LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092234.D
Acq On : 13 Jan 2017 4:46
Operator : UM/SJ
Sample : I1131-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW-003

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-BF122116.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 | 4.733 | 245 | 249 | 259 | rBV | 1572503 | 2832339 | 49.88% | 6.457% |
| 2 | 5.201 | 287 | 290 | 292 | rBV | 3989119 | 5678345 | 100.00% | 12.946% |
| 3 | 6.264 | 380 | 383 | 390 | rBV | 4730678 | 5187312 | 91.35% | 11.826% |
| 4 | 6.367 | 390 | 392 | 395 | rVV | 4727969 | 4914626 | 86.55% | 11.204% |
| 5 | 6.596 | 410 | 412 | 414 | rBV | 954415 | 888597 | 15.65% | 2.026% |
| 6 | 6.756 | 423 | 426 | 428 | rBV | 2952596 | 3621069 | 63.77% | 8.255% |
| 7 | 7.167 | 459 | 462 | 464 | rBV | 2627647 | 2652741 | 46.72% | 6.048% |
| 8 | 7.876 | 522 | 524 | 527 | rBV | 844420 | 1013968 | 17.86% | 2.312% |
| 9 | 8.962 | 616 | 619 | 621 | rBV | 4596339 | 4464474 | 78.62% | 10.178% |
| 10 | 9.362 | 651 | 654 | 656 | rBV | 1108608 | 944412 | 16.63% | 2.153% |
| 11 | 9.625 | 675 | 677 | 679 | rBV | 1236002 | 1240601 | 21.85% | 2.828% |
| 12 | 10.082 | 715 | 717 | 718 | rVB | 65639 | 69367 | 1.22% | 0.158% |
| 13 | 10.299 | 732 | 736 | 738 | rBV | 35141 | 60346 | 1.06% | 0.138% |
| 14 | 10.413 | 744 | 746 | 749 | rBV2 | 2057297 | 2758933 | 48.59% | 6.290% |
| 15 | 10.550 | 756 | 758 | 764 | rVB | 108225 | 153396 | 2.70% | 0.350% |
| 16 | 10.996 | 795 | 797 | 798 | rBV2 | 69592 | 74286 | 1.31% | 0.169% |
| 17 | 11.111 | 804 | 807 | 811 | rVB2 | 748885 | 1145182 | 20.17% | 2.611% |
| 18 | 11.659 | 853 | 855 | 858 | rVV2 | 197617 | 226326 | 3.99% | 0.516% |
| 19 | 12.311 | 910 | 912 | 914 | rBV | 180490 | 161219 | 2.84% | 0.368% |
| 20 | 12.539 | 929 | 932 | 934 | rBV | 137245 | 175896 | 3.10% | 0.401% |
| 21 | 12.688 | 943 | 945 | 948 | rVB | 2689065 | 3059108 | 53.87% | 6.974% |
| 22 | 13.602 | 1022 | 1025 | 1031 | rBV2 | 150339 | 269610 | 4.75% | 0.615% |
| 23 | 13.728 | 1034 | 1036 | 1039 | rBV | 821974 | 1015582 | 17.89% | 2.315% |
| 24 | 14.585 | 1109 | 1111 | 1113 | rBV | 49966 | 57245 | 1.01% | 0.131% |
| 25 | 14.722 | 1121 | 1123 | 1127 | rBV | 74857 | 140577 | 2.48% | 0.320% |
| 26 | 15.042 | 1149 | 1151 | 1153 | rBV | 57931 | 75892 | 1.34% | 0.173% |
| 27 | 15.088 | 1153 | 1155 | 1158 | rBV | 752237 | 915082 | 16.12% | 2.086% |
| 28 | 15.568 | 1194 | 1197 | 1200 | rBV4 | 30299 | 66896 | 1.18% | 0.153% |

