LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087700.D
Acq On : 5 Jun 2016 10:41
Operator : UM/SJ
Sample : H3312-04
Misc :
ALS Vial : 42 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW1

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-BF060416.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 | 1.770 | 15 | 16 | 26 | rVV | 345240 | 590138 | 13.10% | 1.890% |
| 2 | 1.907 | 26 | 28 | 47 | rVB | 2431522 | 4505781 | 100.00% | 14.427% |
| 3 | 5.039 | 300 | 302 | 306 | rBV | 162667 | 190303 | 4.22% | 0.609% |
| 4 | 5.450 | 335 | 338 | 340 | rBV | 1706003 | 1568491 | 34.81% | 5.022% |
| 5 | 6.479 | 425 | 428 | 430 | rBV | 1247014 | 1072688 | 23.81% | 3.435% |
| 6 | 6.627 | 438 | 441 | 443 | rBV | 2427567 | 2847392 | 63.19% | 9.117% |
| 7 | 6.856 | 459 | 461 | 465 | rVB | 866543 | 758398 | 16.83% | 2.428% |
| 8 | 7.016 | 472 | 475 | 477 | rBV | 2556602 | 2392773 | 53.10% | 7.662% |
| 9 | 7.382 | 505 | 507 | 508 | rBV | 61156 | 62232 | 1.38% | 0.199% |
| 10 | 7.427 | 508 | 511 | 513 | rVB | 1923560 | 2268016 | 50.34% | 7.262% |
| 11 | 7.530 | 519 | 520 | 523 | rVB | 65177 | 90472 | 2.01% | 0.290% |
| 12 | 8.147 | 571 | 574 | 576 | rBV | 932360 | 1047383 | 23.25% | 3.354% |
| 13 | 8.479 | 599 | 603 | 608 | rBV2 | 26649 | 54549 | 1.21% | 0.175% |
| 14 | 9.222 | 665 | 668 | 671 | rVV | 2996585 | 3699968 | 82.12% | 11.847% |
| 15 | 9.622 | 700 | 703 | 705 | rVB | 214243 | 301848 | 6.70% | 0.967% |
| 16 | 9.828 | 719 | 721 | 725 | rBV | 152433 | 148643 | 3.30% | 0.476% |
| 17 | 9.896 | 725 | 727 | 730 | rVB | 1193043 | 1102310 | 24.46% | 3.530% |
| 18 | 10.319 | 762 | 764 | 771 | rBV3 | 43180 | 75059 | 1.67% | 0.240% |
| 19 | 10.639 | 788 | 792 | 793 | rBV3 | 27071 | 47619 | 1.06% | 0.152% |
| 20 | 10.685 | 793 | 796 | 799 | rBV | 1977344 | 2229212 | 49.47% | 7.138% |
| 21 | 11.256 | 844 | 846 | 850 | rBV2 | 40923 | 64852 | 1.44% | 0.208% |
| 22 | 11.382 | 854 | 857 | 859 | rVB | 1193638 | 1095418 | 24.31% | 3.507% |
| 23 | 11.919 | 902 | 904 | 910 | rBV2 | 272775 | 336372 | 7.47% | 1.077% |
| 24 | 12.708 | 971 | 973 | 979 | rBV | 220079 | 250386 | 5.56% | 0.802% |
| 25 | 12.799 | 979 | 981 | 983 | rVB | 67601 | 61235 | 1.36% | 0.196% |
| 26 | 12.971 | 993 | 996 | 998 | rBV | 2891803 | 2816886 | 62.52% | 9.020% |
| 27 | 13.874 | 1073 | 1075 | 1078 | rVB | 81611 | 81917 | 1.82% | 0.262% |
| 28 | 14.011 | 1084 | 1087 | 1090 | rBV | 907182 | 835723 | 18.55% | 2.676% |
| 29 | 15.440 | 1209 | 1212 | 1215 | rBV | 538540 | 634749 | 14.09% | 2.032% |

