

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
 Data File : BF089007.D  
 Acq On : 15 Jul 2016 1:51  
 Operator : UM/SJ  
 Sample : H3995-02  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 LSS-SB-SB12(0-2in)

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-BF063016.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         | 1.655       | 5             | 6           | 15           | rVV      | 147682         | 312399        | 19.00%          | 1.437%        |
| 2         | 1.781       | 15            | 17          | 23           | rVV      | 960184         | 1287426       | 78.31%          | 5.921%        |
| 3         | 1.861       | 23            | 24          | 38           | rVB      | 68623          | 150974        | 9.18%           | 0.694%        |
| 4         | 2.833       | 107           | 109         | 123          | rVB2     | 11769          | 26369         | 1.60%           | 0.121%        |
| 5         | 4.844       | 282           | 285         | 290          | rBV      | 111636         | 180902        | 11.00%          | 0.832%        |
| 6         | 5.004       | 290           | 299         | 302          | rBV      | 15056          | 61193         | 3.72%           | 0.281%        |
| 7         | 5.050       | 302           | 303         | 317          | rVB      | 11578          | 25718         | 1.56%           | 0.118%        |
| 8         | 5.290       | 321           | 324         | 326          | rBV      | 1548927        | 1573176       | 95.70%          | 7.235%        |
| 9         | 6.342       | 413           | 416         | 419          | rBV      | 1130112        | 1584354       | 96.38%          | 7.287%        |
| 10        | 6.467       | 424           | 427         | 429          | rBV      | 1209367        | 1643920       | 100.00%         | 7.561%        |
| 11        | 6.684       | 444           | 446         | 448          | rBV      | 336038         | 305266        | 18.57%          | 1.404%        |
| 12        | 6.845       | 457           | 460         | 462          | rVB      | 1433572        | 1221572       | 74.31%          | 5.618%        |
| 13        | 7.256       | 493           | 496         | 498          | rBV      | 989486         | 910866        | 55.41%          | 4.189%        |
| 14        | 7.976       | 556           | 559         | 561          | rBV      | 419530         | 381781        | 23.22%          | 1.756%        |
| 15        | 8.685       | 619           | 621         | 623          | rBV      | 19142          | 17973         | 1.09%           | 0.083%        |
| 16        | 9.050       | 650           | 653         | 655          | rBV      | 1706557        | 1424985       | 86.68%          | 6.554%        |
| 17        | 9.382       | 680           | 682         | 684          | rBV      | 53256          | 42244         | 2.57%           | 0.194%        |
| 18        | 9.450       | 685           | 688         | 690          | rVB      | 150277         | 188506        | 11.47%          | 0.867%        |
| 19        | 9.576       | 697           | 699         | 703          | rVB      | 27029          | 23853         | 1.45%           | 0.110%        |
| 20        | 9.725       | 708           | 712         | 713          | rVV      | 283258         | 403199        | 24.53%          | 1.854%        |
| 21        | 9.771       | 713           | 716         | 719          | rVB      | 30269          | 35989         | 2.19%           | 0.166%        |
| 22        | 10.182      | 749           | 752         | 754          | rVB2     | 18876          | 34101         | 2.07%           | 0.157%        |
| 23        | 10.239      | 754           | 757         | 758          | rBV      | 14191          | 16586         | 1.01%           | 0.076%        |
| 24        | 10.433      | 771           | 774         | 776          | rVB2     | 11283          | 18021         | 1.10%           | 0.083%        |
| 25        | 10.502      | 778           | 780         | 783          | rVV2     | 640786         | 753676        | 45.85%          | 3.466%        |
| 26        | 10.593      | 785           | 788         | 789          | rBV2     | 12591          | 17105         | 1.04%           | 0.079%        |
| 27        | 10.639      | 789           | 792         | 796          | rVB2     | 17083          | 35764         | 2.18%           | 0.164%        |
| 28        | 10.719      | 798           | 799         | 801          | rBV2     | 23354          | 22026         | 1.34%           | 0.101%        |
| 29        | 10.856      | 810           | 811         | 815          | rBV3     | 19026          | 31111         | 1.89%           | 0.143%        |
| 30        | 11.074      | 829           | 830         | 834          | rBV2     | 41991          | 63799         | 3.88%           | 0.293%        |
| 31        | 11.165      | 836           | 838         | 839          | rBV      | 43490          | 40657         | 2.47%           | 0.187%        |
| 32        | 11.199      | 839           | 841         | 844          | rVV2     | 357520         | 439041        | 26.71%          | 2.019%        |
| 33        | 11.268      | 844           | 847         | 849          | rVB2     | 75581          | 97458         | 5.93%           | 0.448%        |
| 34        | 11.348      | 853           | 854         | 859          | rVB4     | 12812          | 27490         | 1.67%           | 0.126%        |

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
 Data File : BF089007.D  
 Acq On : 15 Jul 2016 1:51  
 Operator : UM/SJ  
 Sample : H3995-02  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 LSS-SB-SB12(0-2in)

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-BF063016.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 35 | 11.428 | 859  | 861  | 864  | rBV2 | 35200  | 36745   | 2.24%  | 0.169% |
| 36 | 11.508 | 867  | 868  | 872  | rVB2 | 36203  | 52477   | 3.19%  | 0.241% |
| 37 | 11.599 | 875  | 876  | 879  | rVB  | 22698  | 20175   | 1.23%  | 0.093% |
| 38 | 11.702 | 880  | 885  | 887  | rBV2 | 47534  | 135361  | 8.23%  | 0.623% |
| 39 | 11.748 | 887  | 889  | 890  | rVV  | 187717 | 170232  | 10.36% | 0.783% |
| 40 | 11.805 | 892  | 894  | 898  | rVB  | 34168  | 55356   | 3.37%  | 0.255% |
| 41 | 11.908 | 899  | 903  | 906  | rVB4 | 12259  | 29299   | 1.78%  | 0.135% |
| 42 | 12.011 | 908  | 912  | 916  | rBV2 | 25232  | 49660   | 3.02%  | 0.228% |
| 43 | 12.239 | 931  | 932  | 934  | rBV  | 19860  | 29779   | 1.81%  | 0.137% |
| 44 | 12.331 | 938  | 940  | 941  | rVV2 | 42175  | 46278   | 2.82%  | 0.213% |
| 45 | 12.399 | 944  | 946  | 948  | rVV  | 308515 | 269614  | 16.40% | 1.240% |
| 46 | 12.468 | 948  | 952  | 953  | rVV3 | 17984  | 41605   | 2.53%  | 0.191% |
| 47 | 12.525 | 956  | 957  | 960  | rVV3 | 15586  | 27914   | 1.70%  | 0.128% |
| 48 | 12.628 | 963  | 966  | 967  | rBV  | 208370 | 222627  | 13.54% | 1.024% |
| 49 | 12.662 | 967  | 969  | 973  | rVB4 | 25177  | 59872   | 3.64%  | 0.275% |
| 50 | 12.777 | 977  | 979  | 982  | rVV  | 964961 | 1153154 | 70.15% | 5.303% |
| 51 | 12.845 | 982  | 985  | 989  | rVV4 | 19438  | 38493   | 2.34%  | 0.177% |
| 52 | 12.994 | 996  | 998  | 1000 | rBV  | 30212  | 62110   | 3.78%  | 0.286% |
| 53 | 13.062 | 1002 | 1004 | 1008 | rVV2 | 28717  | 58183   | 3.54%  | 0.268% |
| 54 | 13.234 | 1017 | 1019 | 1020 | rBV  | 24836  | 32023   | 1.95%  | 0.147% |
| 55 | 13.257 | 1020 | 1021 | 1023 | rVB  | 74191  | 55993   | 3.41%  | 0.258% |
| 56 | 13.565 | 1046 | 1048 | 1050 | rBV2 | 29834  | 52332   | 3.18%  | 0.241% |
| 57 | 13.691 | 1056 | 1059 | 1062 | rBV2 | 125520 | 203188  | 12.36% | 0.934% |
| 58 | 13.817 | 1067 | 1070 | 1076 | rBV2 | 368882 | 588740  | 35.81% | 2.708% |
| 59 | 14.320 | 1111 | 1114 | 1119 | rBV  | 194331 | 335208  | 20.39% | 1.542% |
| 60 | 14.731 | 1148 | 1150 | 1153 | rBV  | 150522 | 139276  | 8.47%  | 0.641% |
| 61 | 14.811 | 1155 | 1157 | 1163 | rVB  | 77080  | 135078  | 8.22%  | 0.621% |
| 62 | 14.902 | 1163 | 1165 | 1171 | rBV2 | 367372 | 835698  | 50.84% | 3.843% |
| 63 | 15.131 | 1183 | 1185 | 1188 | rBV  | 70737  | 86695   | 5.27%  | 0.399% |
| 64 | 15.188 | 1188 | 1190 | 1192 | rBV  | 153039 | 194882  | 11.85% | 0.896% |
| 65 | 15.417 | 1207 | 1210 | 1212 | rBV  | 226137 | 312998  | 19.04% | 1.440% |
| 66 | 15.623 | 1225 | 1228 | 1231 | rBV  | 758694 | 1319545 | 80.27% | 6.069% |
| 67 | 15.668 | 1231 | 1232 | 1237 | rVB  | 164296 | 180106  | 10.96% | 0.828% |
| 68 | 16.308 | 1286 | 1288 | 1294 | rVB2 | 80784  | 148405  | 9.03%  | 0.683% |
| 69 | 16.571 | 1309 | 1311 | 1314 | rVB  | 65252  | 108543  | 6.60%  | 0.499% |
| 70 | 16.628 | 1314 | 1316 | 1323 | rVB7 | 48408  | 134276  | 8.17%  | 0.618% |
| 71 | 16.983 | 1344 | 1347 | 1352 | rBV2 | 95139  | 231989  | 14.11% | 1.067% |

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

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-BF063016.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 72 | 17.874 | 1422 | 1425 | 1432 | rVB2 | 107310 | 289092 | 17.59% | 1.330% |
| 73 | 18.126 | 1444 | 1447 | 1450 | rVB  | 44037  | 95676  | 5.82%  | 0.440% |
| 74 | 18.274 | 1458 | 1460 | 1473 | rVB2 | 88025  | 305345 | 18.57% | 1.404% |

