LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092316\
Data File : BF090206.D
Acq On : 23 Sep 2016 19:11
Operator : UM/SJ
Sample : H4887-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TRACK-D-GRID-17A

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-BF092016.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 | 1.655 | 5 | 6 | 49 | rVB | 3299832 | 8978885 | 100.00% | 26.818% |
| 2 | 4.581 | 259 | 262 | 272 | rVB | 346450 | 572017 | 6.37% | 1.709% |
| 3 | 5.062 | 301 | 304 | 307 | rBV | 2232572 | 2405285 | 26.79% | 7.184% |
| 4 | 6.159 | 397 | 400 | 402 | rBV | 2364146 | 2723476 | 30.33% | 8.135% |
| 5 | 6.262 | 406 | 409 | 411 | rBV | 2689287 | 2581542 | 28.75% | 7.711% |
| 6 | 6.490 | 427 | 429 | 432 | rBV | 800939 | 701158 | 7.81% | 2.094% |
| 7 | 6.650 | 440 | 443 | 445 | rBV | 2290677 | 2249107 | 25.05% | 6.718% |
| 8 | 7.062 | 476 | 479 | 482 | rBV | 1460862 | 1464277 | 16.31% | 4.374% |
| 9 | 7.210 | 489 | 492 | 494 | rVB | 78240 | 97502 | 1.09% | 0.291% |
| 10 | 7.782 | 539 | 542 | 544 | rBV | 881069 | 898447 | 10.01% | 2.683% |
| 11 | 8.856 | 634 | 636 | 639 | rBV | 2777842 | 2698754 | 30.06% | 8.061% |
| 12 | 9.256 | 669 | 671 | 674 | rBV | 892479 | 812842 | 9.05% | 2.428% |
| 13 | 9.519 | 692 | 694 | 696 | rVV | 1133073 | 950159 | 10.58% | 2.838% |
| 14 | 10.308 | 760 | 763 | 765 | rBV2 | 1026454 | 1386948 | 15.45% | 4.143% |
| 15 | 10.445 | 773 | 775 | 779 | rBV | 96856 | 143242 | 1.60% | 0.428% |
| 16 | 10.982 | 820 | 822 | 826 | rBV2 | 614543 | 762759 | 8.50% | 2.278% |
| 17 | 11.245 | 843 | 845 | 850 | rVV | 123835 | 111517 | 1.24% | 0.333% |
| 18 | 12.411 | 945 | 947 | 949 | rVB | 96248 | 110605 | 1.23% | 0.330% |
| 19 | 12.571 | 959 | 961 | 964 | rBV | 1985832 | 1931348 | 21.51% | 5.769% |
| 20 | 13.485 | 1039 | 1041 | 1045 | rVV2 | 146502 | 169589 | 1.89% | 0.507% |
| 21 | 13.600 | 1048 | 1051 | 1057 | rBV | 735927 | 889307 | 9.90% | 2.656% |
| 22 | 14.582 | 1135 | 1137 | 1141 | rBV | 71556 | 134101 | 1.49% | 0.401% |
| 23 | 14.925 | 1164 | 1167 | 1172 | rVB | 608764 | 707640 | 7.88% | 2.114% |

