

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF060517\  
 Data File : BF095686.D  
 Acq On : 5 Jun 2017 22:09  
 Operator : SJ/MA  
 Sample : I3444-07  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 BU-RO-298-060117

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-BF060517.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         | 1.601       | 8             | 11          | 46           | rVB      | 812458         | 1586188       | 4.98%           | 2.347%        |
| 2         | 5.289       | 634           | 638         | 670          | rBV      | 562546         | 1246815       | 3.92%           | 1.845%        |
| 3         | 6.948       | 916           | 920         | 934          | rBV      | 685174         | 1200090       | 3.77%           | 1.776%        |
| 4         | 7.048       | 934           | 937         | 949          | rVB      | 908122         | 1416803       | 4.45%           | 2.097%        |
| 5         | 7.395       | 993           | 996         | 1010         | rBV      | 420776         | 589091        | 1.85%           | 0.872%        |
| 6         | 7.630       | 1032          | 1036        | 1060         | rBV      | 759981         | 1103601       | 3.47%           | 1.633%        |
| 7         | 8.307       | 1148          | 1151        | 1170         | rBV      | 477468         | 734929        | 2.31%           | 1.088%        |
| 8         | 9.430       | 1334          | 1342        | 1355         | rBV      | 645225         | 889694        | 2.79%           | 1.317%        |
| 9         | 11.207      | 1639          | 1644        | 1651         | rBV      | 1287525        | 1529196       | 4.80%           | 2.263%        |
| 10        | 12.248      | 1817          | 1821        | 1826         | rBV2     | 740296         | 893975        | 2.81%           | 1.323%        |
| 11        | 13.542      | 2037          | 2041        | 2049         | rBV      | 503024         | 735981        | 2.31%           | 1.089%        |
| 12        | 14.642      | 2225          | 2228        | 2241         | rVB      | 605226         | 857265        | 2.69%           | 1.269%        |
| 13        | 15.477      | 2357          | 2370        | 2373         | rBV      | 4999438        | 11541849      | 36.25%          | 17.079%       |
| 14        | 16.500      | 2522          | 2544        | 2546         | rBV6     | 5711625        | 31835365      | 100.00%         | 47.108%       |
| 15        | 16.606      | 2556          | 2562        | 2565         | rBV      | 4104724        | 5599247       | 17.59%          | 8.285%        |
| 16        | 16.636      | 2565          | 2567        | 2569         | rVV      | 579995         | 524295        | 1.65%           | 0.776%        |
| 17        | 16.659      | 2569          | 2571        | 2586         | rVB3     | 368731         | 510275        | 1.60%           | 0.755%        |
| 18        | 17.024      | 2629          | 2633        | 2638         | rVB      | 979654         | 997386        | 3.13%           | 1.476%        |
| 19        | 17.330      | 2677          | 2685        | 2687         | rBV2     | 264337         | 429574        | 1.35%           | 0.636%        |
| 20        | 17.430      | 2699          | 2702        | 2712         | rVB2     | 406789         | 624202        | 1.96%           | 0.924%        |
| 21        | 17.547      | 2716          | 2722        | 2730         | rBV2     | 671789         | 1047179       | 3.29%           | 1.550%        |
| 22        | 18.353      | 2855          | 2859        | 2863         | rBV      | 513528         | 593524        | 1.86%           | 0.878%        |
| 23        | 18.400      | 2863          | 2867        | 2871         | rVB      | 533354         | 598438        | 1.88%           | 0.886%        |
| 24        | 20.018      | 3138          | 3142        | 3150         | rVB      | 382555         | 494211        | 1.55%           | 0.731%        |

