LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083830.D
Acq On : 15 Dec 2015 23:03
Operator : UM/IZ
Sample : G4782-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

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 | 4.441 | 203 | 206 | 209 | rBV | 60026 | 76541 | 3.16% | 0.535% |
| 2 | 5.081 | 259 | 262 | 264 | rBV | 353500 | 386140 | 15.93% | 2.701% |
| 3 | 5.504 | 297 | 299 | 301 | rBV | 731201 | 638384 | 26.33% | 4.466% |
| 4 | 5.904 | 332 | 334 | 337 | rBB | 65464 | 56087 | 2.31% | 0.392% |
| 5 | 6.522 | 386 | 388 | 392 | rBV | 353925 | 374831 | 15.46% | 2.622% |
| 6 | 6.670 | 398 | 401 | 403 | rBV | 1331306 | 1228482 | 50.67% | 8.594% |
| 7 | 6.899 | 419 | 421 | 424 | rBB | 583989 | 503283 | 20.76% | 3.521% |
| 8 | 7.059 | 433 | 435 | 438 | rBB | 1938303 | 1689049 | 69.66% | 11.816% |
| 9 | 7.459 | 467 | 470 | 473 | rBV | 1087840 | 1238181 | 51.07% | 8.662% |
| 10 | 8.190 | 531 | 534 | 536 | rBV | 586323 | 611415 | 25.22% | 4.277% |
| 11 | 9.265 | 625 | 628 | 630 | rBV | 2689715 | 2424702 | 100.00% | 16.963% |
| 12 | 9.653 | 660 | 662 | 667 | rVB | 30110 | 31836 | 1.31% | 0.223% |
| 13 | 9.939 | 685 | 687 | 690 | rBV | 624572 | 595733 | 24.57% | 4.168% |
| 14 | 10.373 | 724 | 725 | 727 | rVB | 22677 | 26716 | 1.10% | 0.187% |
| 15 | 10.728 | 753 | 756 | 758 | rBV | 759953 | 783063 | 32.30% | 5.478% |
| 16 | 10.853 | 764 | 767 | 771 | rVB | 30071 | 42994 | 1.77% | 0.301% |
| 17 | 11.425 | 815 | 817 | 819 | rBV | 533882 | 536283 | 22.12% | 3.752% |
| 18 | 12.831 | 938 | 940 | 944 | rBV | 67871 | 59251 | 2.44% | 0.415% |
| 19 | 13.002 | 953 | 955 | 958 | rBV | 1782343 | 2041674 | 84.20% | 14.283% |
| 20 | 13.539 | 1000 | 1002 | 1004 | rBV | 58639 | 52272 | 2.16% | 0.366% |
| 21 | 13.917 | 1032 | 1035 | 1039 | rBV | 17589 | 32176 | 1.33% | 0.225% |
| 22 | 14.054 | 1044 | 1047 | 1054 | rBV | 505615 | 516805 | 21.31% | 3.615% |
| 23 | 15.494 | 1170 | 1173 | 1184 | rBV | 187354 | 348554 | 14.38% | 2.438% |

