

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\  
 Data File : BF097706.D  
 Acq On : 15 Aug 2017 22:22  
 Operator : SJ/JU  
 Sample : I4751-16  
 Misc :  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-24-COMP

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-BF081517.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 4.987       | 486           | 493         | 501          | rBV      | 195704         | 271471        | 8.36%           | 0.886%        |
| 2         | 5.392       | 557           | 562         | 565          | rBV      | 3041093        | 3040456       | 93.63%          | 9.928%        |
| 3         | 6.410       | 729           | 735         | 743          | rVB      | 2867044        | 3247345       | 100.00%         | 10.603%       |
| 4         | 6.551       | 754           | 759         | 762          | rBV      | 3174324        | 3005900       | 92.56%          | 9.815%        |
| 5         | 6.781       | 795           | 798         | 802          | rBV      | 1045600        | 883062        | 27.19%          | 2.883%        |
| 6         | 6.939       | 821           | 825         | 828          | rBV      | 2647508        | 2218570       | 68.32%          | 7.244%        |
| 7         | 7.345       | 889           | 894         | 897          | rBV      | 2098202        | 1873999       | 57.71%          | 6.119%        |
| 8         | 8.063       | 1012          | 1016        | 1020         | rBV      | 1289870        | 1187452       | 36.57%          | 3.877%        |
| 9         | 9.145       | 1195          | 1200        | 1203         | rBV      | 3415678        | 2949796       | 90.84%          | 9.632%        |
| 10        | 9.539       | 1263          | 1267        | 1270         | rBV      | 445760         | 377879        | 11.64%          | 1.234%        |
| 11        | 9.822       | 1310          | 1315        | 1318         | rVB      | 1309538        | 1215693       | 37.44%          | 3.970%        |
| 12        | 10.257      | 1387          | 1389        | 1392         | rVB      | 54226          | 44404         | 1.37%           | 0.145%        |
| 13        | 10.604      | 1443          | 1448        | 1451         | rBV      | 1877334        | 1652807       | 50.90%          | 5.397%        |
| 14        | 10.733      | 1467          | 1470        | 1478         | rBV      | 66424          | 68663         | 2.11%           | 0.224%        |
| 15        | 11.180      | 1543          | 1546        | 1549         | rBV      | 44619          | 37549         | 1.16%           | 0.123%        |
| 16        | 11.304      | 1563          | 1567        | 1569         | rBV      | 1187680        | 1123468       | 34.60%          | 3.668%        |
| 17        | 11.704      | 1632          | 1635        | 1639         | rVB      | 693437         | 582443        | 17.94%          | 1.902%        |
| 18        | 11.833      | 1654          | 1657        | 1665         | rVB3     | 121660         | 119627        | 3.68%           | 0.391%        |
| 19        | 12.392      | 1748          | 1752        | 1754         | rBV      | 1415967        | 1273480       | 39.22%          | 4.158%        |
| 20        | 12.416      | 1754          | 1756        | 1758         | rVV      | 1593033        | 1269299       | 39.09%          | 4.145%        |
| 21        | 12.433      | 1758          | 1759        | 1763         | rVV3     | 145558         | 105419        | 3.25%           | 0.344%        |
| 22        | 12.498      | 1767          | 1770        | 1775         | rVV2     | 339355         | 301828        | 9.29%           | 0.986%        |
| 23        | 12.733      | 1805          | 1810        | 1814         | rBV2     | 51769          | 67654         | 2.08%           | 0.221%        |
| 24        | 12.886      | 1832          | 1836        | 1840         | rBV      | 2004650        | 1908313       | 58.77%          | 6.231%        |
| 25        | 13.792      | 1987          | 1990        | 1994         | rBV      | 74219          | 73787         | 2.27%           | 0.241%        |
| 26        | 13.933      | 2010          | 2014        | 2017         | rBV      | 979202         | 854545        | 26.32%          | 2.790%        |
| 27        | 15.362      | 2252          | 2257        | 2262         | rBV      | 614666         | 787743        | 24.26%          | 2.572%        |
| 28        | 15.427      | 2265          | 2268        | 2272         | rVB2     | 34335          | 41990         | 1.29%           | 0.137%        |
| 29        | 15.851      | 2337          | 2340        | 2344         | rVB3     | 30548          | 41143         | 1.27%           | 0.134%        |

