LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099883.D
Acq On : 27 Oct 2017 17:55
Operator : SJ/JU
Sample : I6113-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-01-102417

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-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.998 | 493 | 495 | 505 | rBV | 27820 | 37948 | 3.43% | 0.398% |
| 2 | 5.416 | 563 | 566 | 579 | rBV | 188096 | 267927 | 24.23% | 2.809% |
| 3 | 6.439 | 737 | 740 | 759 | rBV | 229649 | 310335 | 28.06% | 3.254% |
| 4 | 6.569 | 759 | 762 | 768 | rBV | 349249 | 337657 | 30.53% | 3.540% |
| 5 | 6.792 | 797 | 800 | 810 | rBV | 607879 | 523597 | 47.35% | 5.490% |
| 6 | 6.945 | 823 | 826 | 842 | rBB | 261053 | 260076 | 23.52% | 2.727% |
| 7 | 7.363 | 894 | 897 | 913 | rBV | 174098 | 186520 | 16.87% | 1.956% |
| 8 | 8.075 | 1015 | 1018 | 1031 | rBV | 831386 | 717499 | 64.88% | 7.523% |
| 9 | 8.639 | 1111 | 1114 | 1121 | rBB | 20611 | 19611 | 1.77% | 0.206% |
| 10 | 9.151 | 1197 | 1201 | 1210 | rBV | 537168 | 433975 | 39.24% | 4.550% |
| 11 | 9.551 | 1266 | 1269 | 1277 | rVB | 91137 | 78107 | 7.06% | 0.819% |
| 12 | 9.839 | 1313 | 1318 | 1322 | rBV | 879739 | 792523 | 71.66% | 8.310% |
| 13 | 10.257 | 1386 | 1389 | 1392 | rVB | 17827 | 14642 | 1.32% | 0.154% |
| 14 | 10.551 | 1436 | 1439 | 1445 | rVB | 128067 | 97949 | 8.86% | 1.027% |
| 15 | 10.633 | 1450 | 1453 | 1461 | rBV | 221393 | 204936 | 18.53% | 2.149% |
| 16 | 10.727 | 1466 | 1469 | 1477 | rBV2 | 28716 | 35250 | 3.19% | 0.370% |
| 17 | 11.180 | 1543 | 1546 | 1548 | rBV | 28211 | 23192 | 2.10% | 0.243% |
| 18 | 11.333 | 1568 | 1572 | 1574 | rBV | 811781 | 748524 | 67.68% | 7.848% |
| 19 | 11.357 | 1574 | 1576 | 1581 | rVB | 63863 | 54862 | 4.96% | 0.575% |
| 20 | 11.604 | 1615 | 1618 | 1621 | rVB | 25909 | 17385 | 1.57% | 0.182% |
| 21 | 11.710 | 1633 | 1636 | 1639 | rBV | 322692 | 235808 | 21.32% | 2.472% |
| 22 | 11.851 | 1655 | 1660 | 1661 | rBV2 | 27828 | 38028 | 3.44% | 0.399% |
| 23 | 11.868 | 1661 | 1663 | 1666 | rVB | 20461 | 18224 | 1.65% | 0.191% |
| 24 | 11.945 | 1673 | 1676 | 1679 | rBV2 | 16493 | 19284 | 1.74% | 0.202% |
| 25 | 12.015 | 1684 | 1688 | 1691 | rBV | 23280 | 22749 | 2.06% | 0.239% |
| 26 | 12.398 | 1749 | 1753 | 1755 | rBV | 1221069 | 1105910 | 100.00% | 11.596% |
| 27 | 12.421 | 1755 | 1757 | 1763 | rVB2 | 859713 | 769634 | 69.59% | 8.070% |
| 28 | 12.504 | 1767 | 1771 | 1775 | rVB | 168676 | 138151 | 12.49% | 1.449% |
| 29 | 12.551 | 1775 | 1779 | 1783 | rBV | 83695 | 101980 | 9.22% | 1.069% |
| 30 | 12.639 | 1791 | 1794 | 1798 | rBV4 | 14201 | 19329 | 1.75% | 0.203% |
| 31 | 12.739 | 1807 | 1811 | 1814 | rBV4 | 19387 | 22078 | 2.00% | 0.231% |
| 32 | 12.780 | 1814 | 1818 | 1825 | rVB2 | 71601 | 95616 | 8.65% | 1.003% |
| 33 | 12.915 | 1837 | 1841 | 1844 | rVB | 412350 | 347218 | 31.40% | 3.641% |
| 34 | 13.004 | 1852 | 1856 | 1858 | rBV3 | 8790 | 12208 | 1.10% | 0.128% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099883.D
Acq On : 27 Oct 2017 17:55
Operator : SJ/JU
Sample : I6113-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-01-102417