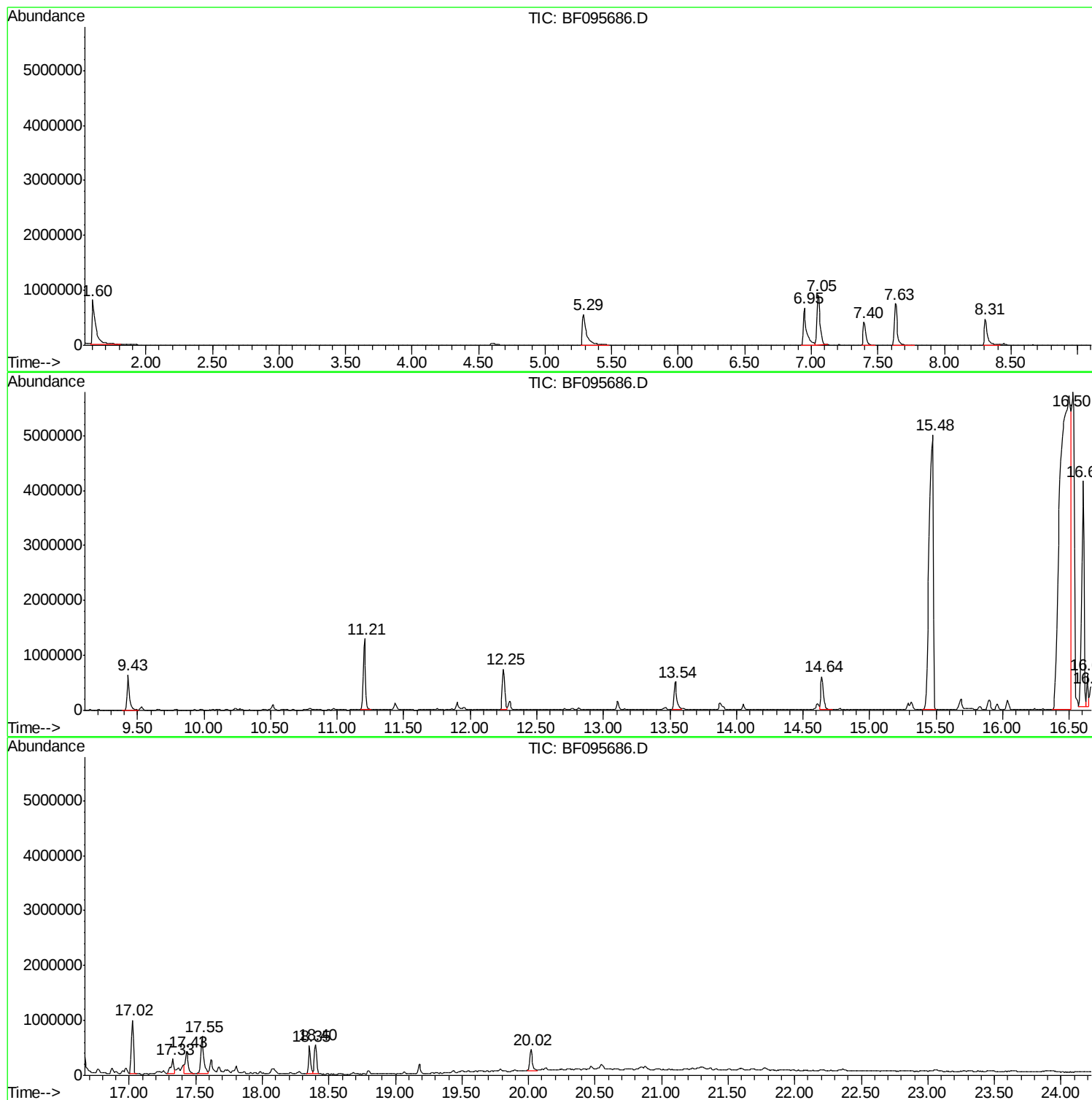
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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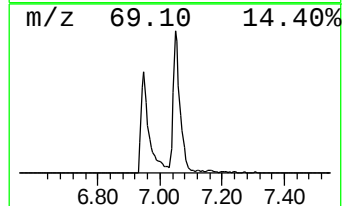
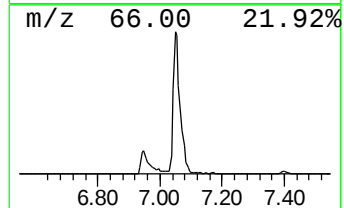
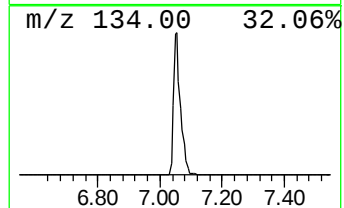
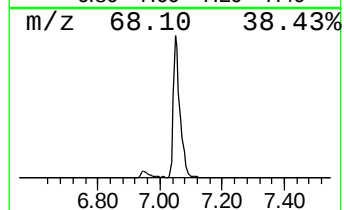
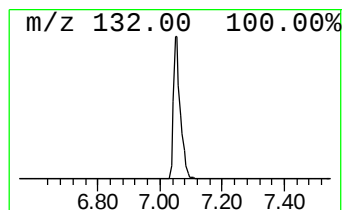
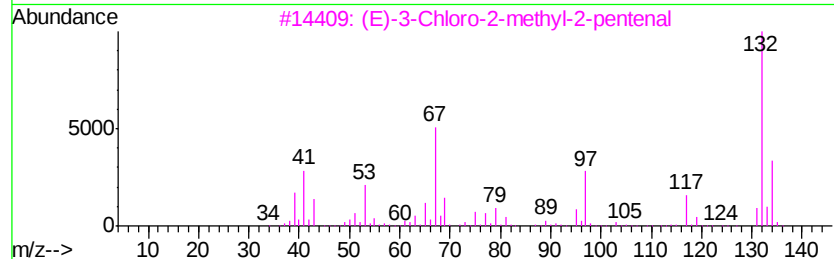
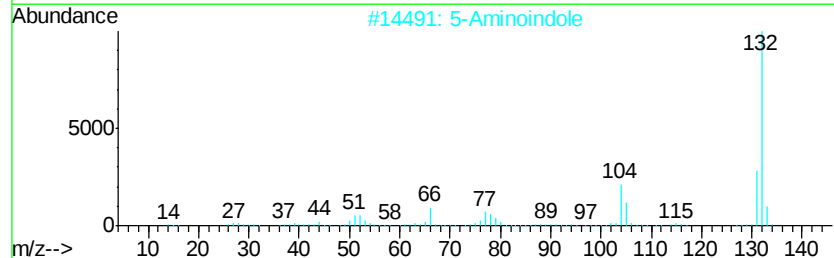
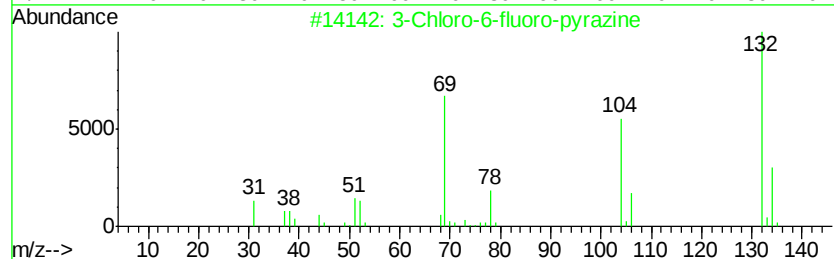
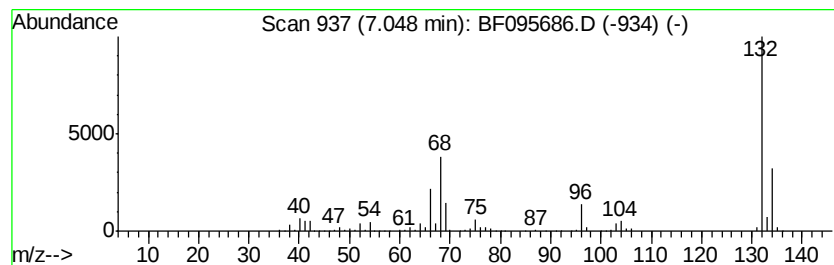
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown7.05 Concentration Rank 5

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.05 | 48.10 ng | 1416800 | 1,4-Dichlorobenzene-d4 | 7.40 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 16   |
| 2    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 3    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 12   |
| 4    |    | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6  | 10   |
| 5    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 10   |



