LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

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-BF092317.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 | 2.146 | 7 | 10 | 31 | rVB | 468236 | 784720 | 22.94% | 3.601% |
| 2 | 2.281 | 31 | 33 | 50 | rVB4 | 45758 | 111406 | 3.26% | 0.511% |
| 3 | 5.081 | 506 | 509 | 517 | rBV | 158536 | 165366 | 4.83% | 0.759% |
| 4 | 5.487 | 574 | 578 | 591 | rBV | 1164308 | 1103258 | 32.25% | 5.063% |
| 5 | 6.492 | 745 | 749 | 758 | rVB | 747884 | 708018 | 20.69% | 3.249% |
| 6 | 6.634 | 769 | 773 | 776 | rBV | 2209006 | 1850755 | 54.10% | 8.493% |
| 7 | 6.863 | 808 | 812 | 815 | rBV | 902171 | 708860 | 20.72% | 3.253% |
| 8 | 7.022 | 834 | 839 | 842 | rBV | 2732476 | 2438959 | 71.29% | 11.192% |
| 9 | 7.428 | 903 | 908 | 911 | rBV | 1790209 | 1960945 | 57.32% | 8.998% |
| 10 | 8.145 | 1026 | 1030 | 1033 | rBV | 1206972 | 967226 | 28.27% | 4.438% |
| 11 | 8.263 | 1044 | 1050 | 1054 | rBV3 | 32124 | 35553 | 1.04% | 0.163% |
| 12 | 8.316 | 1054 | 1059 | 1065 | rBV8 | 18278 | 51408 | 1.50% | 0.236% |
| 13 | 8.686 | 1119 | 1122 | 1129 | rVB | 77849 | 72468 | 2.12% | 0.333% |
| 14 | 8.898 | 1151 | 1158 | 1161 | rBV | 143481 | 140281 | 4.10% | 0.644% |
| 15 | 9.222 | 1204 | 1213 | 1216 | rBV | 3590352 | 3421206 | 100.00% | 15.699% |
| 16 | 9.328 | 1227 | 1231 | 1235 | rVB3 | 35976 | 40877 | 1.19% | 0.188% |
| 17 | 9.398 | 1240 | 1243 | 1247 | rBV2 | 50546 | 45445 | 1.33% | 0.209% |
| 18 | 9.610 | 1276 | 1279 | 1282 | rBV | 333891 | 265328 | 7.76% | 1.218% |
| 19 | 9.822 | 1310 | 1315 | 1317 | rBV2 | 50172 | 49809 | 1.46% | 0.229% |
| 20 | 9.851 | 1317 | 1320 | 1322 | rVV | 143837 | 131487 | 3.84% | 0.603% |
| 21 | 9.898 | 1324 | 1328 | 1332 | rVB | 1141399 | 999806 | 29.22% | 4.588% |
| 22 | 10.245 | 1386 | 1387 | 1391 | rVB2 | 44648 | 35275 | 1.03% | 0.162% |
| 23 | 10.316 | 1396 | 1399 | 1402 | rBV2 | 84639 | 88078 | 2.57% | 0.404% |
| 24 | 10.692 | 1459 | 1463 | 1466 | rBV | 1272854 | 1243947 | 36.36% | 5.708% |
| 25 | 10.792 | 1477 | 1480 | 1485 | rVB2 | 74887 | 74369 | 2.17% | 0.341% |
| 26 | 11.239 | 1554 | 1556 | 1559 | rBV2 | 53009 | 59609 | 1.74% | 0.274% |
| 27 | 11.386 | 1578 | 1581 | 1585 | rBV | 1019882 | 847181 | 24.76% | 3.887% |
| 28 | 11.916 | 1667 | 1671 | 1674 | rBV2 | 267017 | 297403 | 8.69% | 1.365% |
| 29 | 12.698 | 1802 | 1804 | 1808 | rBV | 157347 | 153382 | 4.48% | 0.704% |
| 30 | 12.974 | 1847 | 1851 | 1854 | rBV | 1867768 | 1801381 | 52.65% | 8.266% |
| 31 | 14.033 | 2028 | 2031 | 2034 | rVB | 630798 | 553924 | 16.19% | 2.542% |
| 32 | 15.510 | 2278 | 2282 | 2287 | rVB | 465990 | 585004 | 17.10% | 2.684% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