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-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.063 | 1863 | 1866 | 1868 | rBV3 | 26271 | 23491 | 2.12% | 0.246% |
| 36 | 13.133 | 1876 | 1878 | 1880 | rBV2 | 17133 | 13417 | 1.21% | 0.141% |
| 37 | 13.227 | 1890 | 1894 | 1898 | rVB4 | 22667 | 25307 | 2.29% | 0.265% |
| 38 | 13.345 | 1911 | 1914 | 1919 | rVB4 | 14165 | 16584 | 1.50% | 0.174% |
| 39 | 13.474 | 1933 | 1936 | 1939 | rBV | 17067 | 19017 | 1.72% | 0.199% |
| 40 | 13.668 | 1965 | 1969 | 1970 | rBV4 | 7723 | 11958 | 1.08% | 0.125% |
| 41 | 13.804 | 1988 | 1992 | 1996 | rVB5 | 26799 | 30473 | 2.76% | 0.320% |
| 42 | 13.898 | 2006 | 2008 | 2010 | rBV2 | 14127 | 12571 | 1.14% | 0.132% |
| 43 | 13.986 | 2018 | 2023 | 2026 | rBV | 579814 | 570281 | 51.57% | 5.979% |
| 44 | 14.121 | 2043 | 2046 | 2048 | rVB2 | 18710 | 16154 | 1.46% | 0.169% |
| 45 | 14.209 | 2059 | 2061 | 2064 | rBV4 | 9821 | 13691 | 1.24% | 0.144% |
| 46 | 14.421 | 2093 | 2097 | 2101 | rBV7 | 24317 | 44587 | 4.03% | 0.468% |
| 47 | 15.333 | 2250 | 2252 | 2256 | rBV | 16560 | 21503 | 1.94% | 0.225% |
| 48 | 15.456 | 2269 | 2273 | 2284 | rVB | 428724 | 550043 | 49.74% | 5.767% |
| 49 | 16.098 | 2379 | 2382 | 2386 | rVB6 | 19188 | 23079 | 2.09% | 0.242% |
| 50 | 17.592 | 2634 | 2636 | 2646 | rVB10 | 18364 | 36395 | 3.29% | 0.382% |

Sum of corrected areas: 9537283

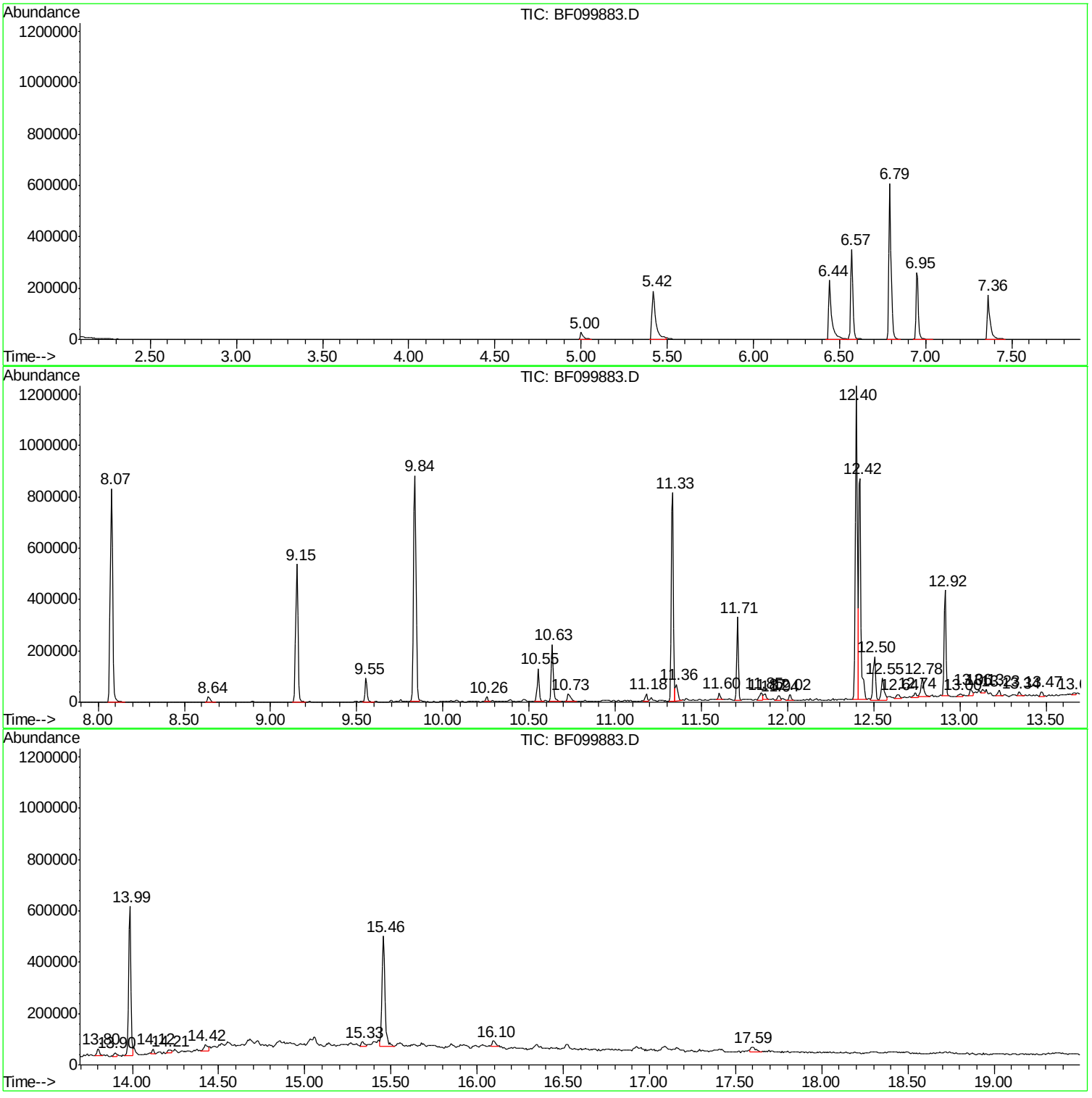
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099883.D
Acq On : 27 Oct 2017 17:55
Operator : SJ/JU
Sample : I6113-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-01-102417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099883.D
Acq On : 27 Oct 2017 17:55
Operator : SJ/JU
Sample : I6113-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-01-102417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