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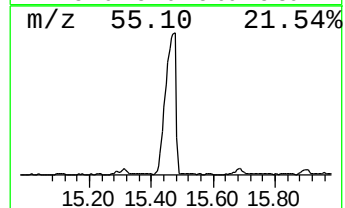
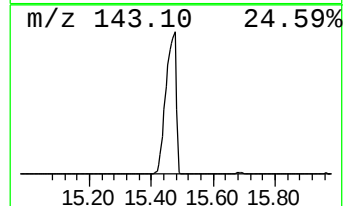
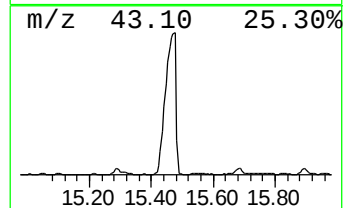
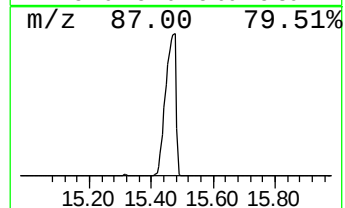
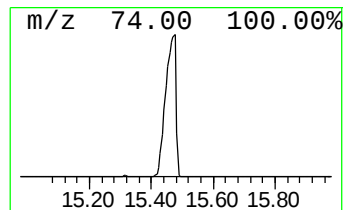
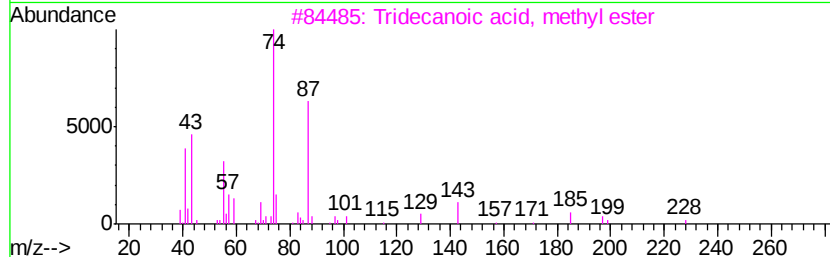
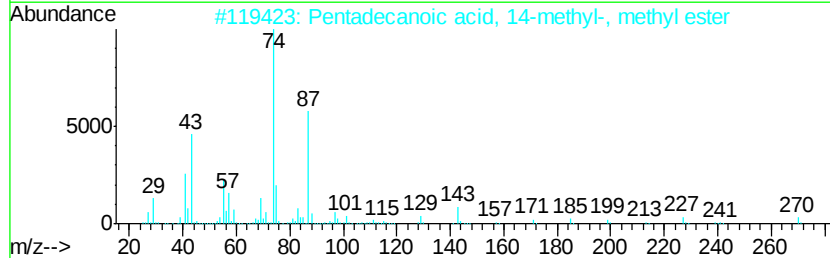
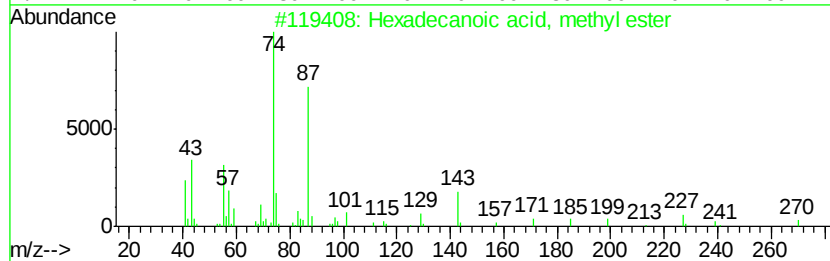
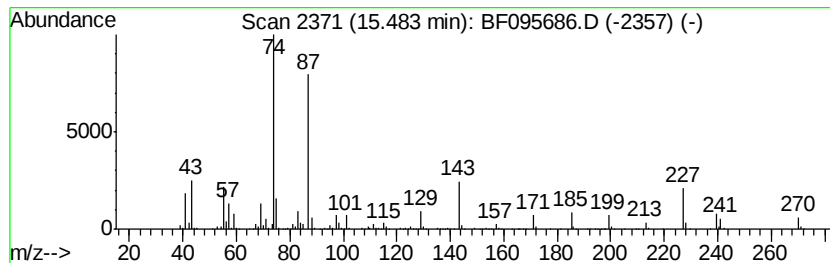
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 2

| R.T.  | EstConc   | Area     | Relative to ISTD | R.T.  |
|-------|-----------|----------|------------------|-------|
| 15.48 | 269.27 ng | 11541800 | Phenanthrene-d10 | 14.64 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Hexadecanoic acid, methyl ester     | 270 | C17H34O2 | 000112-39-0 | 99   |
| 2    |    | Pentadecanoic acid, 14-methyl-, ... | 270 | C17H34O2 | 005129-60-2 | 93   |
| 3    |    | Tridecanoic acid, methyl ester      | 228 | C14H28O2 | 001731-88-0 | 92   |
| 4    |    | Pentadecanoic acid, methyl ester    | 256 | C16H32O2 | 007132-64-1 | 86   |
| 5    |    | Decanoic acid, methyl ester         | 186 | C11H22O2 | 000110-42-9 | 83   |



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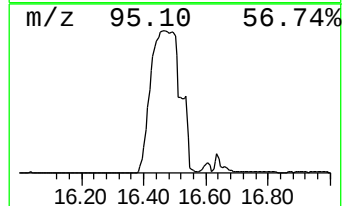
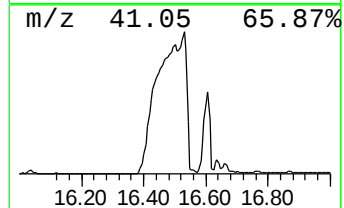
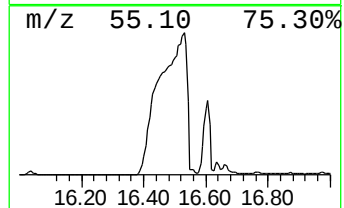
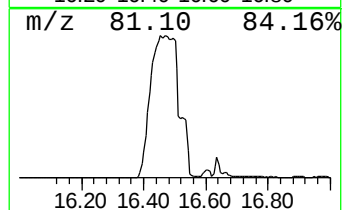
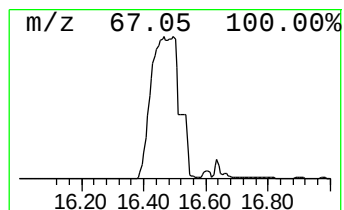
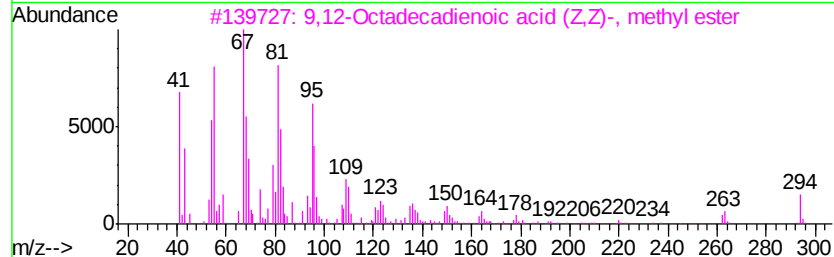
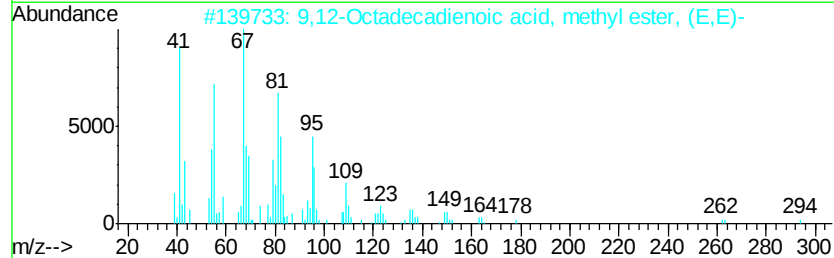
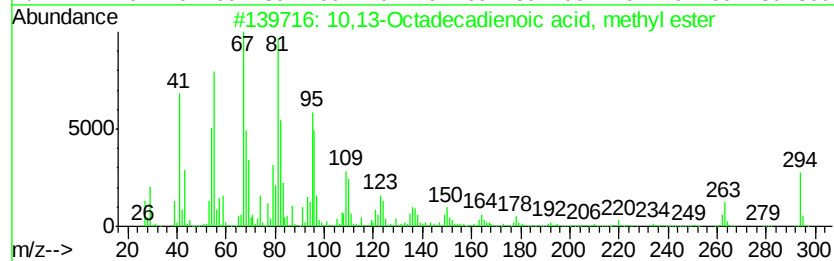
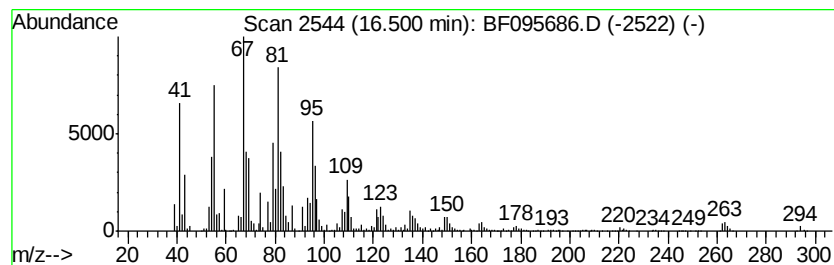
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 10,13-Octadecadienoic acid,... Concentration Rank 1