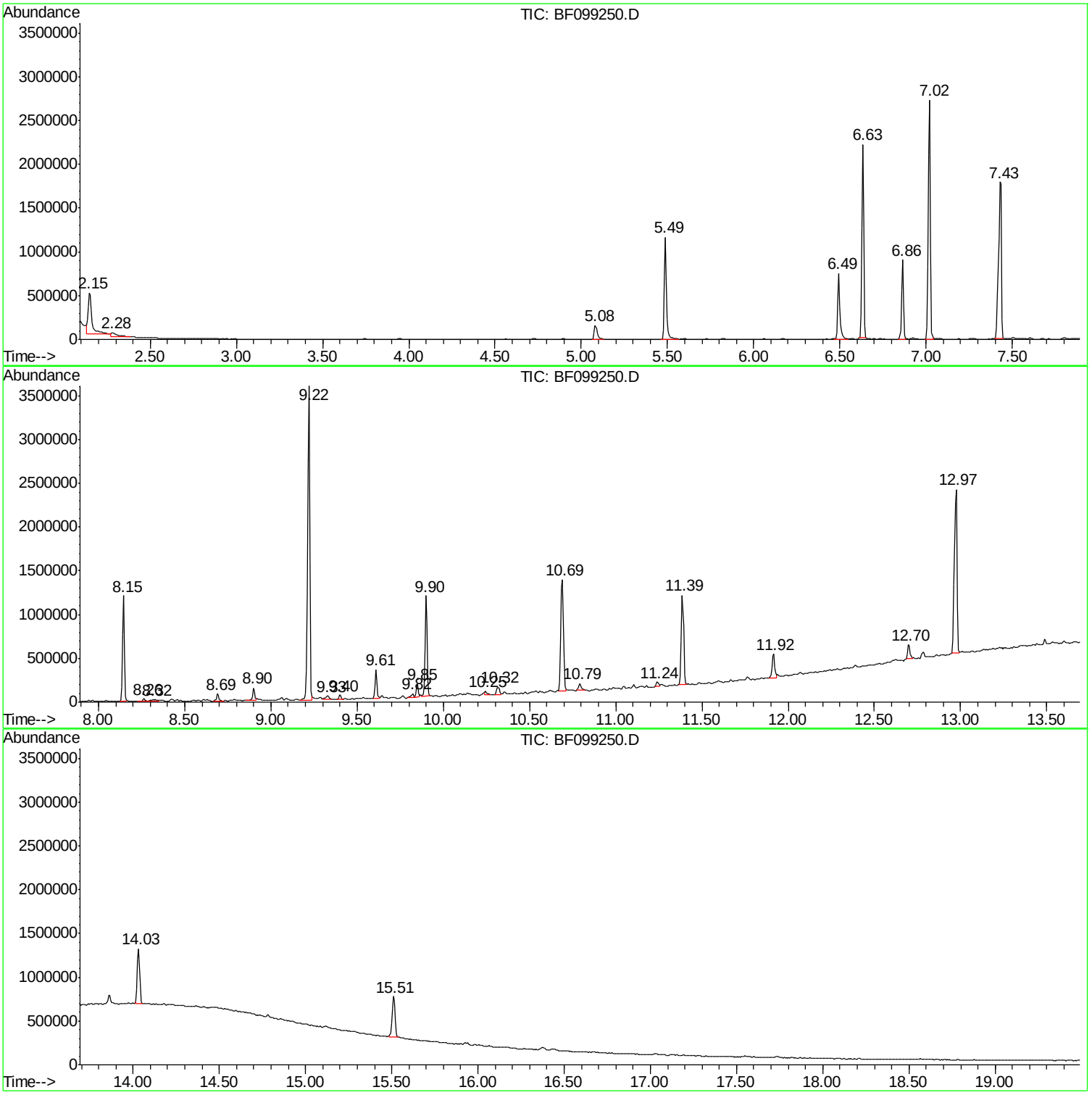
Sum of corrected areas: 21792734

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

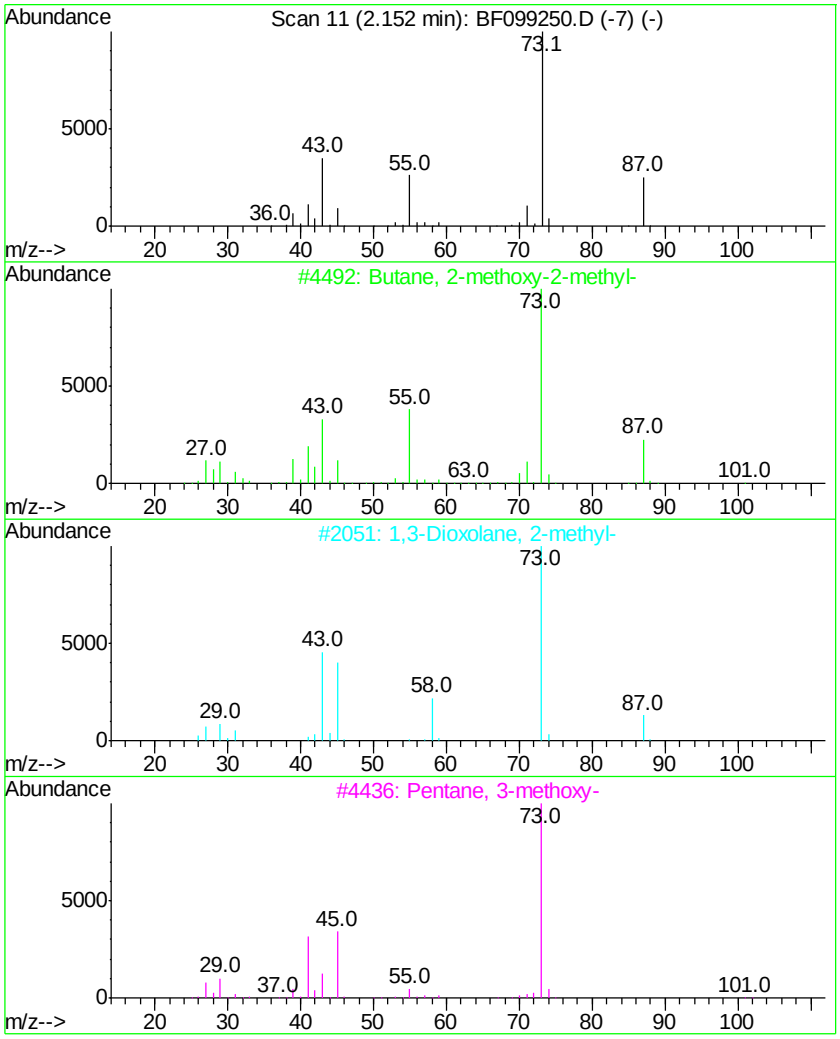
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

