LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081482.D
Acq On : 6 Sep 2015 00:32
Operator : UM/IZ
Sample : G3555-07
Misc :
ALS Vial : 59 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-7

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-BF090115.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 | 4.399 | 243 | 246 | 260 | rVB | 613908 | 1405942 | 65.24% | 7.804% |
| 2 | 4.901 | 288 | 290 | 293 | rBV | 1387286 | 1857462 | 86.19% | 10.311% |
| 3 | 6.033 | 386 | 389 | 391 | rBV | 1632593 | 2155004 | 100.00% | 11.962% |
| 4 | 6.124 | 395 | 397 | 399 | rBV | 1962001 | 1826354 | 84.75% | 10.138% |
| 5 | 6.353 | 415 | 417 | 420 | rVB | 405301 | 362544 | 16.82% | 2.012% |
| 6 | 6.513 | 429 | 431 | 433 | rBV | 1521183 | 1333924 | 61.90% | 7.405% |
| 7 | 6.936 | 465 | 468 | 470 | rBV | 1294164 | 1283962 | 59.58% | 7.127% |
| 8 | 7.645 | 528 | 530 | 532 | rBV | 545860 | 455729 | 21.15% | 2.530% |
| 9 | 8.730 | 622 | 625 | 627 | rBV | 2216949 | 2029044 | 94.15% | 11.263% |
| 10 | 9.130 | 658 | 660 | 663 | rBV | 443653 | 371313 | 17.23% | 2.061% |
| 11 | 9.382 | 680 | 682 | 685 | rVB | 511310 | 465629 | 21.61% | 2.585% |
| 12 | 10.171 | 748 | 751 | 753 | rBV | 1288933 | 1266014 | 58.75% | 7.028% |
| 13 | 10.319 | 762 | 764 | 767 | rBV | 31919 | 35225 | 1.63% | 0.196% |
| 14 | 10.765 | 801 | 803 | 804 | rBV | 28628 | 23231 | 1.08% | 0.129% |
| 15 | 10.845 | 808 | 810 | 813 | rBV | 482286 | 455222 | 21.12% | 2.527% |
| 16 | 11.428 | 859 | 861 | 867 | rBV | 60737 | 76702 | 3.56% | 0.426% |
| 17 | 12.296 | 934 | 937 | 939 | rBV | 94098 | 132384 | 6.14% | 0.735% |
| 18 | 12.365 | 942 | 943 | 946 | rVB | 31929 | 28238 | 1.31% | 0.157% |
| 19 | 12.434 | 946 | 949 | 952 | rBV | 1705192 | 1609358 | 74.68% | 8.934% |
| 20 | 12.994 | 995 | 998 | 1000 | rBV | 99235 | 95959 | 4.45% | 0.533% |
| 21 | 13.359 | 1028 | 1030 | 1036 | rBV | 71556 | 142452 | 6.61% | 0.791% |
| 22 | 13.451 | 1036 | 1038 | 1041 | rBV | 317334 | 313128 | 14.53% | 1.738% |
| 23 | 13.679 | 1056 | 1058 | 1060 | rBV | 27673 | 29218 | 1.36% | 0.162% |
| 24 | 13.977 | 1082 | 1084 | 1086 | rBV | 27189 | 25556 | 1.19% | 0.142% |
| 25 | 14.765 | 1151 | 1153 | 1155 | rBV | 208384 | 235262 | 10.92% | 1.306% |