| R.T.  | EstConc    | Area     | Relative to ISTD | R.T.  |
|-------|------------|----------|------------------|-------|
| 16.50 | 1072.76 ng | 31835400 | Chrysene-d12     | 18.35 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 10,13-Octadecadienoic acid, meth... | 294 | C19H34O2 | 056554-62-2 | 99   |
| 2    |    | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4 | 99   |
| 3    |    | 9,12-Octadecadienoic acid (Z,Z)-... | 294 | C19H34O2 | 000112-63-0 | 98   |
| 4    |    | 9,15-Octadecadienoic acid, methy... | 294 | C19H34O2 | 017309-05-6 | 98   |
| 5    |    | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002462-85-3 | 98   |



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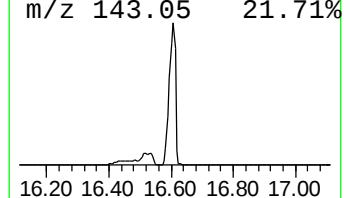
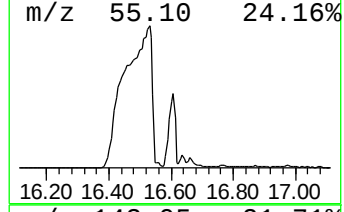
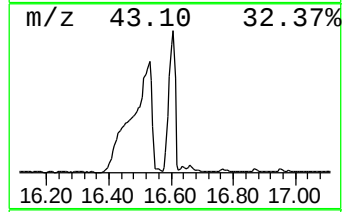
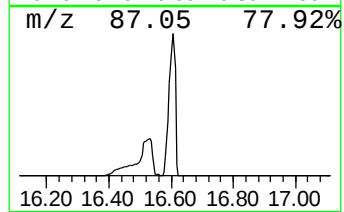
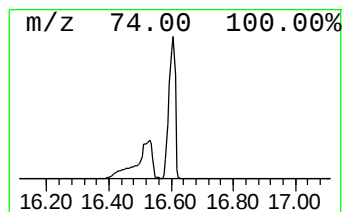
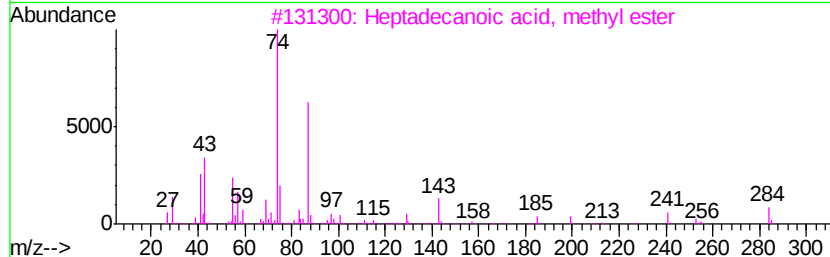
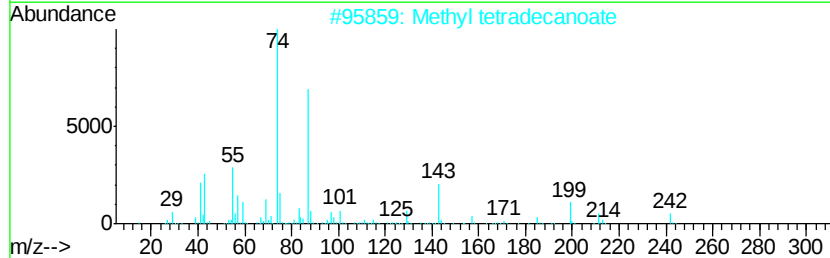
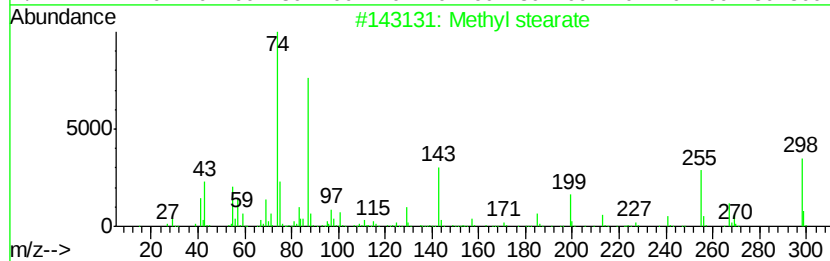
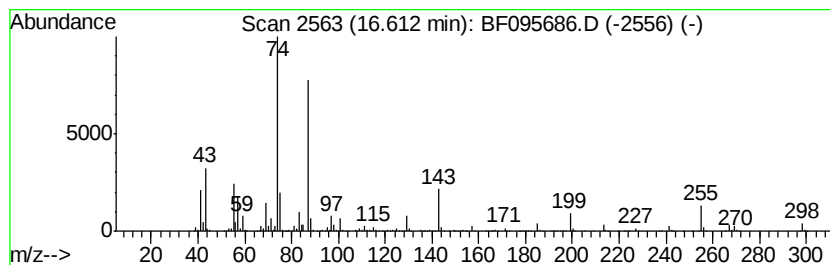
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 Methyl stearate Concentration Rank 3

| R.T.  | EstConc   | Area    | Relative to ISTD | R.T.  |
|-------|-----------|---------|------------------|-------|
| 16.61 | 188.68 ng | 5599250 | Chrysene-d12     | 18.35 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Methyl stearate                     | 298 | C19H38O2 | 000112-61-8 | 98   |
| 2    |    | Methyl tetradecanoate               | 242 | C15H30O2 | 000124-10-7 | 94   |
| 3    |    | Heptadecanoic acid, methyl ester    | 284 | C18H36O2 | 001731-92-6 | 91   |
| 4    |    | Heptadecanoic acid, 16-methyl-, ... | 298 | C19H38O2 | 005129-61-3 | 90   |
| 5    |    | Pentadecanoic acid, methyl ester    | 256 | C16H32O2 | 007132-64-1 | 90   |