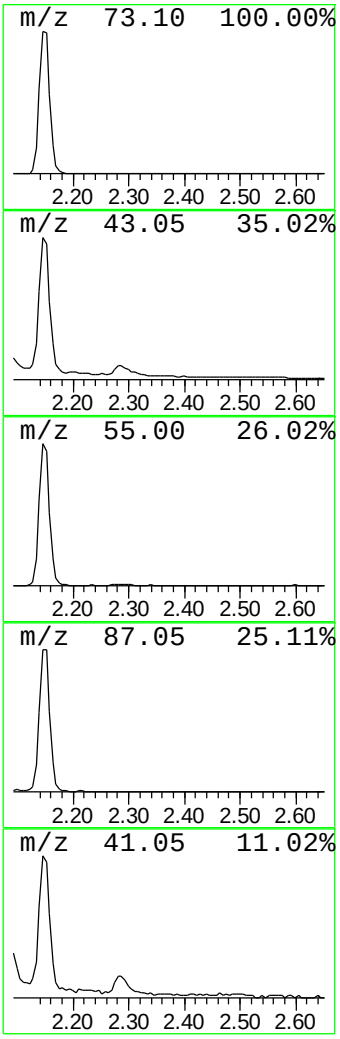
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.15 | 22.14 ng | 784720 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 23 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 12 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

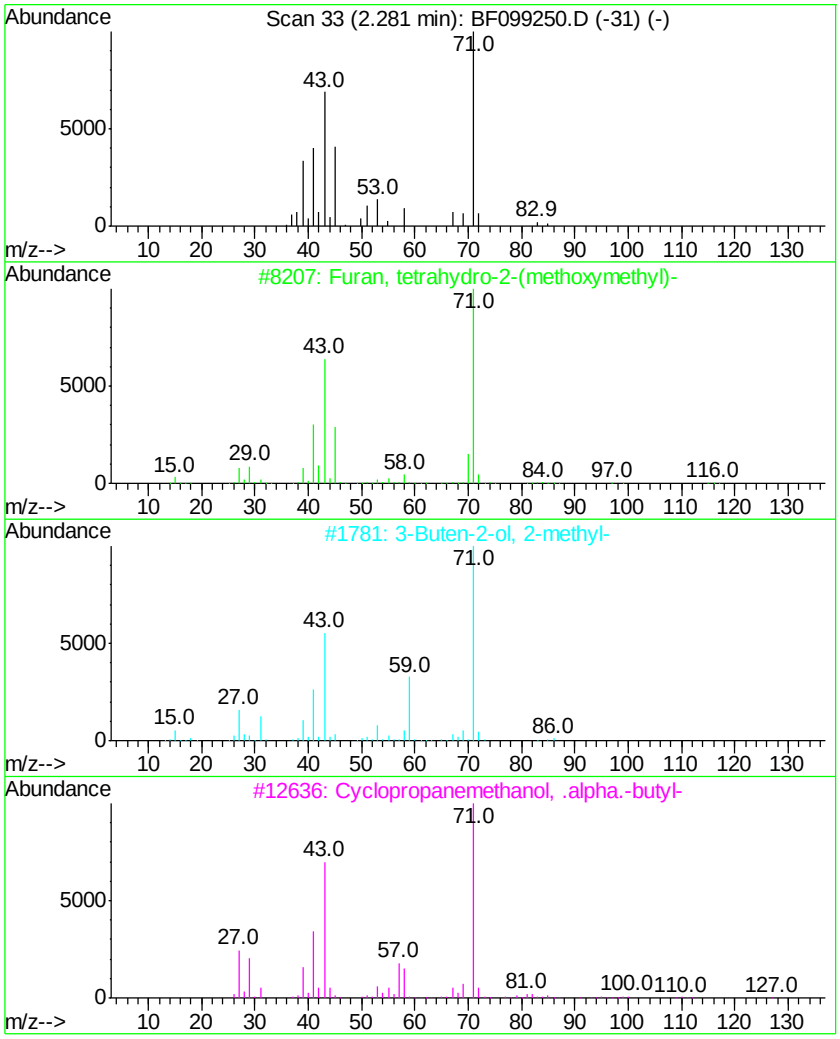
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