Sum of corrected areas: 33480507

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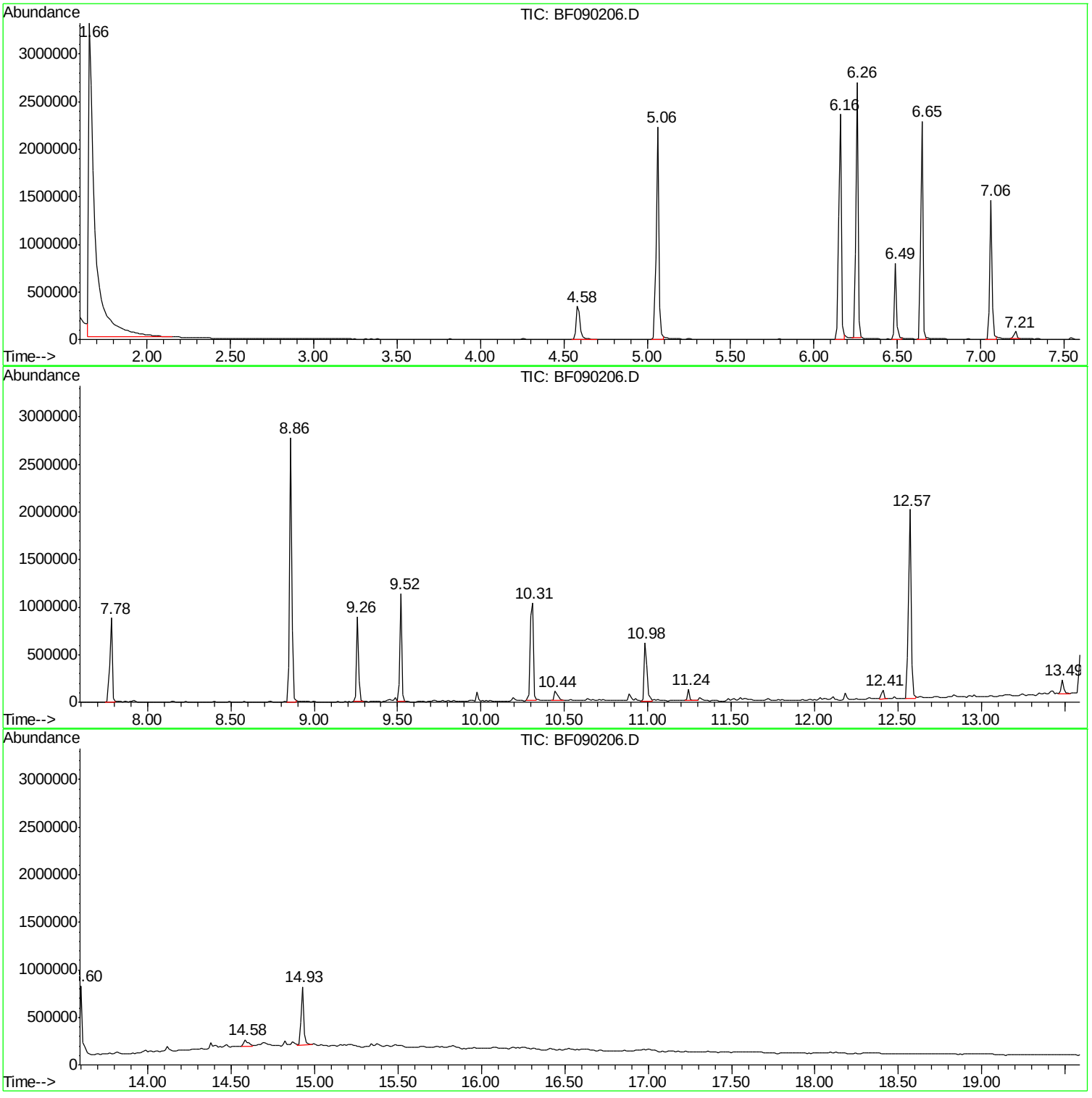
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TRACK-D-GRID-17A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF090206.D
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Operator : UM/SJ
Sample : H4887-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TRACK-D-GRID-17A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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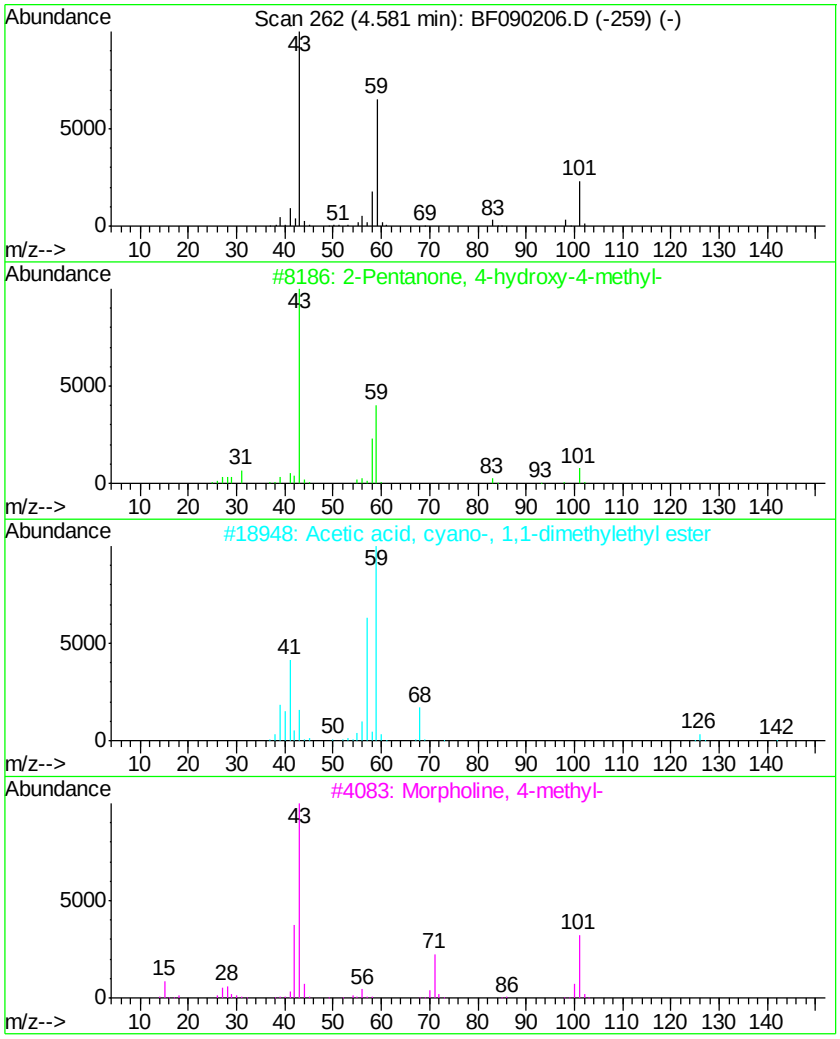
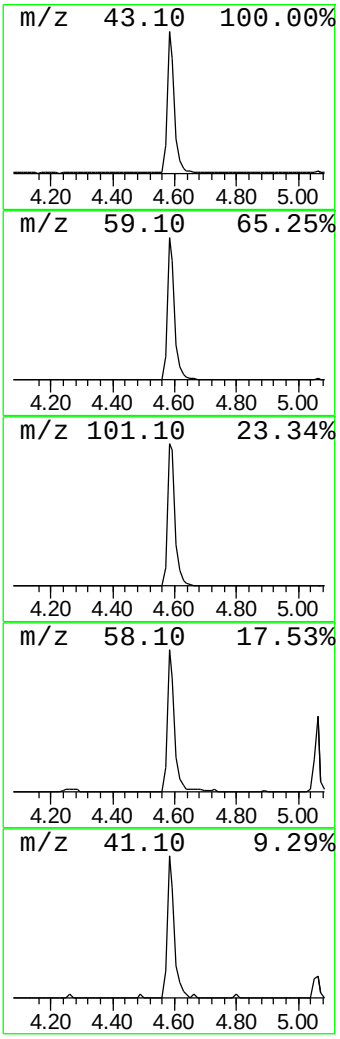
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.58 | 16.32 ng | 572017 | 1,4-Dichlorobenzene-d4 | 6.49 |