Sum of corrected areas: 43863427

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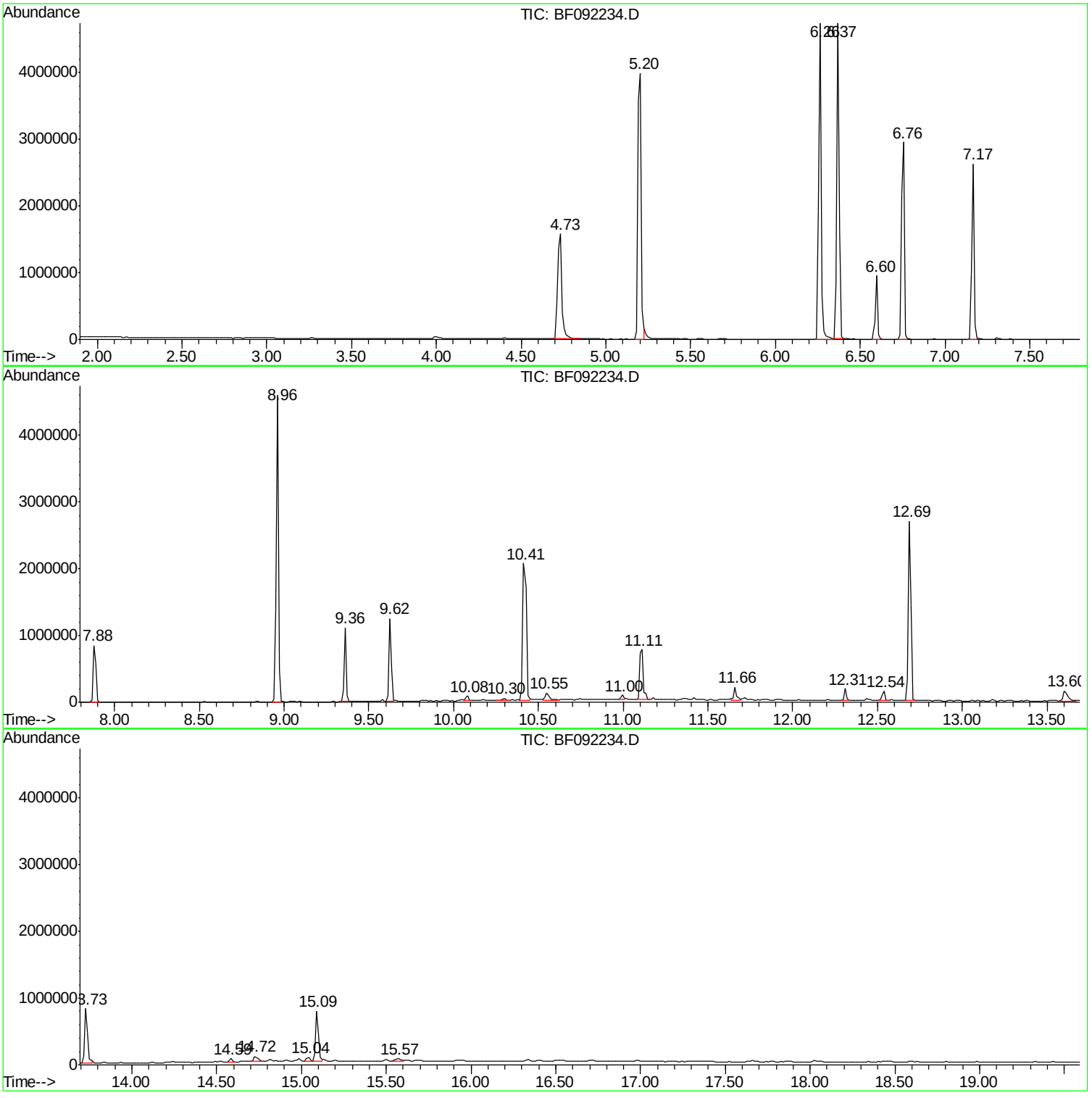
Sample : I1131-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SW-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092234.D
Acq On : 13 Jan 2017 4:46
Operator : UM/SJ
Sample : I1131-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