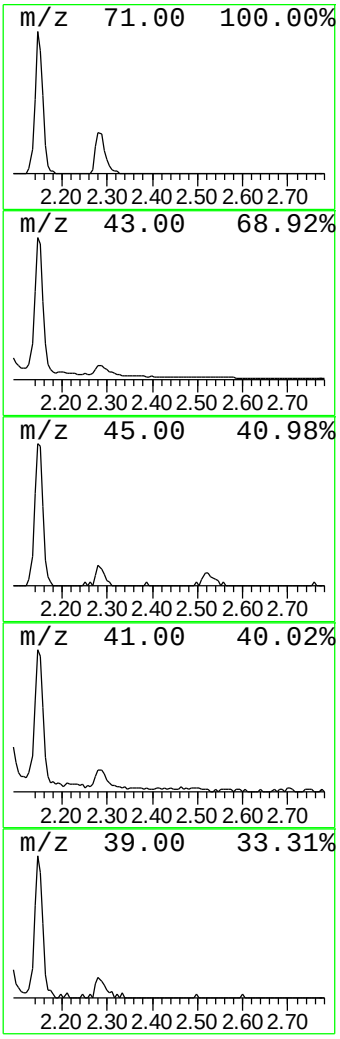
**********

Peak Number 2 Furan, tetrahydro-2-(methox... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.28 | 3.14 ng | 111406 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Furan, tetrahydro-2-(methoxymeth... | 116 | C6H12O2 | 019354-27-9 | 50 |
| 2 | 3-Buten-2-ol, 2-methyl- | 86 | C5H10O | 000115-18-4 | 40 |
| 3 | Cyclopropanemethanol, .alpha.-bu... | 128 | C8H16O | 004379-16-2 | 38 |
| 4 | 2-Furanmethanol, tetrahydro- | 102 | C5H10O2 | 000097-99-4 | 37 |
| 5 | Butanoic acid, anhydride | 158 | C8H14O3 | 000106-31-0 | 28 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

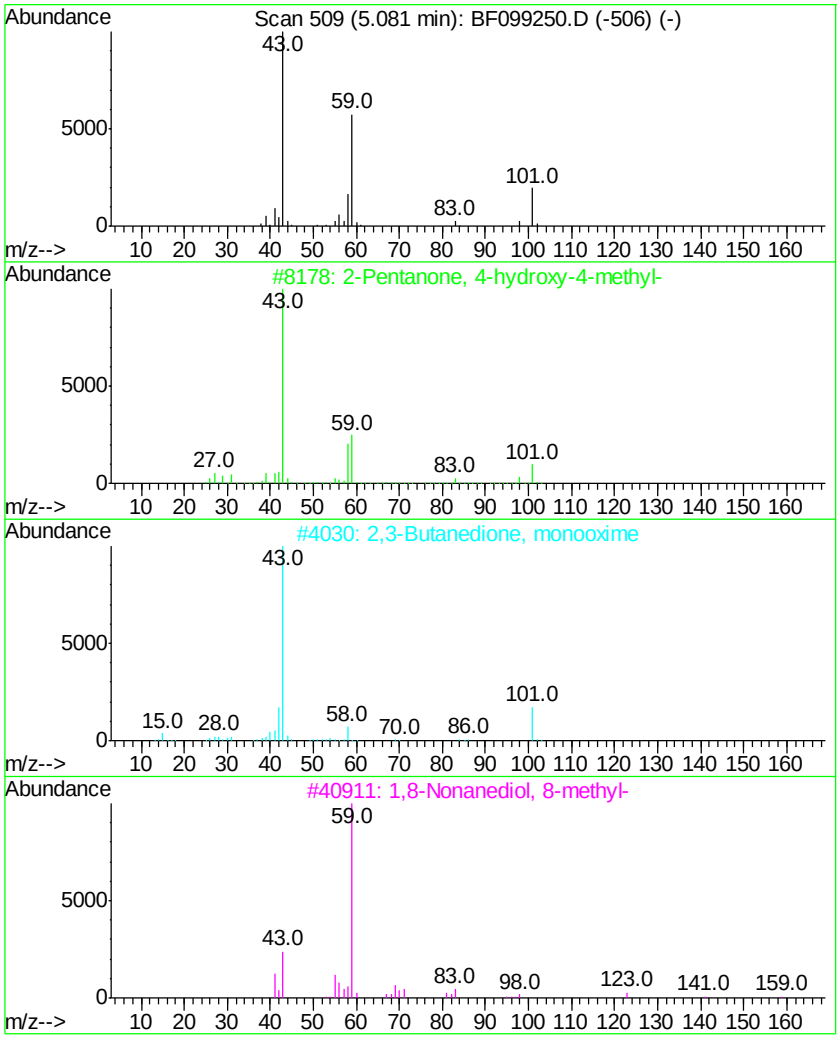
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