| 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 | 17 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092316\
Data File : BF090206.D
Acq On : 23 Sep 2016 19:11
Operator : UM/SJ
Sample : H4887-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TRACK-D-GRID-17A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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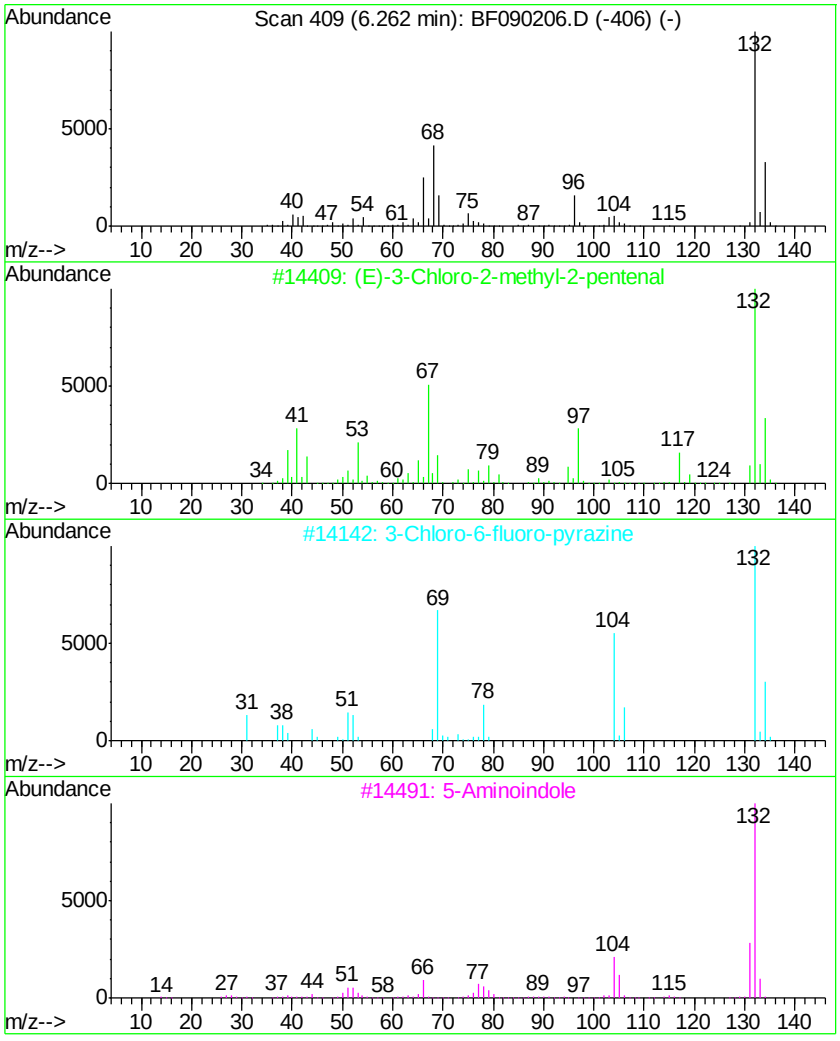
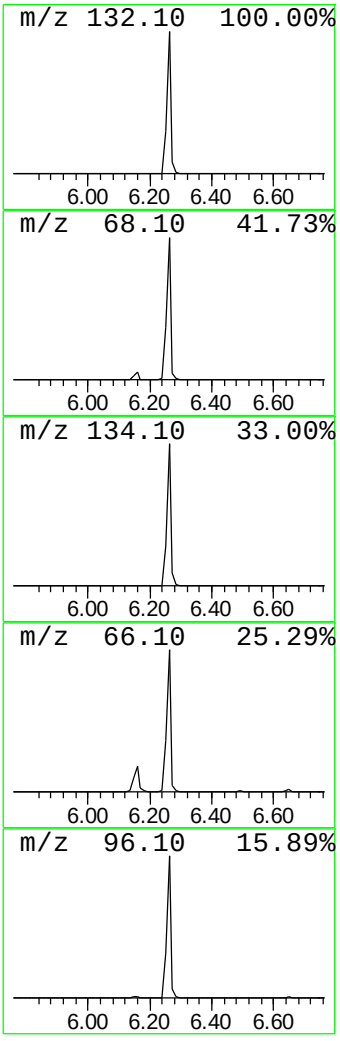
Peak Number 3 unknown6.26 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.26 | 73.64 ng | 2581540 | 1,4-Dichlorobenzene-d4 | 6.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 10 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092316\
Data File : BF090206.D
Acq On : 23 Sep 2016 19:11
Operator : UM/SJ
Sample : H4887-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TRACK-D-GRID-17A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