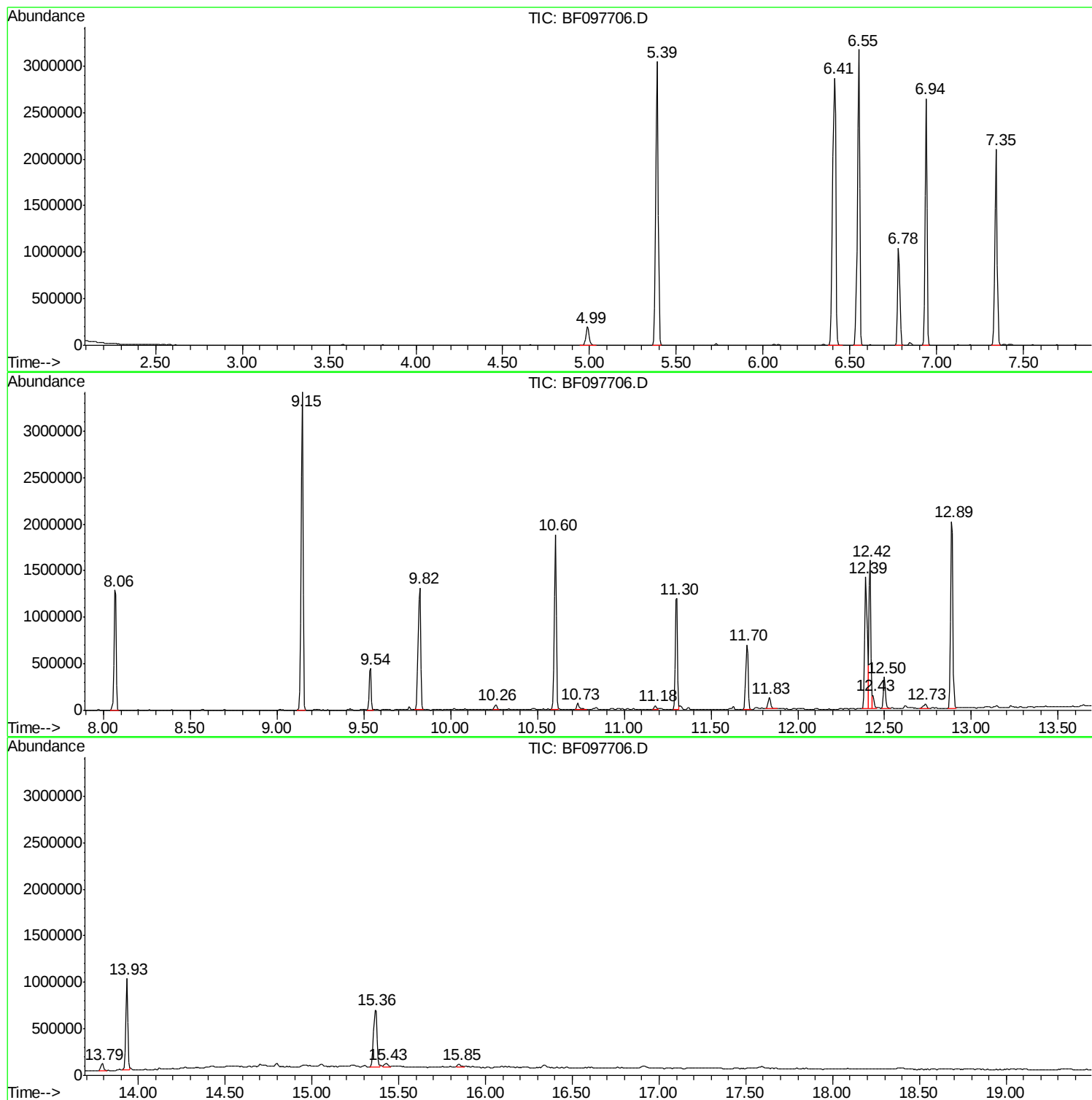
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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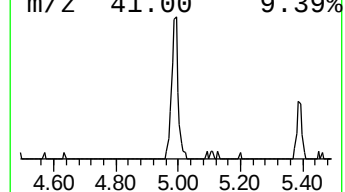
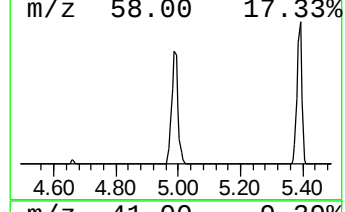
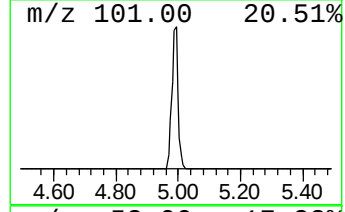
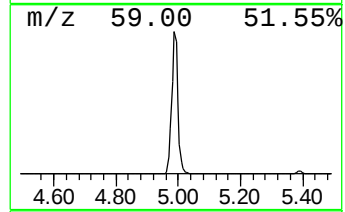
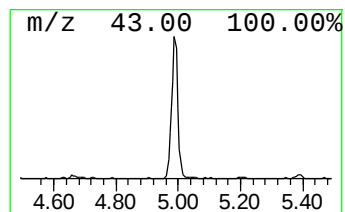
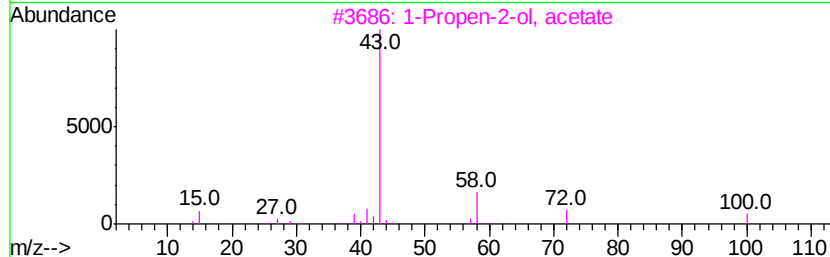
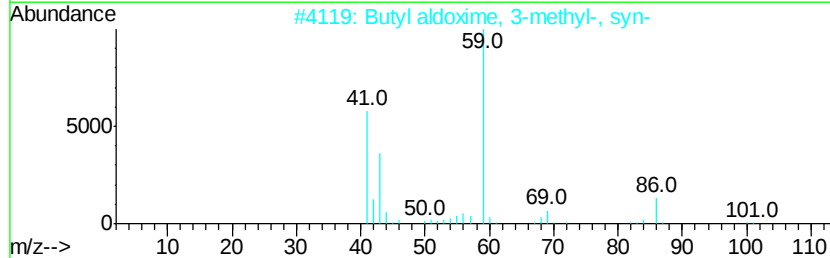
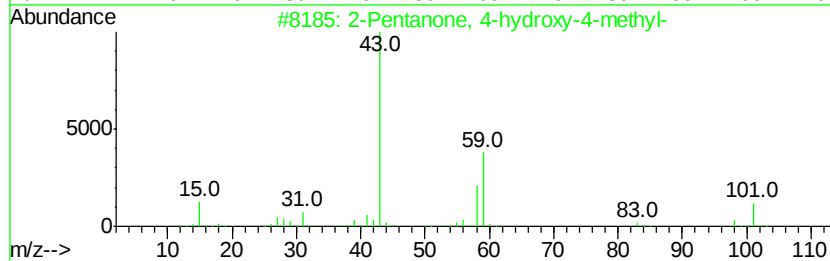
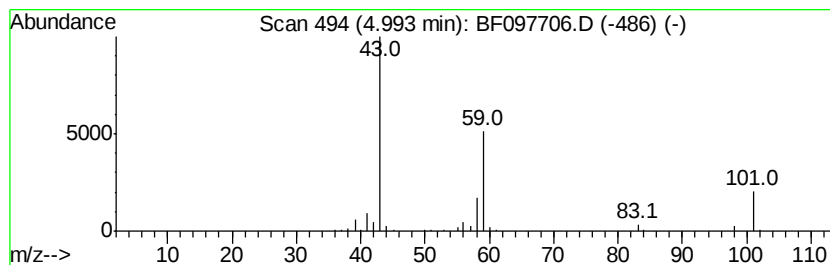
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.99 | 6.15 ng | 271471 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# | of | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|------|----|----------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2  | 000123-42-2 | 59   |
| 2    |    | Butyl aldoxime, 3-methyl-, syn-  | 101 | C5H11NO  | 005780-40-5 | 23   |
| 3    |    | 1-Propen-2-ol, acetate           | 100 | C5H8O2   | 000108-22-5 | 10   |
| 4    |    | 2,3-Butanedione, monooxime       | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 5    |    | 1,8-Nonanediol, 8-methyl-        | 174 | C10H22O2 | 054725-73-4 | 9    |