Sum of corrected areas: 14294452

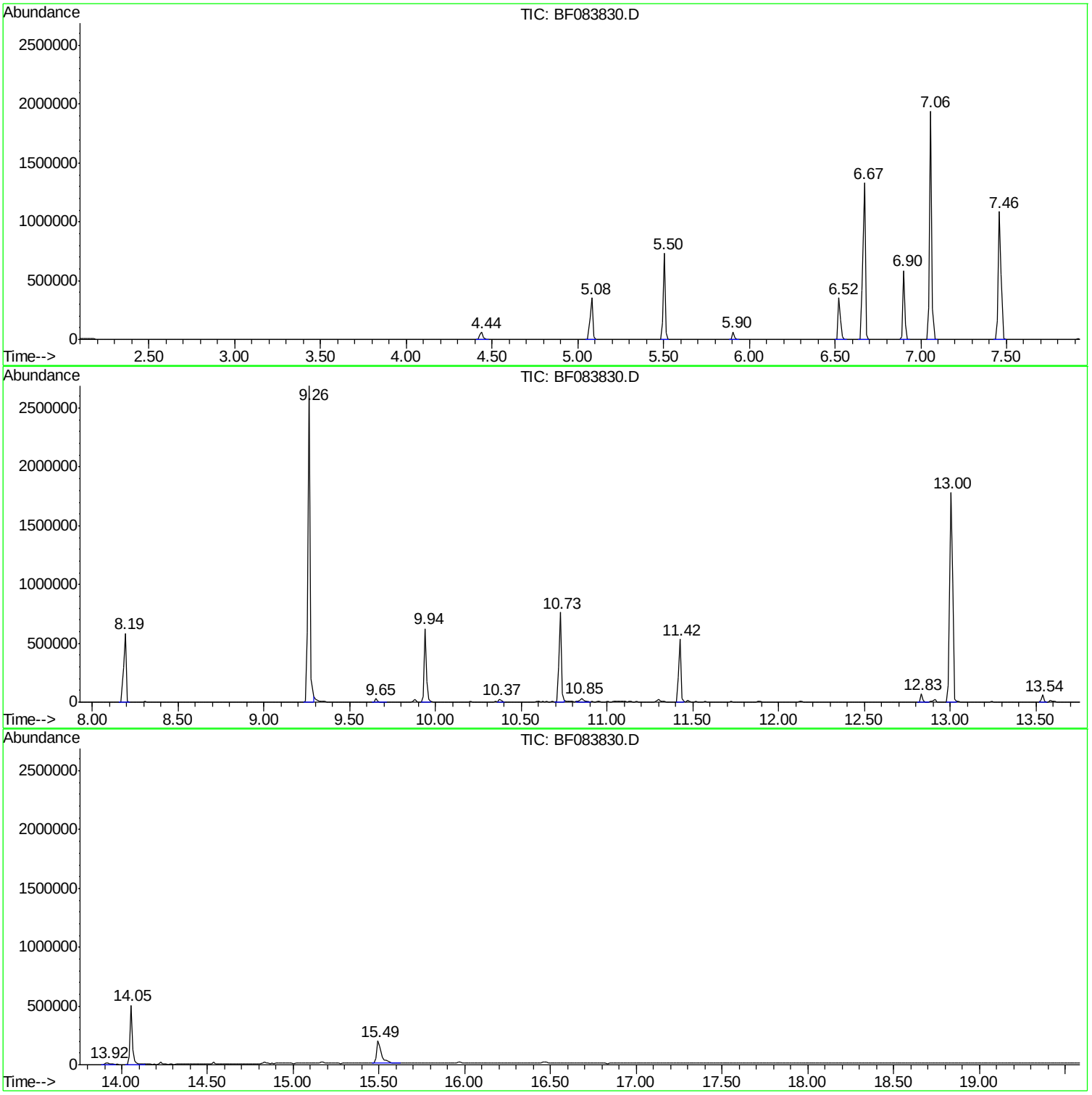
LSC Report - Integrated Chromatogram

Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083830.D
Acq On : 15 Dec 2015 23:03
Operator : UM/IZ
Sample : G4782-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

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 : BF083830.D
Acq On : 15 Dec 2015 23:03
Operator : UM/IZ
Sample : G4782-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

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

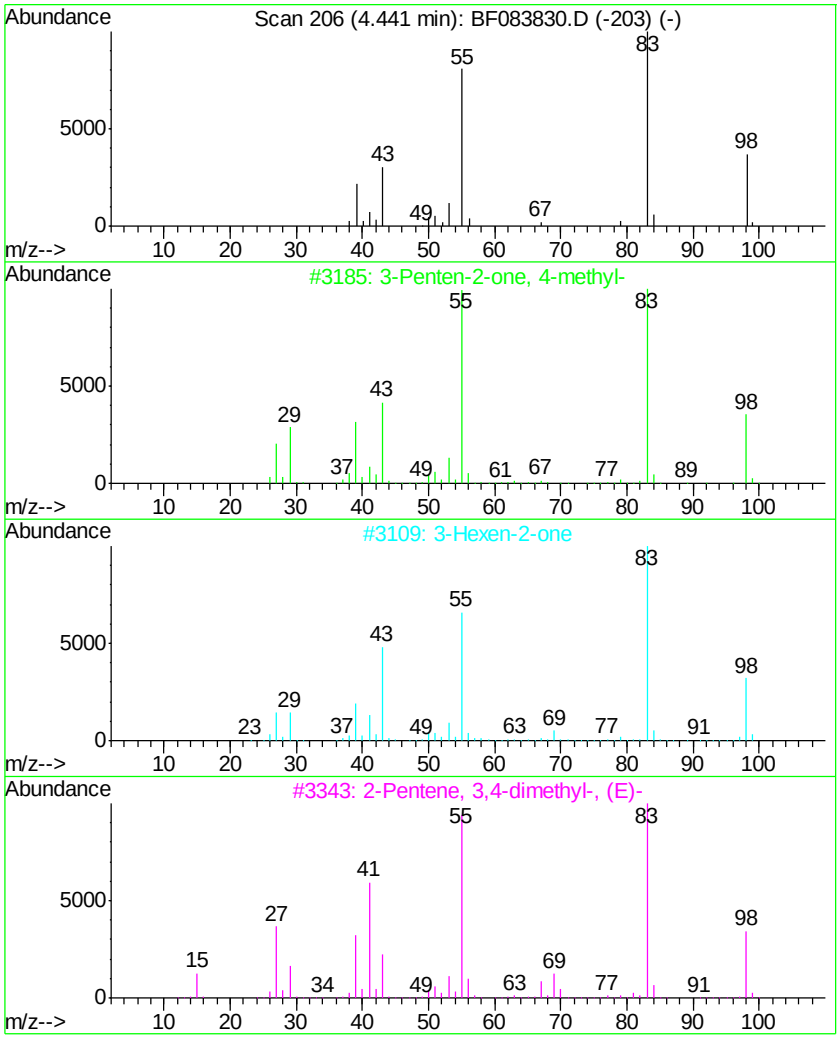
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

