LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083831.D
Acq On : 15 Dec 2015 23:31
Operator : UM/IZ
Sample : G4782-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121115-D534-F-D-S

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-BF121315.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 | 4.430 | 203 | 205 | 210 | rVB | 54147 | 77366 | 2.93% | 0.495% |
| 2 | 5.081 | 259 | 262 | 264 | rBV | 350926 | 421407 | 15.95% | 2.695% |
| 3 | 5.504 | 297 | 299 | 301 | rBV | 798568 | 730824 | 27.65% | 4.674% |
| 4 | 5.904 | 332 | 334 | 336 | rBB | 67445 | 56343 | 2.13% | 0.360% |
| 5 | 6.522 | 386 | 388 | 391 | rBV | 402779 | 440424 | 16.67% | 2.817% |
| 6 | 6.670 | 398 | 401 | 403 | rBV | 1484793 | 1349689 | 51.07% | 8.632% |
| 7 | 6.899 | 419 | 421 | 424 | rVB | 597153 | 512203 | 19.38% | 3.276% |
| 8 | 7.059 | 433 | 435 | 437 | rBV | 2013886 | 1732946 | 65.57% | 11.083% |
| 9 | 7.459 | 467 | 470 | 473 | rBV | 1103643 | 1299408 | 49.17% | 8.311% |
| 10 | 8.190 | 531 | 534 | 536 | rBV | 656615 | 657004 | 24.86% | 4.202% |
| 11 | 9.265 | 625 | 628 | 630 | rBV | 2946403 | 2642808 | 100.00% | 16.903% |
| 12 | 9.653 | 661 | 662 | 667 | rVB | 35507 | 36976 | 1.40% | 0.236% |
| 13 | 9.882 | 679 | 682 | 685 | rBV | 31378 | 28202 | 1.07% | 0.180% |
| 14 | 9.939 | 685 | 687 | 690 | rBV | 708852 | 668255 | 25.29% | 4.274% |
| 15 | 10.373 | 724 | 725 | 727 | rVB | 27437 | 31559 | 1.19% | 0.202% |
| 16 | 10.728 | 753 | 756 | 758 | rBV | 941869 | 927708 | 35.10% | 5.933% |
| 17 | 10.853 | 764 | 767 | 773 | rVB | 43222 | 58679 | 2.22% | 0.375% |
| 18 | 11.425 | 815 | 817 | 819 | rBV | 629805 | 612294 | 23.17% | 3.916% |
| 19 | 12.831 | 938 | 940 | 943 | rVB | 103377 | 91895 | 3.48% | 0.588% |
| 20 | 13.002 | 953 | 955 | 958 | rBV | 1667477 | 2288303 | 86.59% | 14.635% |
| 21 | 13.539 | 1000 | 1002 | 1004 | rBV | 73345 | 65506 | 2.48% | 0.419% |
| 22 | 13.917 | 1032 | 1035 | 1042 | rBV2 | 19792 | 39618 | 1.50% | 0.253% |
| 23 | 14.054 | 1044 | 1047 | 1054 | rVV | 469846 | 508168 | 19.23% | 3.250% |
| 24 | 15.494 | 1170 | 1173 | 1183 | rBV | 179102 | 357929 | 13.54% | 2.289% |