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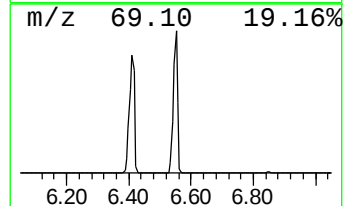
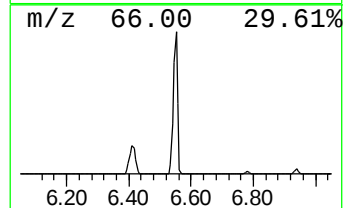
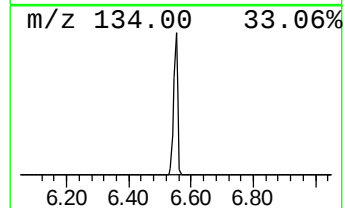
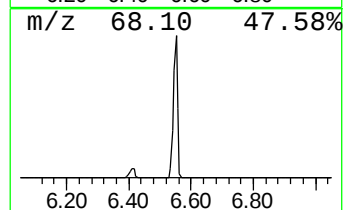
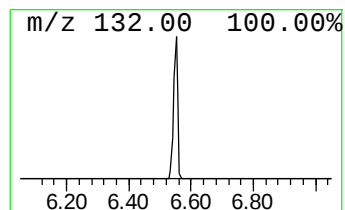
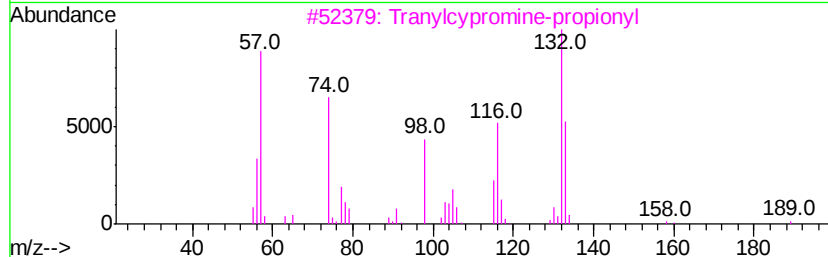
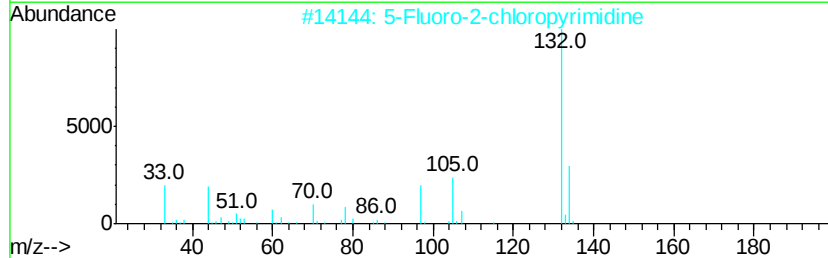
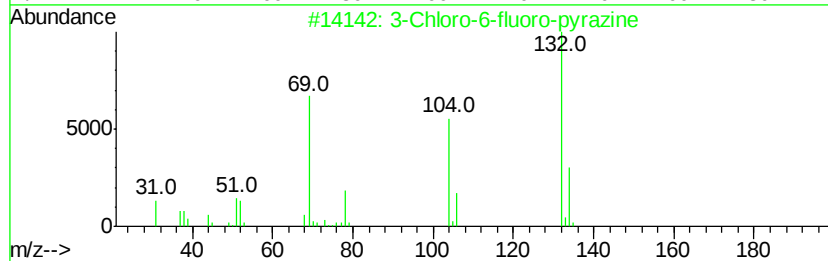
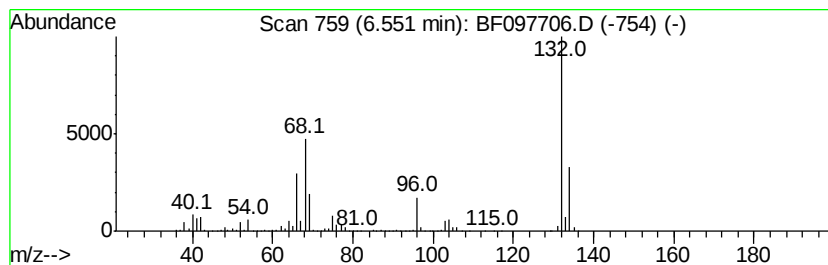
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 2 unknown6.55 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.55 | 68.08 ng | 3005900 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 16   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 3    |    | Tranvlcypropine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 10   |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