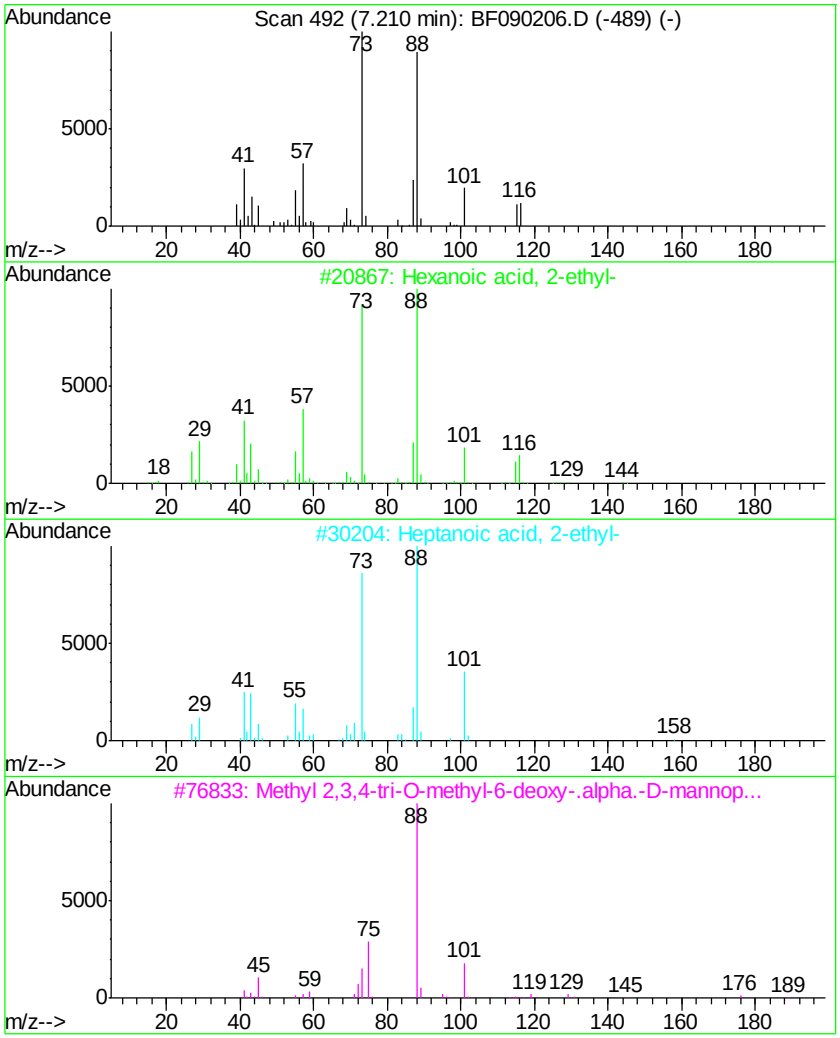
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