Sum of corrected areas: 15635514

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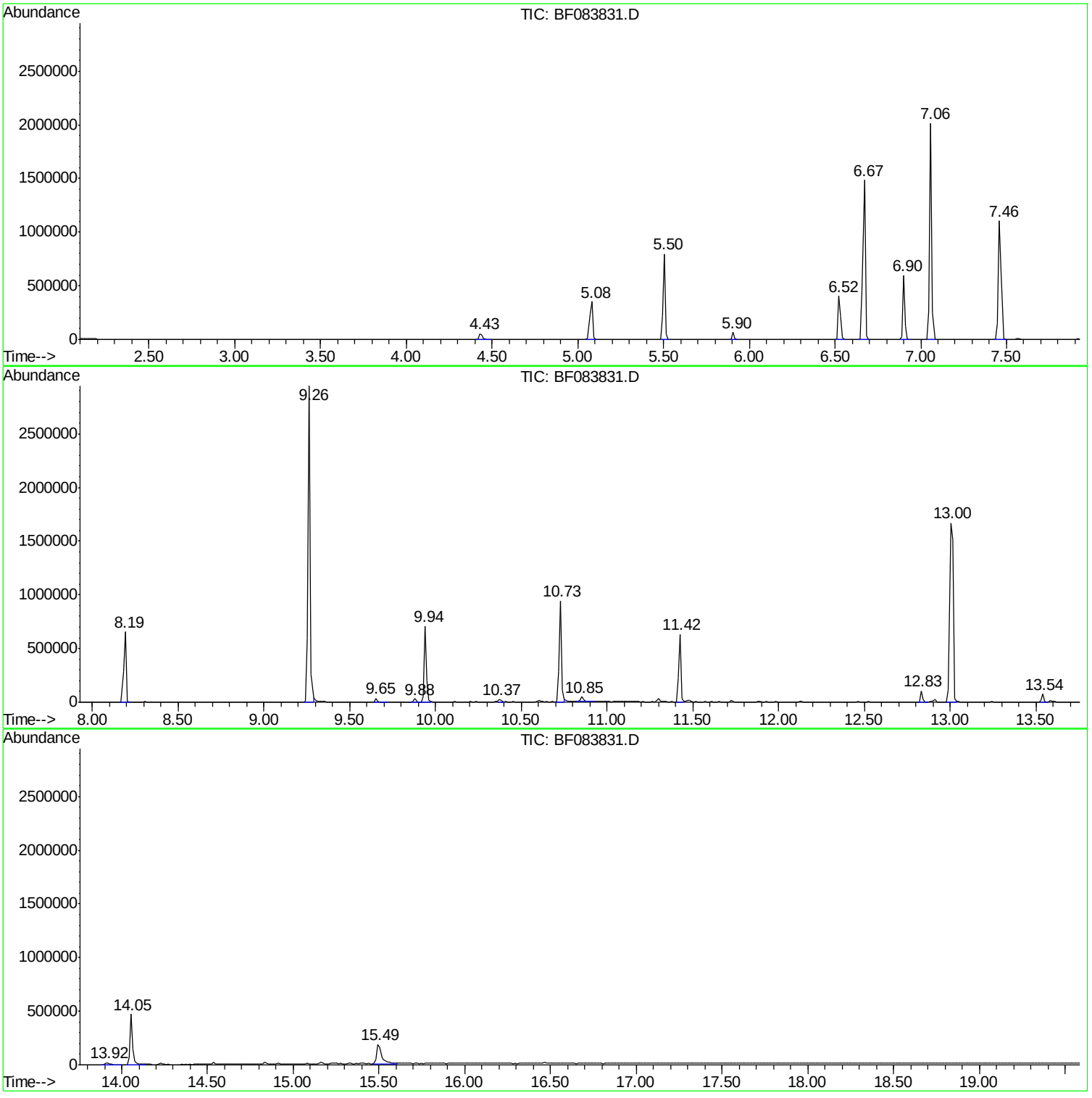
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
121115-D534-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083831.D
Acq On : 15 Dec 2015 23:31
Operator : UM/IZ
Sample : G4782-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121115-D534-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

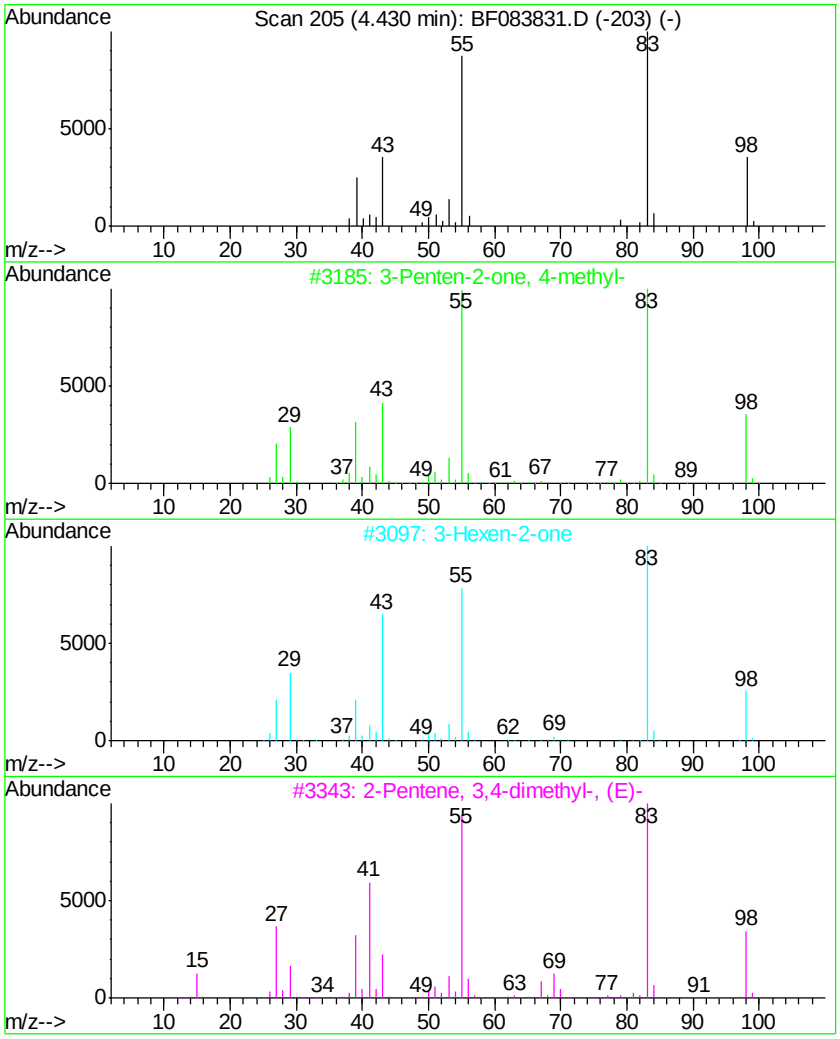
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