**Instrument :** BNA_F
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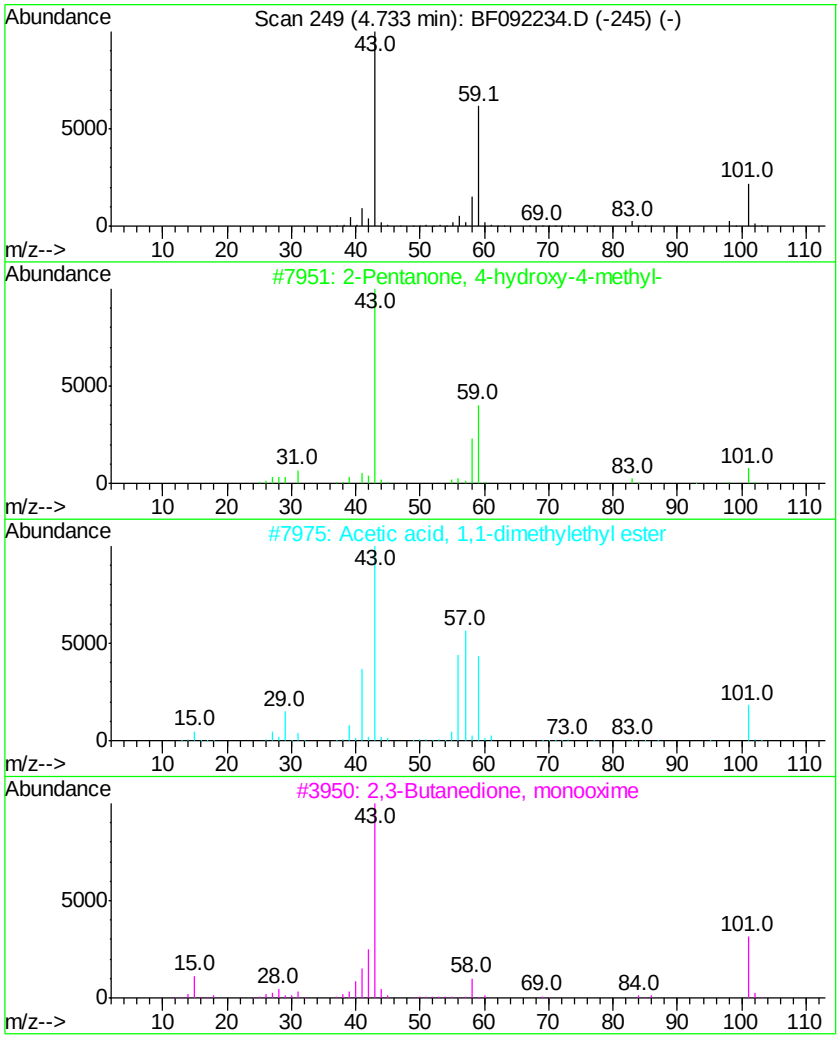
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

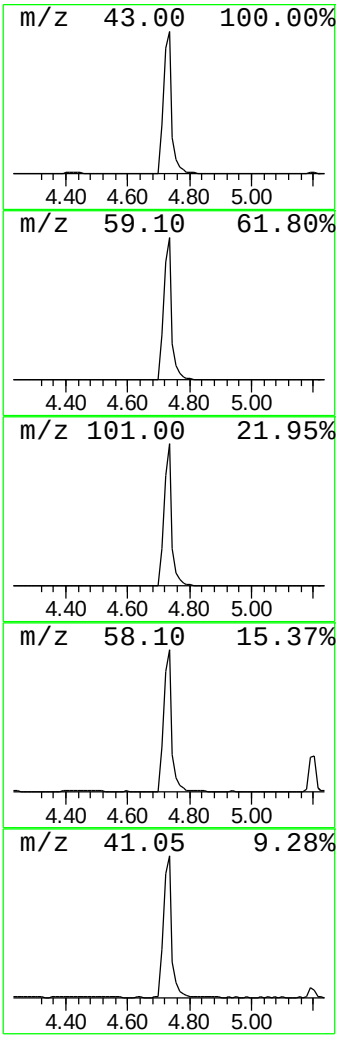
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.73 | 63.75 ng | 2832340 | 1,4-Dichlorobenzene-d4 | 6.60 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 25 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



# Library Search Compound Report

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Data File : BF092234.D
Acq On : 13 Jan 2017 4:46
Operator : UM/SJ
Sample : I1131-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