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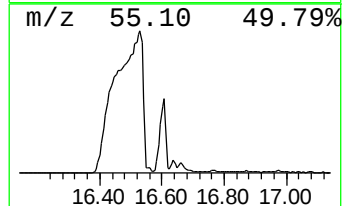
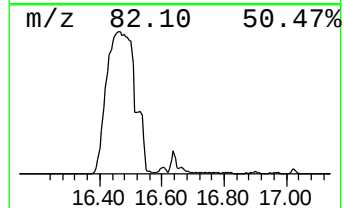
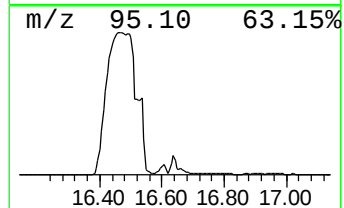
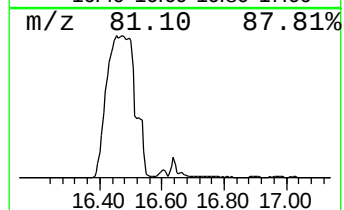
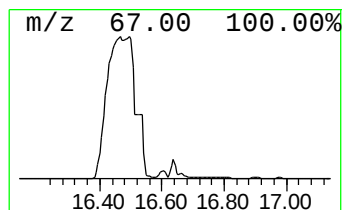
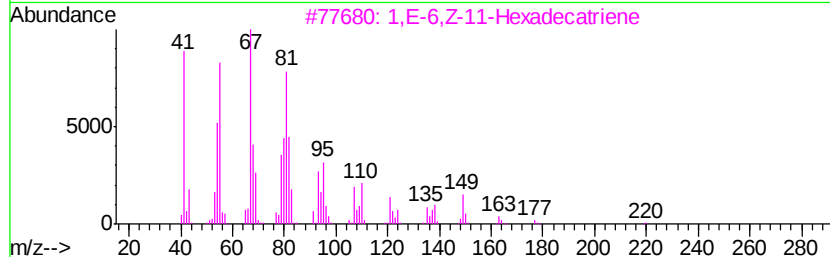
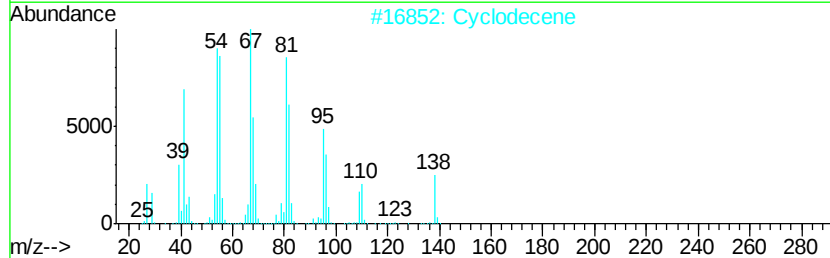
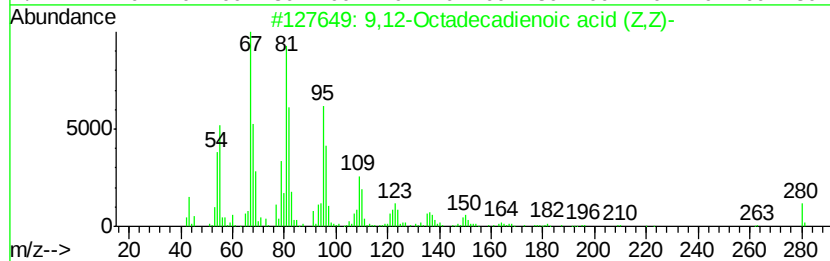
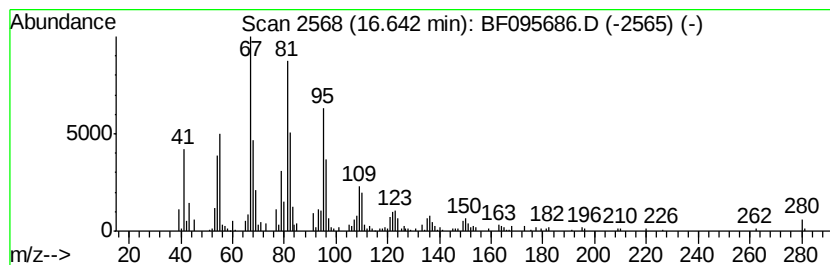
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 7 9,12-Octadecadienoic acid (... Concentration Rank 9

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 16.64 | 17.67 ng | 524295 | Chrysene-d12     | 18.35 |

| Hit# | of | Tentative ID                      | MW  | MolForm  | CAS#        | Qual |
|------|----|-----------------------------------|-----|----------|-------------|------|
| 1    | 5  | 9,12-Octadecadienoic acid (Z,Z)-  | 280 | C18H32O2 | 000060-33-3 | 99   |
| 2    |    | Cyclodecene                       | 138 | C10H18   | 003618-12-0 | 95   |
| 3    |    | 1,E-6,Z-11-Hexadecatriene         | 220 | C16H28   | 083483-55-0 | 81   |
| 4    |    | 7-Tetradecyne                     | 194 | C14H26   | 035216-11-6 | 80   |
| 5    |    | 9-Octadecynoic acid, methyl ester | 294 | C19H34O2 | 001120-32-7 | 80   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF060517\  
Data File : BF095686.D  
Acq On : 5 Jun 2017 22:09  
Operator : SJ/MA  
Sample : I3444-07  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BU-RO-298-060117