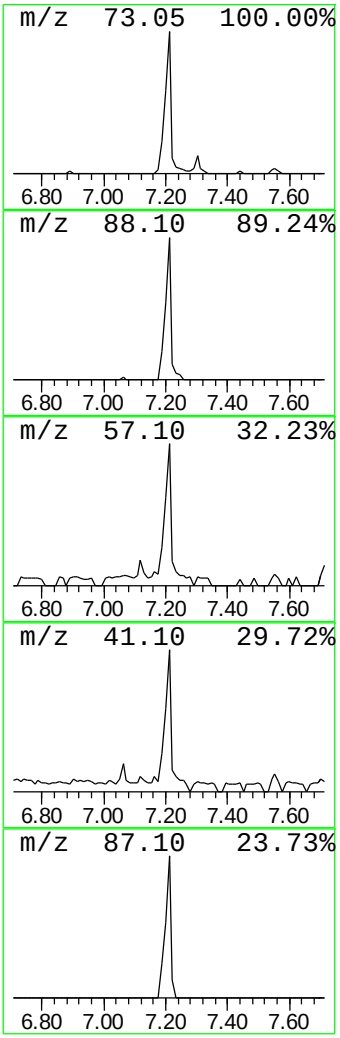
**********

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.21 | 2.17 ng | 97502 | Naphthalene-d8 | 7.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanoic acid, 2-ethyl- | 144 | C8H16O2 | 000149-57-5 | 86 |
| 2 | Heptanoic acid, 2-ethyl- | 158 | C9H18O2 | 003274-29-1 | 53 |
| 3 | Methyl 2,3,4-tri-O-methyl-6-deox... | 220 | C10H20O5 | 072983-16-5 | 33 |
| 4 | Butanoic acid, 2-ethyl-, 1,2,3-p... | 386 | C21H38O6 | 056554-54-2 | 32 |
| 5 | 1,4-Dioxane | 88 | C4H8O2 | 000123-91-1 | 32 |