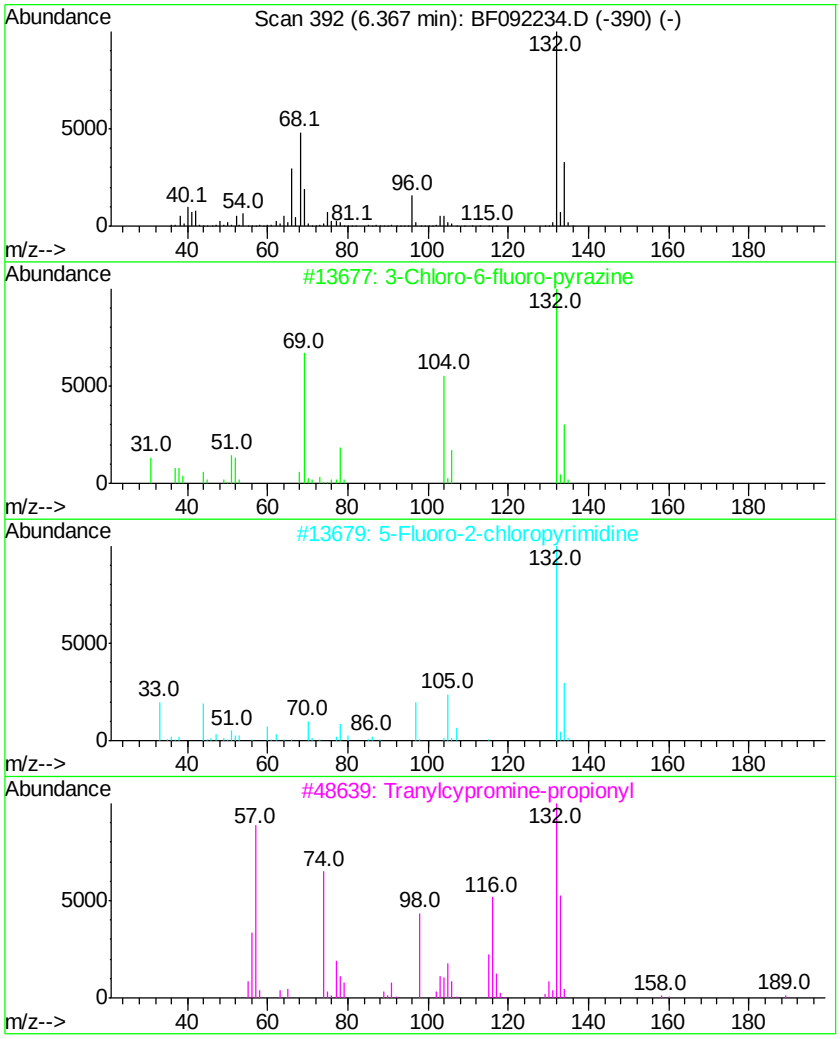
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

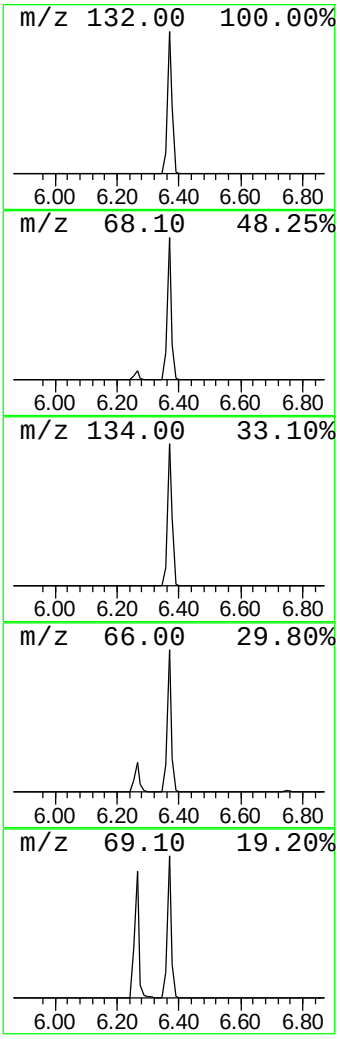
**********

Peak Number 2 unknown6.37 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.37 | 110.62 ng | 4914630 | 1,4-Dichlorobenzene-d4 | 6.60 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |



# Library Search Compound Report

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Operator : UM/SJ
Sample : I1131-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