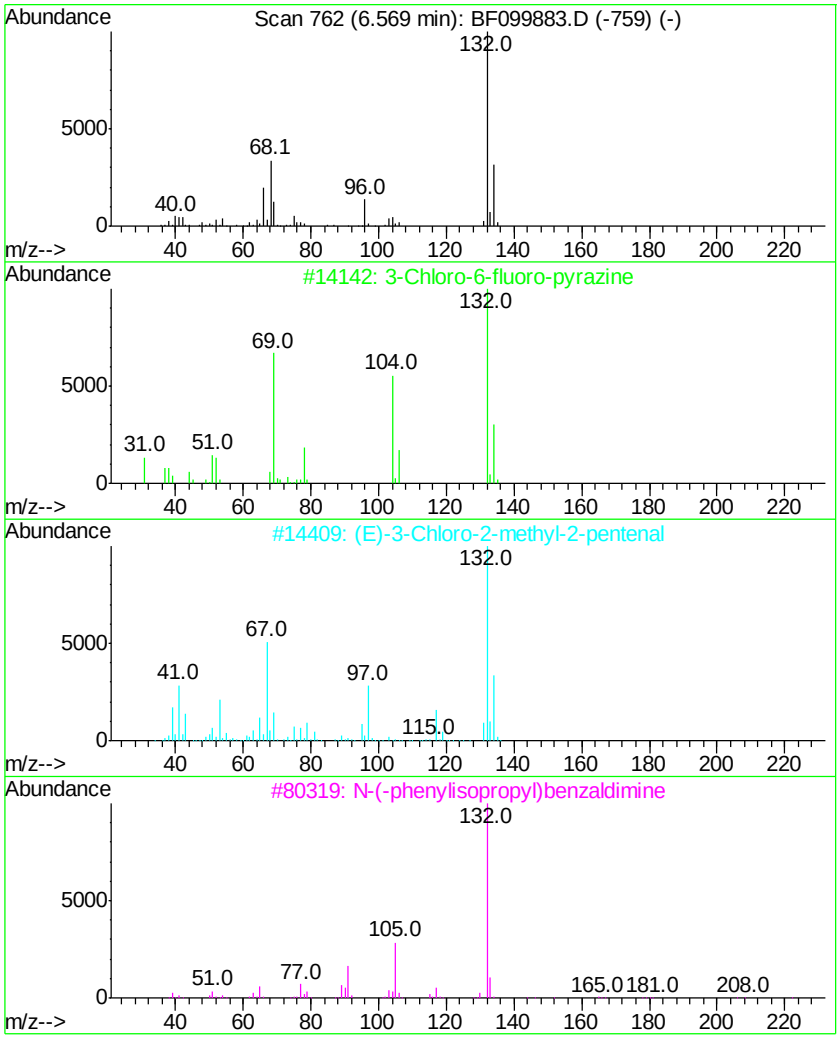
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

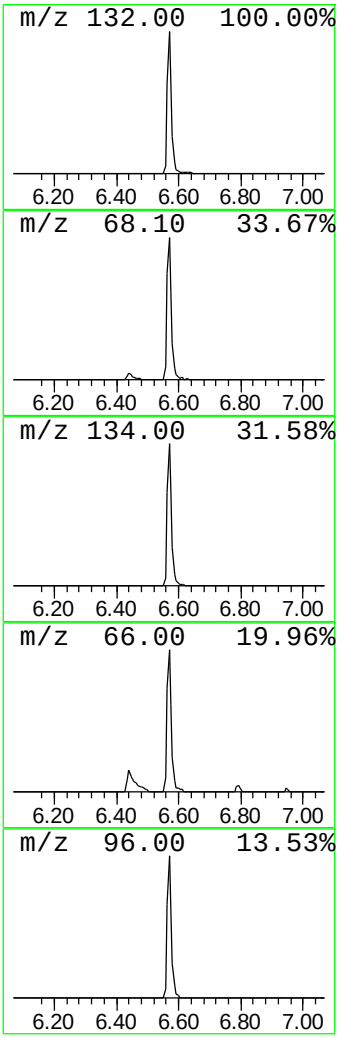
**********

Peak Number 1 unknown6.57 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.57 | 12.90 ng | 337657 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 25 |
| 3 | N-(-phenylisopropyl)benzaldimine | 223 | C16H17N | 1000379-01-3 | 12 |
| 4 | Amphetaminil | 250 | C17H18N2 | 017590-01-1 | 12 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099883.D
Acq On : 27 Oct 2017 17:55
Operator : SJ/JU
Sample : I6113-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-01-102417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