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

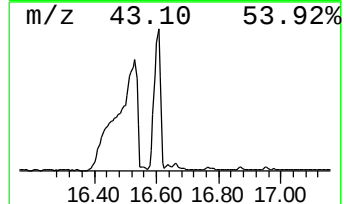
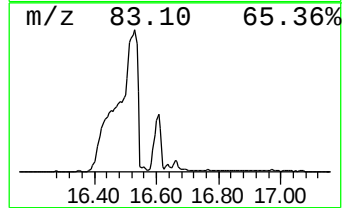
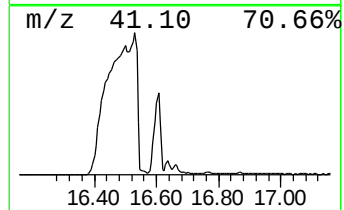
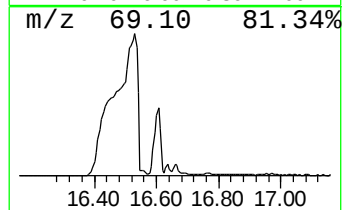
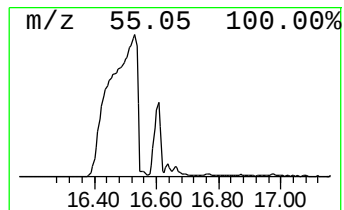
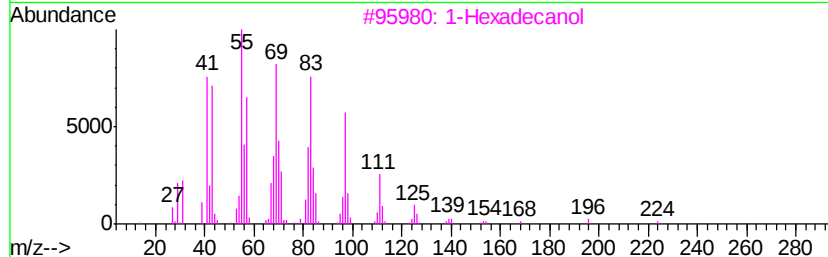
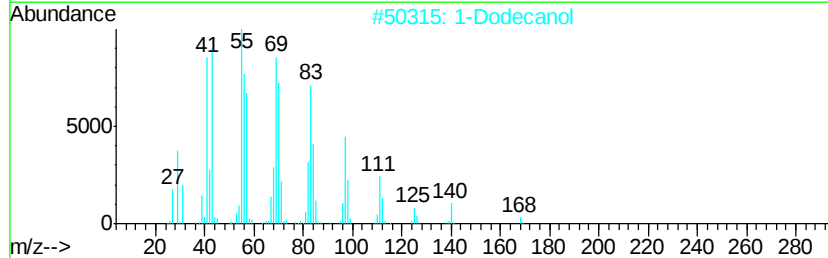
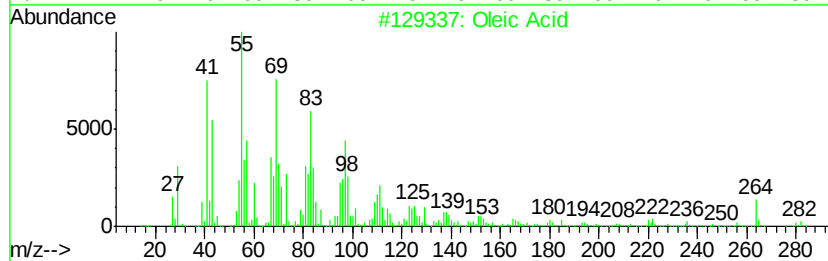
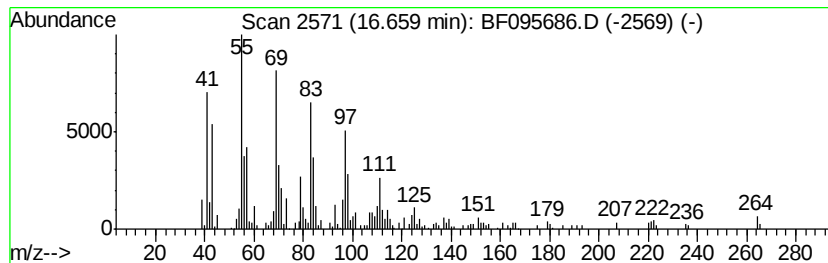
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 8 Oleic Acid Concentration Rank 10

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 16.66 | 17.19 ng | 510275 | Chrysene-d12     | 18.35 |

| Hit# | of | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---------------------|-----|----------|-------------|------|
| 1    | 5  | Oleic Acid          | 282 | C18H34O2 | 000112-80-1 | 90   |
| 2    |    | 1-Dodecanol         | 186 | C12H26O  | 000112-53-8 | 80   |
| 3    |    | 1-Hexadecanol       | 242 | C16H34O  | 036653-82-4 | 72   |
| 4    |    | Cyclopentadecane    | 210 | C15H30   | 000295-48-7 | 72   |
| 5    |    | 17-Pentatriacontene | 491 | C35H70   | 006971-40-0 | 72   |



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Data File : BF095686.D  
Acq On : 5 Jun 2017 22:09  
Operator : SJ/MA  
Sample : I3444-07  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

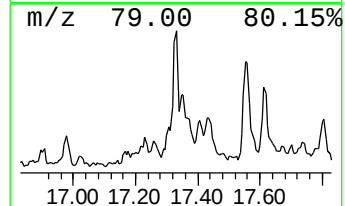
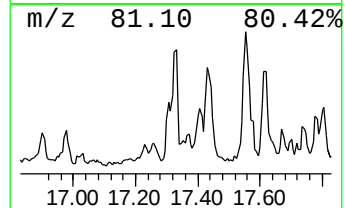
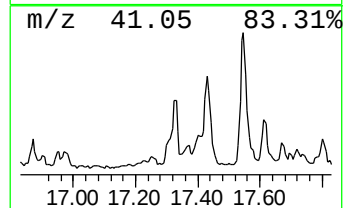
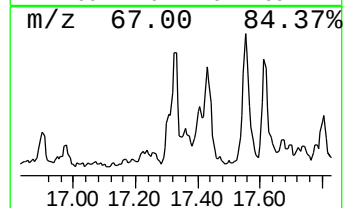
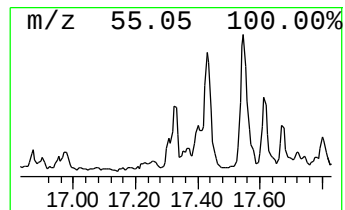
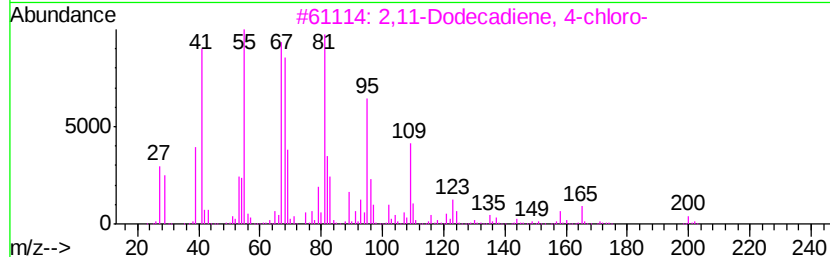
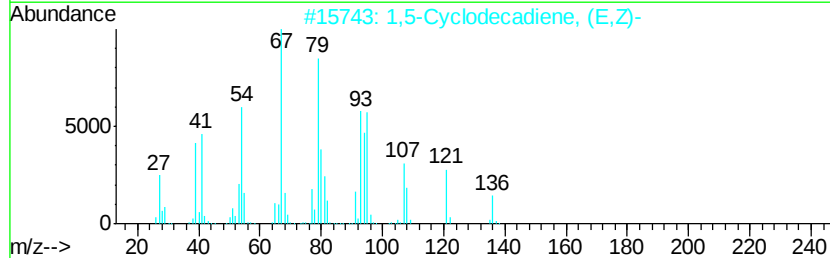
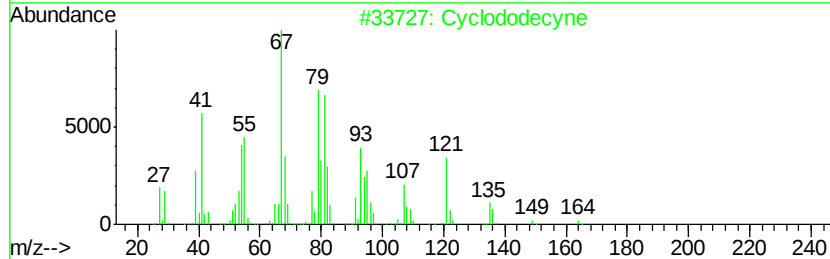
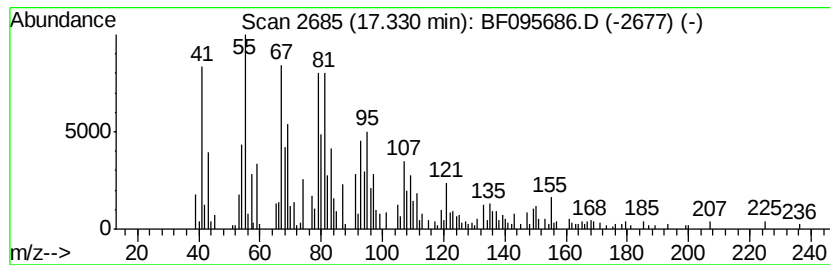
Instrument :  
BNA\_F  
ClientSampleId :  
BU-RO-298-060117