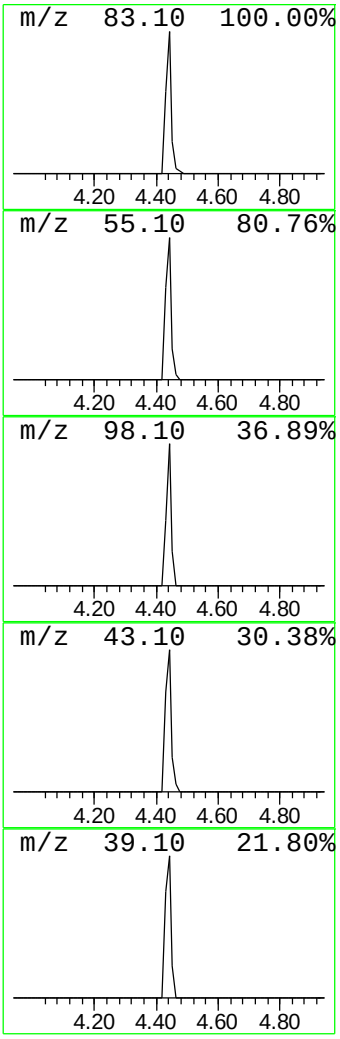
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.44 | 3.04 ng | 76541 | 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 | 90 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 90 |
| 4 | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14 | 004914-91-4 | 86 |
| 5 | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14 | 000690-08-4 | 78 |



Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083830.D
Acq On : 15 Dec 2015 23:03
Operator : UM/IZ
Sample : G4782-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

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

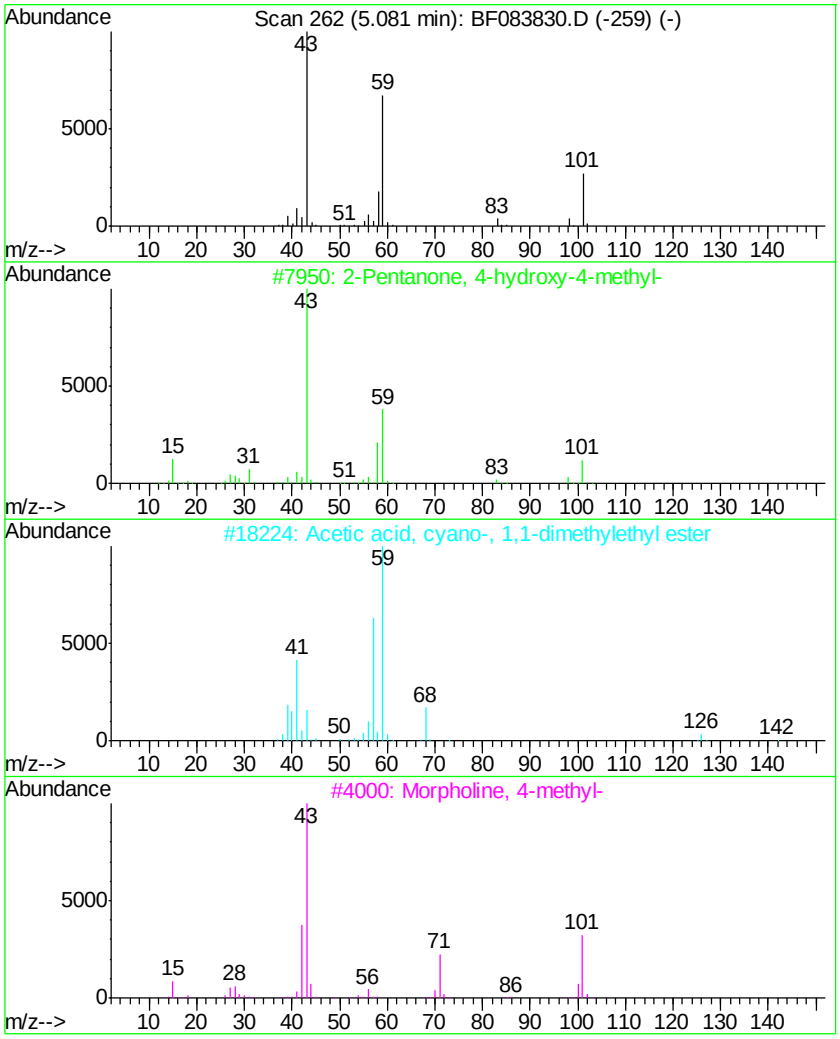
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