Sum of corrected areas: 18014856

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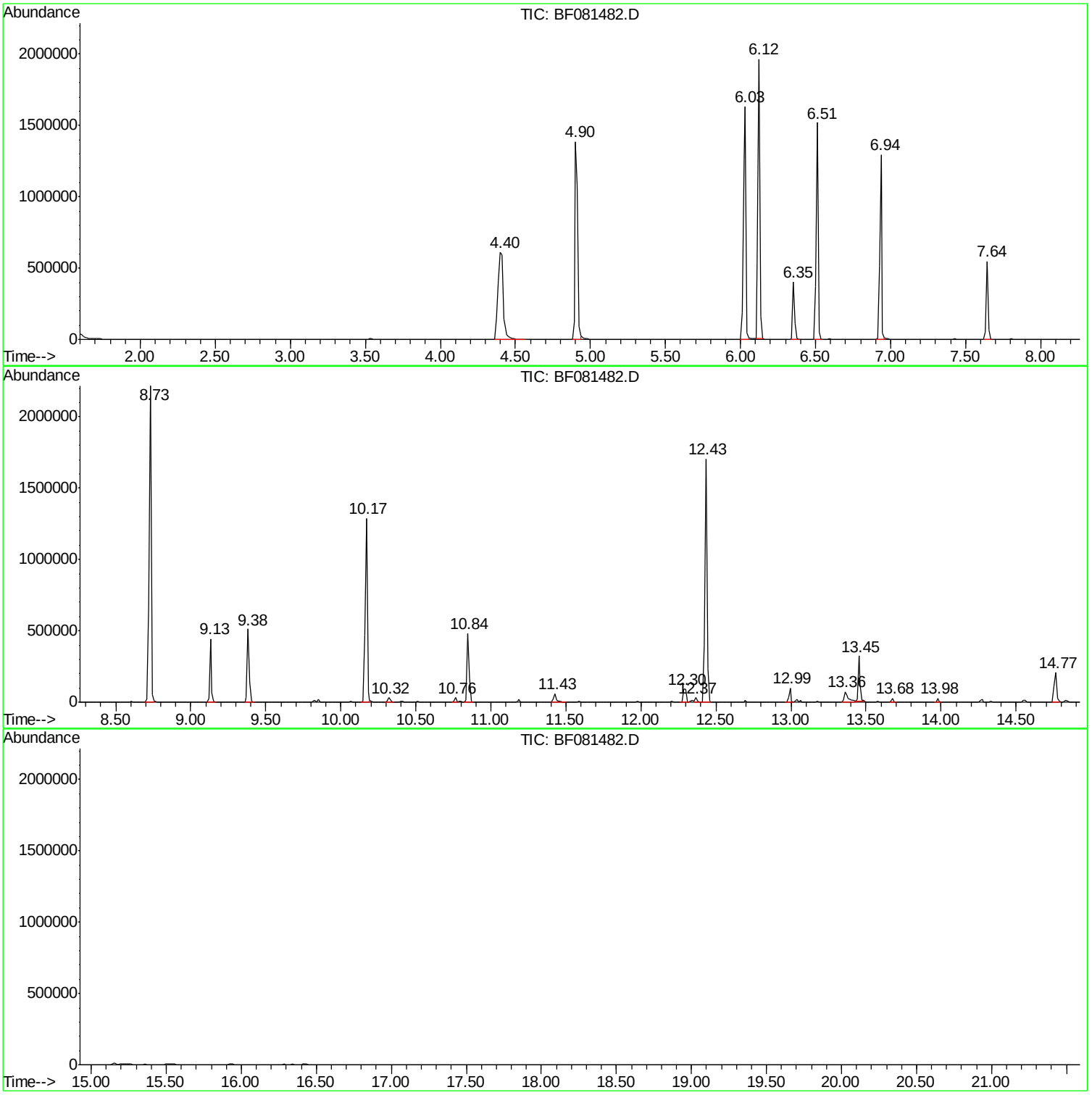
Sample : G3555-07
Misc :
ALS Vial : 59 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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\BF090515\
Data File : BF081482.D
Acq On : 6 Sep 2015 00:32
Operator : UM/IZ
Sample : G3555-07
Misc :
ALS Vial : 59 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

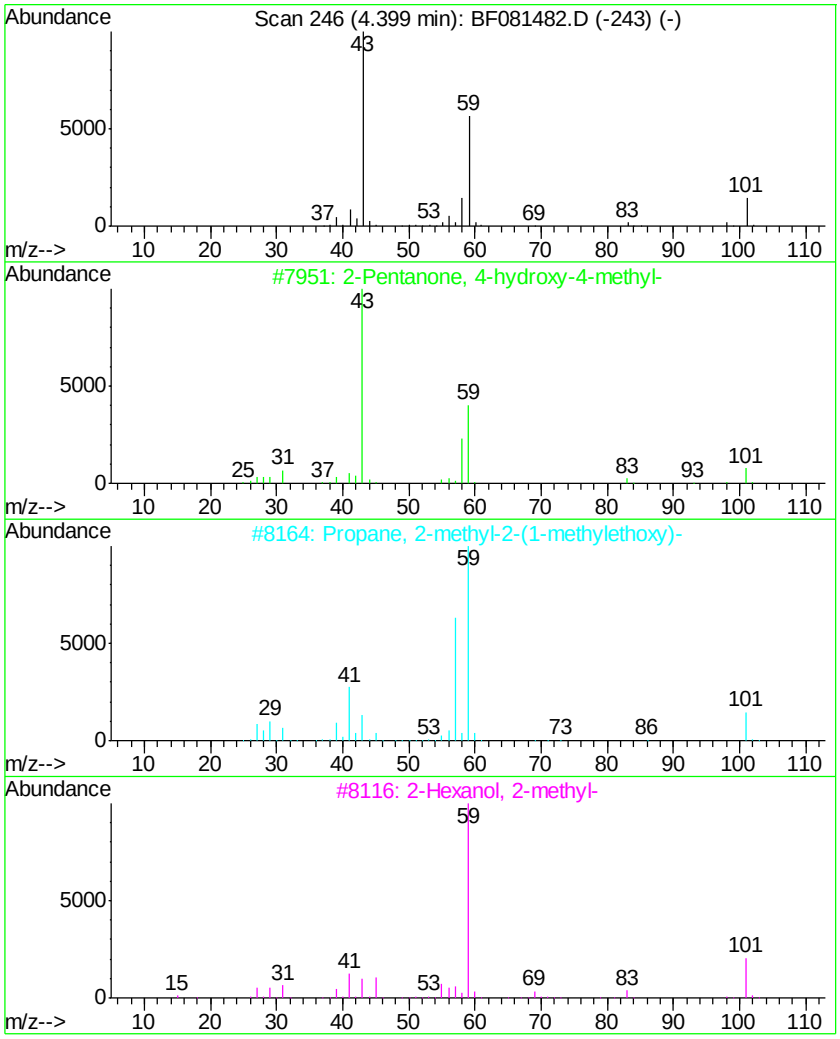
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