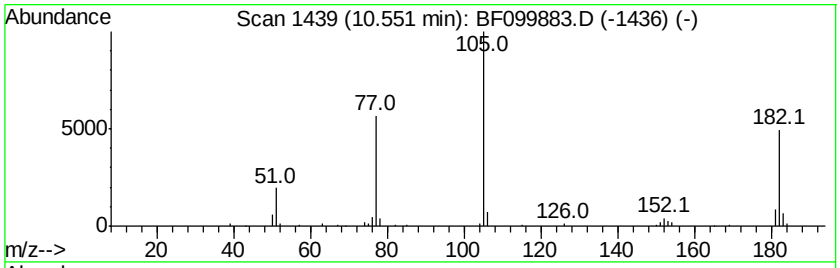
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

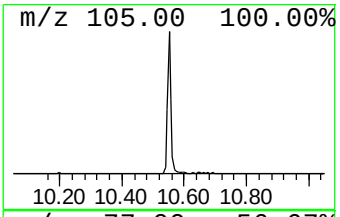
**********

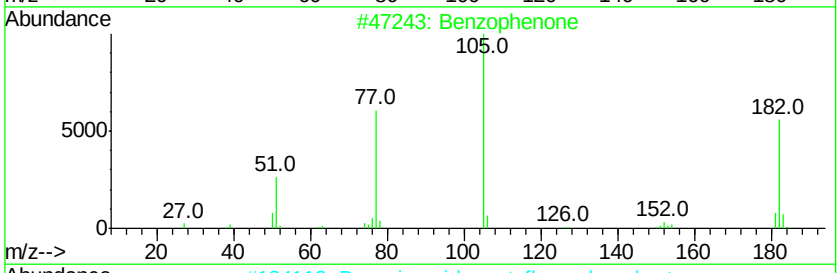
Peak Number 3 Benzophenone Concentration Rank 9

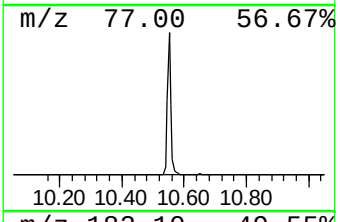
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.55 | 2.47 ng | 97949 | Acenaphthene-d10 | 9.84 |

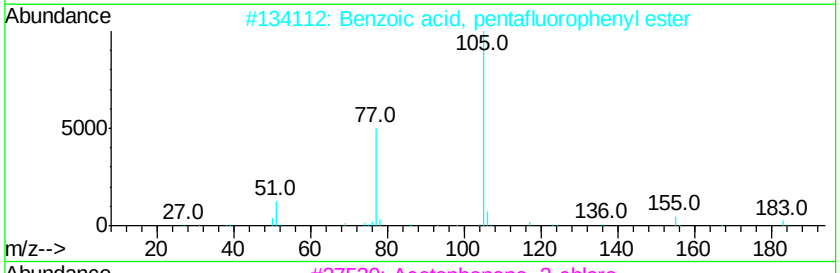
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 97 |
| 2 | Benzoic acid, pentafluorophenyl ... | 288 | C13H5F5O2 | 1000360-67-9 | 50 |
| 3 | Acetophenone, 2-chloro- | 154 | C8H7ClO | 000532-27-4 | 49 |
| 4 | 2-(2-Oxo-2-phenyl-ethyl)-malonon... | 184 | C11H8N2O | 1000296-76-9 | 47 |
| 5 | N-Methoxy-N-methylbenzamide | 165 | C9H11NO2 | 006919-61-5 | 47 |

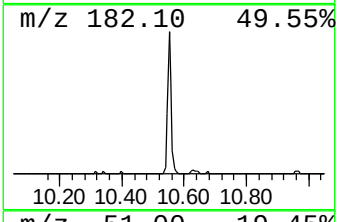


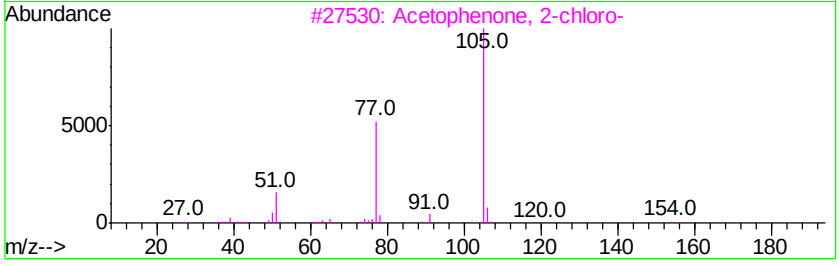



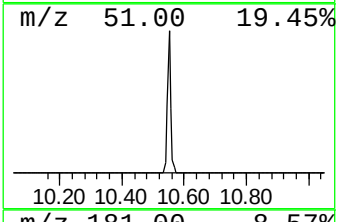



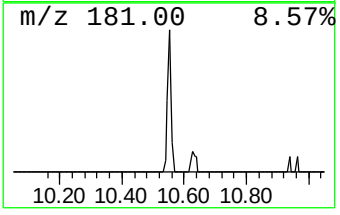



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Data File : BF099883.D
Acq On : 27 Oct 2017 17:55
Operator : SJ/JU
Sample : I6113-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-01-102417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