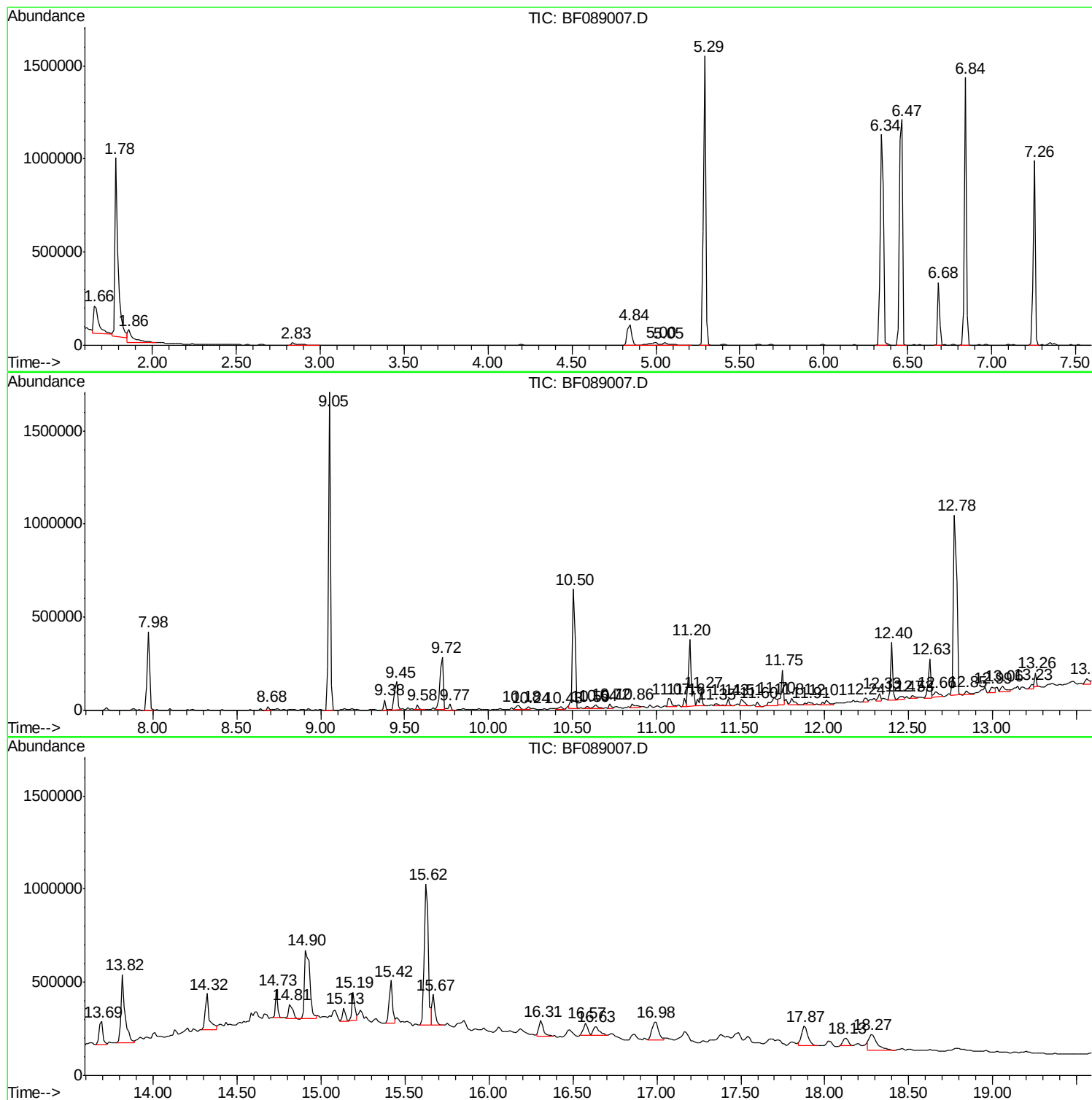
Sum of corrected areas: 21743522

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

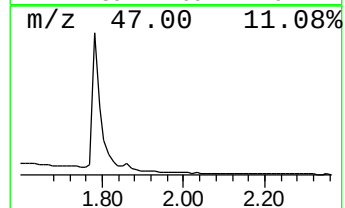
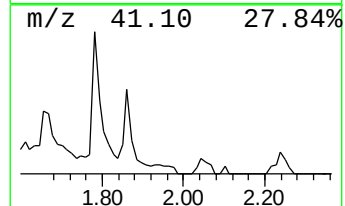
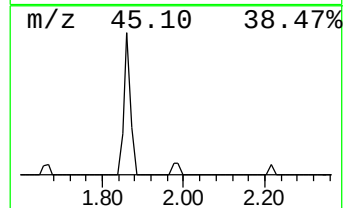
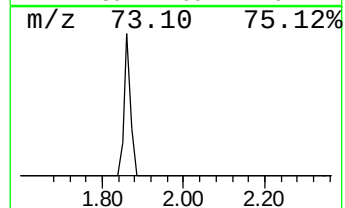
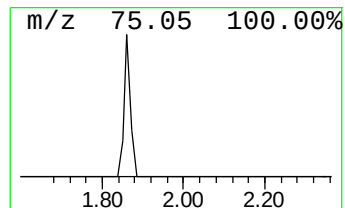
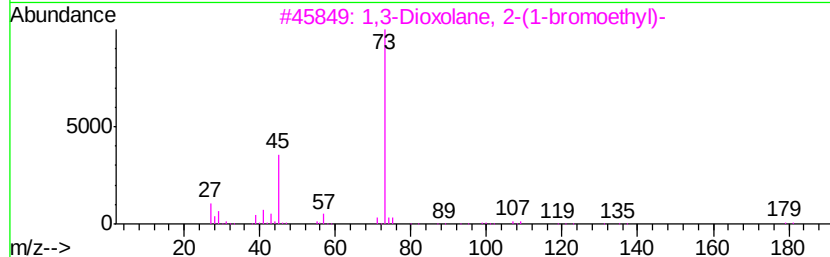
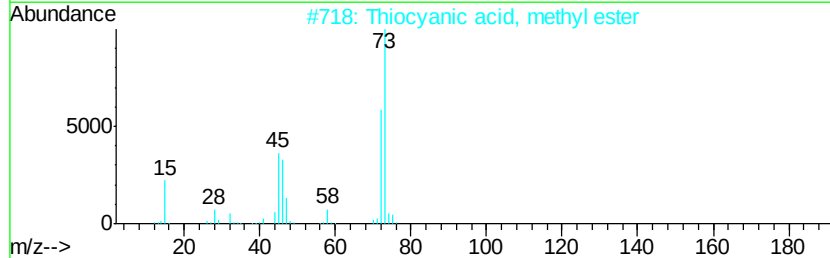
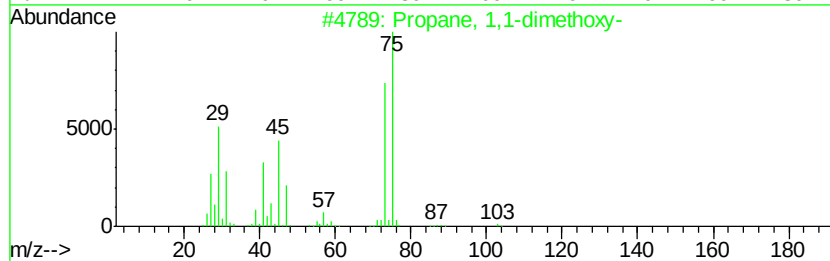
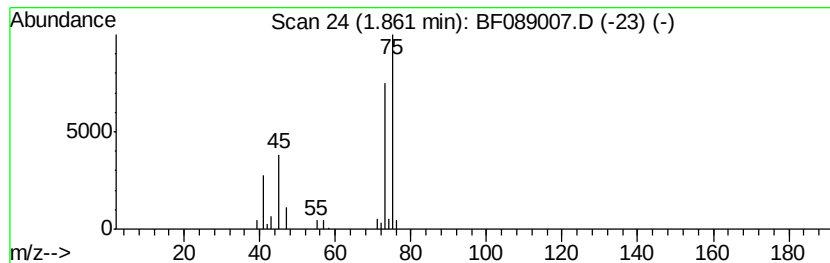
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 unknown1.86 Concentration Rank 18

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 1.86 | 9.89 ng | 150974 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|------|----|----------------------------------|-----|----------|-------------|------|
| 1    | 5  | Propane, 1,1-dimethoxy-          | 104 | C5H12O2  | 004744-10-9 | 40   |
| 2    |    | Thiocyanic acid, methyl ester    | 73  | C2H3NS   | 000556-64-9 | 25   |
| 3    |    | 1,3-Dioxolane, 2-(1-bromoethyl)- | 180 | C5H9BrO2 | 005267-73-2 | 12   |
| 4    |    | Pentane, 3-methoxy-              | 102 | C6H14O   | 036839-67-5 | 12   |
| 5    |    | Glycine                          | 75  | C2H5NO2  | 000056-40-6 | 7    |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

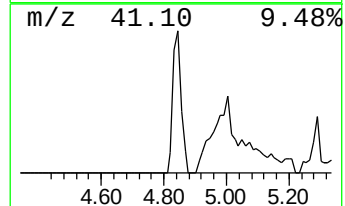
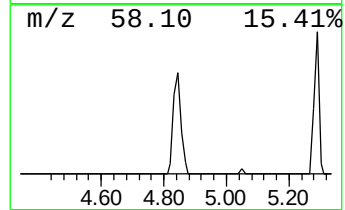
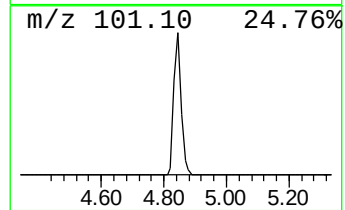
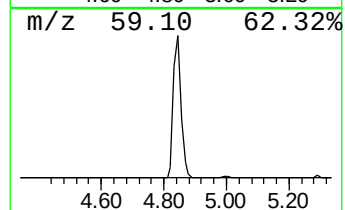
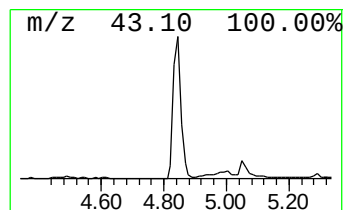
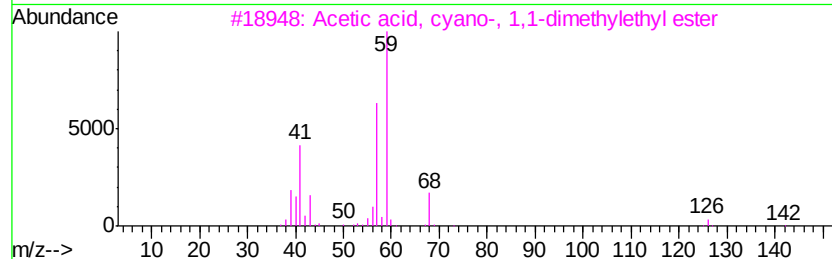
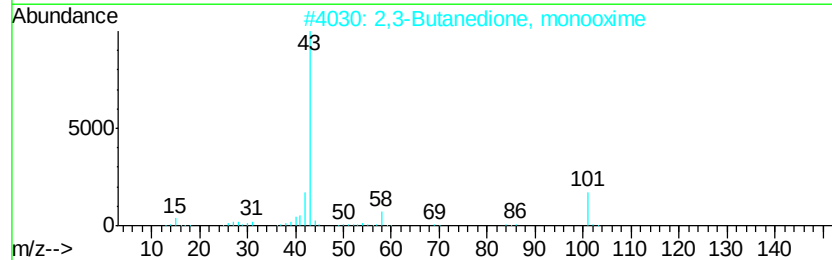
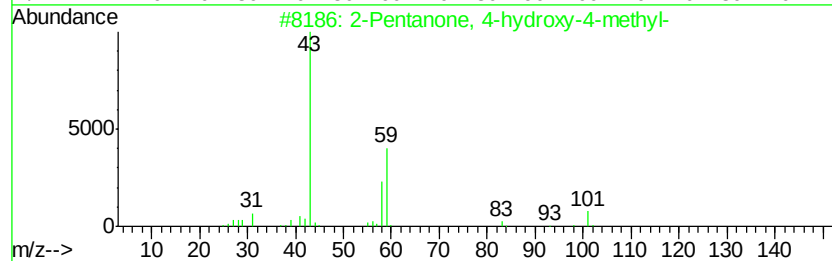
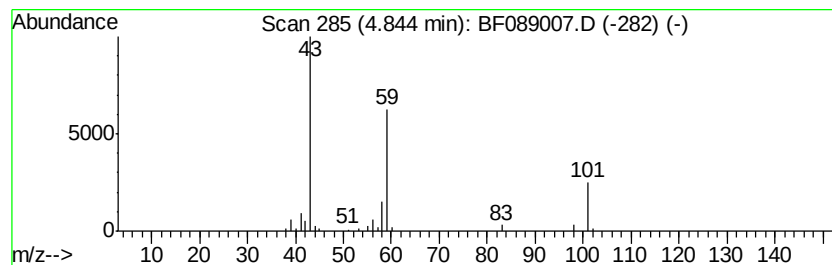
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 15

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.84 | 11.85 ng | 180902 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of                                   | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|--------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2      | 000123-42-2 | 56      |      |      |
| 2    | 2,3-Butanedione, monooxime           | 101 | C4H7NO2      | 000057-71-6 | 35      |      |      |
| 3    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2     | 001116-98-9 | 17      |      |      |
| 4    | Morpholine, 4-methyl-                | 101 | C5H11NO      | 000109-02-4 | 9       |      |      |
| 5    | 5-Hexen-2-one                        | 98  | C6H10O       | 000109-49-9 | 9       |      |      |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