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Data File : BF090206.D
Acq On : 23 Sep 2016 19:11
Operator : UM/SJ
Sample : H4887-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TRACK-D-GRID-17A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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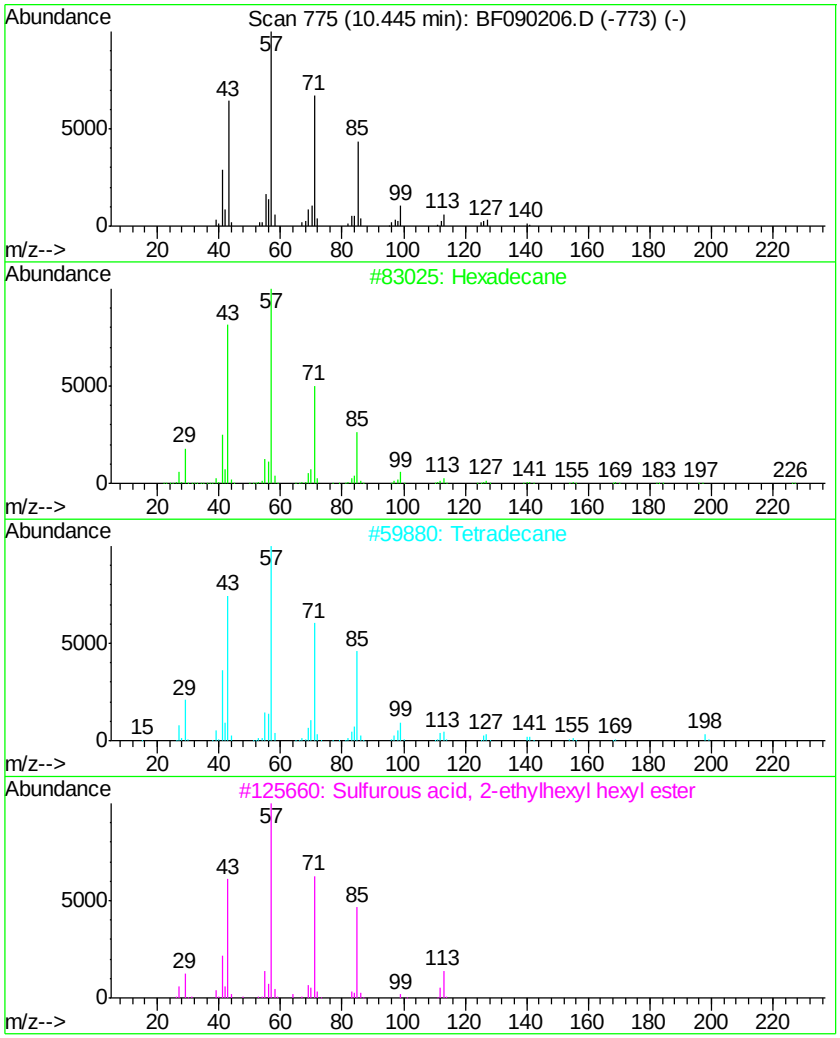
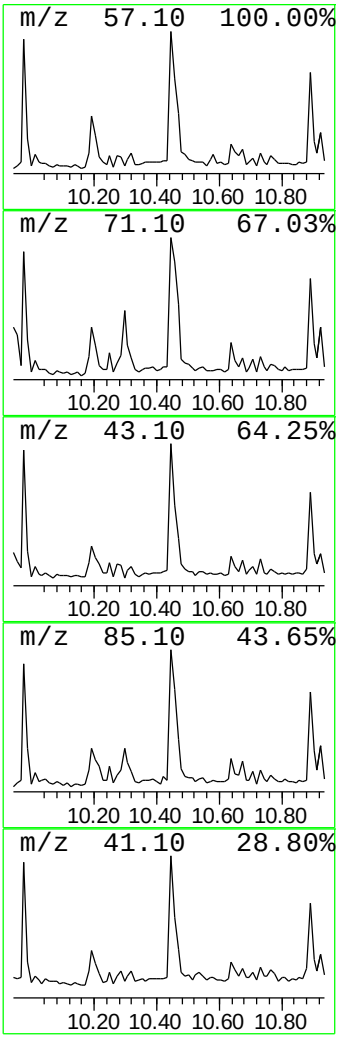
Peak Number 6 Hexadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.44 | 3.76 ng | 143242 | Phenanthrene-d10 | 10.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 80 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 78 |
| 3 | Sulfurous acid, 2-ethylhexyl hex... | 278 | C14H30O3S | 1000309-20-2 | 72 |
| 4 | Decane, 5-propyl- | 184 | C13H28 | 017312-62-8 | 72 |
| 5 | Nonane, 5-butyl- | 184 | C13H28 | 017312-63-9 | 72 |



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Operator : UM/SJ
Sample : H4887-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TRACK-D-GRID-17A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