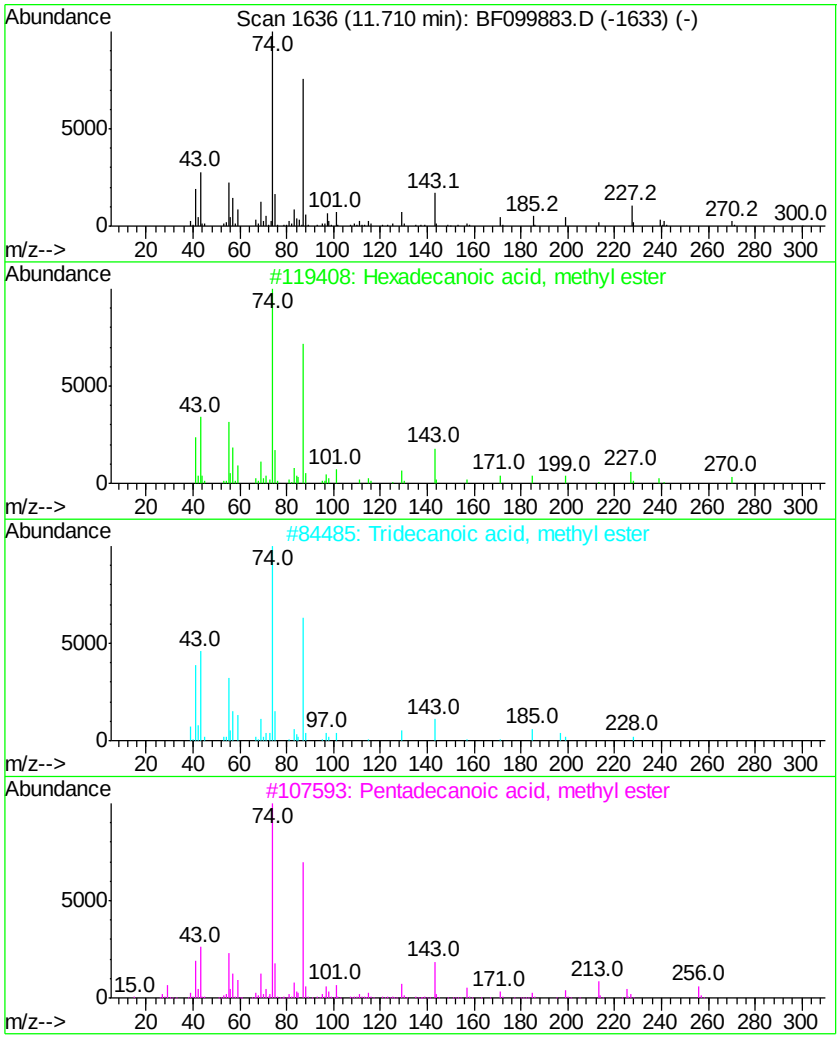
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

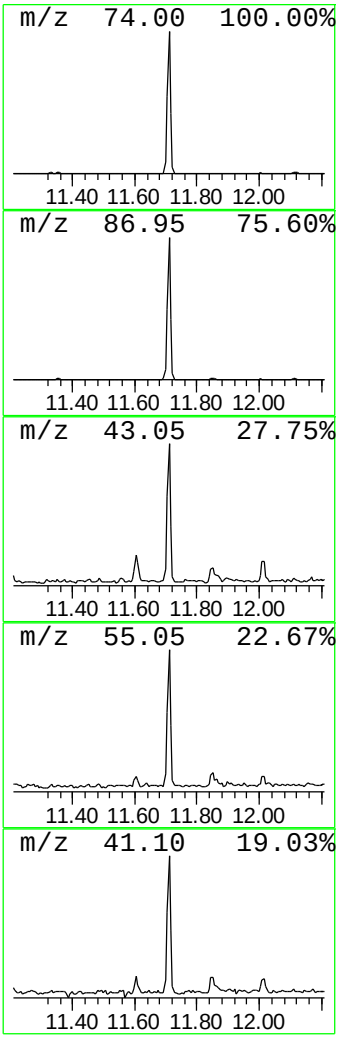
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.71 | 6.30 ng | 235808 | Phenanthrene-d10 | 11.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 97 |
| 2 | Tridecanoic acid, methyl ester | 228 | C14H28O2 | 001731-88-0 | 91 |
| 3 | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 86 |
| 4 | Methyl tetradecanoate | 242 | C15H30O2 | 000124-10-7 | 86 |
| 5 | Decanoic acid, methyl ester | 186 | C11H22O2 | 000110-42-9 | 83 |