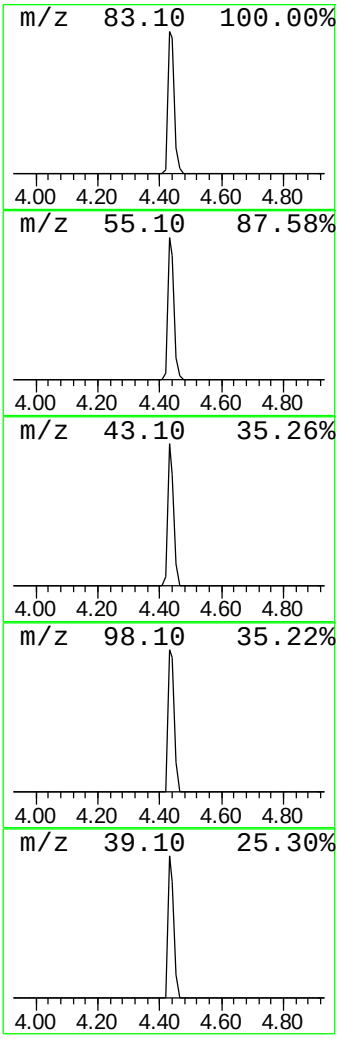
**********

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.43 | 3.02 ng | 77366 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 91 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 91 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 90 |
| 4 | 2-Pentene, 2,4-dimethyl- | 98 | C7H14 | 000625-65-0 | 86 |
| 5 | 2-Pentene, 4,4-dimethyl-, (Z)- | 98 | C7H14 | 000762-63-0 | 86 |



# Library Search Compound Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083831.D
Acq On : 15 Dec 2015 23:31
Operator : UM/IZ
Sample : G4782-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
121115-D534-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

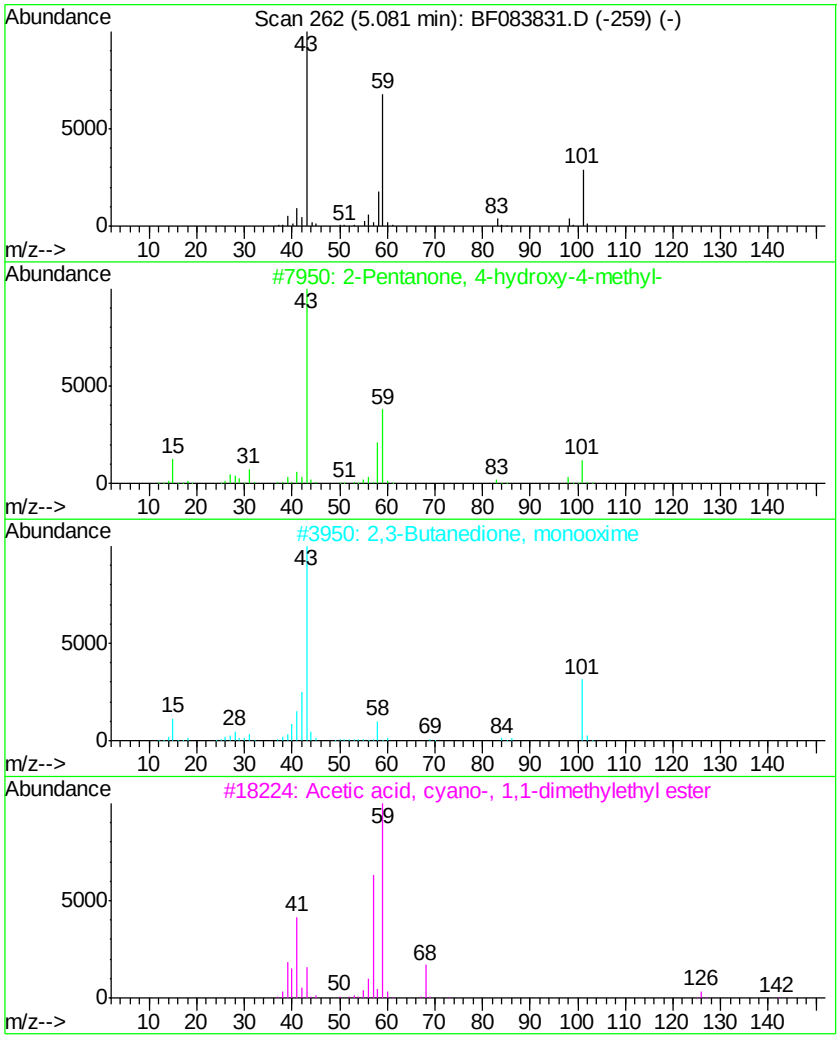
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