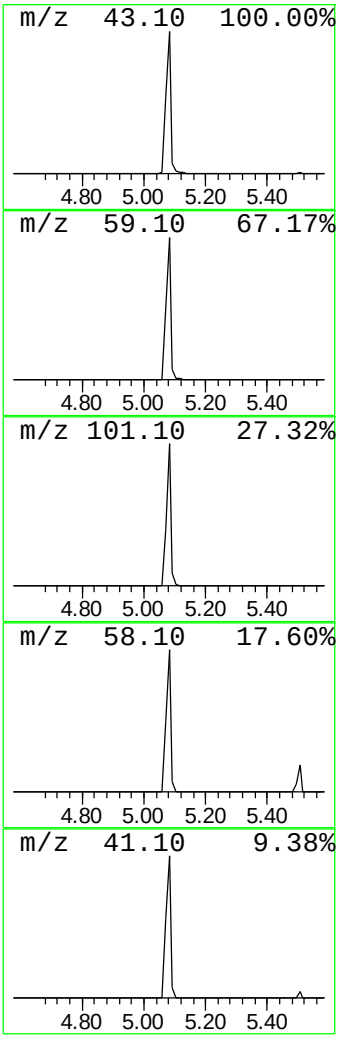
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.08 | 15.34 ng | 386140 | 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 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |



Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083830.D
Acq On : 15 Dec 2015 23:03
Operator : UM/IZ
Sample : G4782-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

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

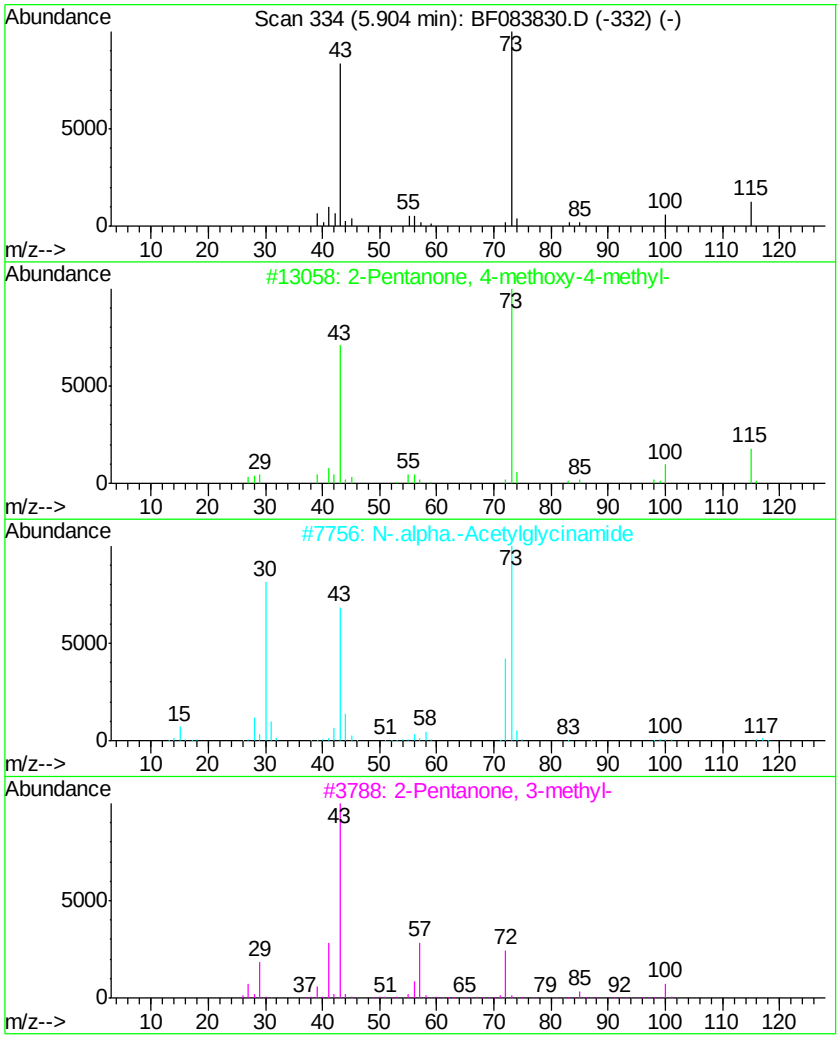
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