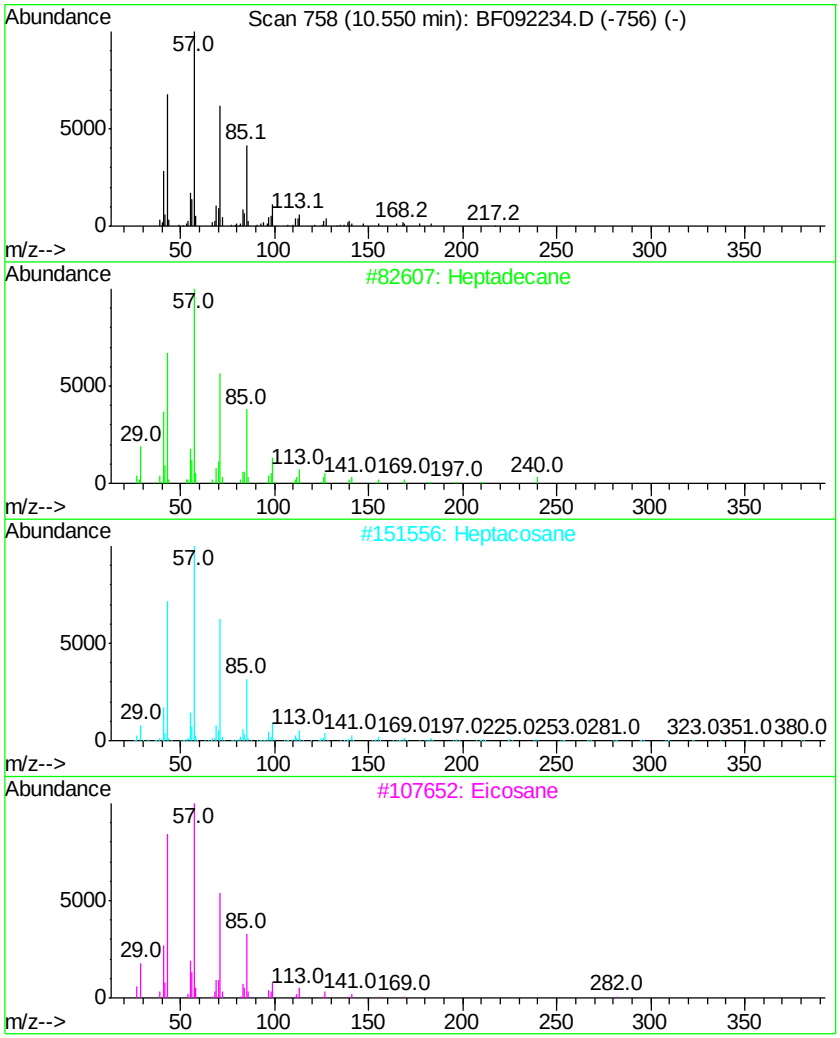
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

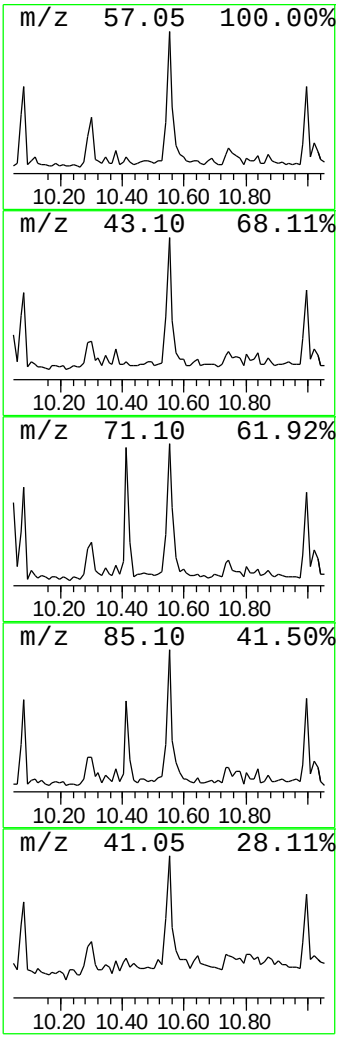
**********

Peak Number 4 Heptadecane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.55 | 2.68 ng | 153396 | Phenanthrene-d10 | 11.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 91 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 3 | Eicosane | 282 | C20H42 | 000112-95-8 | 90 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
Data File : BF092234.D
Acq On : 13 Jan 2017 4:46
Operator : UM/SJ
Sample : I1131-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