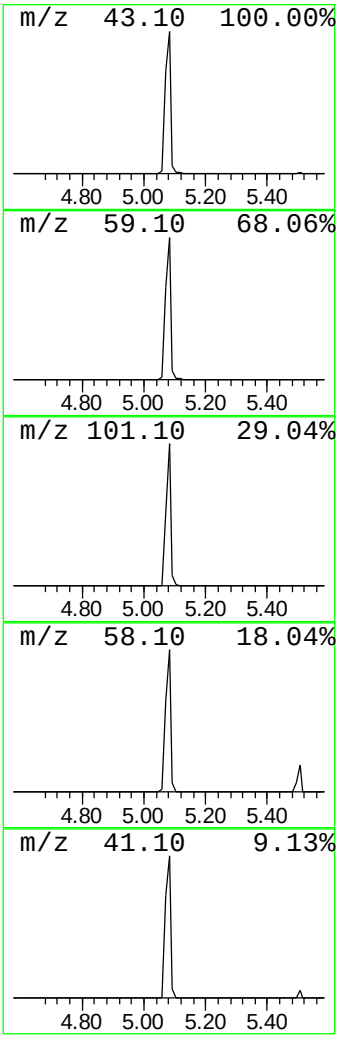
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.08 | 16.45 ng | 421407 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 25 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083831.D
Acq On : 15 Dec 2015 23:31
Operator : UM/IZ
Sample : G4782-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121115-D534-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

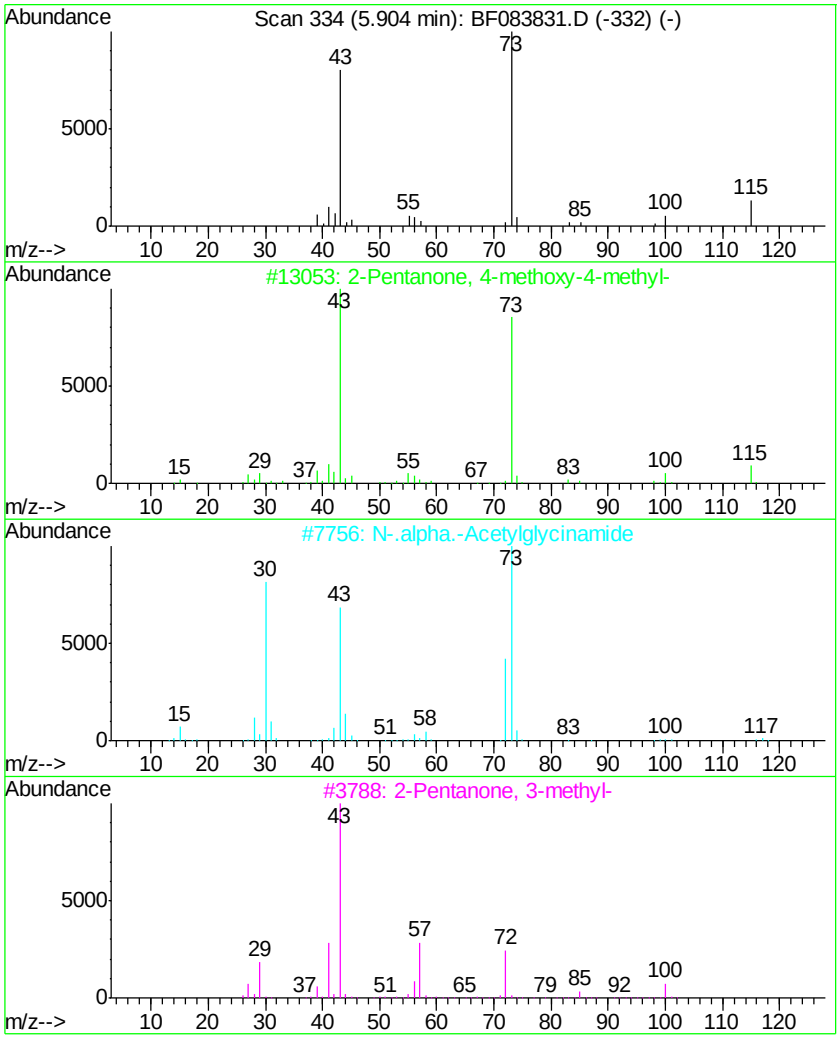
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