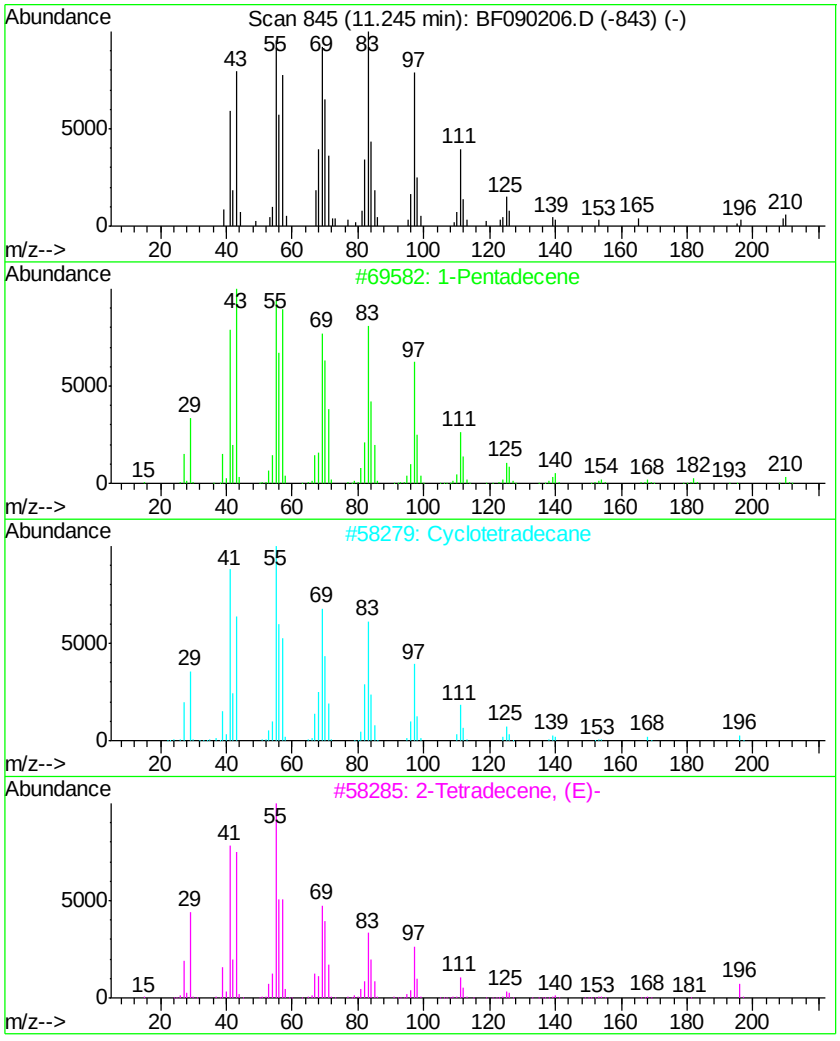
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

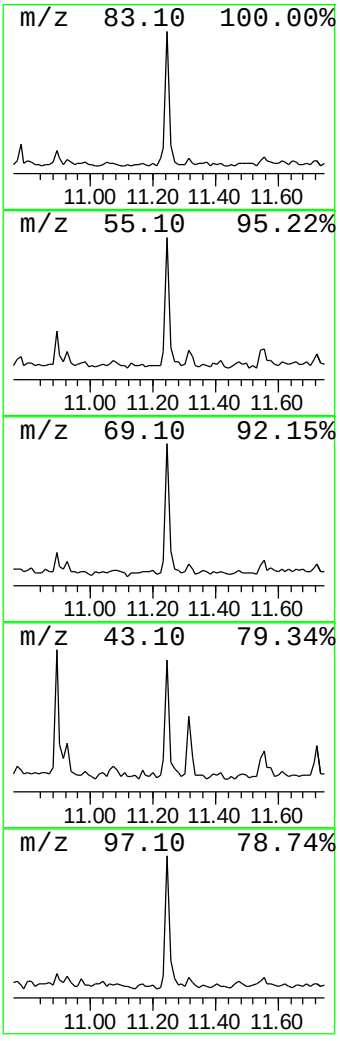
**********

Peak Number 7 1-Pentadecene Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.25 | 2.92 ng | 111517 | Phenanthrene-d10 | 10.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Pentadecene | 210 | C15H30 | 013360-61-7 | 96 |
| 2 | Cyclotetradecane | 196 | C14H28 | 000295-17-0 | 96 |
| 3 | 2-Tetradecene, (E)- | 196 | C14H28 | 035953-54-9 | 95 |
| 4 | n-Pentadecanol | 228 | C15H32O | 000629-76-5 | 95 |
| 5 | 1-Tetradecanol | 214 | C14H30O | 000112-72-1 | 95 |