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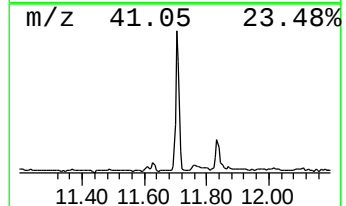
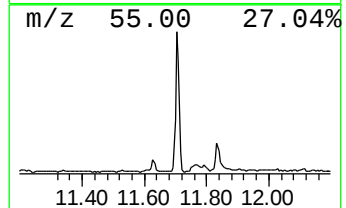
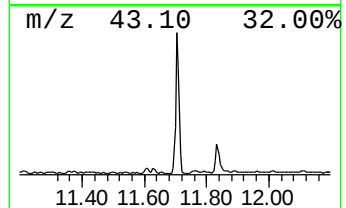
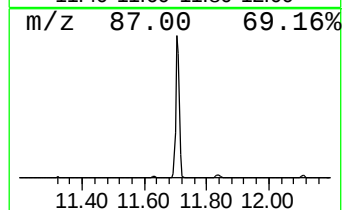
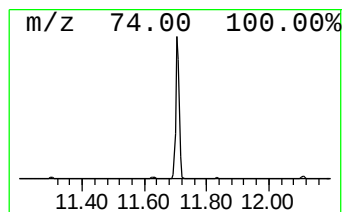
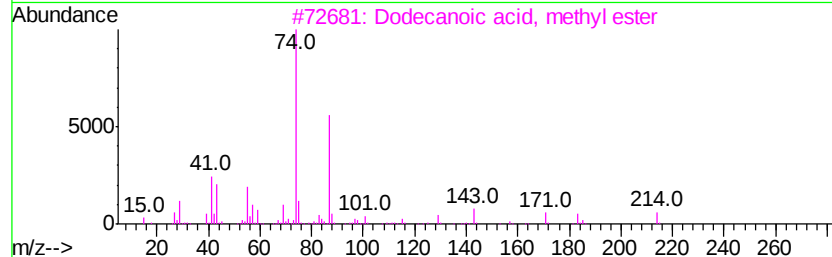
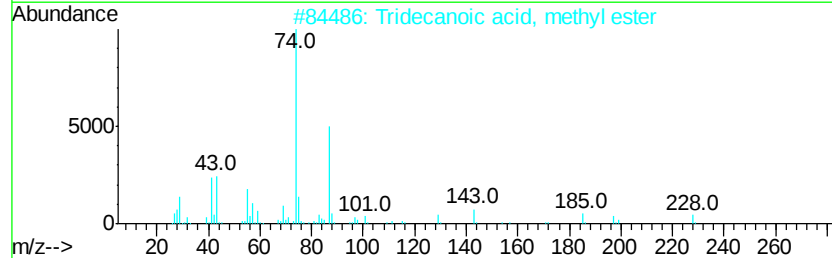
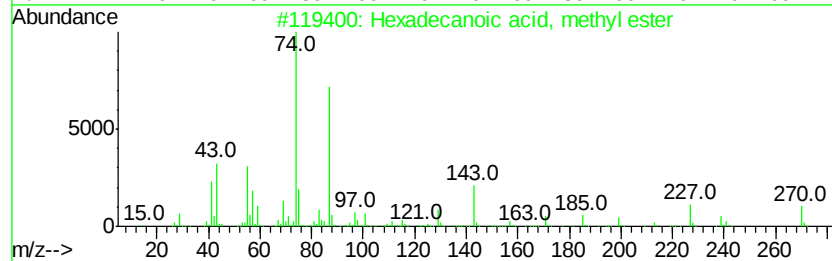
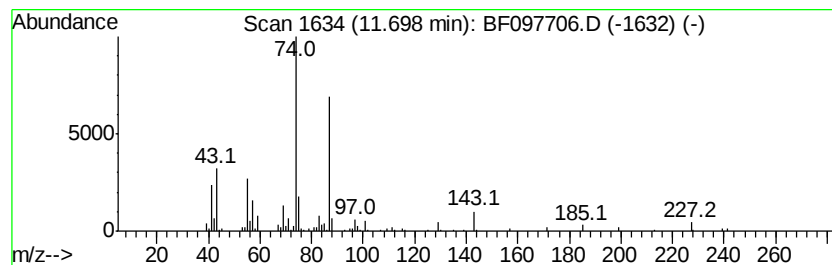
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 11.70 | 10.37 ng | 582443 | Phenanthrene-d10 | 11.30 |

| Hit# of | 5 | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|---------|---|----------------------------------|-----|----------|-------------|------|
| 1       |   | Hexadecanoic acid, methyl ester  | 270 | C17H34O2 | 000112-39-0 | 98   |
| 2       |   | Tridecanoic acid, methyl ester   | 228 | C14H28O2 | 001731-88-0 | 91   |
| 3       |   | Dodecanoic acid, methyl ester    | 214 | C13H26O2 | 000111-82-0 | 91   |
| 4       |   | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 90   |
| 5       |   | Methyl tetradecanoate            | 242 | C15H30O2 | 000124-10-7 | 90   |