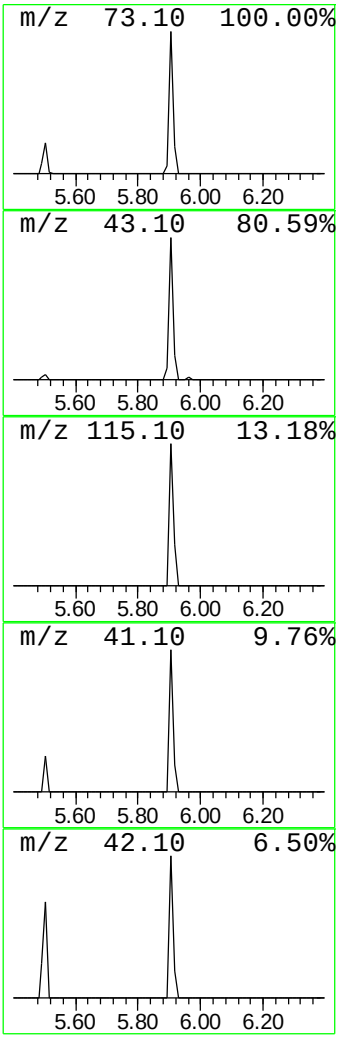
**********

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.90 | 2.20 ng | 56343 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-methoxy-4-methyl- | 130 | C7H14O2 | 000107-70-0 | 83 |
| 2 | N-.alpha.-Acetylglycinamide | 116 | C4H8N2O2 | 002620-63-5 | 33 |
| 3 | 2-Pentanone, 3-methyl- | 100 | C6H12O | 000565-61-7 | 25 |
| 4 | Borane, dimethoxy- | 74 | C2H7BO2 | 004542-61-4 | 9 |
| 5 | 2-Propyn-1-ol, acetate | 98 | C5H6O2 | 000627-09-8 | 9 |



Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083831.D
Acq On : 15 Dec 2015 23:31
Operator : UM/IZ
Sample : G4782-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121115-D534-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