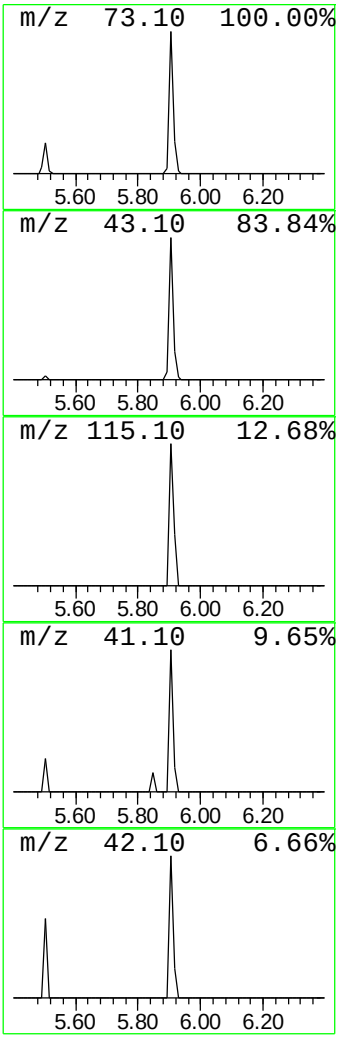
**********

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.90 | 2.23 ng | 56087 | 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 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |
| 5 | Borane, dimethoxy- | 74 | C2H7BO2 | 004542-61-4 | 9 |



Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083830.D
Acq On : 15 Dec 2015 23:03
Operator : UM/IZ
Sample : G4782-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