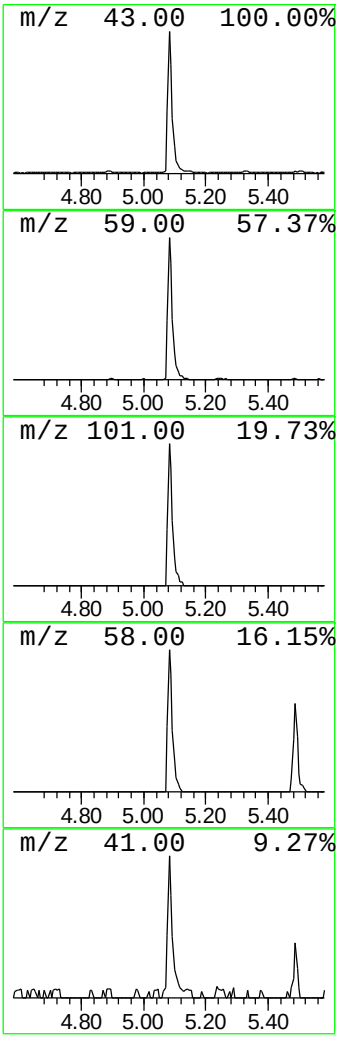
**********

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.08 | 4.67 ng | 165366 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 25 |
| 3 | 1,8-Nonanediol, 8-methyl- | 174 | C10H22O2 | 054725-73-4 | 25 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 10 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

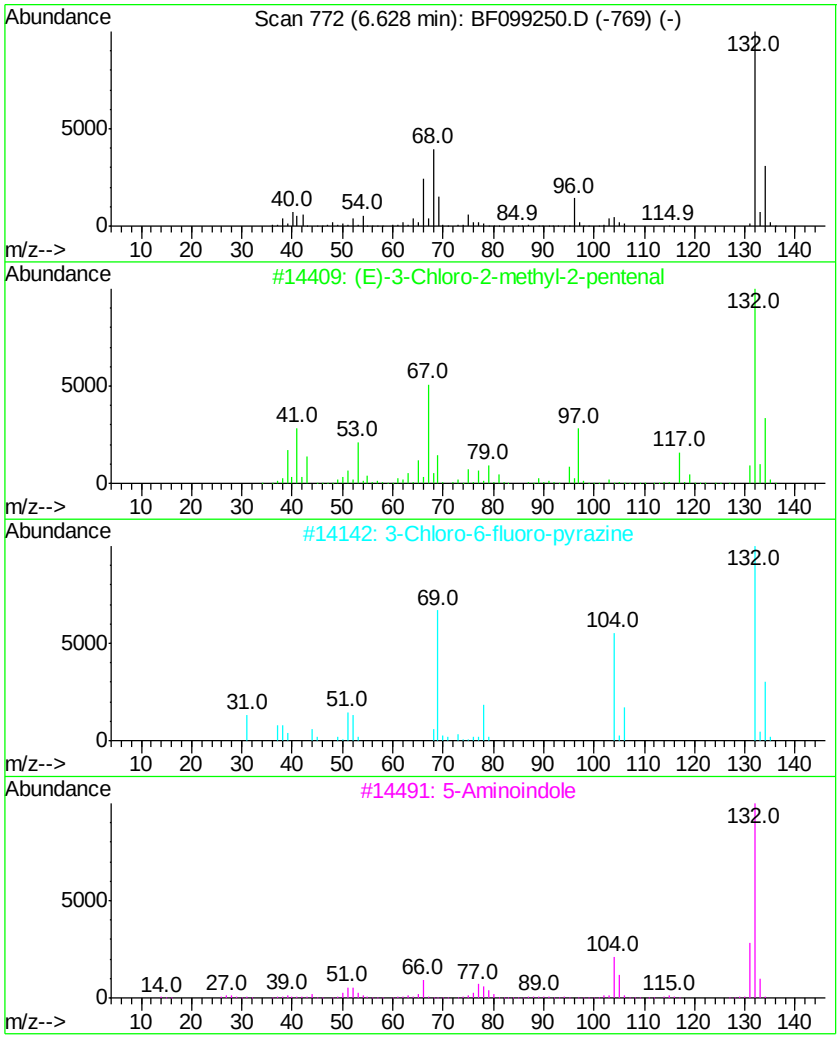
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

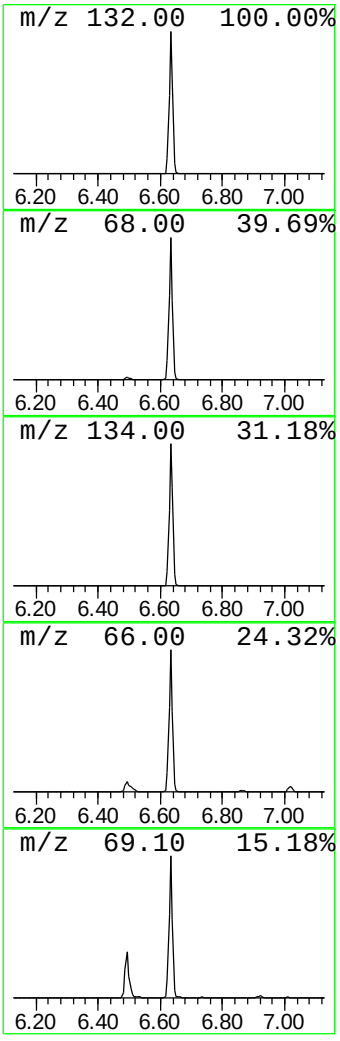
**********

Peak Number 4 unknown6.63 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.63 | 52.22 ng | 1850760 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 35 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 25 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 5 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