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060517.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 9 Cyclododecyne Concentration Rank 11

| R.T.    | EstConc  | Area                            | Relative to ISTD | R.T.            |
|---------|----------|---------------------------------|------------------|-----------------|
| 17.33   | 14.48 ng | 429574                          | Chrysene-d12     | 18.35           |
| Hit# of | 5        | Tentative ID                    | MW MolForm       | CAS# Qual       |
| 1       |          | Cyclododecyne                   | 164 C12H20       | 001129-90-4 89  |
| 2       |          | 1,5-Cyclodecadiene, (E,Z)-      | 136 C10H16       | 001124-78-3 78  |
| 3       |          | 2,11-Dodecadiene, 4-chloro-     | 200 C12H21Cl     | 1000155-54-5 60 |
| 4       |          | 1-Methyl-2-methylenecyclohexane | 110 C8H14        | 002808-75-5 50  |
| 5       |          | 11-Hexadecynal                  | 236 C16H28O      | 086426-73-5 49  |



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Operator : SJ/MA  
Sample : I3444-07  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BU-RO-298-060117

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

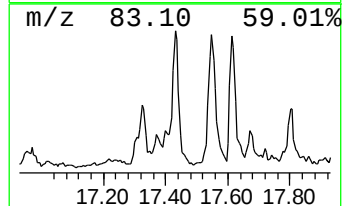
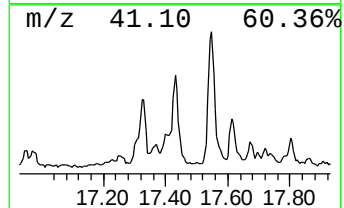
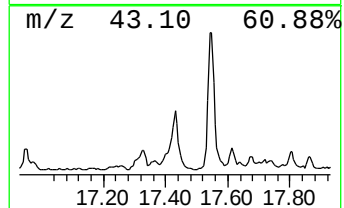
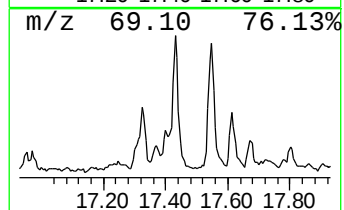
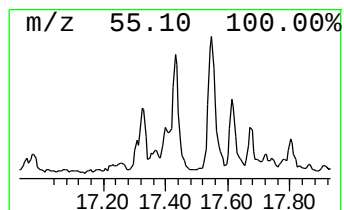
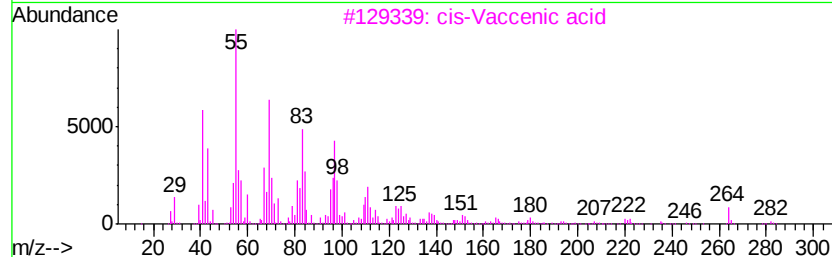
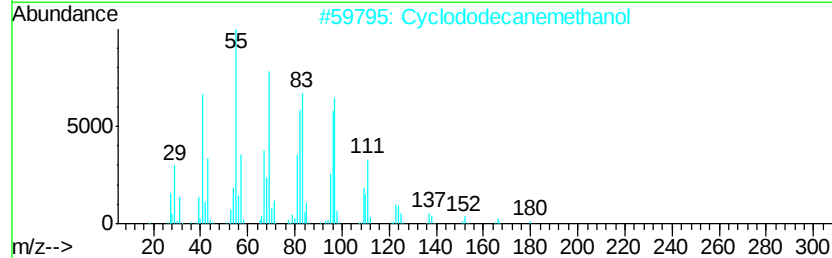
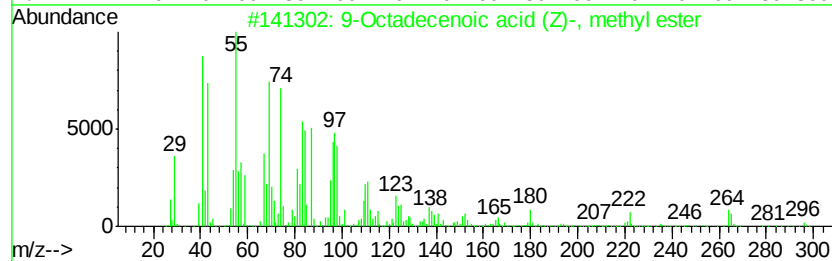
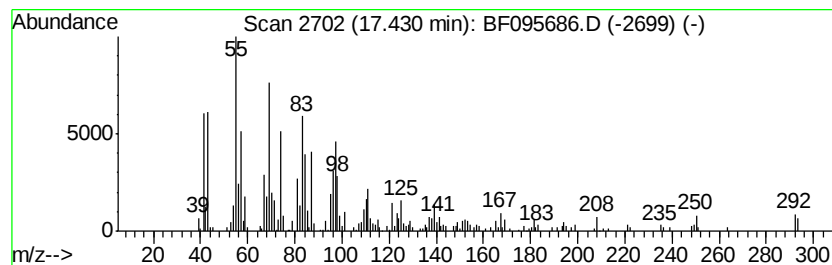
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 10 9-Octadecenoic acid (Z)-, m... Concentration Rank 8

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 17.43 | 21.03 ng | 624202 | Chrysene-d12     | 18.35 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 58   |
| 2    |    | Cyclododecanemethanol               | 198 | C13H26O  | 001892-12-2 | 49   |
| 3    |    | cis-Vaccenic acid                   | 282 | C18H34O2 | 000506-17-2 | 46   |
| 4    |    | Cyclobutanone, 2-(1,1-dimethylet... | 126 | C8H14O   | 004579-31-1 | 42   |
| 5    |    | Cyclohexane, 1-(cyclohexylmethyl... | 208 | C15H28   | 054934-92-8 | 41   |