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

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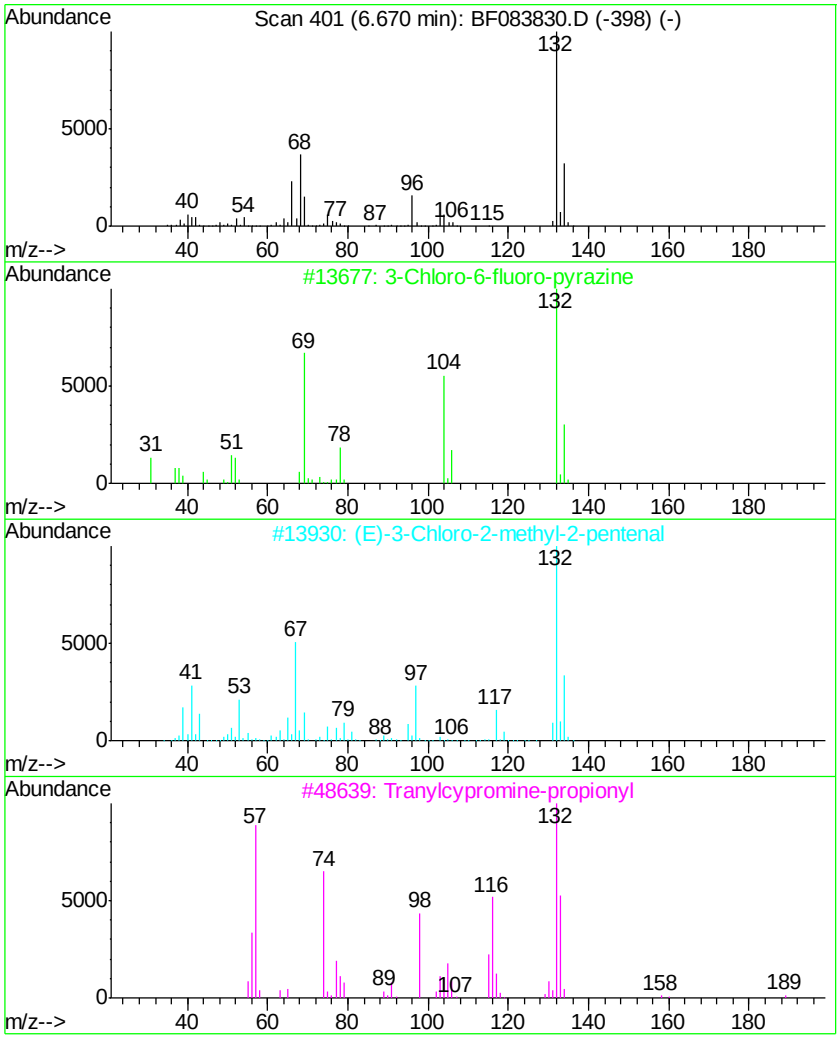
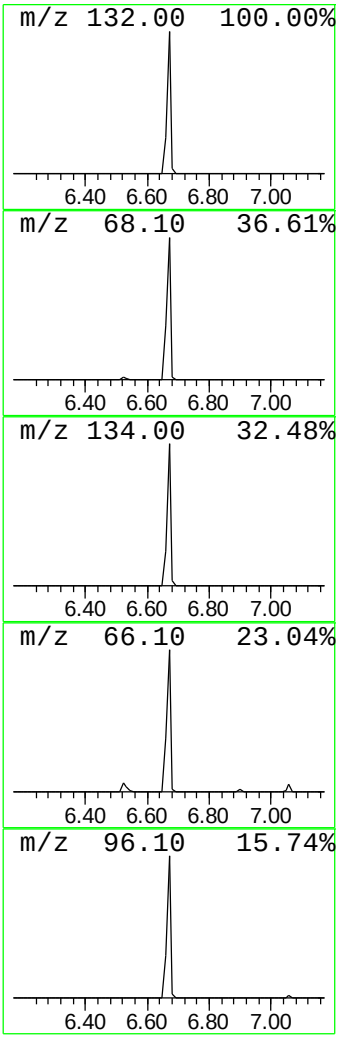
Peak Number 4 unknown6.67 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.67 | 48.82 ng | 1228480 | 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 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 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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Data File : BF083830.D
Acq On : 15 Dec 2015 23:03
Operator : UM/IZ
Sample : G4782-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

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

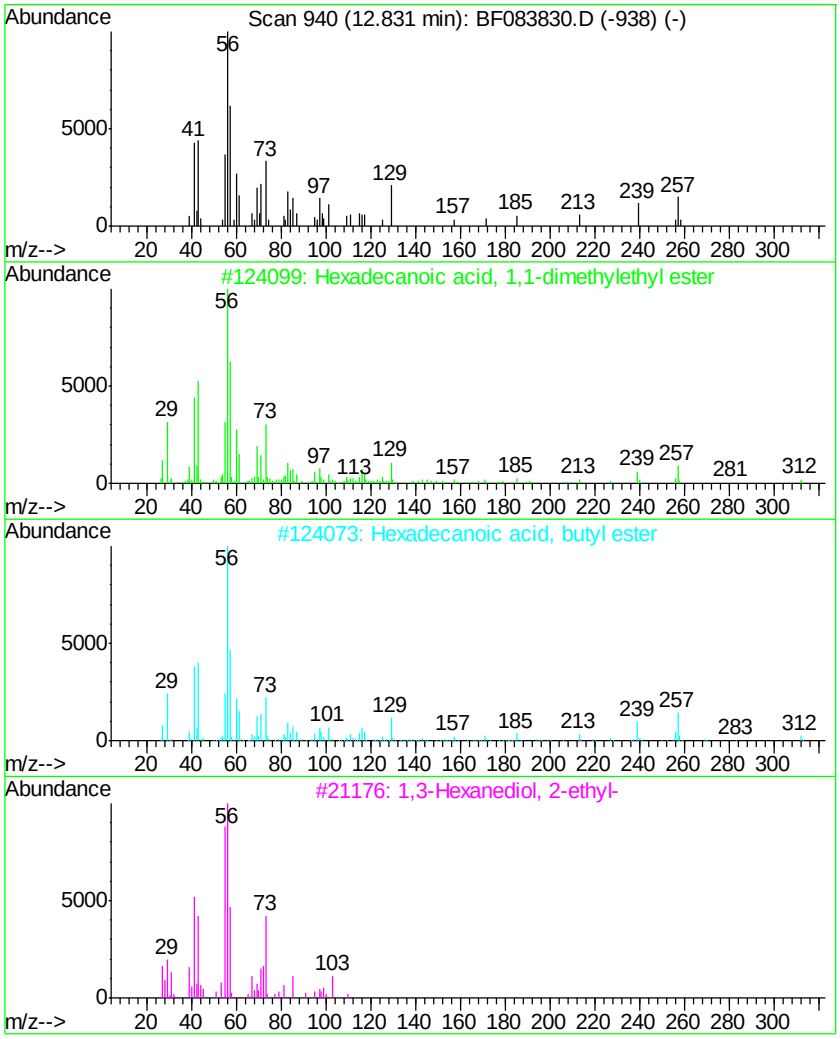
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