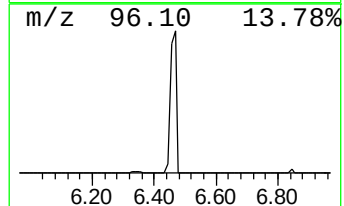
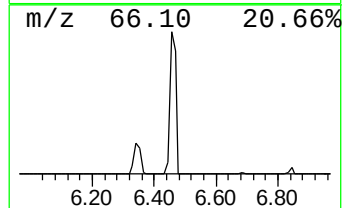
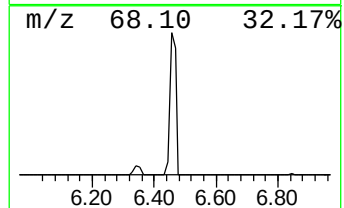
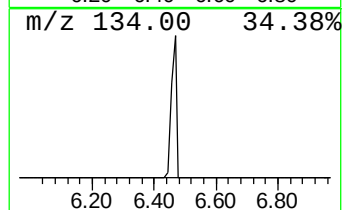
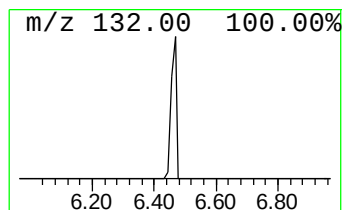
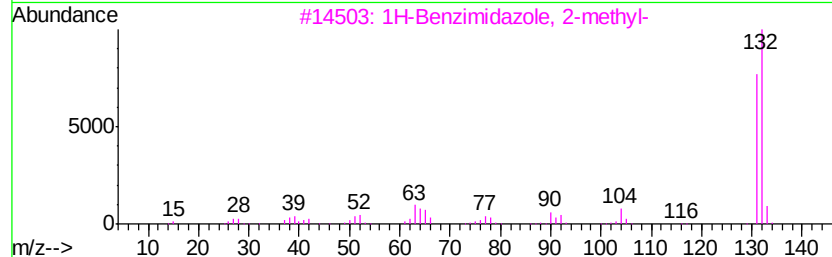
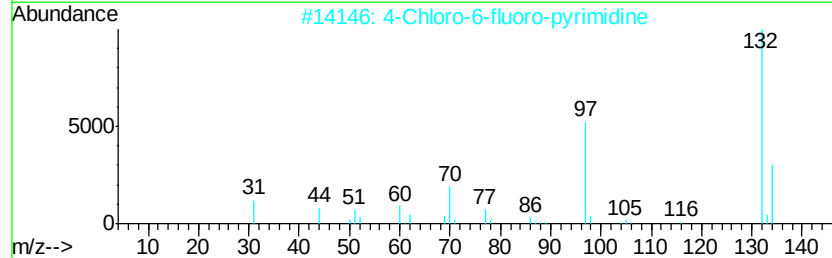
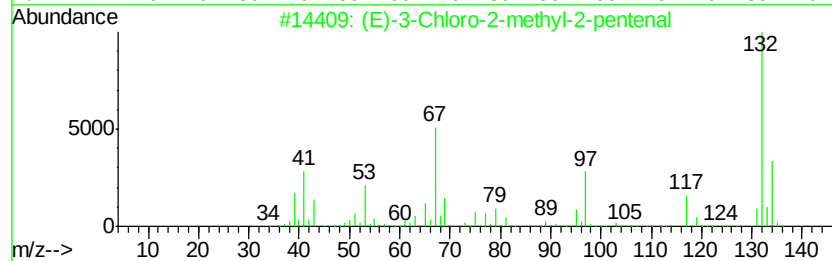
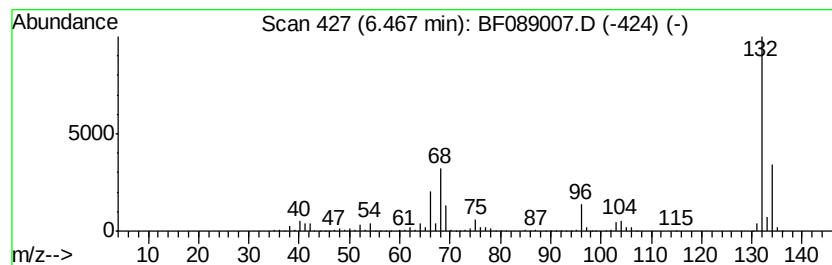
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 unknown6.47 Concentration Rank 2

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 6.47 | 107.70 ng | 1643920 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 25   |
| 2    |    | 4-Chloro-6-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-01-6  | 9    |
| 3    |    | 1H-Benzimidazole, 2-methyl-         | 132 | C8H8N2    | 000615-15-6  | 9    |
| 4    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |
| 5    |    | (5-Methyl-2-pyridyl)acetonitrile    | 132 | C8H8N2    | 1000241-93-9 | 9    |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

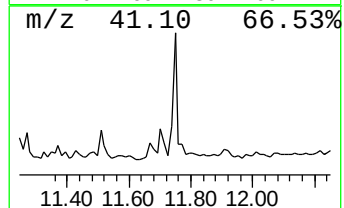
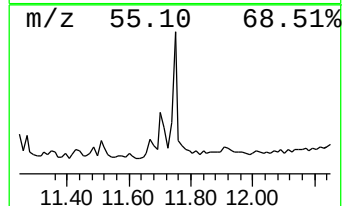
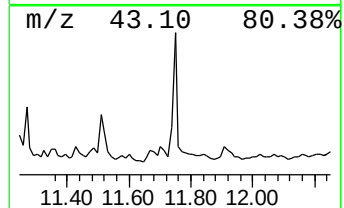
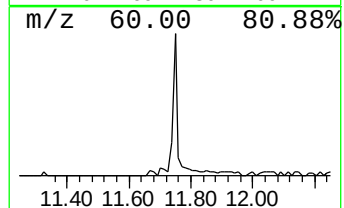
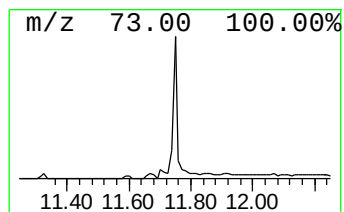
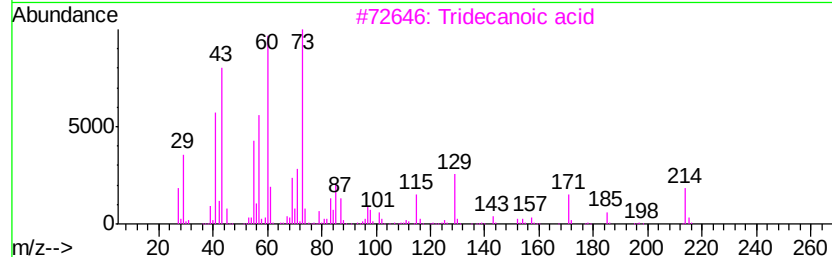
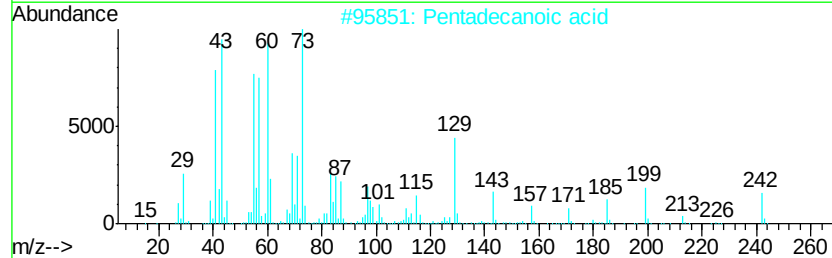
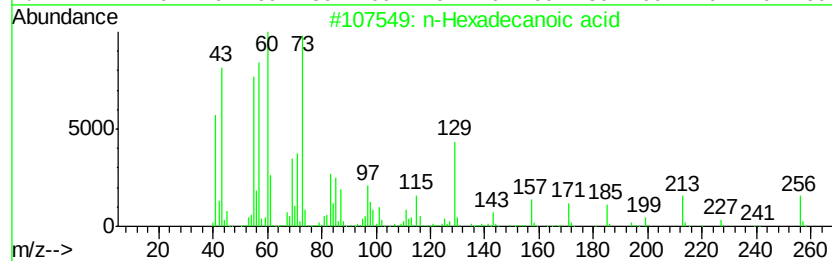
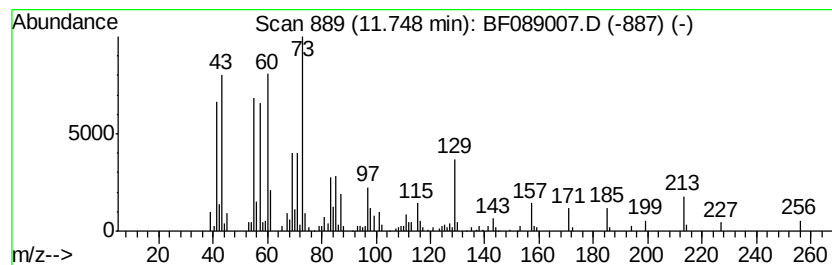
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 7 n-Hexadecanoic acid Concentration Rank 20

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.75 | 7.75 ng | 170232 | Phenanthrene-d10 | 11.20 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | n-Hexadecanoic acid                 | 256 | C16H32O2  | 000057-10-3  | 99   |
| 2    |    | Pentadecanoic acid                  | 242 | C15H30O2  | 001002-84-2  | 93   |
| 3    |    | Tridecanoic acid                    | 214 | C13H26O2  | 000638-53-9  | 91   |
| 4    |    | Tetradecanoic acid                  | 228 | C14H28O2  | 000544-63-8  | 80   |
| 5    |    | Sulfurous acid, 2-propyl tridecy... | 306 | C16H34O3S | 1000309-12-4 | 18   |





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

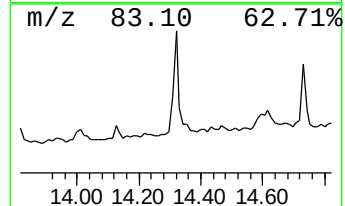
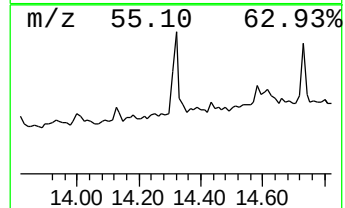
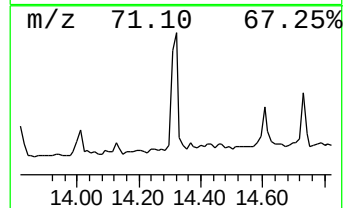
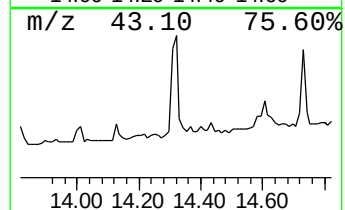
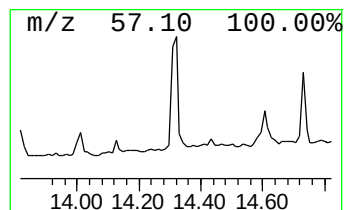
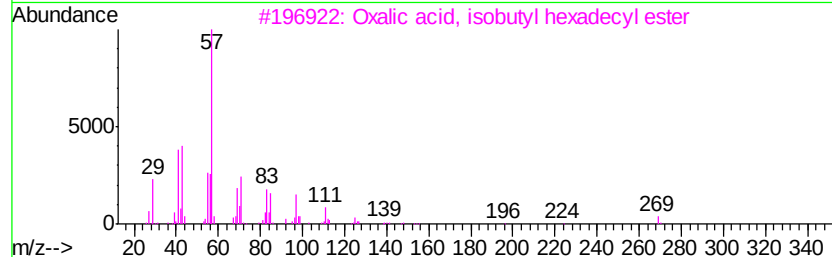
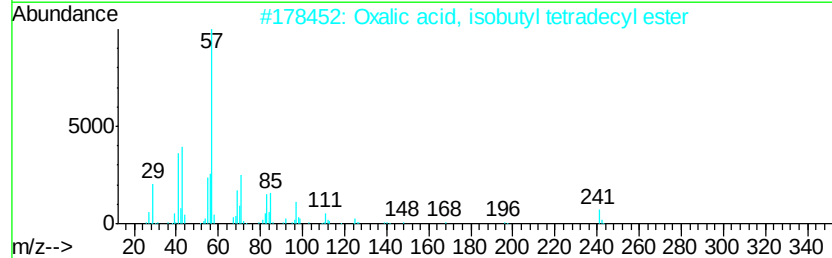
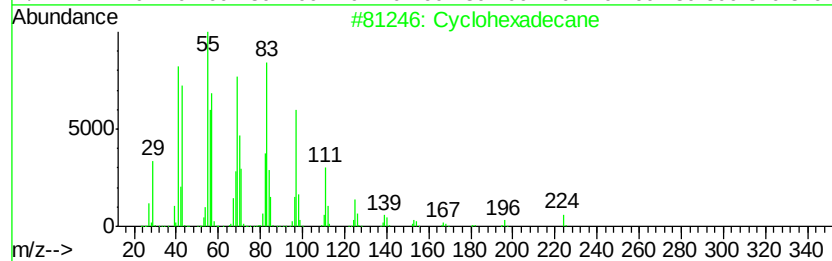
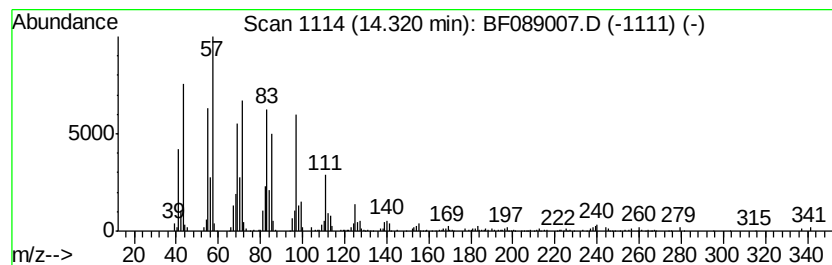
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 8 Cyclohexadecane Concentration Rank 16