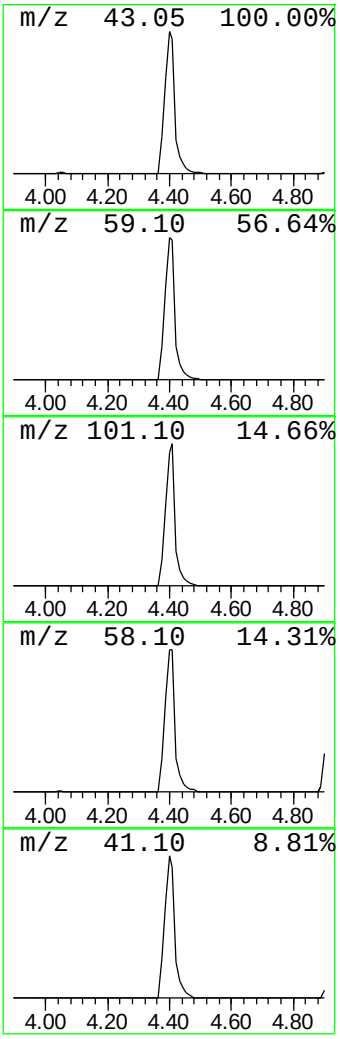
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.40 | 77.56 ng | 1405940 | 1,4-Dichlorobenzene-d4 | 6.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 42 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 4 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081482.D
Acq On : 6 Sep 2015 00:32
Operator : UM/IZ
Sample : G3555-07
Misc :
ALS Vial : 59 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

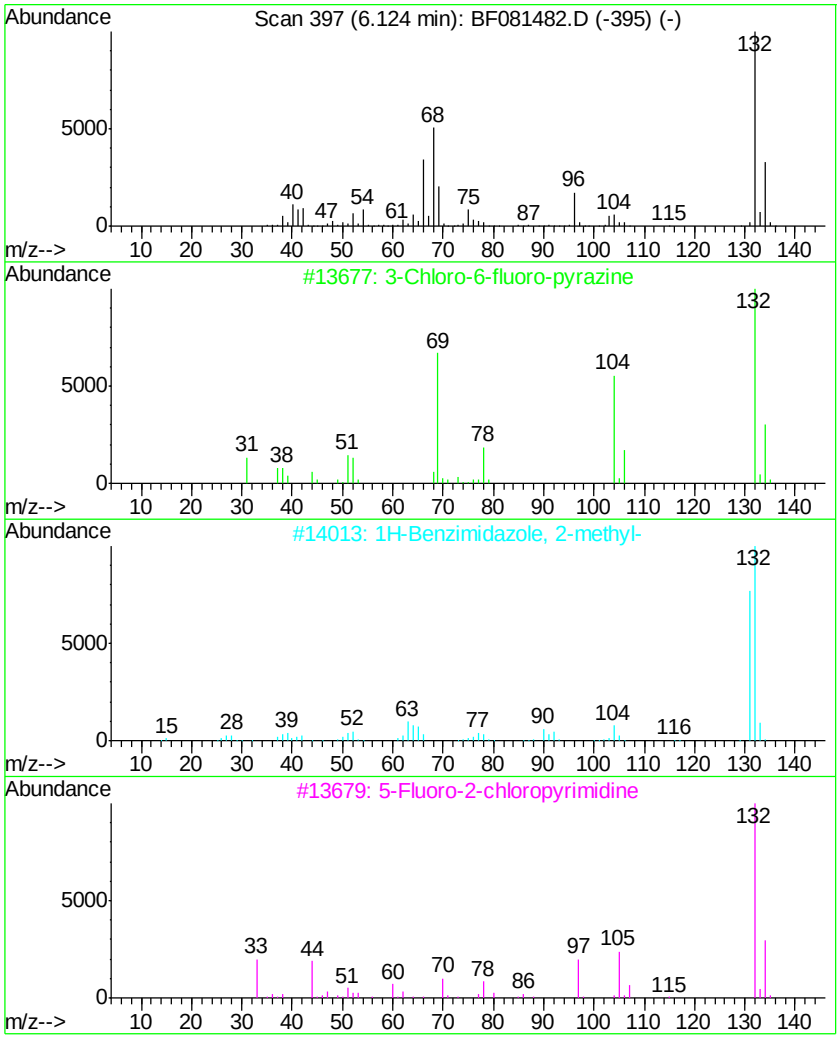
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