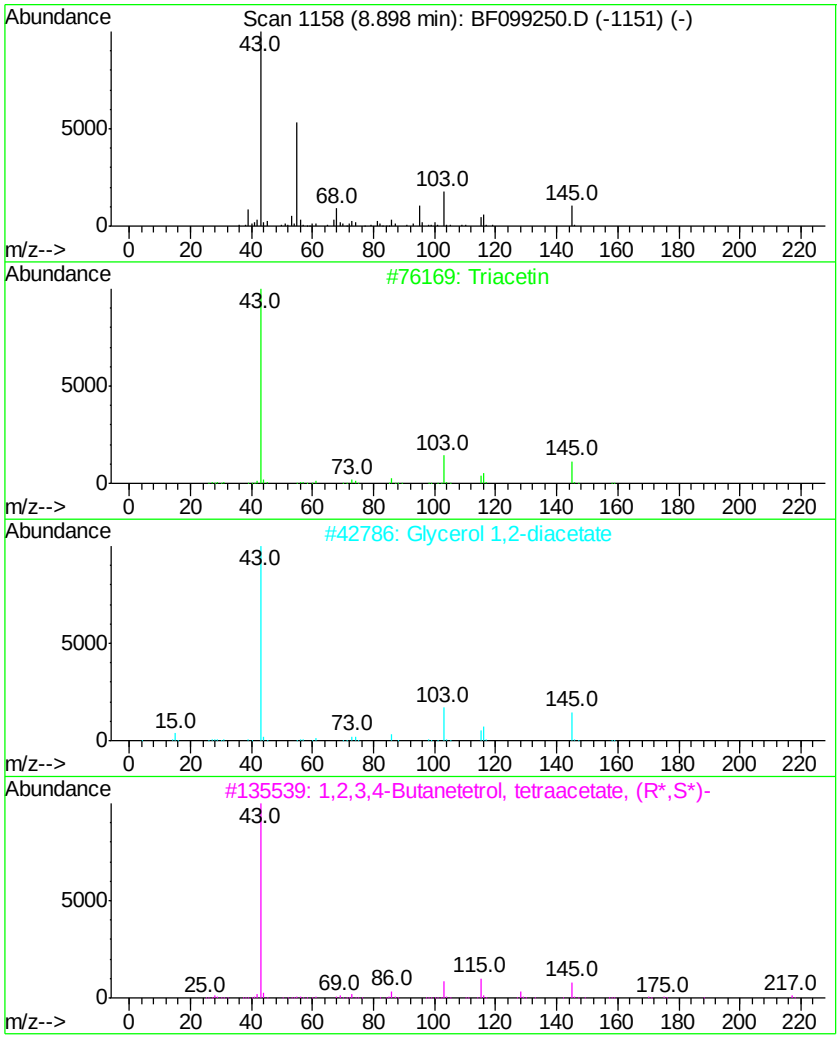
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

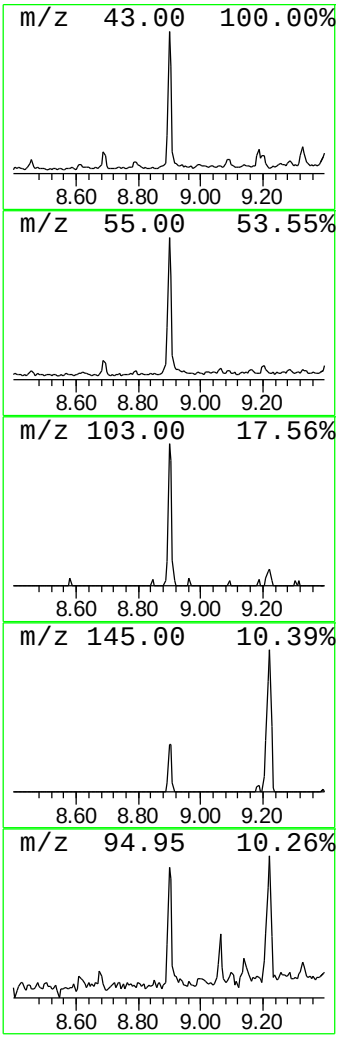
**********

Peak Number 6 Triacetin Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.90 | 2.90 ng | 140281 | Naphthalene-d8 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triacetin | 218 | C9H14O6 | 000102-76-1 | 50 |
| 2 | Glycerol 1,2-diacetate | 176 | C7H12O5 | 000102-62-5 | 50 |
| 3 | 1,2,3,4-Butanetetrol, tetraaceta... | 290 | C12H18O8 | 007208-40-4 | 43 |
| 4 | 1,1,2-Triacetoxyethane | 204 | C8H12O6 | 002983-35-9 | 25 |
| 5 | DL-Arabinose, aldononitrile, tet... | 315 | C13H17NO8 | 1000380-42-1 | 23 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