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SB-24-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M  
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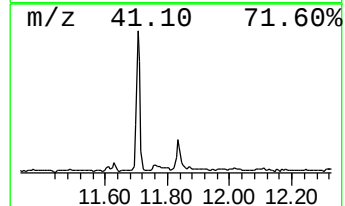
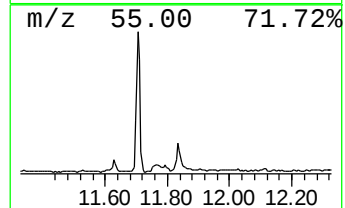
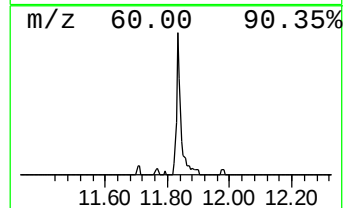
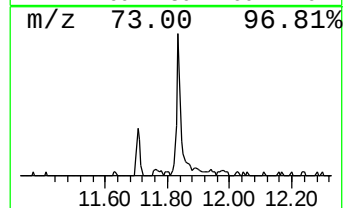
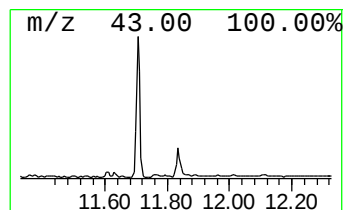
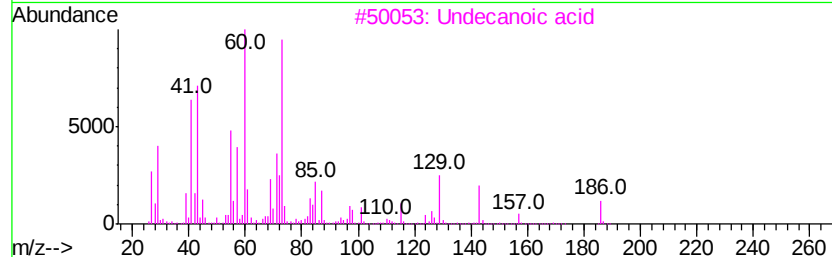
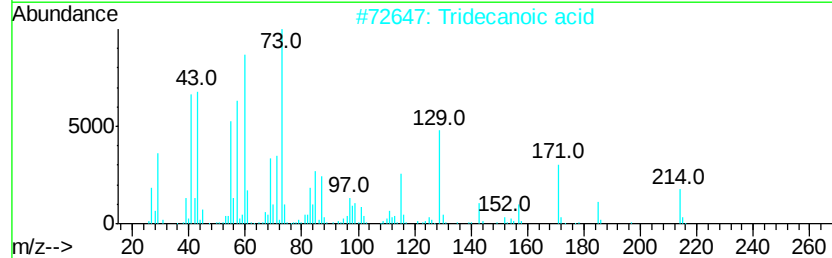
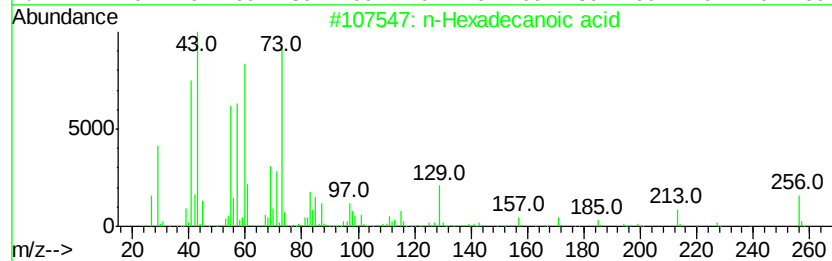
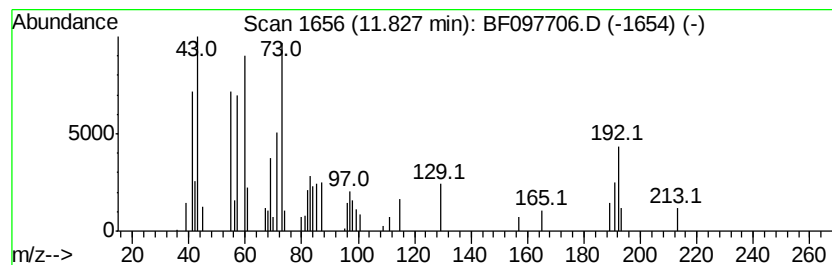
TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.83 | 2.13 ng | 119627 | Phenanthrene-d10 | 11.30 |

| Hit# | of | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---------------------|-----|----------|-------------|------|
| 1    | 5  | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93   |
| 2    |    | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 72   |
| 3    |    | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 72   |
| 4    |    | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 68   |
| 5    |    | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 64   |