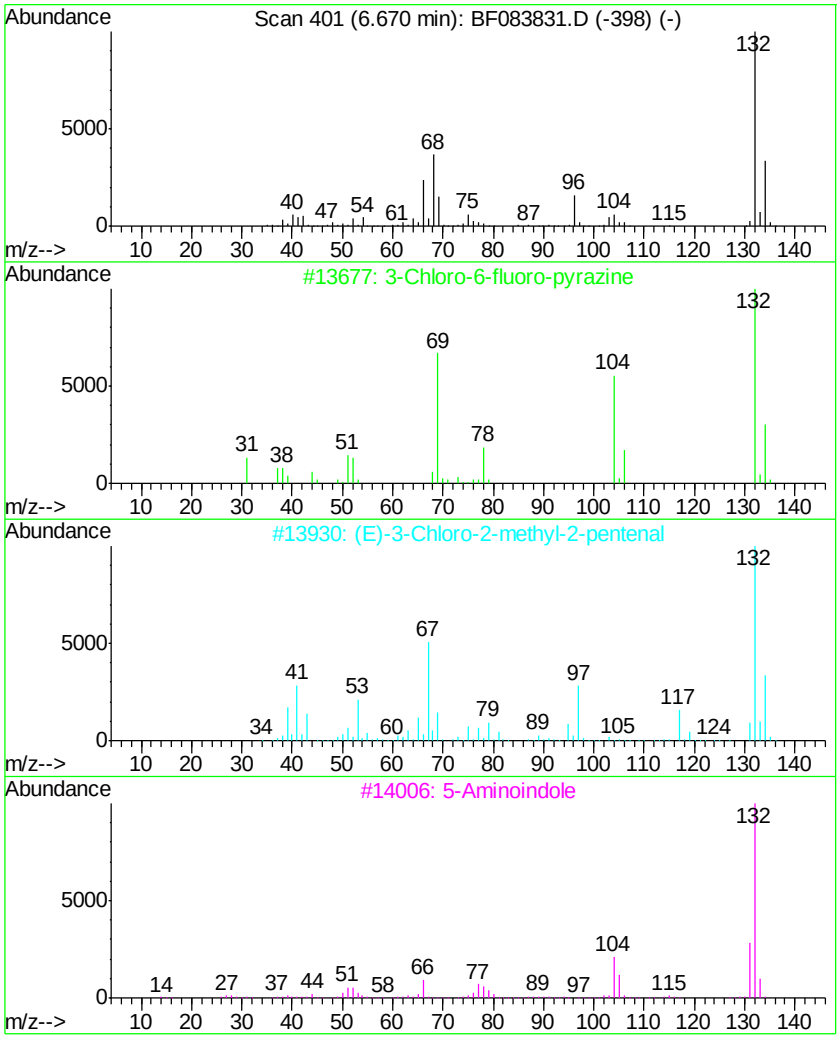
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

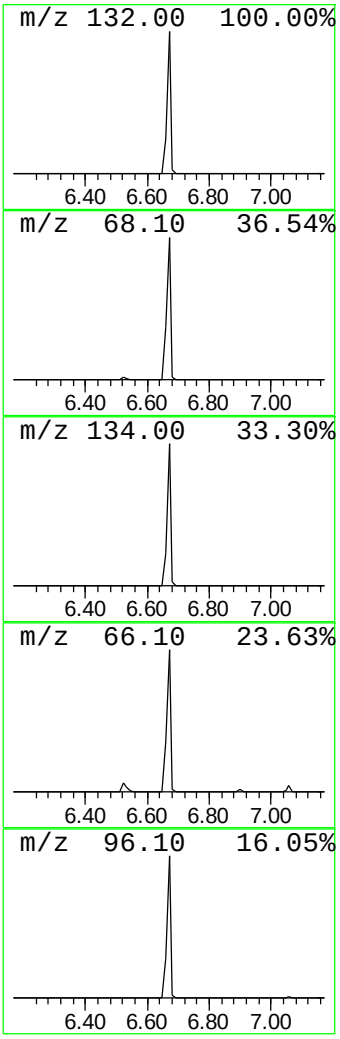
**********

Peak Number 4 unknown6.67 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.67 | 52.70 ng | 1349690 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 10 |
| 5 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 9 |



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Operator : UM/IZ
Sample : G4782-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121115-D534-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

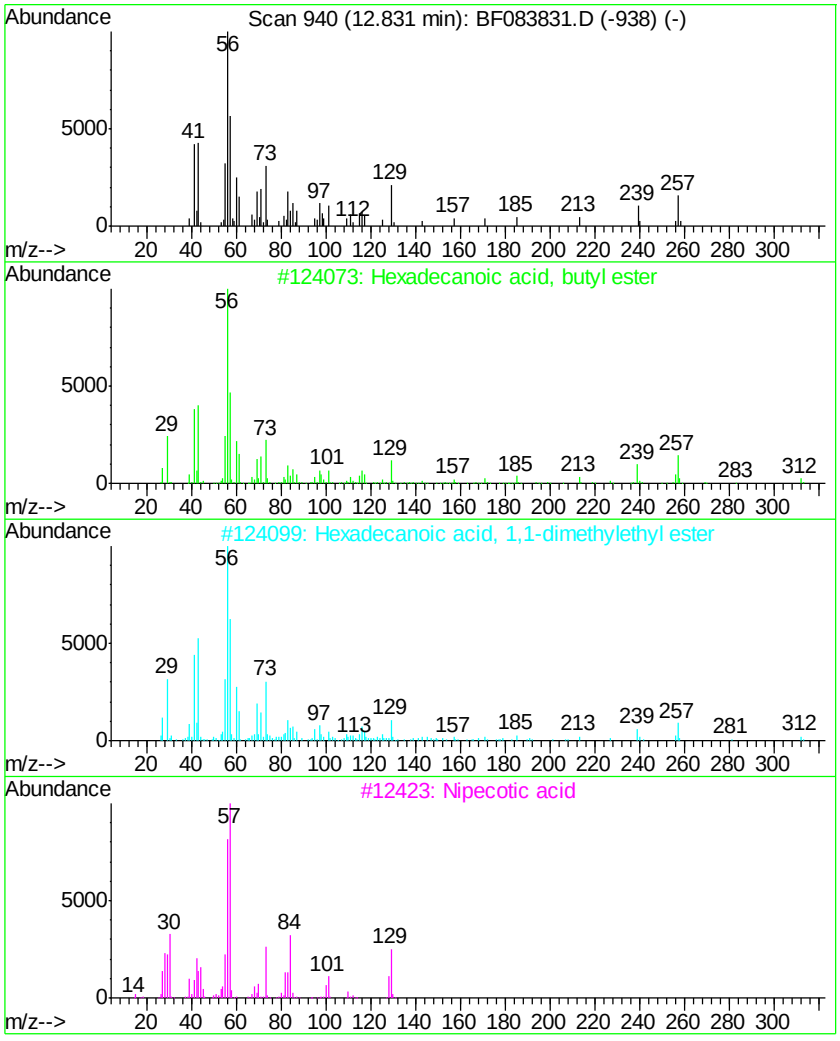
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