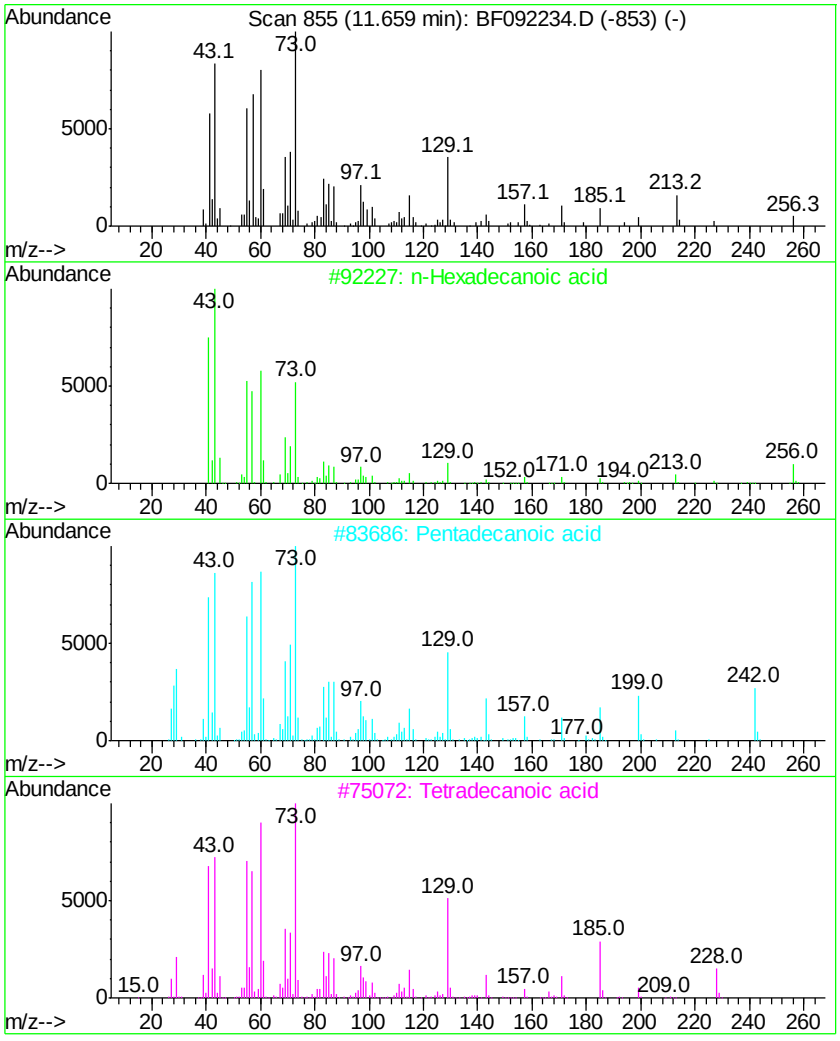
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

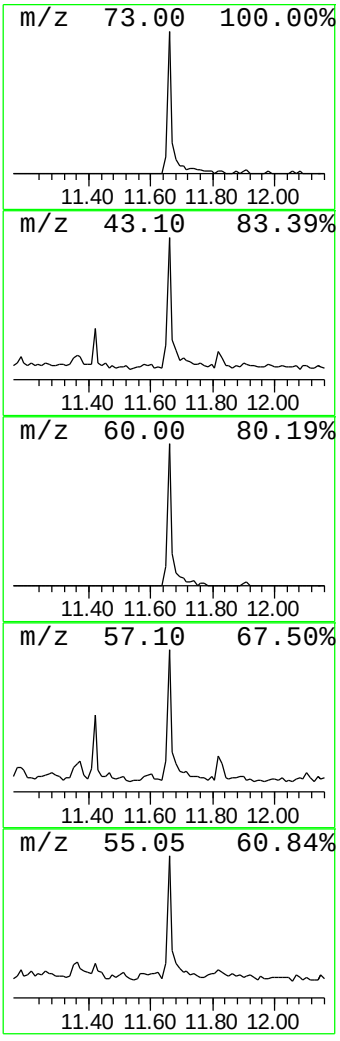
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.66 | 3.95 ng | 226326 | Phenanthrene-d10 | 11.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 83 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 80 |
| 5 | Nonanoic acid | 158 | C9H18O2 | 000112-05-0 | 43 |



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Operator : UM/SJ
Sample : I1131-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