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Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TRACK-D-GRID-17A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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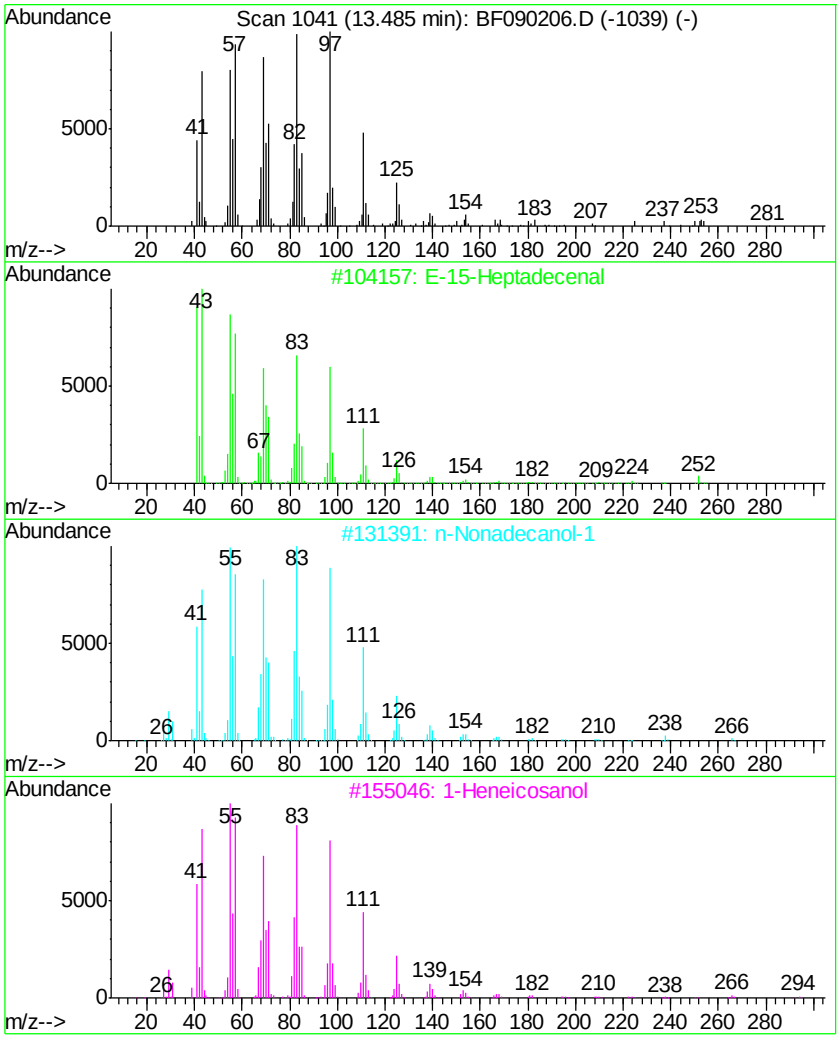
TIC Integration Parameters: LSCINT.P

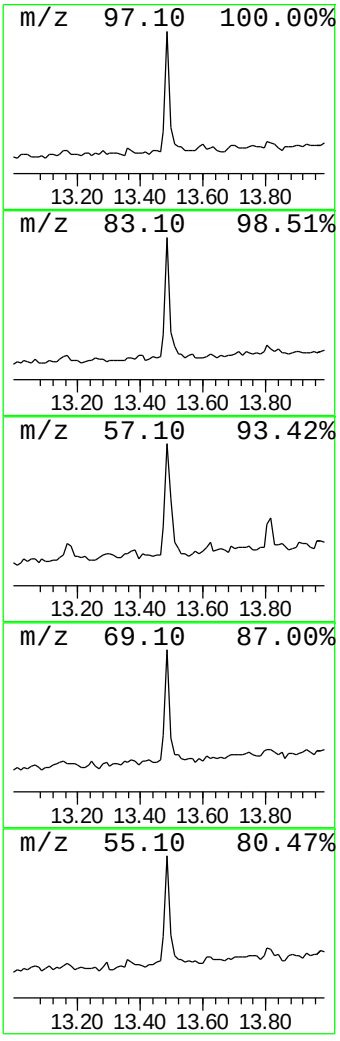
**********

Peak Number 8 E-15-Heptadecenal Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.49 | 3.81 ng | 169589 | Chrysene-d12 | 13.60 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | E-15-Heptadecenal | 252 | C17H32O | 1000130-97-9 | 96 |
| 2 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 95 |
| 3 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 94 |
| 4 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 93 |
| 5 | 13-Tetradecen-1-ol acetate | 254 | C16H30O2 | 056221-91-1 | 92 |



Tentatively Identified Compound (LSC) summary

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**ClientSampleId :** TRACK-D-GRID-17A

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.58 | 16.3 | ng | 572017 | 1 | 6.49 | 701158 | 20.0 |
| unknown6.26 | 6.26 | 73.6 | ng | 2581540 | 1 | 6.49 | 701158 | 20.0 |
| Hexanoic acid, 2-... | 7.21 | 2.2 | ng | 97502 | 2 | 7.78 | 898447 | 20.0 |
| Hexadecane | 10.44 | 3.8 | ng | 143242 | 4 | 10.98 | 762759 | 20.0 |
| 1-Pentadecene | 11.25 | 2.9 | ng | 111517 | 4 | 10.98 | 762759 | 20.0 |
| E-15-Heptadecenal | 13.49 | 3.8 | ng | 169589 | 5 | 13.60 | 889307 | 20.0 |