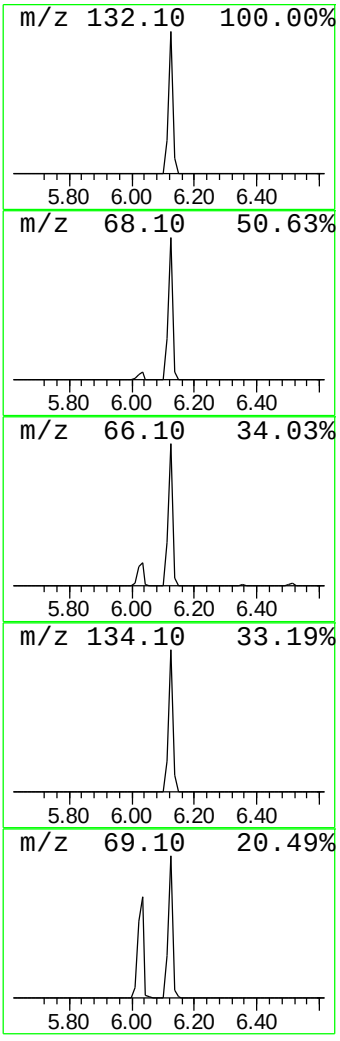
**********

Peak Number 2 unknown6.12 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.12 | 100.75 ng | 1826350 | 1,4-Dichlorobenzene-d4 | 6.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 4 | 2-Cyclohexen-1-one | 96 | C6H8O | 000930-68-7 | 10 |
| 5 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081482.D
Acq On : 6 Sep 2015 00:32
Operator : UM/IZ
Sample : G3555-07
Misc :
ALS Vial : 59 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

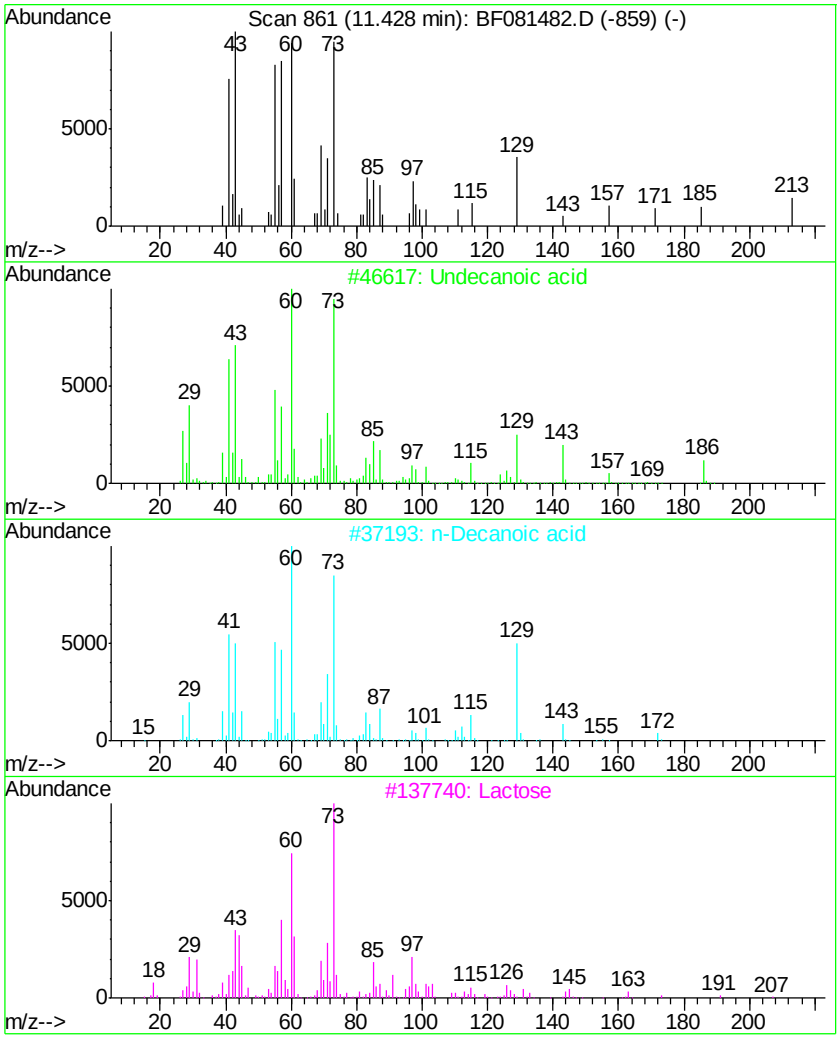
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