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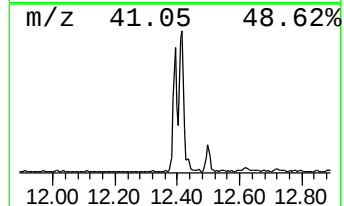
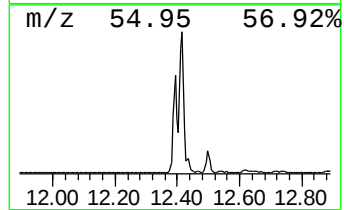
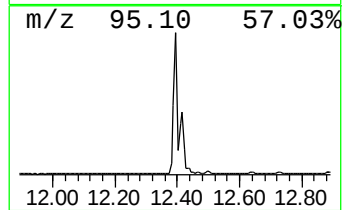
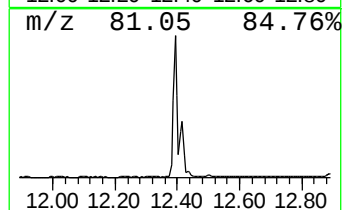
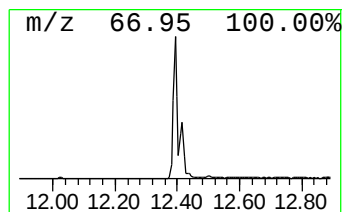
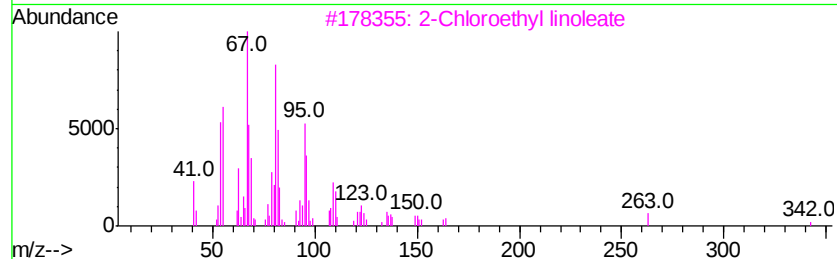
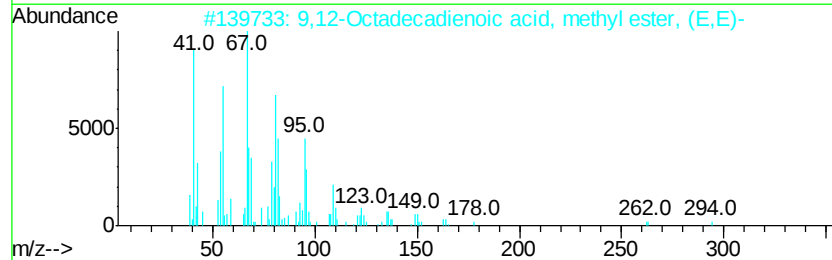
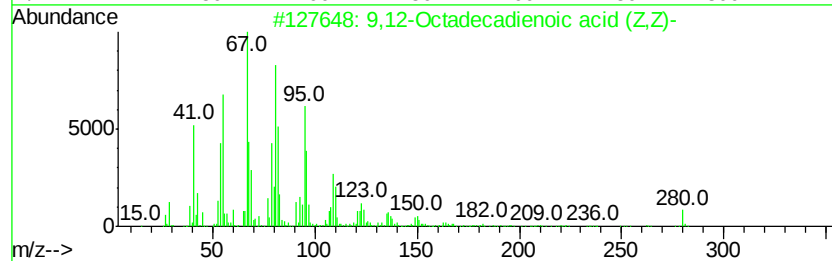
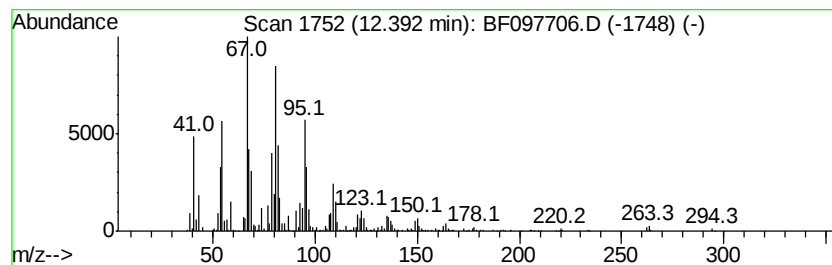
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 9,12-Octadecadienoic acid (... Concentration Rank 3

| R.T.  | EstConc  | Area    | Relative to ISTD | R.T.  |
|-------|----------|---------|------------------|-------|
| 12.39 | 22.67 ng | 1273480 | Phenanthrene-d10 | 11.30 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|-------------------------------------|-----|------------|-------------|------|
| 1    | 5  | 9,12-Octadecadienoic acid (Z,Z)-    | 280 | C18H32O2   | 000060-33-3 | 95   |
| 2    |    | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2   | 002566-97-4 | 93   |
| 3    |    | 2-Chloroethyl linoleate             | 342 | C20H35ClO2 | 025525-76-2 | 91   |
| 4    |    | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2   | 002462-85-3 | 89   |
| 5    |    | 3,4-Octadiene, 7-methyl-            | 124 | C9H16      | 037050-05-8 | 83   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\  
Data File : BF097706.D  
Acq On : 15 Aug 2017 22:22  
Operator : SJ/JU  
Sample : I4751-16  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-24-COMP