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Data File : BF099883.D
Acq On : 27 Oct 2017 17:55
Operator : SJ/JU
Sample : I6113-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-01-102417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

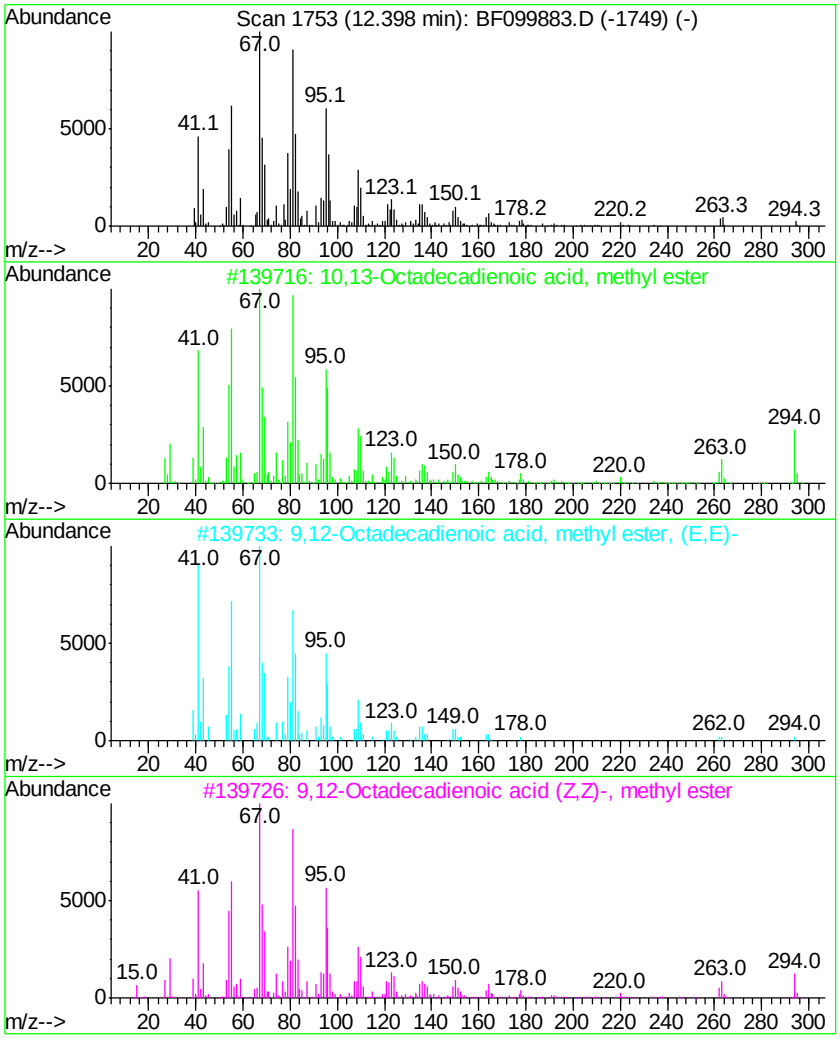
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

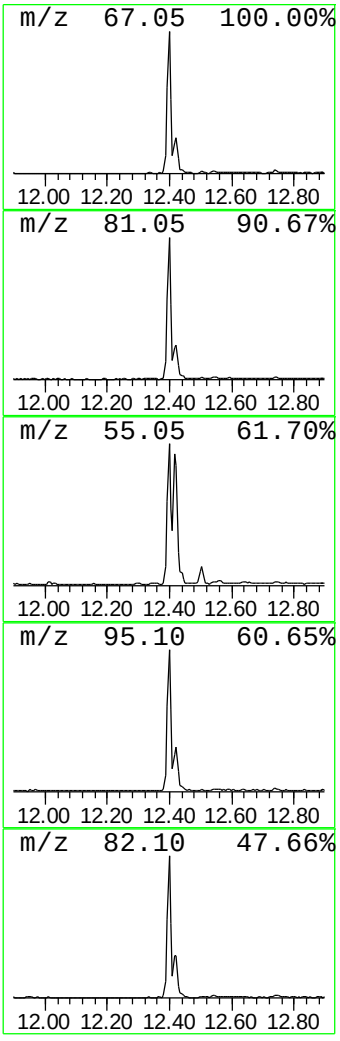
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.40 | 29.55 ng | 1105910 | Phenanthrene-d10 | 11.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 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 | 99 |
| 4 | 8,11-Octadecadienoic acid, methy... | 294 | C19H34O2 | 056599-58-7 | 99 |
| 5 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002462-85-3 | 99 |



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Data File : BF099883.D
Acq On : 27 Oct 2017 17:55
Operator : SJ/JU
Sample : I6113-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-01-102417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

