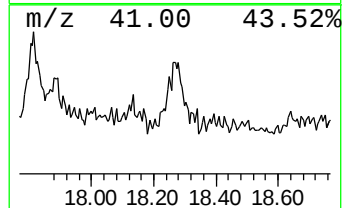
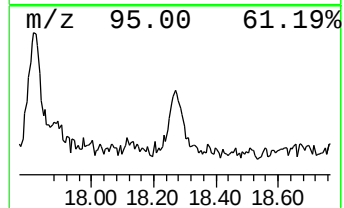
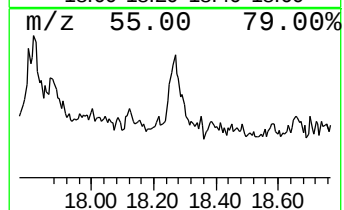
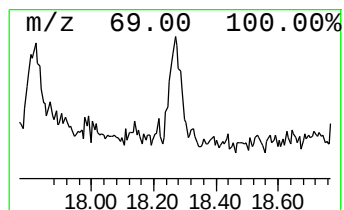
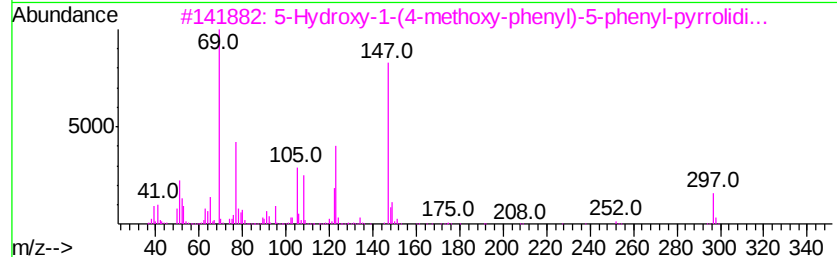
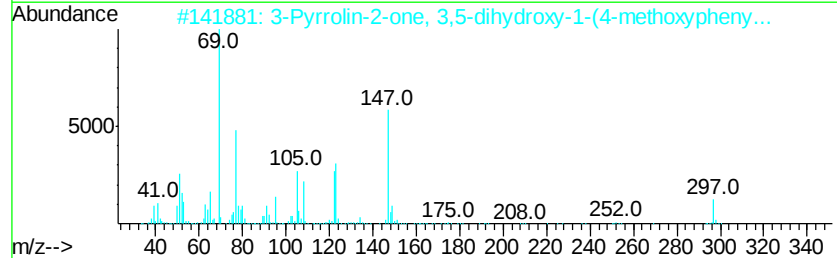
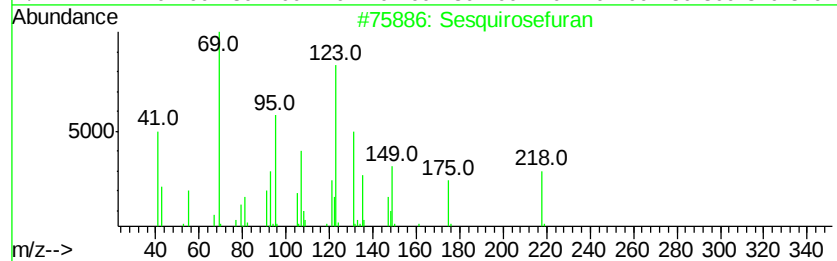
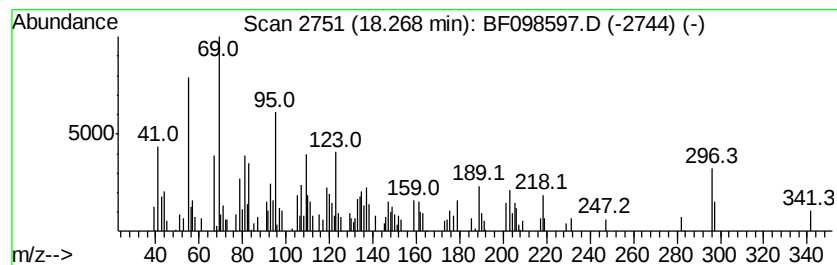
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 20 unknown18.27 Concentration Rank 15

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 18.27 | 7.02 ng | 281111 | Perylene-d12     | 15.17 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | Sesquirosefuran                     | 218 | C15H22O   | 039007-93-7  | 46   |
| 2    |    | 3-Pyrrolin-2-one, 3,5-dihydroxy-... | 297 | C17H15N04 | 1000294-08-5 | 38   |
| 3    |    | 5-Hydroxy-1-(4-methoxy-phenyl)-5... | 297 | C17H15N04 | 1000296-82-7 | 38   |
| 4    |    | 3-Pyrrolin-2-one, 3,5-dihydroxy-... | 297 | C17H15N04 | 1000293-96-4 | 35   |
| 5    |    | Squalene                            | 410 | C30H50    | 000111-02-4  | 35   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF091817\  
 Data File : BF098597.D  
 Acq On : 18 Sep 2017 12:55  
 Operator : SJ/JU  
 Sample : I5229-11  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 UT5400S21

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF091117.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... | 4.82  | 9.9     | ng    | 402262   | 1                     | 6.63  | 813947  | 20.0 |
| unknown6.41          | 6.41  | 96.9    | ng    | 3944670  | 1                     | 6.63  | 813947  | 20.0 |
| n-Hexadecanoic acid  | 11.69 | 4.7     | ng    | 334106   | 4                     | 11.15 | 1413370 | 20.0 |
| Heptafluorobutyri... | 13.63 | 9.0     | ng    | 442431   | 5                     | 13.78 | 983013  | 20.0 |
| 1-Octadecanesulph... | 14.26 | 16.8    | ng    | 826377   | 5                     | 13.78 | 983013  | 20.0 |
| 9-Octadecenamide,... | 14.53 | 10.3    | ng    | 410456   | 6                     | 15.17 | 801247  | 20.0 |
| Squalene             | 14.61 | 4.4     | ng    | 176573   | 6                     | 15.17 | 801247  | 20.0 |
| Oxirane, heptadecyl- | 14.67 | 7.5     | ng    | 300343   | 6                     | 15.17 | 801247  | 20.0 |
| Heptacosane          | 14.85 | 59.9    | ng    | 2400160  | 6                     | 15.17 | 801247  | 20.0 |
| Octadecanal          | 15.37 | 12.6    | ng    | 504850   | 6                     | 15.17 | 801247  | 20.0 |
| Triacontane          | 15.58 | 17.5    | ng    | 700810   | 6                     | 15.17 | 801247  | 20.0 |
| Tetratriacontyl h... | 15.62 | 3.5     | ng    | 141070   | 6                     | 15.17 | 801247  | 20.0 |
| Chloroacetic acid... | 16.62 | 4.3     | ng    | 172339   | 6                     | 15.17 | 801247  | 20.0 |
| .beta.-Sitosterol    | 16.97 | 9.9     | ng    | 398265   | 6                     | 15.17 | 801247  | 20.0 |
| 4,8-Methanoazulen... | 17.68 | 8.2     | ng    | 328944   | 6                     | 15.17 | 801247  | 20.0 |
| unknown17.82         | 17.82 | 8.1     | ng    | 324172   | 6                     | 15.17 | 801247  | 20.0 |
| unknown18.27         | 18.27 | 7.0     | ng    | 281111   | 6                     | 15.17 | 801247  | 20.0 |