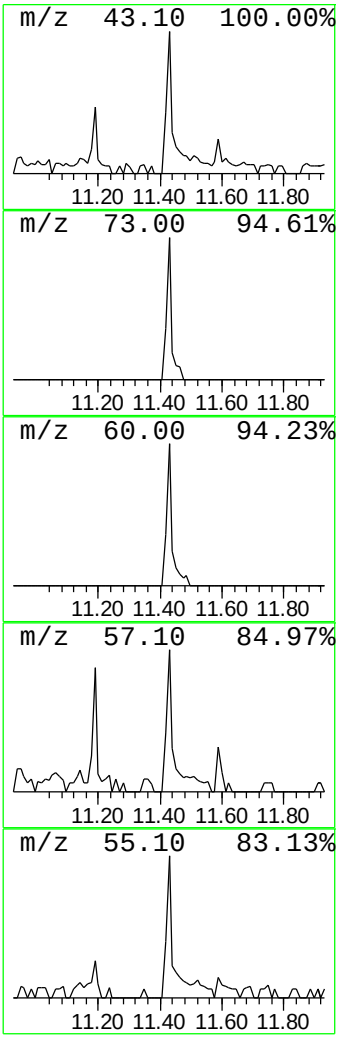
**********

Peak Number 4 Undecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.43 | 3.37 ng | 76702 | Phenanthrene-d10 | 10.84 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 50 |
| 2 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 50 |
| 3 | Lactose | 342 | C12H22O11 | 000063-42-3 | 47 |
| 4 | .alpha.-D-Glucopyranoside, .alph... | 342 | C12H22O11 | 000099-20-7 | 43 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 42 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081482.D
Acq On : 6 Sep 2015 00:32
Operator : UM/IZ
Sample : G3555-07
Misc :
ALS Vial : 59 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

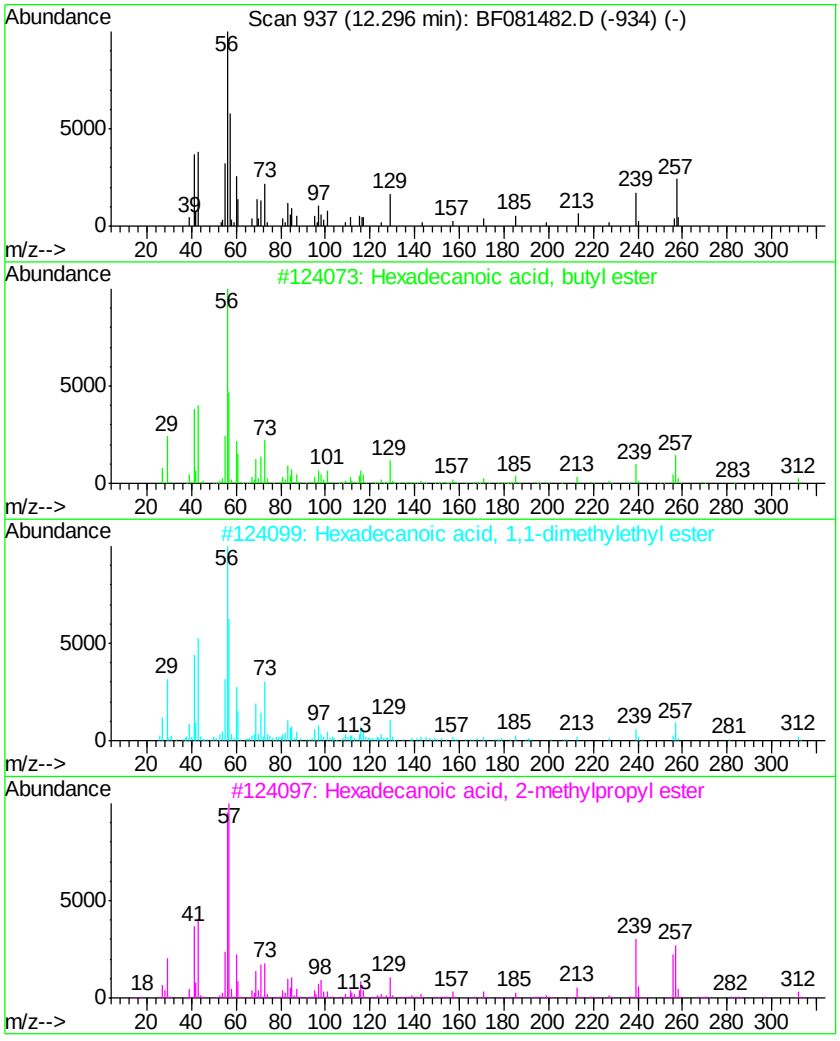
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