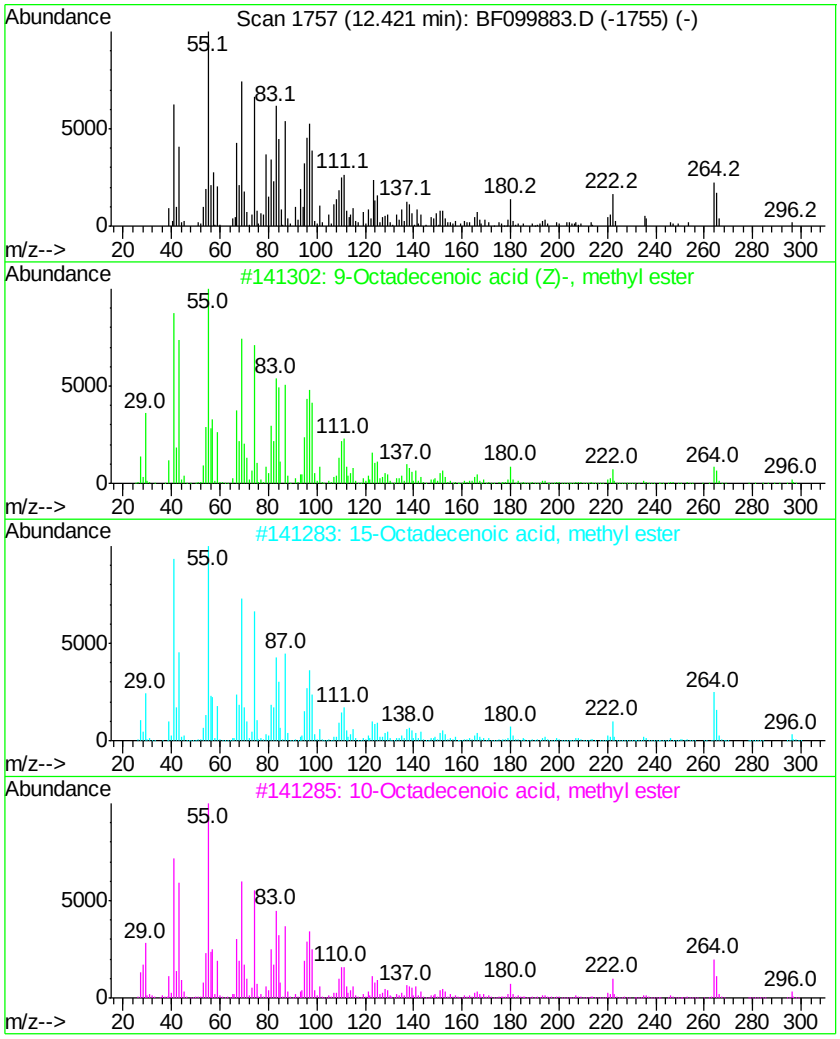
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

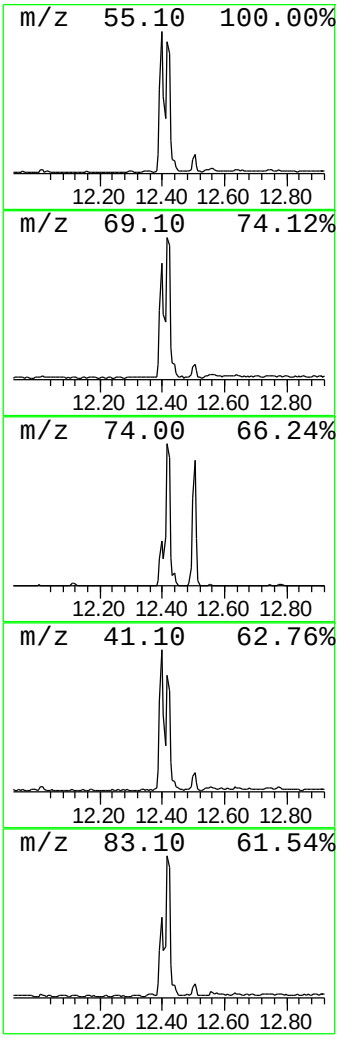
**********

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.42 | 20.56 ng | 769634 | Phenanthrene-d10 | 11.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 99 |
| 2 | 15-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 004764-72-1 | 99 |
| 3 | 10-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 013481-95-3 | 99 |
| 4 | 11-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 052380-33-3 | 99 |
| 5 | 14-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-48-4 | 99 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099883.D
Acq On : 27 Oct 2017 17:55
Operator : SJ/JU
Sample : I6113-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-01-102417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

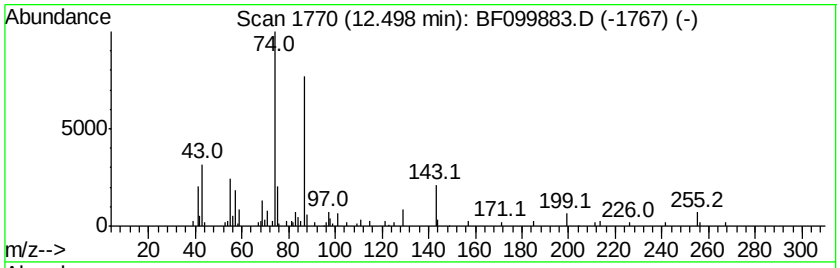
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