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 14.32 | 11.39 ng | 335208 | Chrysene-d12     | 13.82 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | Cyclohexadecane                     | 224 | C16H32     | 000295-65-8  | 99   |
| 2    |    | Oxalic acid, isobutyl tetradecyl... | 342 | C20H38O4   | 1000309-37-9 | 91   |
| 3    |    | Oxalic acid, isobutyl hexadecyl ... | 370 | C22H42O4   | 1000309-38-1 | 91   |
| 4    |    | Triaccontyl pentafluoropropionate   | 584 | C33H61F5O2 | 1000351-80-0 | 81   |
| 5    |    | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5  | 76   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

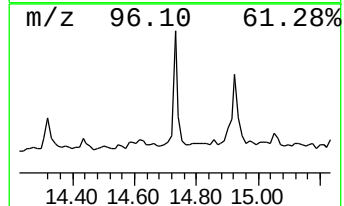
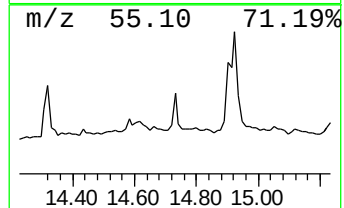
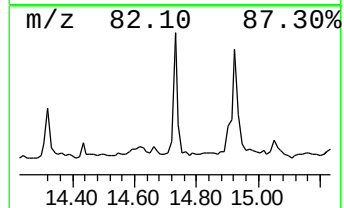
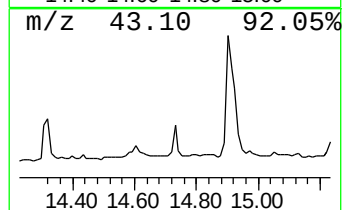
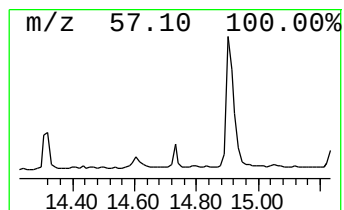
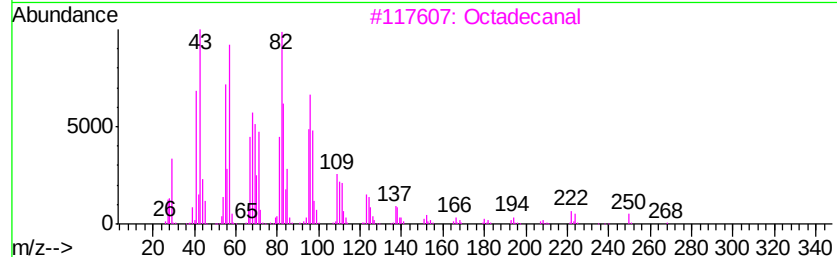
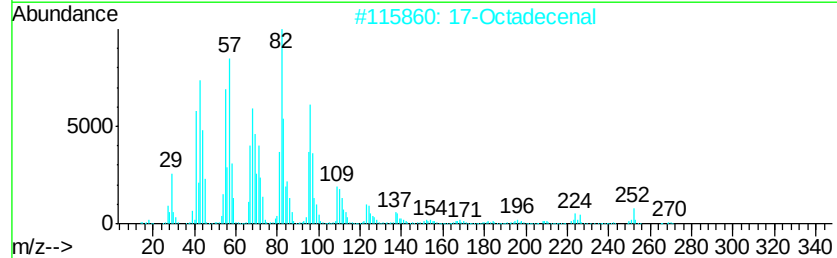
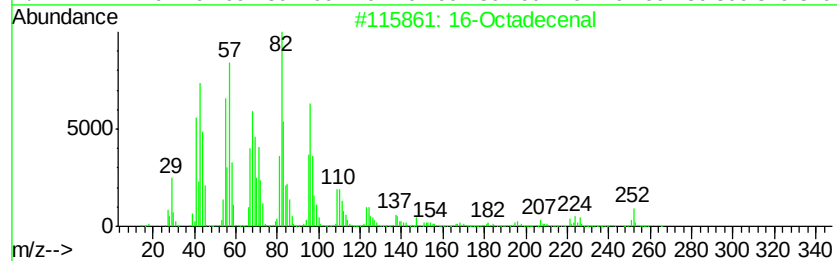
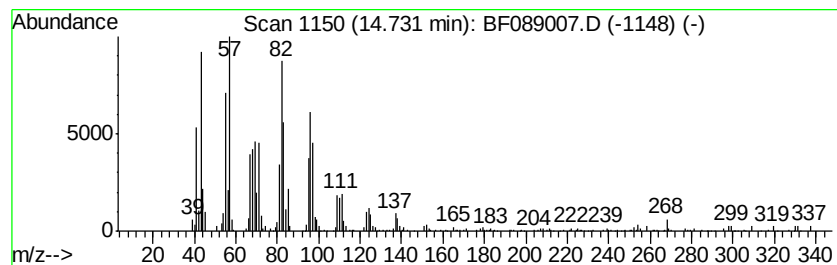
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 9 16-Octadecenal Concentration Rank 13

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 14.73 | 14.29 ng | 139276 | Perylene-d12     | 15.19 |

| Hit# | of | Tentative ID        | MW  | MolForm | CAS#        | Qual |
|------|----|---------------------|-----|---------|-------------|------|
| 1    | 5  | 16-Octadecenal      | 266 | C18H34O | 056554-87-1 | 91   |
| 2    |    | 17-Octadecenal      | 266 | C18H34O | 056554-86-0 | 91   |
| 3    |    | Octadecanal         | 268 | C18H36O | 000638-66-4 | 91   |
| 4    |    | Oxirane, hexadecyl- | 268 | C18H36O | 007390-81-0 | 91   |
| 5    |    | 13-Octadecenal      | 266 | C18H34O | 056554-90-6 | 90   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

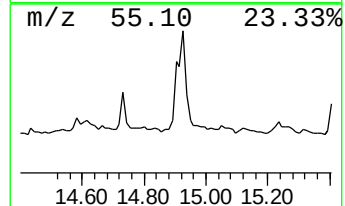
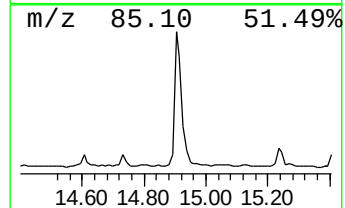
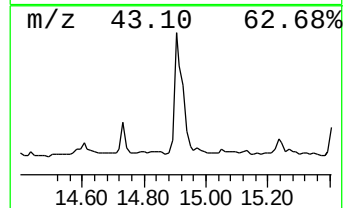
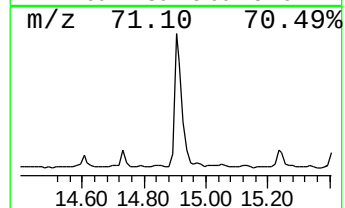
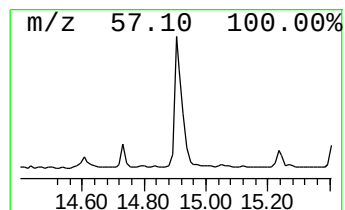
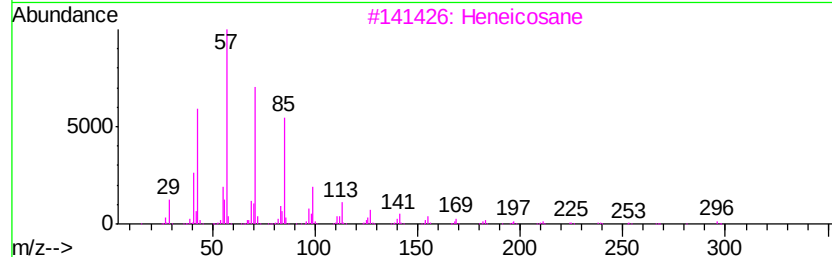
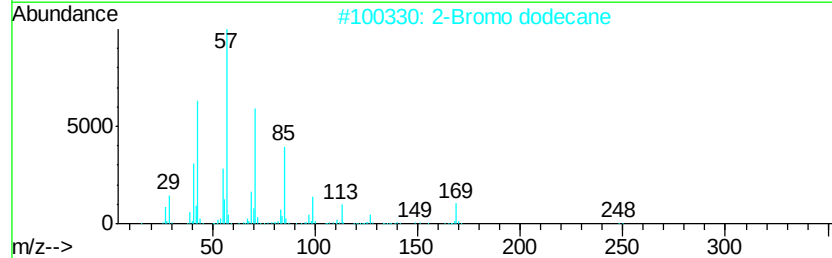
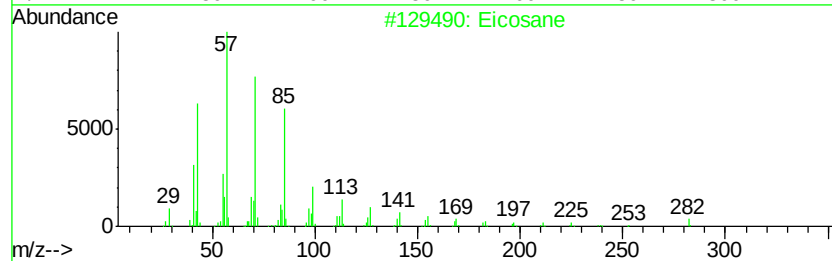
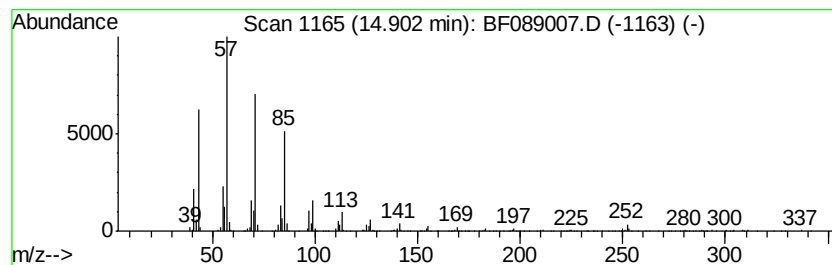
Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 10 Eicosane Concentration Rank 3

| R.T.    | EstConc                      | Area         | Relative to ISTD | R.T.      |
|---------|------------------------------|--------------|------------------|-----------|
| 14.90   | 85.76 ng                     | 835698       | Perylene-d12     | 15.19     |
| Hit# of | 5                            | Tentative ID | MW MolForm       | CAS# Qual |
| 1       | Eicosane                     | 282 C20H42   | 000112-95-8      | 94        |
| 2       | 2-Bromo dodecane             | 248 C12H25Br | 013187-99-0      | 93        |
| 3       | Heneicosane                  | 296 C21H44   | 000629-94-7      | 91        |
| 4       | Tetracosane                  | 338 C24H50   | 000646-31-1      | 90        |
| 5       | Dodecane, 2-methyl-6-propyl- | 226 C16H34   | 055045-08-4      | 87        |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