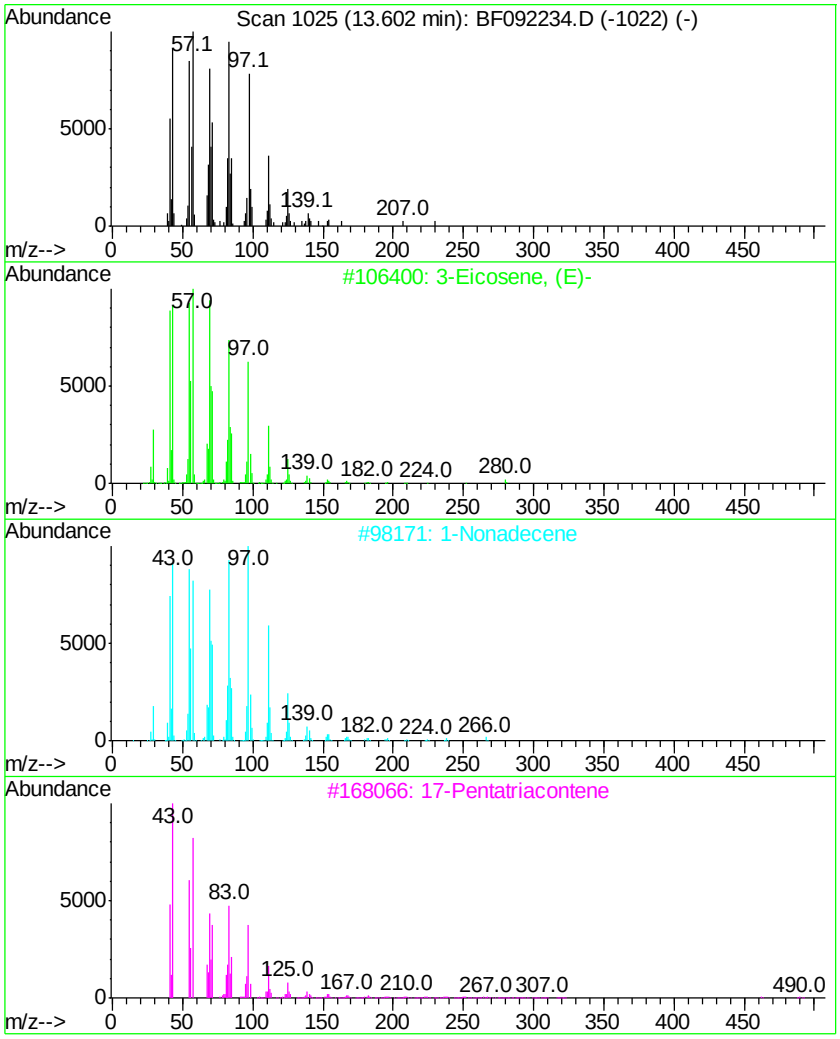
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

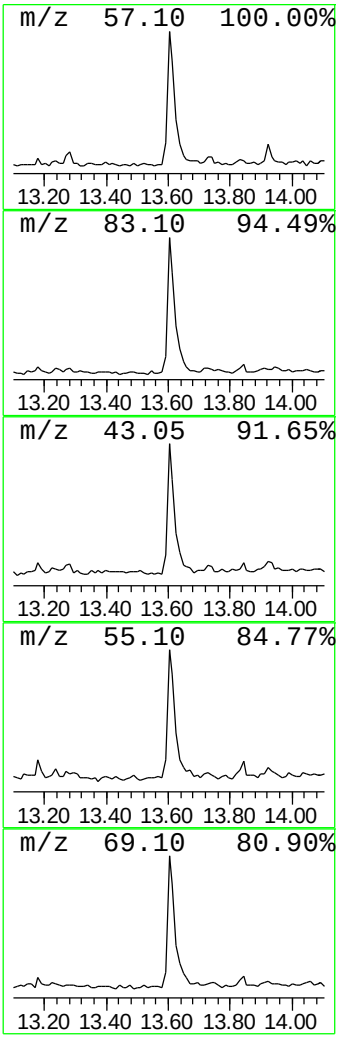
**********

Peak Number 7 3-Eicosene, (E)- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.60 | 5.31 ng | 269610 | Chrysene-d12 | 13.73 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 91 |
| 2 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 91 |
| 3 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 91 |
| 4 | 1-Octadecanol | 270 | C18H38O | 000112-92-5 | 90 |
| 5 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 87 |



# Tentatively Identified Compound (LSC) summary

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Data File : BF092234.D
Acq On : 13 Jan 2017 4:46
Operator : UM/SJ
Sample : I1131-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.73 | 63.8 | ng | 2832340 | 1 | 6.60 | 888597 | 20.0 |
| unknown6.37 | 6.37 | 110.6 | ng | 4914630 | 1 | 6.60 | 888597 | 20.0 |
| Heptadecane | 10.55 | 2.7 | ng | 153396 | 4 | 11.11 | 1145180 | 20.0 |
| n-Hexadecanoic acid | 11.66 | 4.0 | ng | 226326 | 4 | 11.11 | 1145180 | 20.0 |
| 3-Eicosene, (E)- | 13.60 | 5.3 | ng | 269610 | 5 | 13.73 | 1015580 | 20.0 |