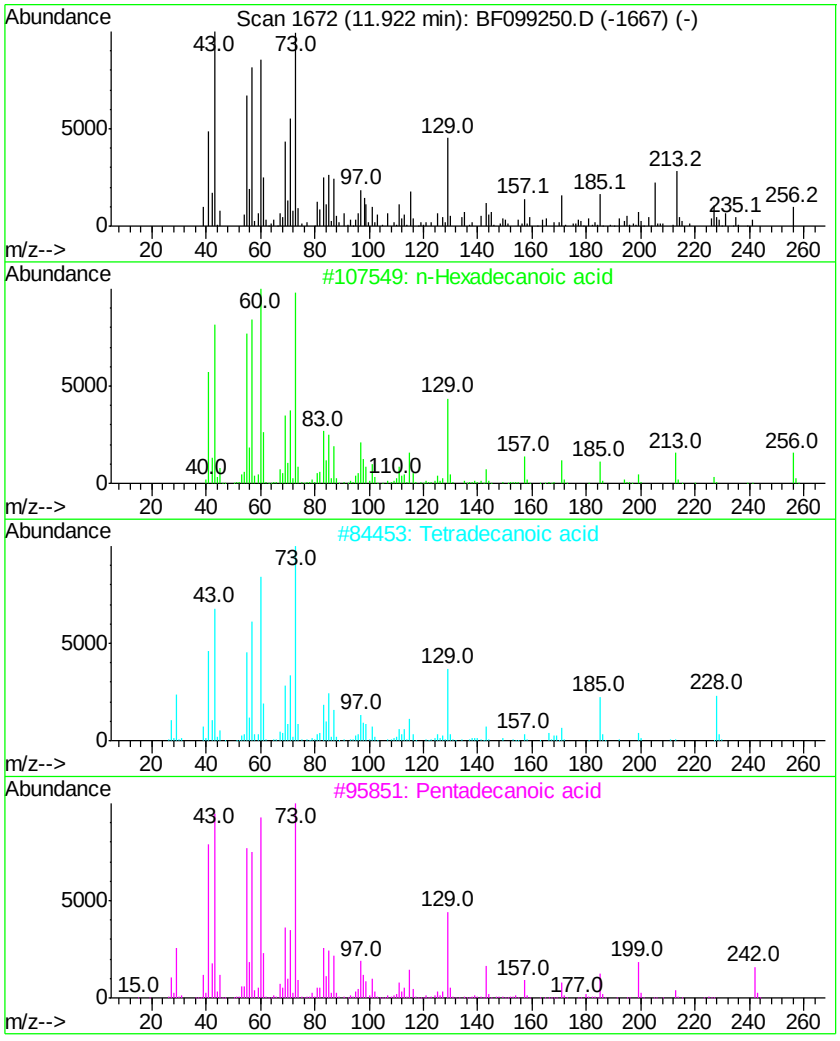
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

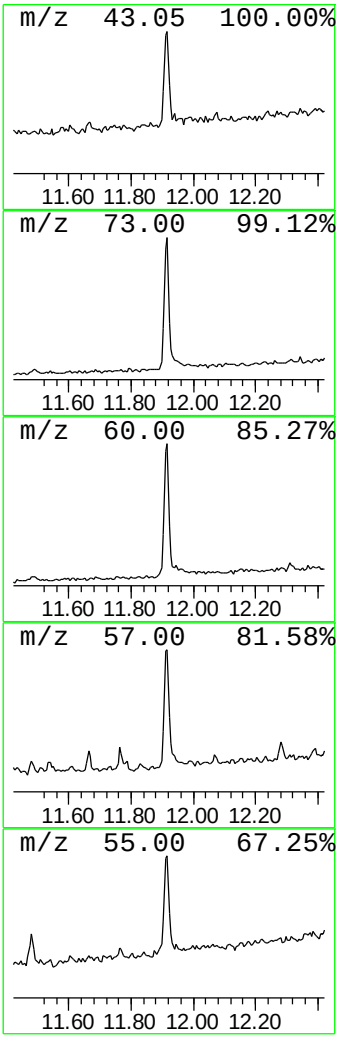
**********

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.92 | 7.02 ng | 297403 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 91 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 86 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 70 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