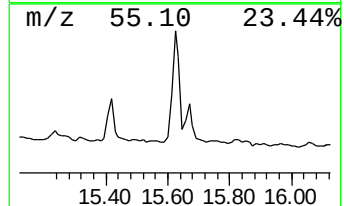
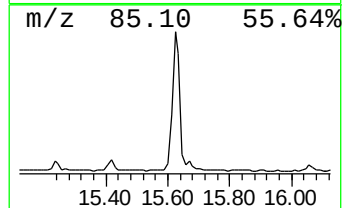
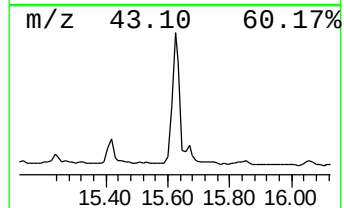
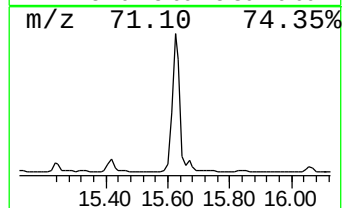
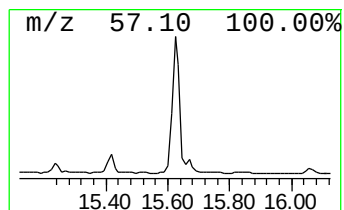
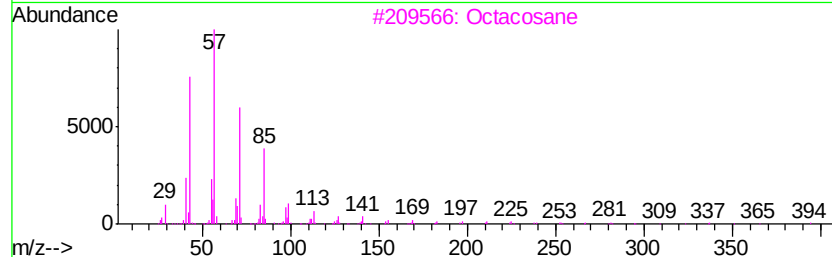
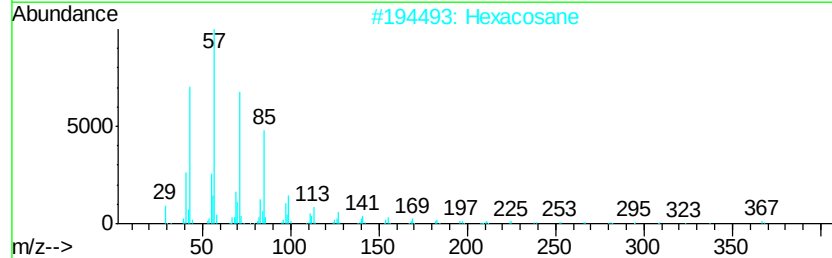
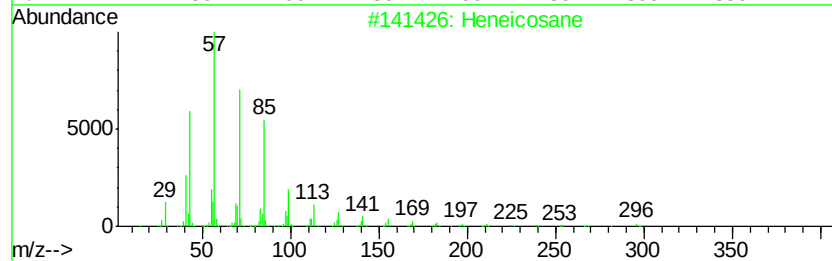
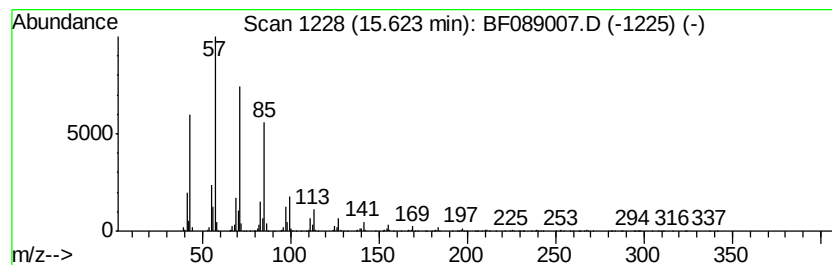
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 12 Heneicosane Concentration Rank 1

| R.T.  | EstConc   | Area    | Relative to ISTD | R.T.  |
|-------|-----------|---------|------------------|-------|
| 15.62 | 135.42 ng | 1319550 | Perylene-d12     | 15.19 |

| Hit# | of | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----|--------------|-----|---------|-------------|------|
| 1    | 5  | Heneicosane  | 296 | C21H44  | 000629-94-7 | 91   |
| 2    |    | Hexacosane   | 366 | C26H54  | 000630-01-3 | 91   |
| 3    |    | Octacosane   | 394 | C28H58  | 000630-02-4 | 91   |
| 4    |    | Eicosane     | 282 | C20H42  | 000112-95-8 | 90   |
| 5    |    | Heptadecane  | 240 | C17H36  | 000629-78-7 | 90   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

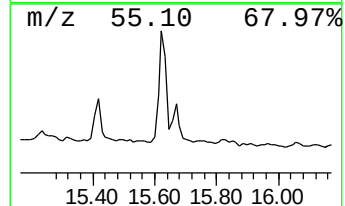
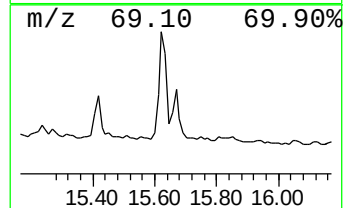
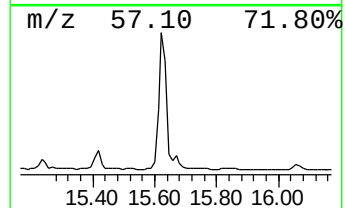
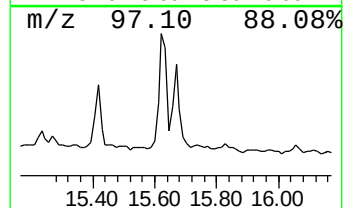
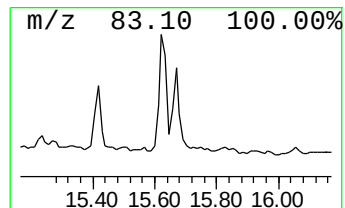
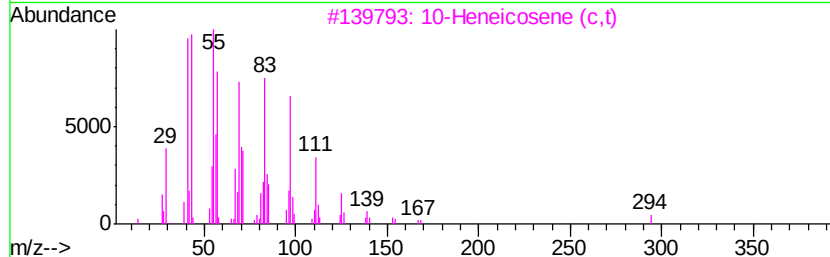
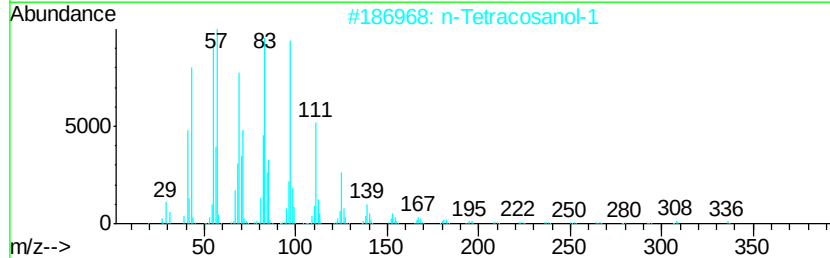
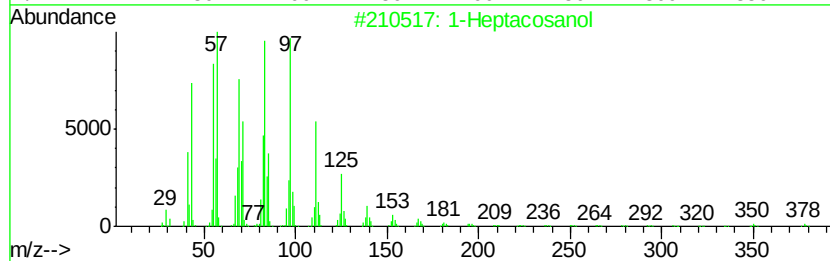
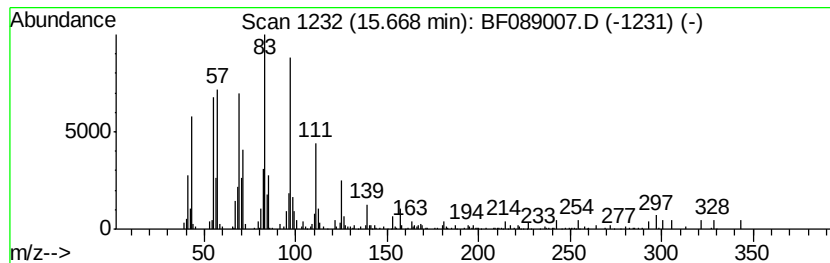
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 13 1-Heptacosanol Concentration Rank 11

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 15.67 | 18.48 ng | 180106 | Perylene-d12     | 15.19 |

| Hit# | of | Tentative ID         | MW  | MolForm  | CAS#        | Qual |
|------|----|----------------------|-----|----------|-------------|------|
| 1    | 5  | 1-Heptacosanol       | 396 | C27H56O  | 002004-39-9 | 93   |
| 2    |    | n-Tetracosanol-1     | 354 | C24H50O  | 000506-51-4 | 89   |
| 3    |    | 10-Heneicosene (c,t) | 294 | C21H42   | 095008-11-0 | 87   |
| 4    |    | Octacosyl acetate    | 452 | C30H60O2 | 018206-97-8 | 81   |
| 5    |    | 1-Docosene           | 308 | C22H44   | 001599-67-3 | 74   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

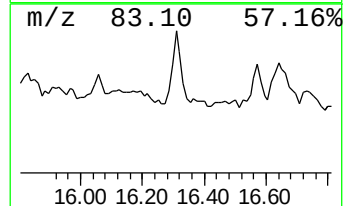
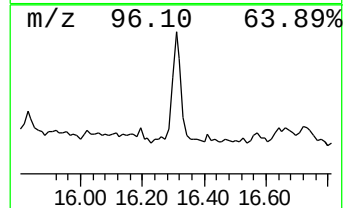
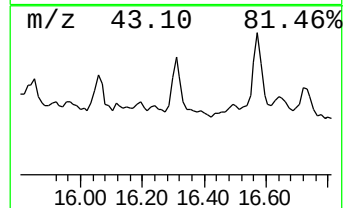
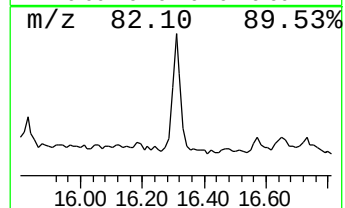
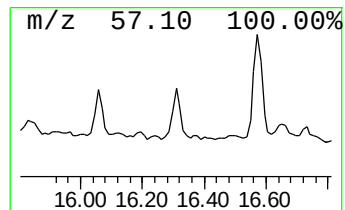
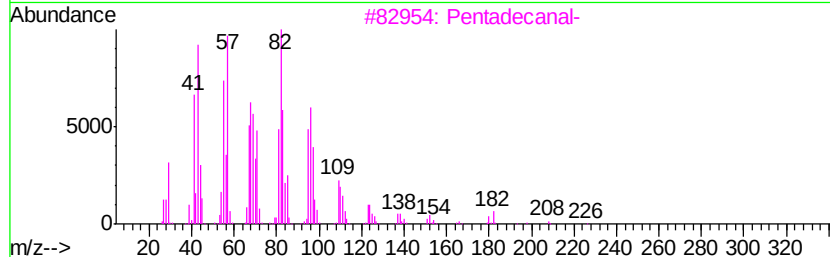
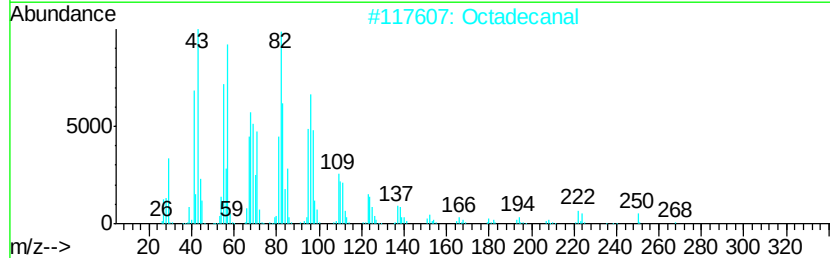
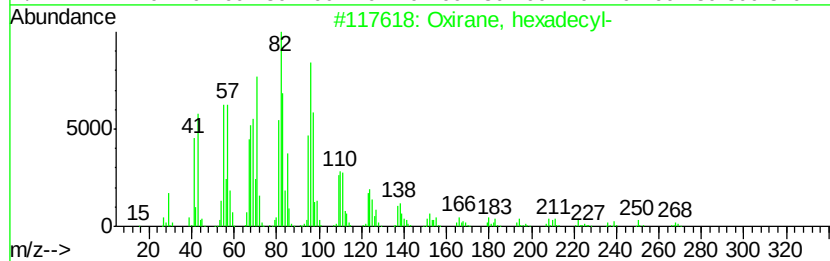
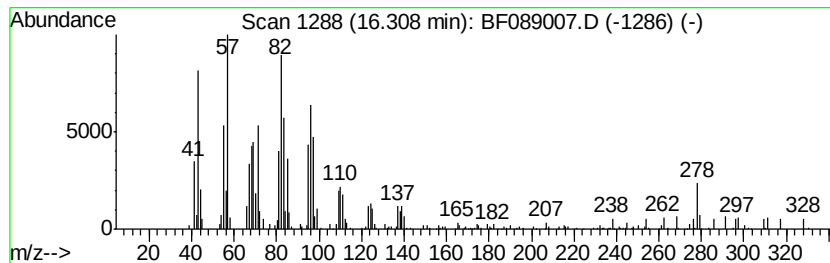
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 14 Oxirane, hexadecyl- Concentration Rank 12