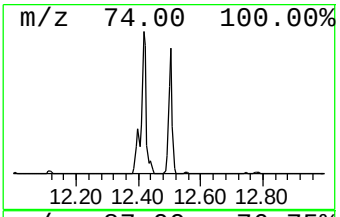
**********

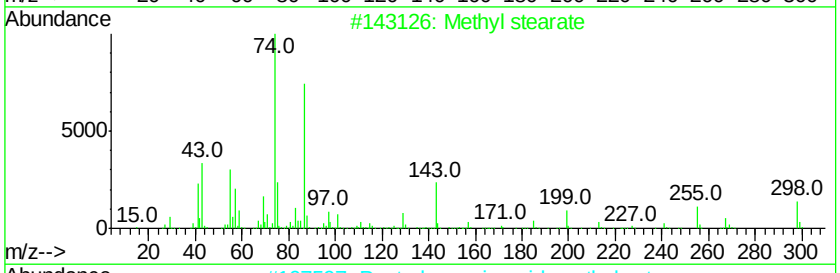
Peak Number 7 Methyl stearate Concentration Rank 6

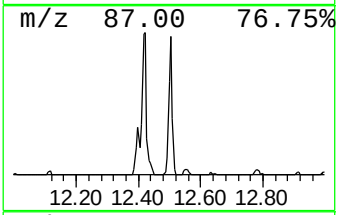
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.50 | 3.69 ng | 138151 | Phenanthrene-d10 | 11.33 |

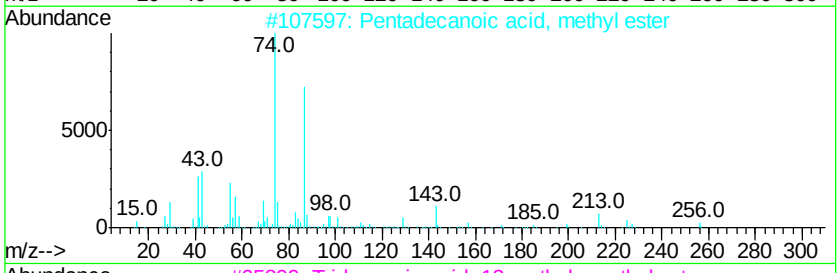
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl stearate | 298 | C19H38O2 | 000112-61-8 | 98 |
| 2 | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 81 |
| 3 | Tridecanoic acid, 12-methyl-, me... | 242 | C15H30O2 | 005129-58-8 | 80 |
| 4 | Heptadecanoic acid, methyl ester | 284 | C18H36O2 | 001731-92-6 | 80 |
| 5 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 80 |

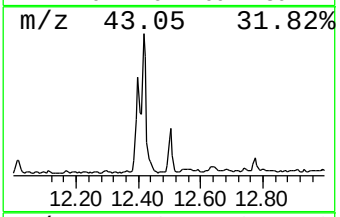


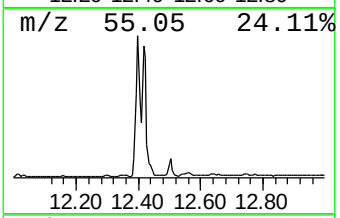



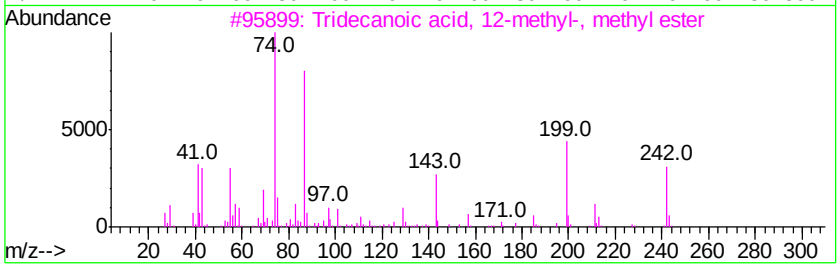



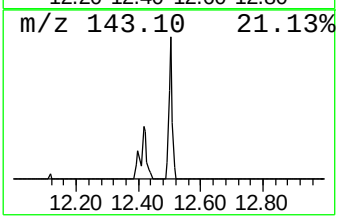



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102717\
Data File : BF099883.D
Acq On : 27 Oct 2017 17:55
Operator : SJ/JU
Sample : I6113-01 5X
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SU-01-102417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown6.57 | 6.57 | 12.9 | ng | 337657 | 1 | 6.79 | 523597 | 20.0 |
| Benzophenone | 10.55 | 2.5 | ng | 97949 | 3 | 9.84 | 792523 | 20.0 |
| Hexadecanoic acid... | 11.71 | 6.3 | ng | 235808 | 4 | 11.33 | 748524 | 20.0 |
| 10,13-Octadecadie... | 12.40 | 29.6 | ng | 1105910 | 4 | 11.33 | 748524 | 20.0 |
| 9-Octadecenoic ac... | 12.42 | 20.6 | ng | 769634 | 4 | 11.33 | 748524 | 20.0 |
| Methyl stearate | 12.50 | 3.7 | ng | 138151 | 4 | 11.33 | 748524 | 20.0 |