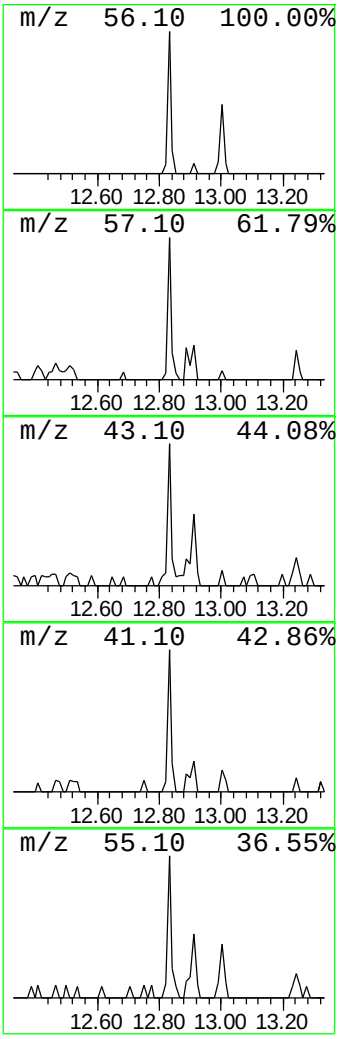
**********

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.83 | 2.29 ng | 59251 | Chrysene-d12 | 14.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 80 |
| 2 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 80 |
| 3 | 1,3-Hexanediol, 2-ethyl- | 146 | C8H18O2 | 000094-96-2 | 32 |
| 4 | Pentadecane, 8-methylene- | 224 | C16H32 | 055668-09-2 | 32 |
| 5 | 1-Hexene, 2,5-dimethyl- | 112 | C8H16 | 006975-92-4 | 27 |



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Operator : UM/IZ
Sample : G4782-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