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 16.31 | 15.23 ng | 148405 | Perylene-d12     | 15.19 |

| Hit# | of | Tentative ID                | MW  | MolForm  | CAS#         | Qual |
|------|----|-----------------------------|-----|----------|--------------|------|
| 1    | 5  | Oxirane, hexadecyl-         | 268 | C18H36O  | 007390-81-0  | 94   |
| 2    |    | Octadecanal                 | 268 | C18H36O  | 000638-66-4  | 91   |
| 3    |    | Pentadecanal-               | 226 | C15H30O  | 002765-11-9  | 91   |
| 4    |    | Oxirane, heptadecyl-        | 282 | C19H38O  | 067860-04-2  | 90   |
| 5    |    | Z-10-Octadecen-1-ol acetate | 310 | C20H38O2 | 1000131-07-2 | 86   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

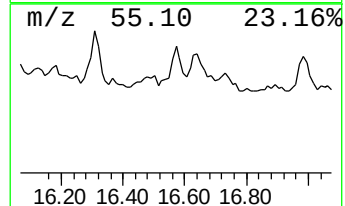
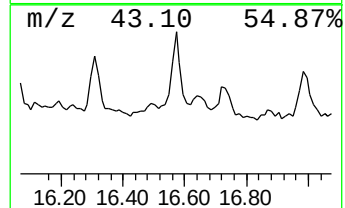
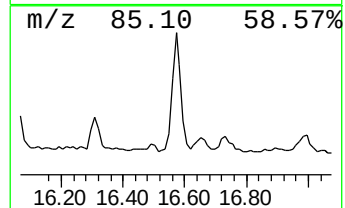
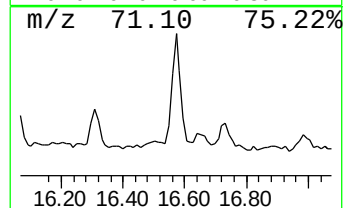
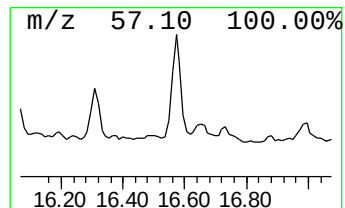
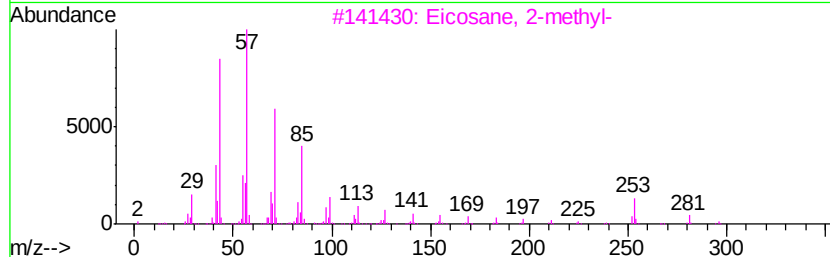
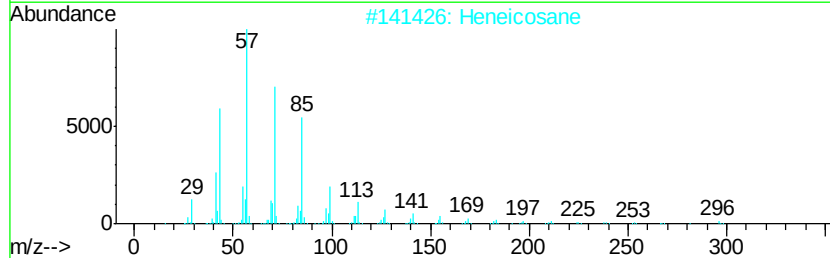
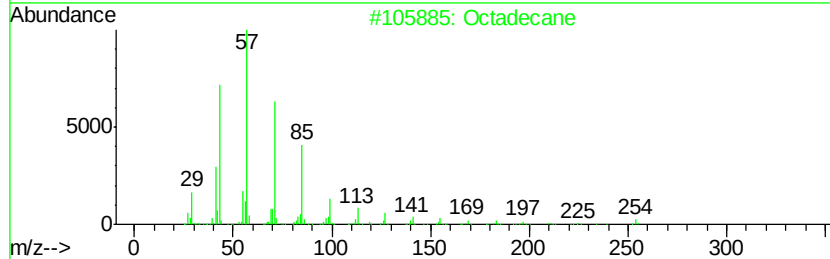
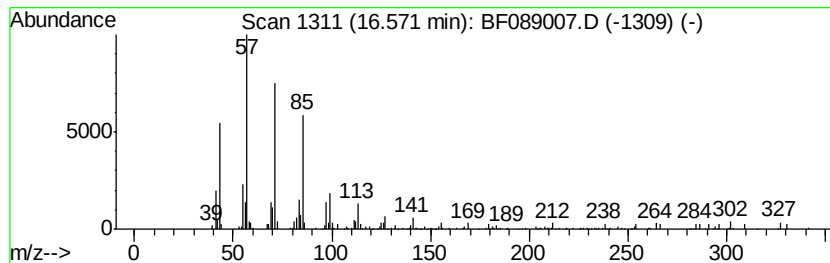
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 15 Octadecane Concentration Rank 17

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 16.57 | 11.14 ng | 108543 | Perylene-d12     | 15.19 |

| Hit# | of | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------|-----|---------|-------------|------|
| 1    | 5  | Octadecane            | 254 | C18H38  | 000593-45-3 | 95   |
| 2    |    | Heneicosane           | 296 | C21H44  | 000629-94-7 | 94   |
| 3    |    | Eicosane, 2-methyl-   | 296 | C21H44  | 001560-84-5 | 93   |
| 4    |    | Hexadecane, 3-methyl- | 240 | C17H36  | 006418-43-5 | 90   |
| 5    |    | Heptadecane           | 240 | C17H36  | 000629-78-7 | 90   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

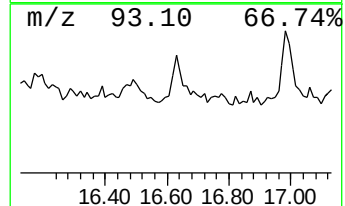
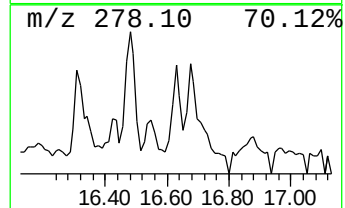
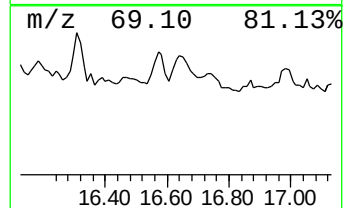
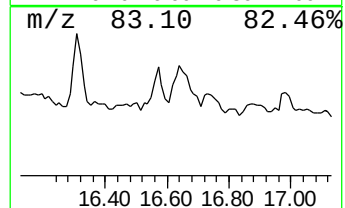
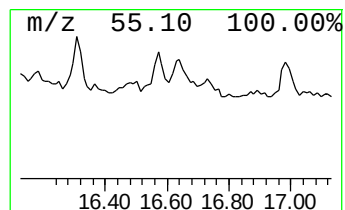
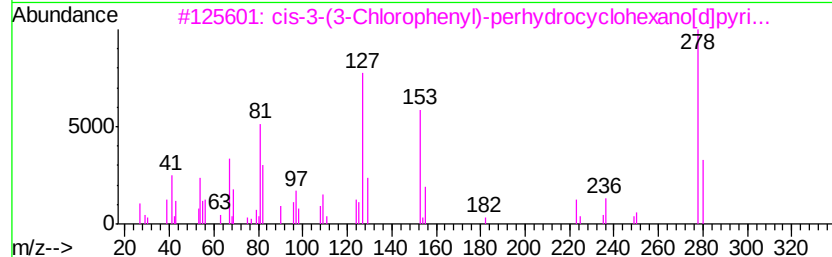
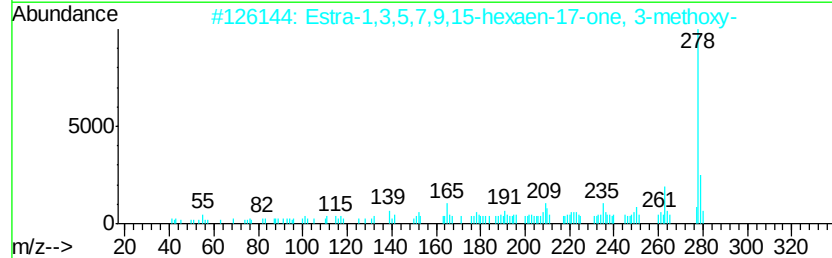
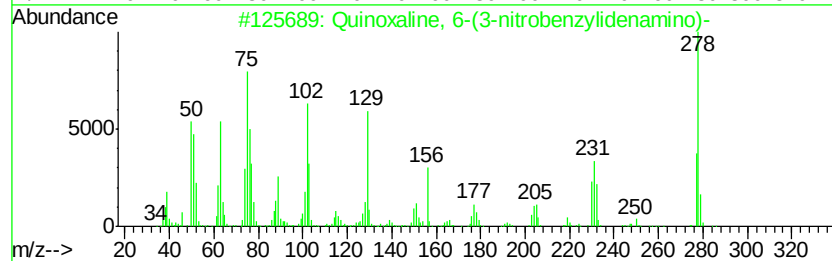
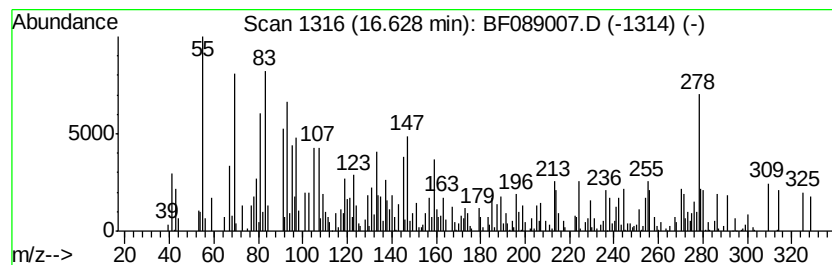
Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 16 Quinoxaline, 6-(3-nitrobenz... Concentration Rank 14

| R.T.    | EstConc  | Area                                  | Relative to ISTD | R.T.         |              |      |
|---------|----------|---------------------------------------|------------------|--------------|--------------|------|
| 16.63   | 13.78 ng | 134276                                | Perylene-d12     | 15.19        |              |      |
| Hit# of | 5        | Tentative ID                          | MW               | MolForm      | CAS#         | Qual |
| 1       |          | Quinoxaline, 6-(3-nitrobenzylidene... | 278              | C15H10N4O2   | 302800-55-1  | 59   |
| 2       |          | Estra-1,3,5,7,9,15-hexaen-17-one...   | 278              | C19H18O2     | 056588-53-5  | 20   |
| 3       |          | cis-3-(3-Chlorophenyl)-perhydroc...   | 278              | C14H15ClN2O2 | 1000148-52-3 | 18   |
| 4       |          | Benzo[bltriphenylene                  | 278              | C22H14       | 000215-58-7  | 15   |
| 5       |          | 2-(4-Methoxyphenyl)-7-methyl-5-o...   | 278              | C17H14N2O2   | 1000303-34-8 | 15   |





Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

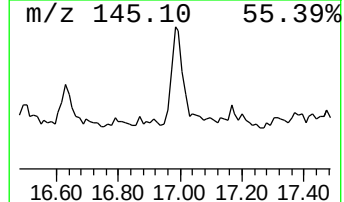
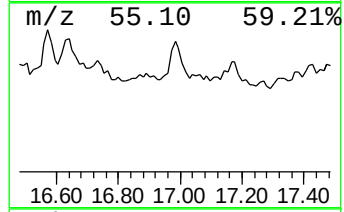
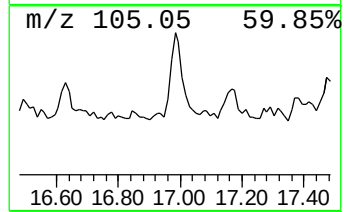
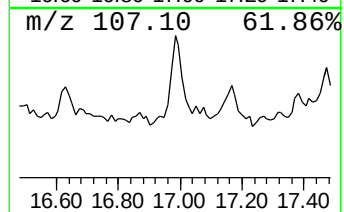
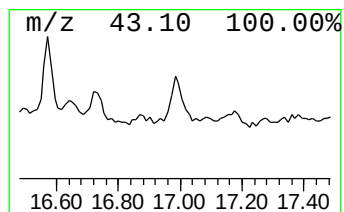
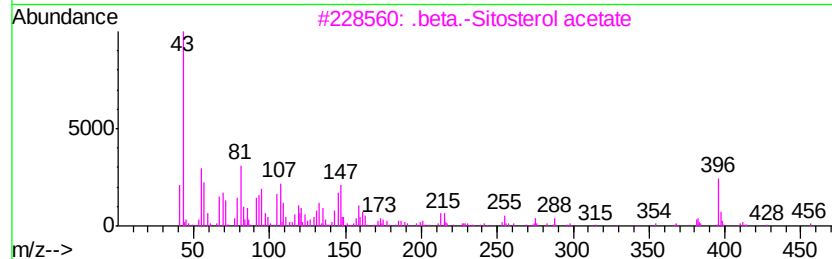
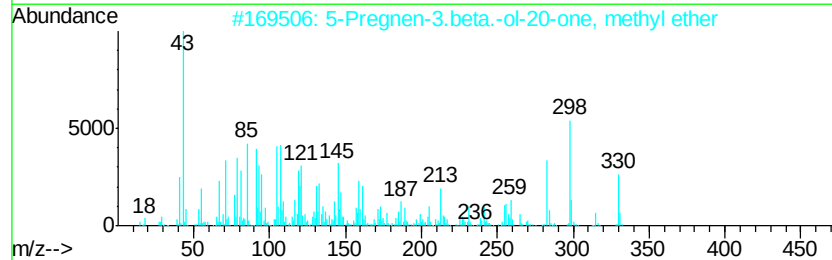
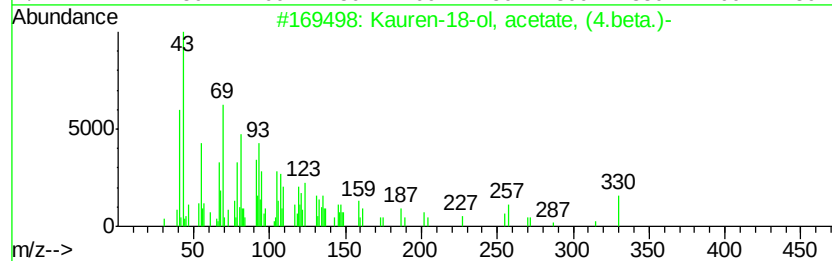
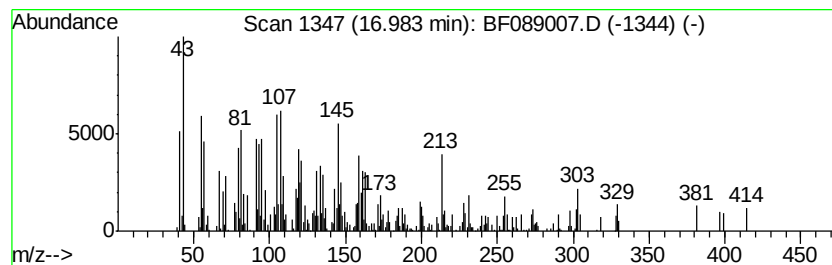
Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 17 Kauren-18-ol, acetate, (4.b... Concentration Rank 9

| R.T.    | EstConc  | Area                                | Relative to ISTD | R.T.      |              |      |
|---------|----------|-------------------------------------|------------------|-----------|--------------|------|
| 16.98   | 23.81 ng | 231989                              | Perylene-d12     | 15.19     |              |      |
| Hit# of | 5        | Tentative ID                        | MW               | MolForm   | CAS#         | Qual |
| 1       |          | Kauren-18-ol, acetate, (4.beta.)-   | 330              | C22H34O2  | 072150-74-4  | 55   |
| 2       |          | 5-Pregnen-3.beta.-ol-20-one, met... | 330              | C22H34O2  | 1000364-94-5 | 40   |
| 3       |          | .beta.-Sitosterol acetate           | 456              | C31H52O2  | 000915-05-9  | 32   |
| 4       |          | Pren-5-en-3-ol, 21-bromo-20-met...  | 394              | C22H35BrO | 055103-80-5  | 22   |
| 5       |          | Bisnor-7-desoxycholic acid          | 364              | C22H36O4  | 1000252-00-7 | 12   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

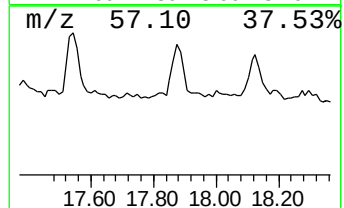
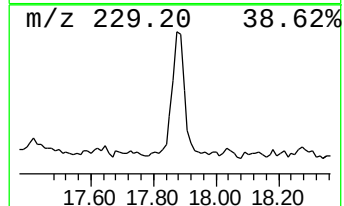
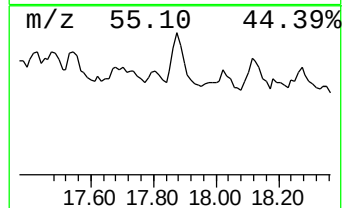
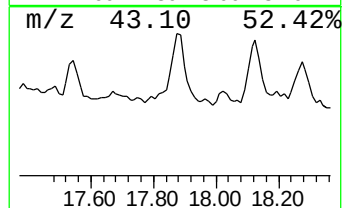
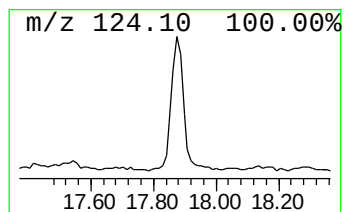
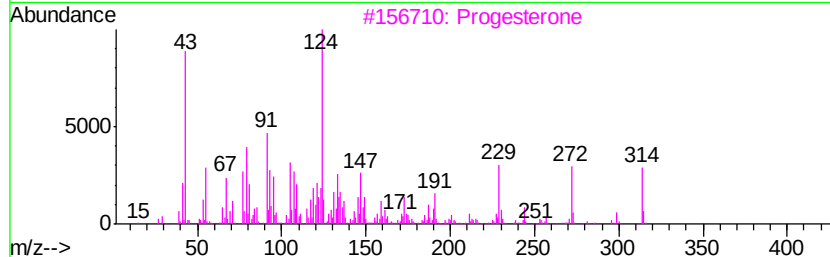
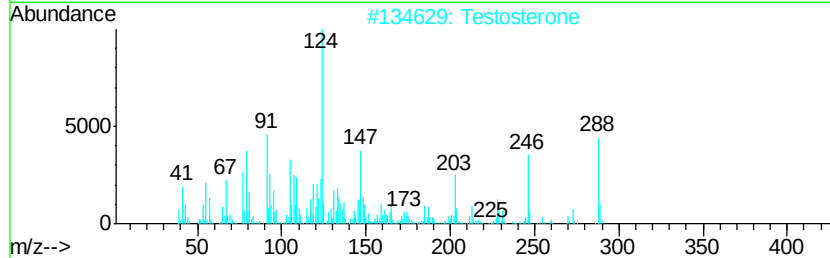
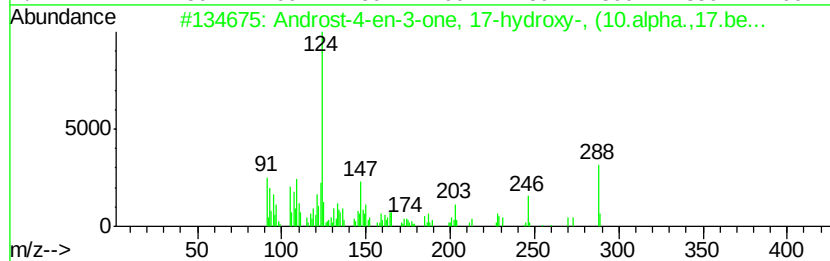
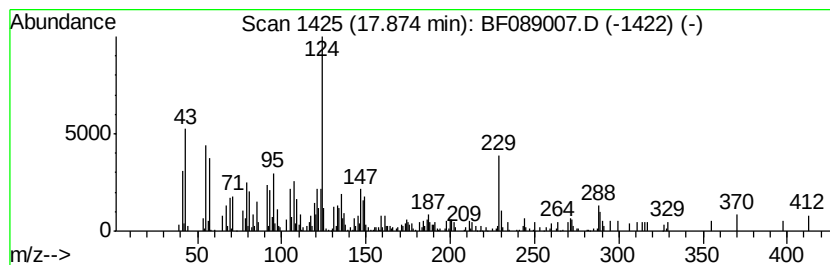
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 18 Androst-4-en-3-one, 17-hydr... Concentration Rank 8

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 17.87 | 29.67 ng | 289092 | Perylene-d12     | 15.19 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#         | Qual |
|------|----|--------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Androst-4-en-3-one, 17-hydroxy-, ... | 288 | C19H28O2 | 000604-39-7  | 83   |
| 2    |    | Testosterone                         | 288 | C19H28O2 | 000058-22-0  | 52   |
| 3    |    | Progesterone                         | 314 | C21H30O2 | 000057-83-0  | 52   |
| 4    |    | (1S,2E,4S,5R,7E,11E)-Cembra-2,7,...  | 306 | C20H34O2 | 1000140-92-3 | 47   |
| 5    |    | Pregn-4-ene-3,20-dione, (8.alpha...  | 314 | C21H30O2 | 003795-19-5  | 45   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