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Operator : SJ/MA  
Sample : I3444-07  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BU-RO-298-060117

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

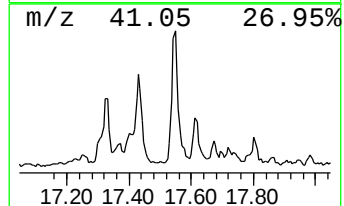
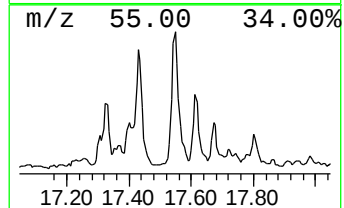
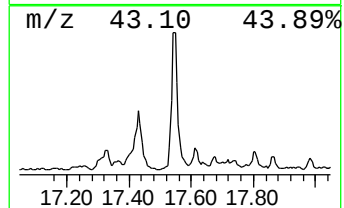
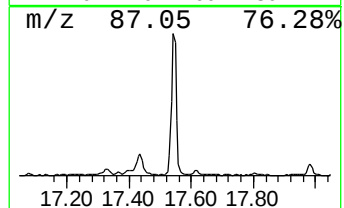
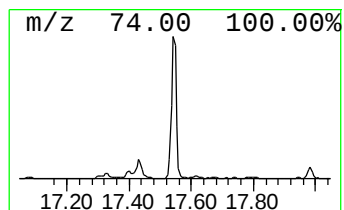
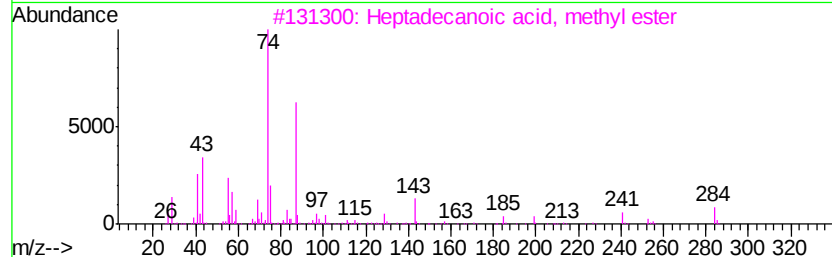
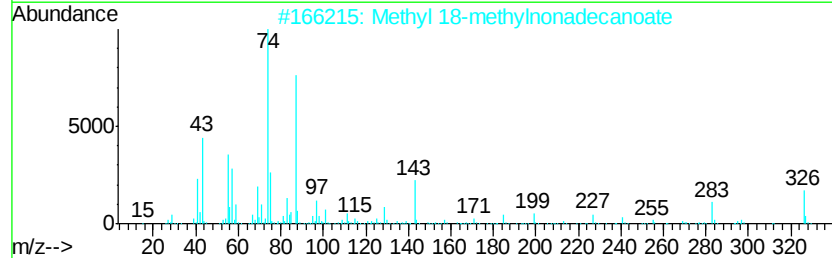
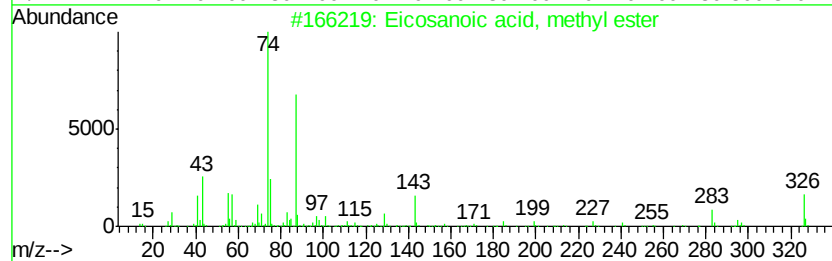
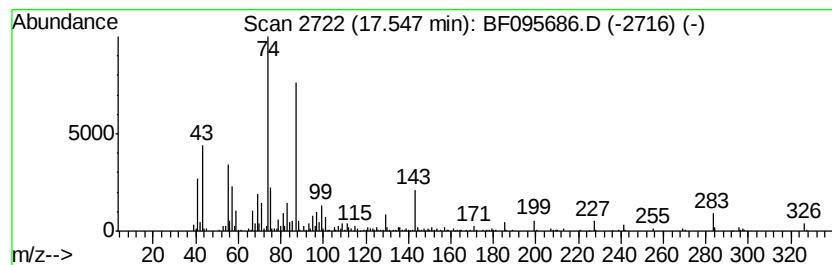
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 11 Eicosanoic acid, methyl ester Concentration Rank 7

| R.T.  | EstConc  | Area    | Relative to ISTD | R.T.  |
|-------|----------|---------|------------------|-------|
| 17.55 | 35.29 ng | 1047180 | Chrysene-d12     | 18.35 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Eicosanoic acid, methyl ester       | 326 | C21H42O2 | 001120-28-1  | 98   |
| 2    |    | Methyl 18-methylnonadecanoate       | 326 | C21H42O2 | 1000352-20-6 | 97   |
| 3    |    | Heptadecanoic acid, methyl ester    | 284 | C18H36O2 | 001731-92-6  | 93   |
| 4    |    | Heptadecanoic acid, 16-methyl-, ... | 298 | C19H38O2 | 005129-61-3  | 93   |
| 5    |    | Hexadecanoic acid, 15-methyl-, m... | 284 | C18H36O2 | 006929-04-0  | 93   |



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Data File : BF095686.D  
Acq On : 5 Jun 2017 22:09  
Operator : SJ/MA  
Sample : I3444-07  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BU-RO-298-060117

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060517.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 |
| unknown7.05          | 7.05  | 48.1    | ng    | 1416800  | 1                     | 7.40  | 589091 | 20.0 |
| Hexadecanoic acid... | 15.48 | 269.3   | ng    | 11541800 | 4                     | 14.64 | 857265 | 20.0 |
| 10,13-Octadecadie... | 16.50 | 1072.8  | ng    | 31835400 | 5                     | 18.35 | 593524 | 20.0 |
| Methyl stearate      | 16.61 | 188.7   | ng    | 5599250  | 5                     | 18.35 | 593524 | 20.0 |
| 9,12-Octadecadien... | 16.64 | 17.7    | ng    | 524295   | 5                     | 18.35 | 593524 | 20.0 |
| Oleic Acid           | 16.66 | 17.2    | ng    | 510275   | 5                     | 18.35 | 593524 | 20.0 |
| Cyclododecyne        | 17.33 | 14.5    | ng    | 429574   | 5                     | 18.35 | 593524 | 20.0 |
| 9-Octadecenoic ac... | 17.43 | 21.0    | ng    | 624202   | 5                     | 18.35 | 593524 | 20.0 |
| Eicosanoic acid, ... | 17.55 | 35.3    | ng    | 1047180  | 5                     | 18.35 | 593524 | 20.0 |