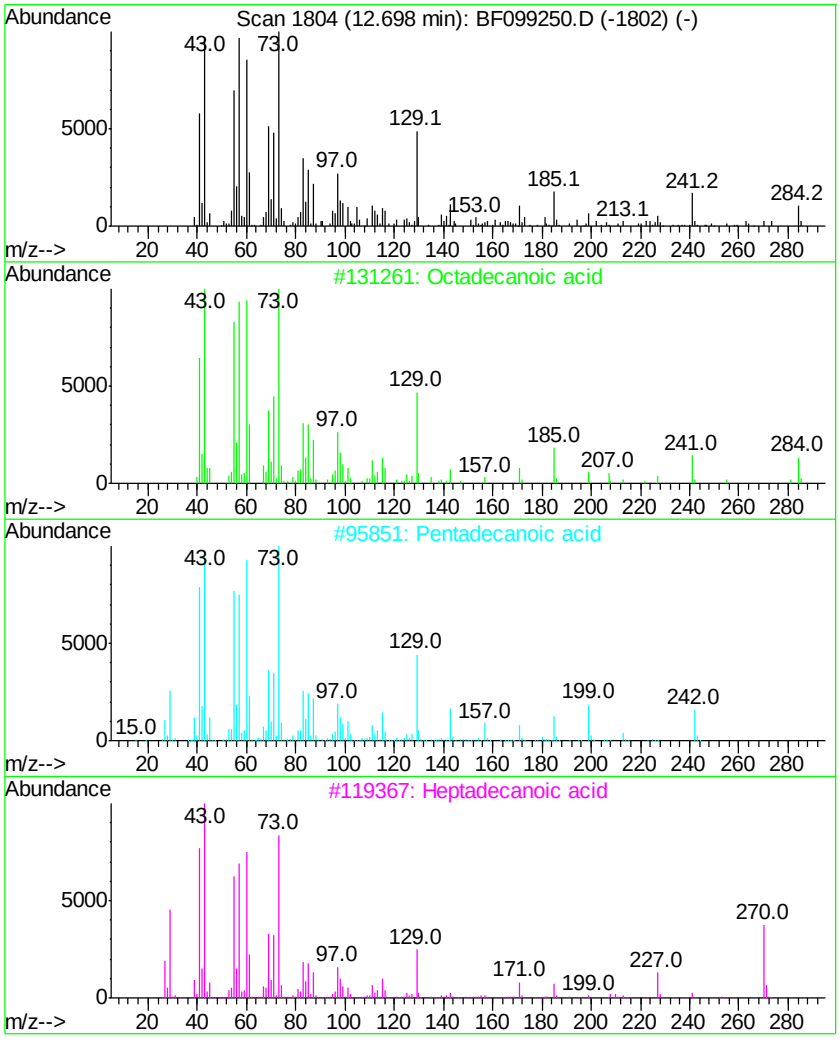
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

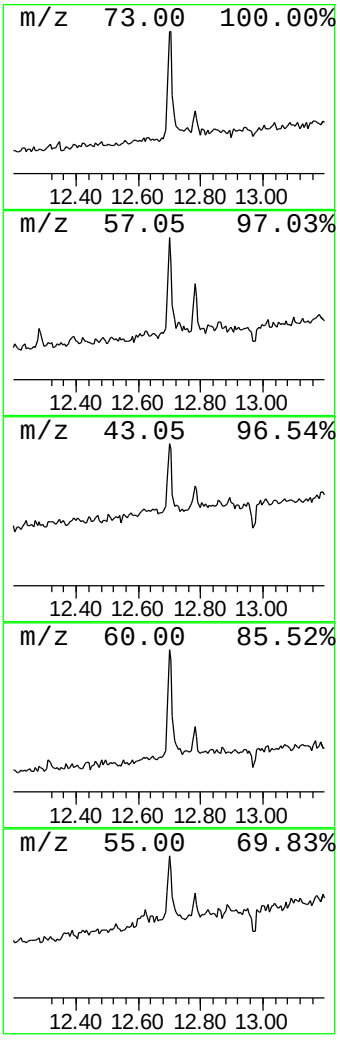
**********

Peak Number 8 Octadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.70 | 3.62 ng | 153382 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 93 |
| 3 | Heptadecanoic acid | 270 | C17H34O2 | 000506-12-7 | 93 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 89 |
| 5 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 87 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100817\
Data File : BF099250.D
Acq On : 9 Oct 2017 00:12
Operator : SJ/JU
Sample : I5706-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MH-23

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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 |
| Butane, 2-methoxy... | 2.15 | 22.1 | ng | 784720 | 1 | 6.86 | 708860 | 20.0 |
| Furan, tetrahydro... | 2.28 | 3.1 | ng | 111406 | 1 | 6.86 | 708860 | 20.0 |
| 2-Pentanone, 4-hy... | 5.08 | 4.7 | ng | 165366 | 1 | 6.86 | 708860 | 20.0 |
| unknown6.63 | 6.63 | 52.2 | ng | 1850760 | 1 | 6.86 | 708860 | 20.0 |
| Triacetin | 8.90 | 2.9 | ng | 140281 | 2 | 8.15 | 967226 | 20.0 |
| n-Hexadecanoic acid | 11.92 | 7.0 | ng | 297403 | 4 | 11.39 | 847181 | 20.0 |
| Octadecanoic acid | 12.70 | 3.6 | ng | 153382 | 4 | 11.39 | 847181 | 20.0 |