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

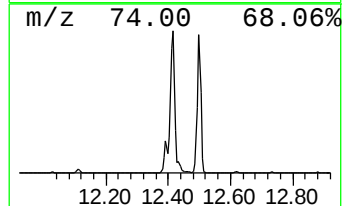
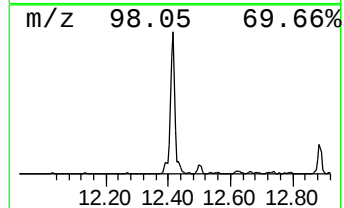
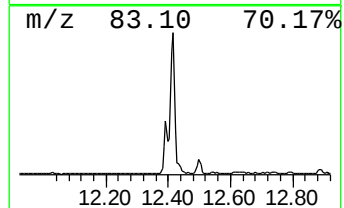
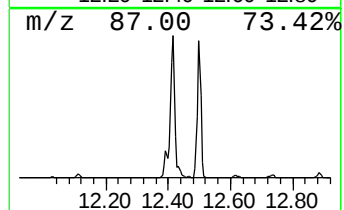
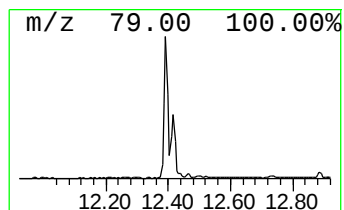
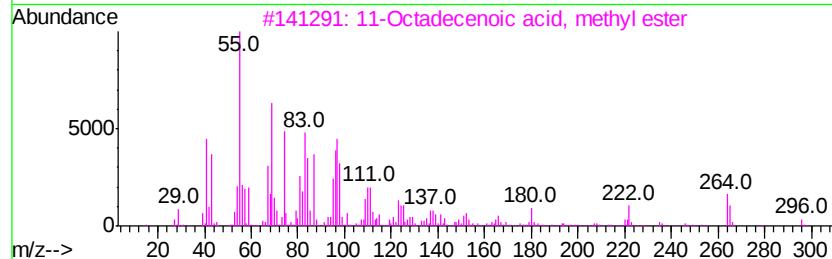
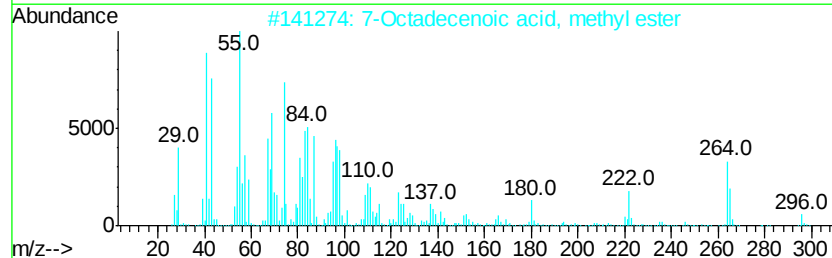
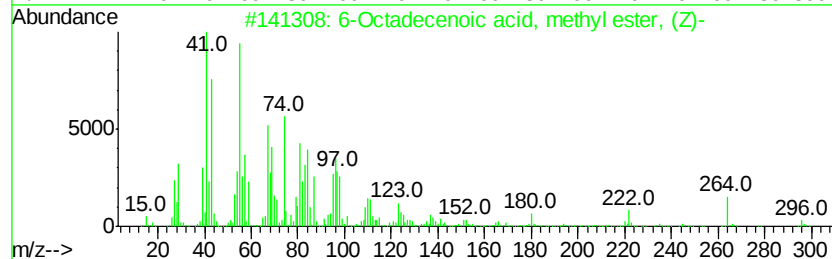
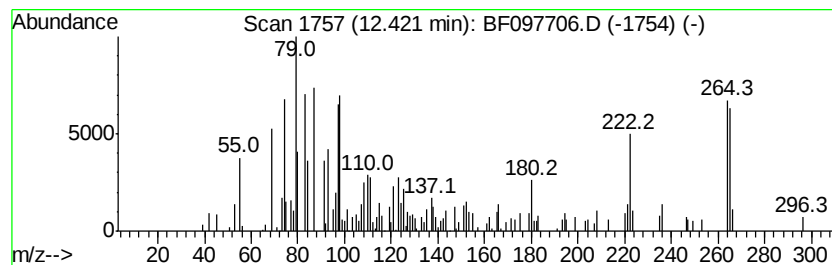
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 6-Octadecenoic acid, methyl... Concentration Rank 4

| R.T.  | EstConc  | Area    | Relative to ISTD | R.T.  |
|-------|----------|---------|------------------|-------|
| 12.42 | 22.60 ng | 1269300 | Phenanthrene-d10 | 11.30 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|---------|---|-------------------------------------|-----|----------|--------------|------|
| 1       |   | 6-Octadecenoic acid, methyl este... | 296 | C19H36O2 | 002777-58-4  | 97   |
| 2       |   | 7-Octadecenoic acid, methyl ester   | 296 | C19H36O2 | 057396-98-2  | 96   |
| 3       |   | 11-Octadecenoic acid, methyl ester  | 296 | C19H36O2 | 052380-33-3  | 96   |
| 4       |   | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9  | 96   |
| 5       |   | cis-13-Octadecenoic acid, methyl... | 296 | C19H36O2 | 1000333-58-3 | 95   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF081517\  
Data File : BF097706.D  
Acq On : 15 Aug 2017 22:22  
Operator : SJ/JU  
Sample : I4751-16  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