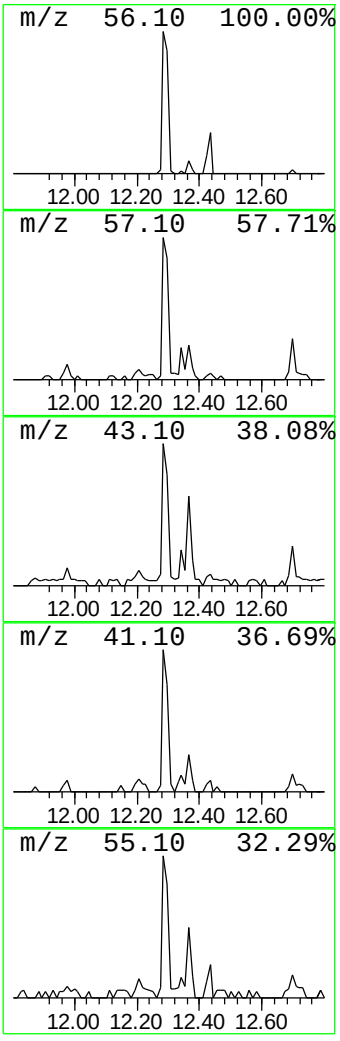
**********

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.30 | 8.46 ng | 132384 | Chrysene-d12 | 13.45 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 91 |
| 2 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 52 |
| 3 | Hexadecanoic acid, 2-methylpropy... | 312 | C20H40O2 | 000110-34-9 | 45 |
| 4 | Pentadecane, 8-methylene- | 224 | C16H32 | 055668-09-2 | 32 |
| 5 | 1-Hexene, 2-methyl- | 98 | C7H14 | 006094-02-6 | 27 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081482.D
Acq On : 6 Sep 2015 00:32
Operator : UM/IZ
Sample : G3555-07
Misc :
ALS Vial : 59 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