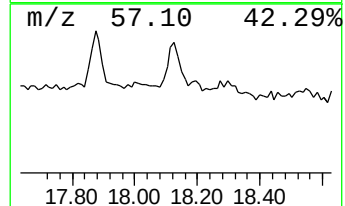
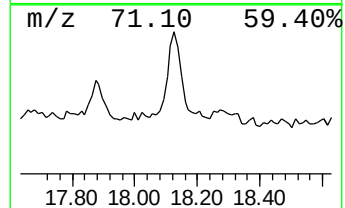
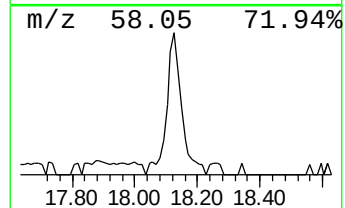
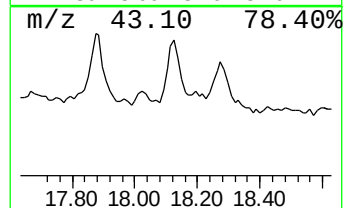
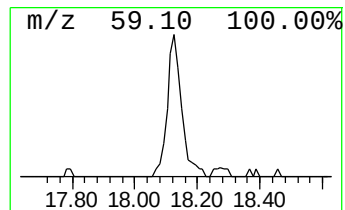
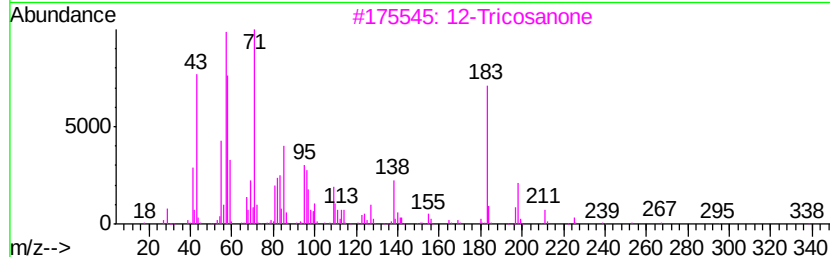
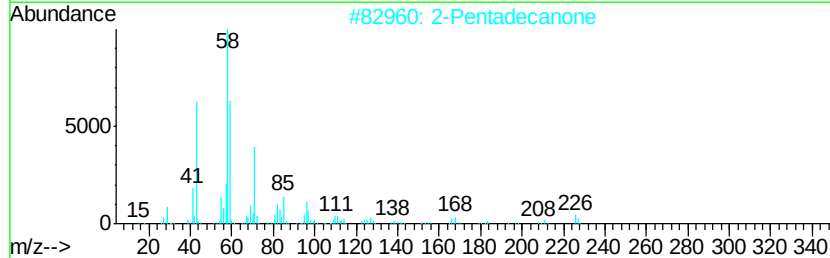
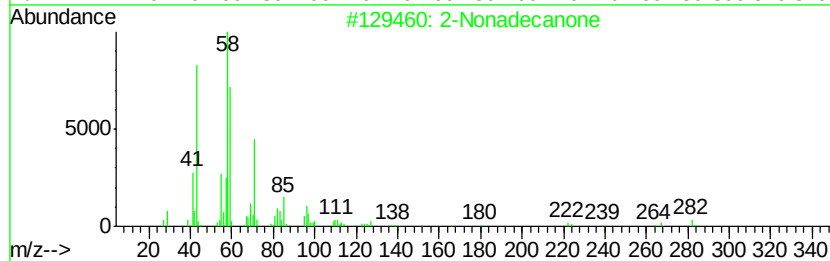
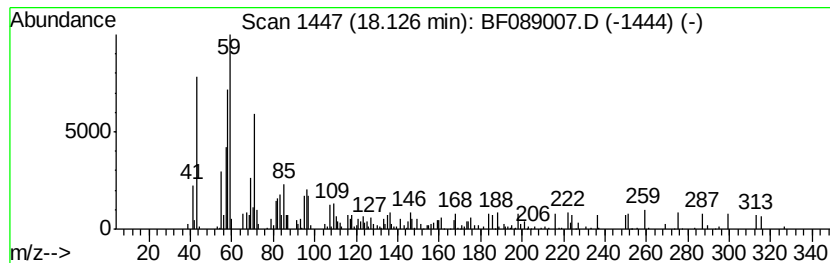
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 19 2-Nonadecanone Concentration Rank 19

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 18.13 | 9.82 ng | 95676 | Perylene-d12     | 15.19 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | 2-Nonadecanone                      | 282 | C19H38O | 000629-66-3  | 53   |
| 2    |    |   | 2-Pentadecanone                     | 226 | C15H30O | 002345-28-0  | 53   |
| 3    |    |   | 12-Tricosanone                      | 338 | C23H46O | 000540-09-0  | 43   |
| 4    |    |   | Carbonic acid, 2-methoxyethyl ne... | 190 | C9H18O4 | 1000331-42-7 | 43   |
| 5    |    |   | 2-Pentanol, 5-methoxy-2-methyl-     | 132 | C7H16O2 | 055724-04-4  | 38   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
Data File : BF089007.D  
Acq On : 15 Jul 2016 1:51  
Operator : UM/SJ  
Sample : H3995-02  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

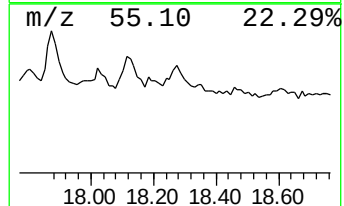
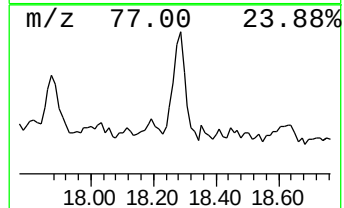
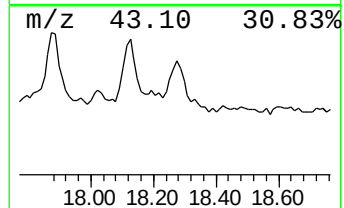
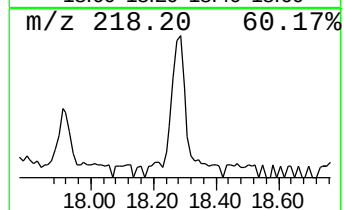
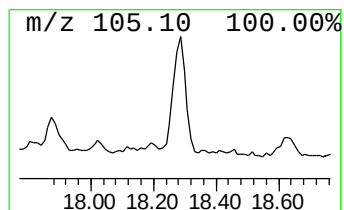
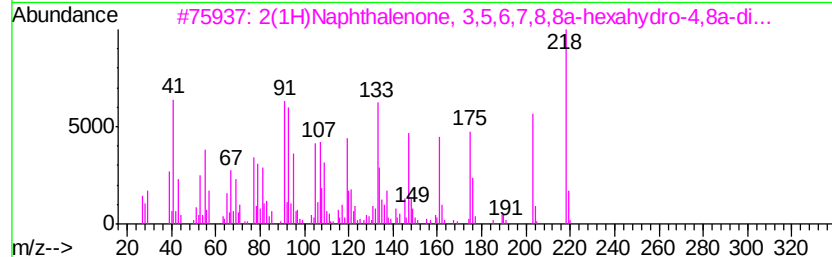
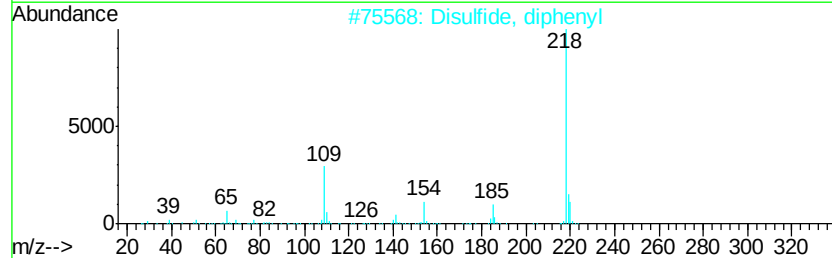
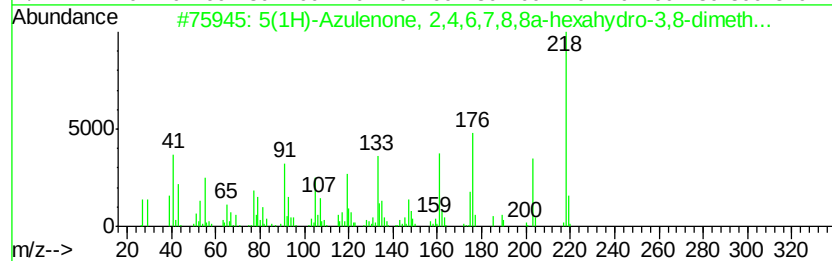
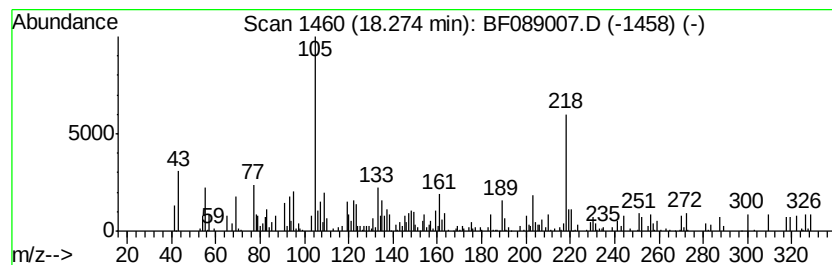
Instrument :  
BNA\_F  
ClientSampleId :  
LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 20 5(1H)-Azulenone, 2,4,6,7,8,... Concentration Rank 7

| R.T.    | EstConc                             | Area         | Relative to ISTD | R.T.         |      |      |
|---------|-------------------------------------|--------------|------------------|--------------|------|------|
| 18.27   | 31.34 ng                            | 305345       | Perylene-d12     | 15.19        |      |      |
| Hit# of | 5                                   | Tentative ID | MW               | MolForm      | CAS# | Qual |
| 1       | 5(1H)-Azulenone, 2,4,6,7,8,8a-he... | 218          | C15H22O          | 006754-66-1  | 56   |      |
| 2       | Disulfide, diphenyl                 | 218          | C12H10S2         | 000882-33-7  | 43   |      |
| 3       | 2(1H)Naphthalenone, 3,5,6,7,8,8a... | 218          | C15H22O          | 1000188-66-5 | 43   |      |
| 4       | Thieno[3,2-b]thiophene-2,5-diimi... | 218          | C8H2N4S2         | 125594-14-1  | 30   |      |
| 5       | 3H-Naphthol[2,3-c]-1,2-dithiol-3... | 218          | C11H6OS2         | 199166-69-3  | 30   |      |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071416\  
 Data File : BF089007.D  
 Acq On : 15 Jul 2016 1:51  
 Operator : UM/SJ  
 Sample : H3995-02  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 LSS-SB-SB12(0-2in)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF063016.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 |
| unknown1.86          | 1.86  | 9.9     | ng    | 150974   | 1                     | 6.68  | 305266 | 20.0 |
| 2-Pentanone, 4-hy... | 4.84  | 11.9    | ng    | 180902   | 1                     | 6.68  | 305266 | 20.0 |
| unknown6.47          | 6.47  | 107.7   | ng    | 1643920  | 1                     | 6.68  | 305266 | 20.0 |
| n-Hexadecanoic acid  | 11.75 | 7.8     | ng    | 170232   | 4                     | 11.20 | 439041 | 20.0 |
| Cyclohexadecane      | 14.32 | 11.4    | ng    | 335208   | 5                     | 13.82 | 588740 | 20.0 |
| 16-Octadecenal       | 14.73 | 14.3    | ng    | 139276   | 6                     | 15.19 | 194882 | 20.0 |
| Eicosane             | 14.90 | 85.8    | ng    | 835698   | 6                     | 15.19 | 194882 | 20.0 |
| Heneicosane          | 15.62 | 135.4   | ng    | 1319550  | 6                     | 15.19 | 194882 | 20.0 |
| 1-Heptacosanol       | 15.67 | 18.5    | ng    | 180106   | 6                     | 15.19 | 194882 | 20.0 |
| Oxirane, hexadecyl-  | 16.31 | 15.2    | ng    | 148405   | 6                     | 15.19 | 194882 | 20.0 |
| Octadecane           | 16.57 | 11.1    | ng    | 108543   | 6                     | 15.19 | 194882 | 20.0 |
| Quinoxaline, 6-(3... | 16.63 | 13.8    | ng    | 134276   | 6                     | 15.19 | 194882 | 20.0 |
| Kauren-18-ol, ace... | 16.98 | 23.8    | ng    | 231989   | 6                     | 15.19 | 194882 | 20.0 |
| Androst-4-en-3-on... | 17.87 | 29.7    | ng    | 289092   | 6                     | 15.19 | 194882 | 20.0 |
| 2-Nonadecanone       | 18.13 | 9.8     | ng    | 95676    | 6                     | 15.19 | 194882 | 20.0 |
| 5(1H)-Azulenone, ... | 18.27 | 31.3    | ng    | 305345   | 6                     | 15.19 | 194882 | 20.0 |