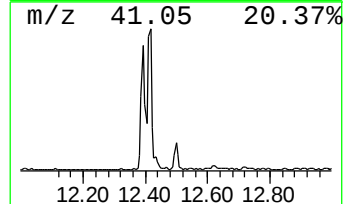
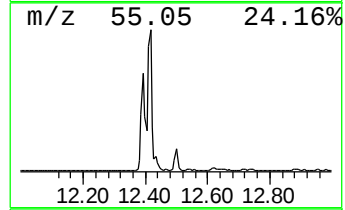
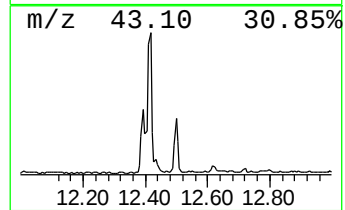
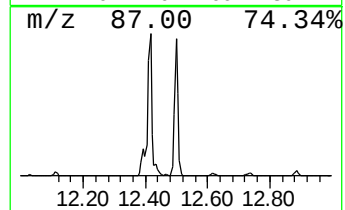
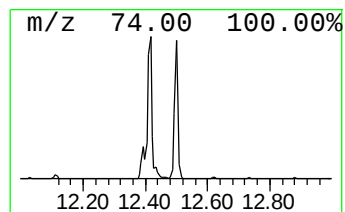
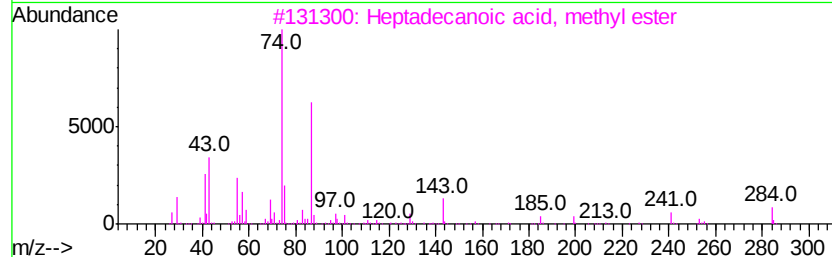
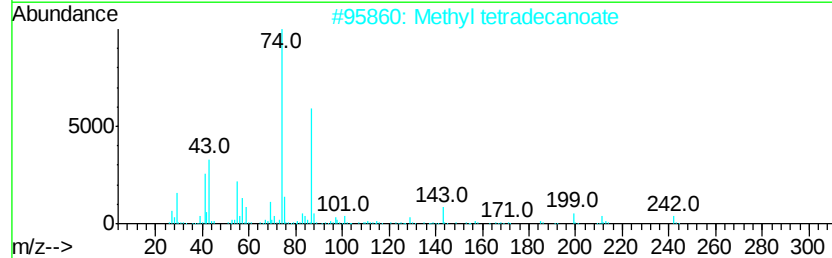
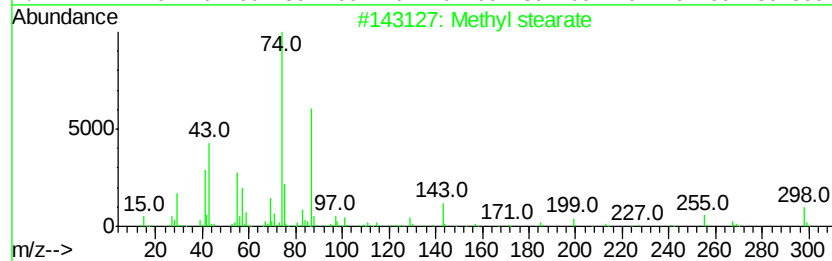
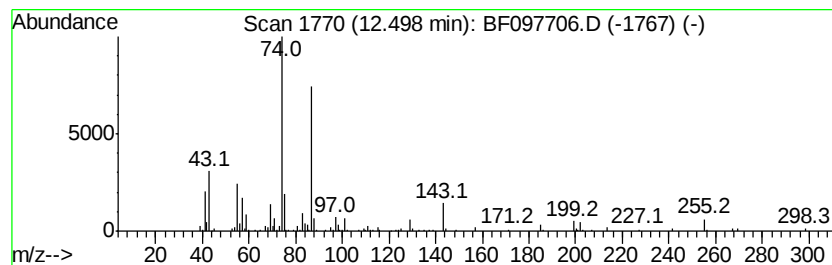
Instrument :  
BNA\_F  
ClientSampleId :  
SB-24-COMP

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081517.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 Methyl stearate Concentration Rank 7

| R.T.    | EstConc | Area                             | Relative to ISTD | R.T.     |             |      |
|---------|---------|----------------------------------|------------------|----------|-------------|------|
| 12.50   | 5.37 ng | 301828                           | Phenanthrene-d10 | 11.30    |             |      |
| Hit# of | 5       | Tentative ID                     | MW               | MolForm  | CAS#        | Qual |
| 1       |         | Methyl stearate                  | 298              | C19H38O2 | 000112-61-8 | 93   |
| 2       |         | Methyl tetradecanoate            | 242              | C15H30O2 | 000124-10-7 | 91   |
| 3       |         | Heptadecanoic acid, methyl ester | 284              | C18H36O2 | 001731-92-6 | 91   |
| 4       |         | Hexadecanoic acid, methyl ester  | 270              | C17H34O2 | 000112-39-0 | 91   |
| 5       |         | Pentadecanoic acid, methyl ester | 256              | C16H32O2 | 007132-64-1 | 90   |



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Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-24-COMP

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081517.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... | 4.99  | 6.2     | ng    | 271471   | 1                     | 6.78  | 883062  | 20.0 |
| unknown6.55          | 6.55  | 68.1    | ng    | 3005900  | 1                     | 6.78  | 883062  | 20.0 |
| Hexadecanoic acid... | 11.70 | 10.4    | ng    | 582443   | 4                     | 11.30 | 1123470 | 20.0 |
| n-Hexadecanoic acid  | 11.83 | 2.1     | ng    | 119627   | 4                     | 11.30 | 1123470 | 20.0 |
| 9,12-Octadecadien... | 12.39 | 22.7    | ng    | 1273480  | 4                     | 11.30 | 1123470 | 20.0 |
| 6-Octadecenoic ac... | 12.42 | 22.6    | ng    | 1269300  | 4                     | 11.30 | 1123470 | 20.0 |
| Methyl stearate      | 12.50 | 5.4     | ng    | 301828   | 4                     | 11.30 | 1123470 | 20.0 |