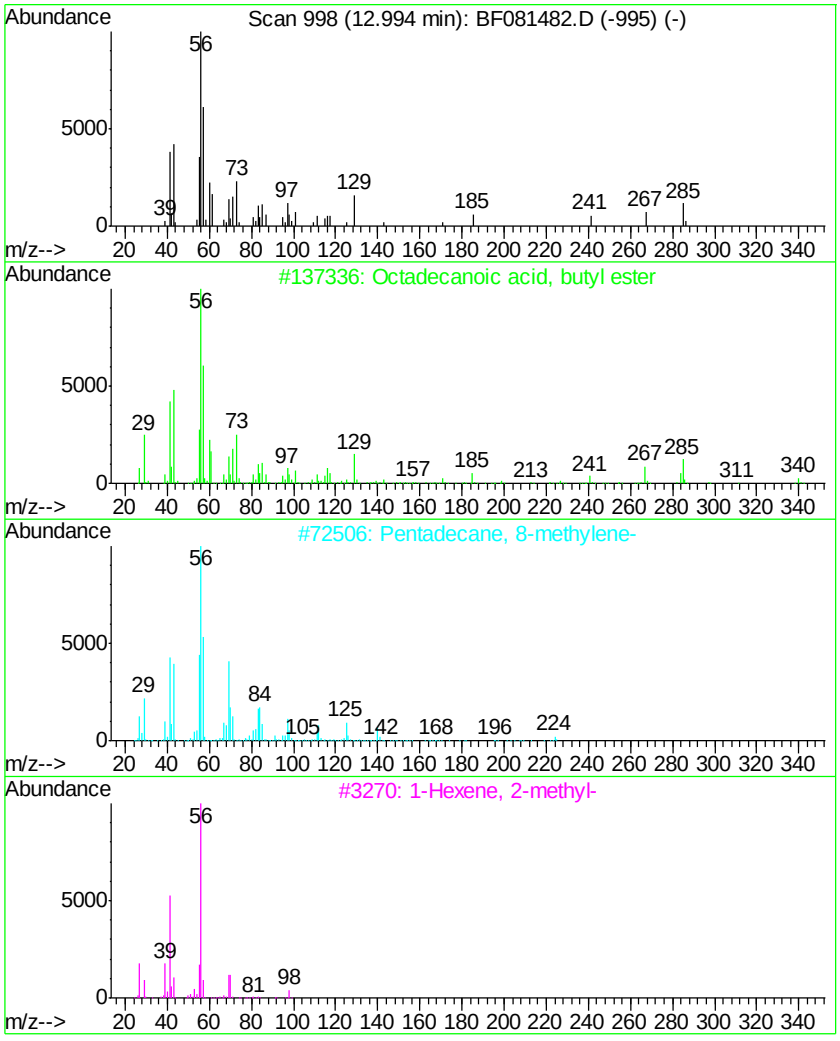
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

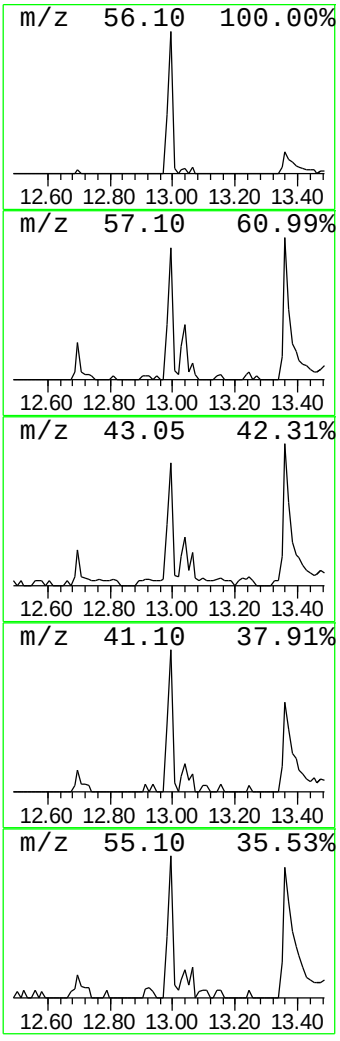
**********

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.99 | 6.13 ng | 95959 | Chrysene-d12 | 13.45 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid, butyl ester | 340 | C22H44O2 | 000123-95-5 | 91 |
| 2 | Pentadecane, 8-methylene- | 224 | C16H32 | 055668-09-2 | 37 |
| 3 | 1-Hexene, 2-methyl- | 98 | C7H14 | 006094-02-6 | 35 |
| 4 | 1-Hexene, 2,5-dimethyl- | 112 | C8H16 | 006975-92-4 | 35 |
| 5 | Propane, 2-cyclopropyl- | 84 | C6H12 | 003638-35-5 | 35 |



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Data File : BF081482.D
Acq On : 6 Sep 2015 00:32
Operator : UM/IZ
Sample : G3555-07
Misc :
ALS Vial : 59 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