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

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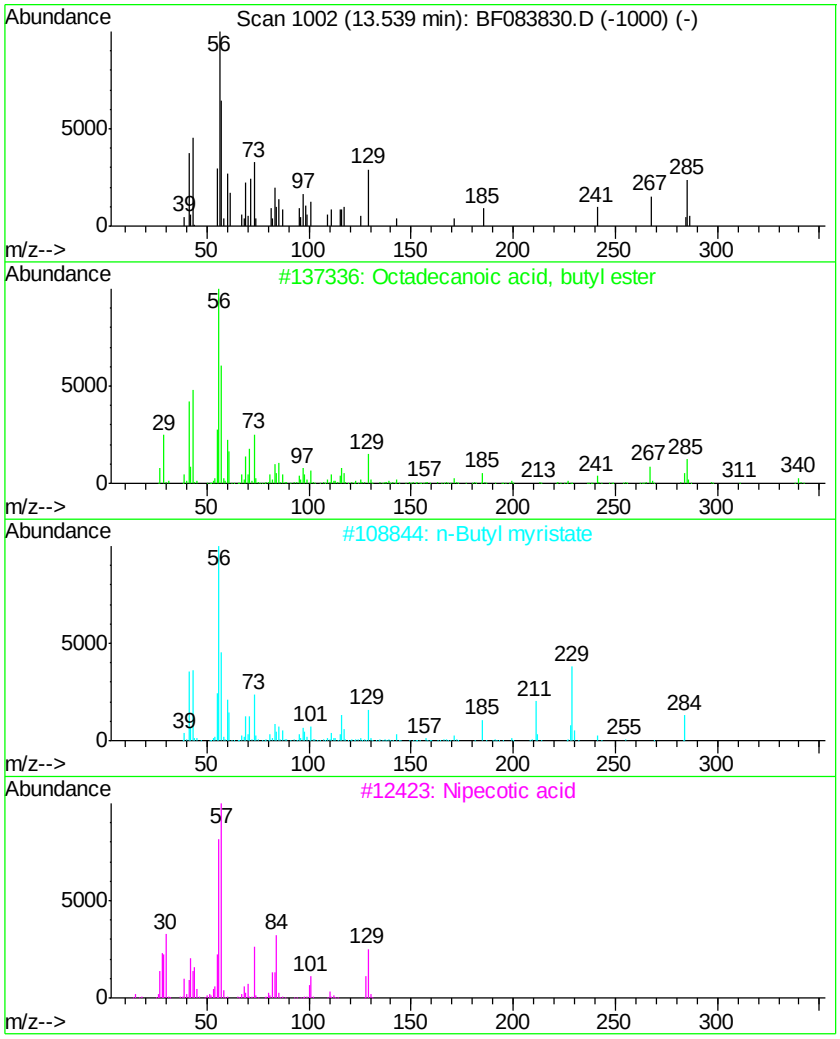
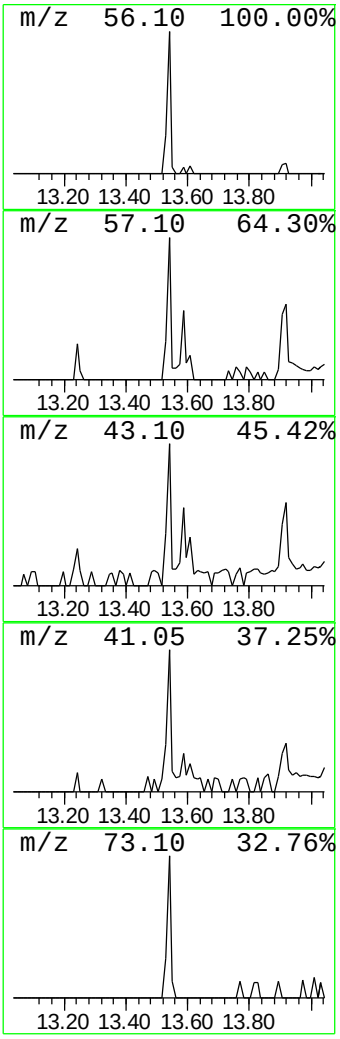
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.54 | 2.02 ng | 52272 | Chrysene-d12 | 14.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid, butyl ester | 340 | C22H44O2 | 000123-95-5 | 80 |
| 2 | n-Butyl myristate | 284 | C18H36O2 | 000110-36-1 | 42 |
| 3 | Nipecotic acid | 129 | C6H11NO2 | 000498-95-3 | 38 |
| 4 | 1-Pentene, 2,4-dimethyl- | 98 | C7H14 | 002213-32-3 | 27 |
| 5 | 7-Heptadecanol, 7-methyl- | 270 | C18H38O | 055723-93-8 | 23 |



Tentatively Identified Compound (LSC) summary

Data Path : V:\HPCHEM1\BNA_F\DATA\BF121515\
Data File : BF083830.D
Acq On : 15 Dec 2015 23:03
Operator : UM/IZ
Sample : G4782-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

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... | 4.44 | 3.0 | ng | 76541 | 1 | 6.90 | 503283 | 20.0 |
| 2-Pentanone, 4-hy... | 5.08 | 15.3 | ng | 386140 | 1 | 6.90 | 503283 | 20.0 |
| 2-Pentanone, 4-me... | 5.90 | 2.2 | ng | 56087 | 1 | 6.90 | 503283 | 20.0 |
| unknown6.67 | 6.67 | 48.8 | ng | 1228480 | 1 | 6.90 | 503283 | 20.0 |
| Hexadecanoic acid... | 12.83 | 2.3 | ng | 59251 | 5 | 14.05 | 516805 | 20.0 |
| Octadecanoic acid... | 13.54 | 2.0 | ng | 52272 | 5 | 14.05 | 516805 | 20.0 |