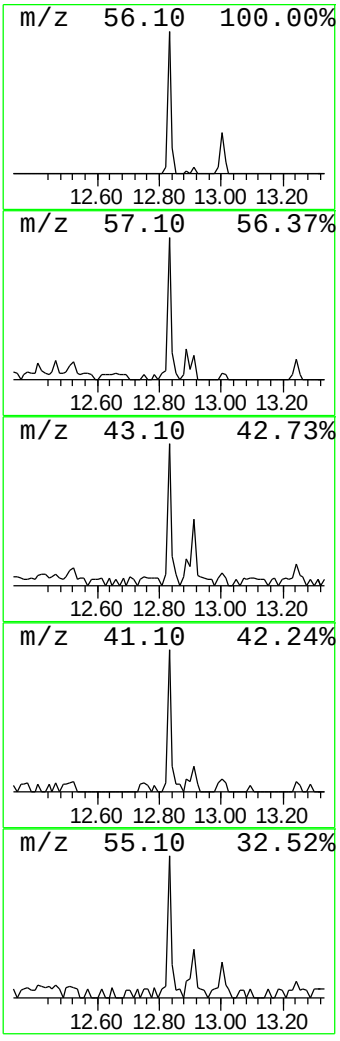
**********

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.83 | 3.62 ng | 91895 | Chrysene-d12 | 14.05 |

| 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 | 86 |
| 3 | Nipecotic acid | 129 | C6H11NO2 | 000498-95-3 | 38 |
| 4 | 1-Pentadecene, 2-methyl- | 224 | C16H32 | 029833-69-0 | 37 |
| 5 | Cyclopropane, 1-(1-methylethyl)-... | 210 | C15H30 | 041977-39-3 | 35 |



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Sample : G4782-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121115-D534-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