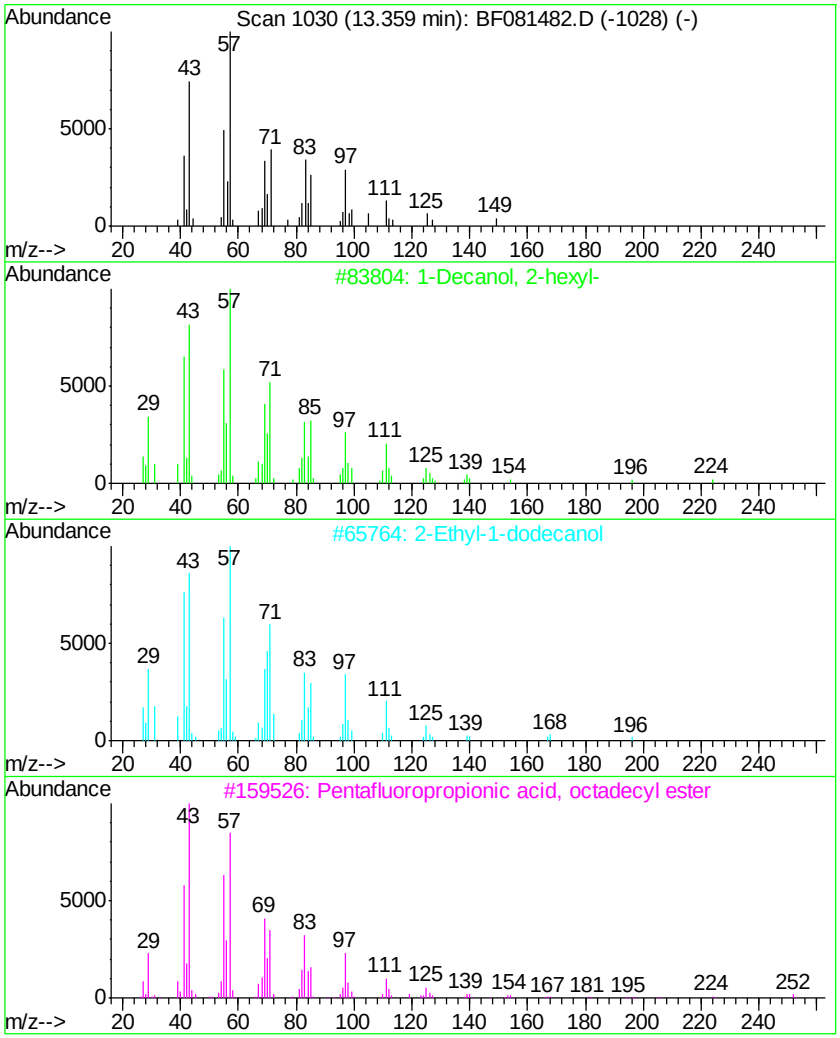
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

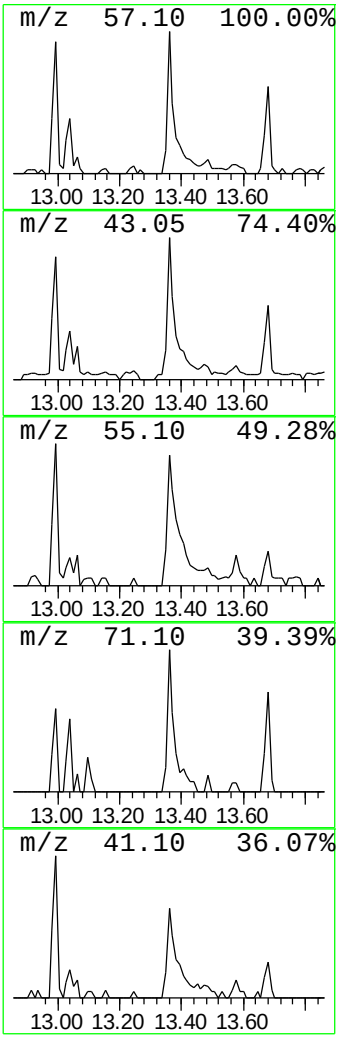
**********

Peak Number 7 1-Decanol, 2-hexyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.36 | 9.10 ng | 142452 | Chrysene-d12 | 13.45 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 86 |
| 2 | 2-Ethyl-1-dodecanol | 214 | C14H30O | 019780-33-7 | 78 |
| 3 | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2 | 1000280-07-7 | 72 |
| 4 | 2-Hexyl-1-octanol | 214 | C14H30O | 019780-79-1 | 64 |
| 5 | Pentafluoropropionic acid, hexad... | 388 | C19H33F5O2 | 006222-07-7 | 58 |



Tentatively Identified Compound (LSC) summary

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Operator : UM/IZ
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Misc :
ALS Vial : 59 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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... | 4.40 | 77.6 | ng | 1405940 | 1 | 6.35 | 362544 | 20.0 |
| unknown6.12 | 6.12 | 100.8 | ng | 1826350 | 1 | 6.35 | 362544 | 20.0 |
| Undecanoic acid | 11.43 | 3.4 | ng | 76702 | 4 | 10.84 | 455222 | 20.0 |
| Hexadecanoic acid... | 12.30 | 8.5 | ng | 132384 | 5 | 13.45 | 313128 | 20.0 |
| Octadecanoic acid... | 12.99 | 6.1 | ng | 95959 | 5 | 13.45 | 313128 | 20.0 |
| 1-Decanol, 2-hexyl- | 13.36 | 9.1 | ng | 142452 | 5 | 13.45 | 313128 | 20.0 |