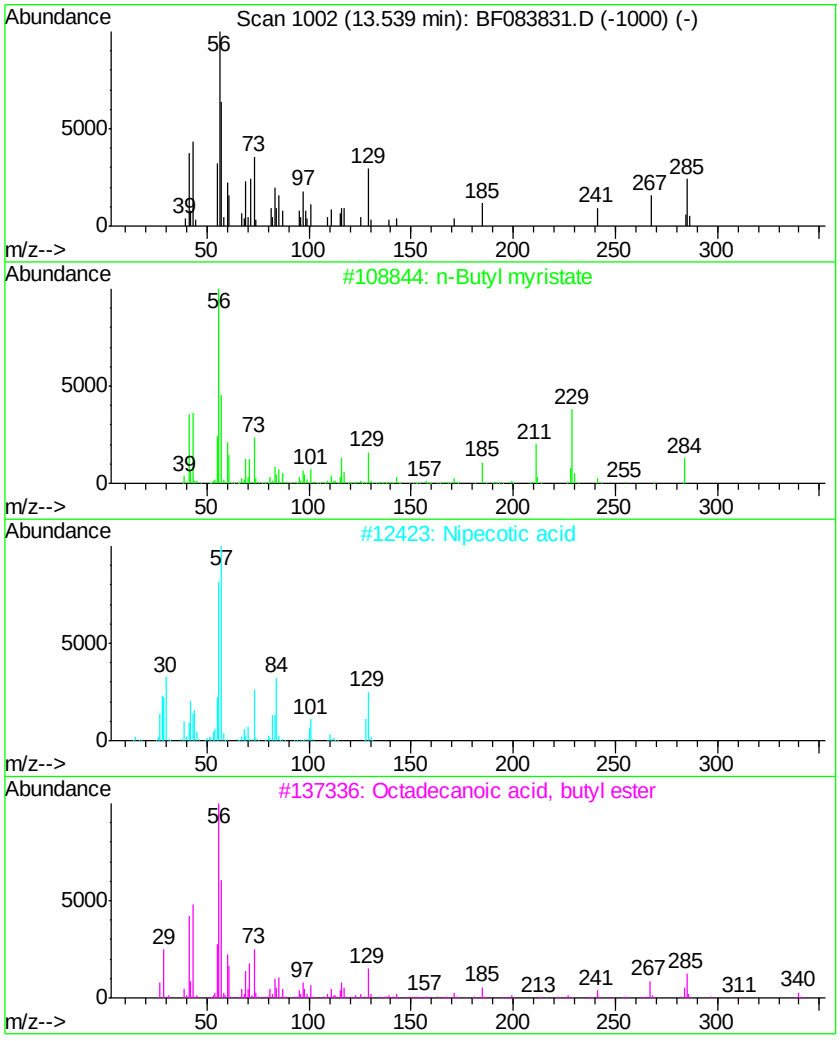
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

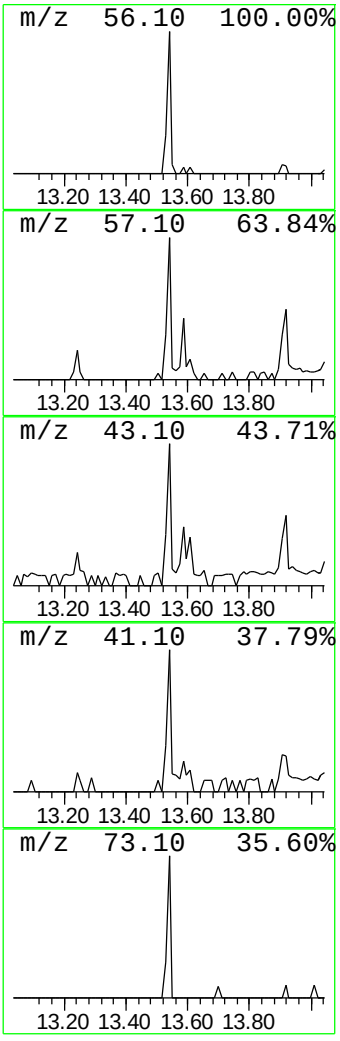
**********

Peak Number 7 n-Butyl myristate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.54 | 2.58 ng | 65506 | Chrysene-d12 | 14.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Butyl myristate | 284 | C18H36O2 | 000110-36-1 | 53 |
| 2 | Nipecotic acid | 129 | C6H11NO2 | 000498-95-3 | 47 |
| 3 | Octadecanoic acid, butyl ester | 340 | C22H44O2 | 000123-95-5 | 38 |
| 4 | 1,3-Pentanediol, 2,2,4-trimethyl- | 146 | C8H18O2 | 000144-19-4 | 32 |
| 5 | 1-Hexene, 2,5-dimethyl- | 112 | C8H16 | 006975-92-4 | 27 |



Tentatively Identified Compound (LSC) summary

Data Path : V:\HPCHEM1\BNA_F\DATA\BF121515\
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Sample : G4782-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 121115-D534-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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 |
| 3-Penten-2-one, 4... | 4.43 | 3.0 | ng | 77366 | 1 | 6.90 | 512203 | 20.0 |
| 2-Pentanone, 4-hy... | 5.08 | 16.4 | ng | 421407 | 1 | 6.90 | 512203 | 20.0 |
| 2-Pentanone, 4-me... | 5.90 | 2.2 | ng | 56343 | 1 | 6.90 | 512203 | 20.0 |
| unknown6.67 | 6.67 | 52.7 | ng | 1349690 | 1 | 6.90 | 512203 | 20.0 |
| Hexadecanoic acid... | 12.83 | 3.6 | ng | 91895 | 5 | 14.05 | 508168 | 20.0 |
| n-Butyl myristate | 13.54 | 2.6 | ng | 65506 | 5 | 14.05 | 508168 | 20.0 |