Sum of corrected areas: 31230813

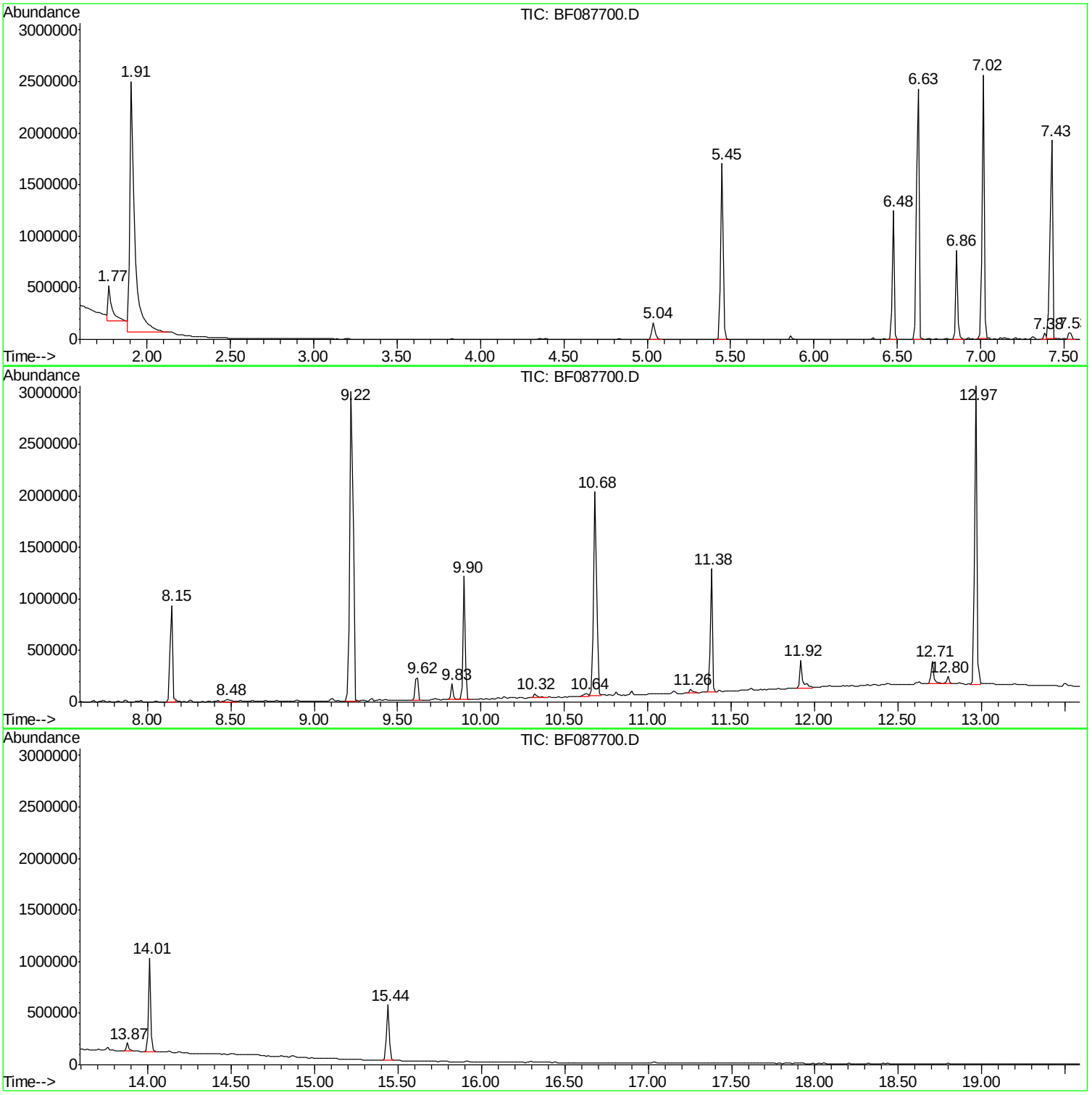
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087700.D
Acq On : 5 Jun 2016 10:41
Operator : UM/SJ
Sample : H3312-04
Misc :
ALS Vial : 42 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087700.D
Acq On : 5 Jun 2016 10:41
Operator : UM/SJ
Sample : H3312-04
Misc :
ALS Vial : 42 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

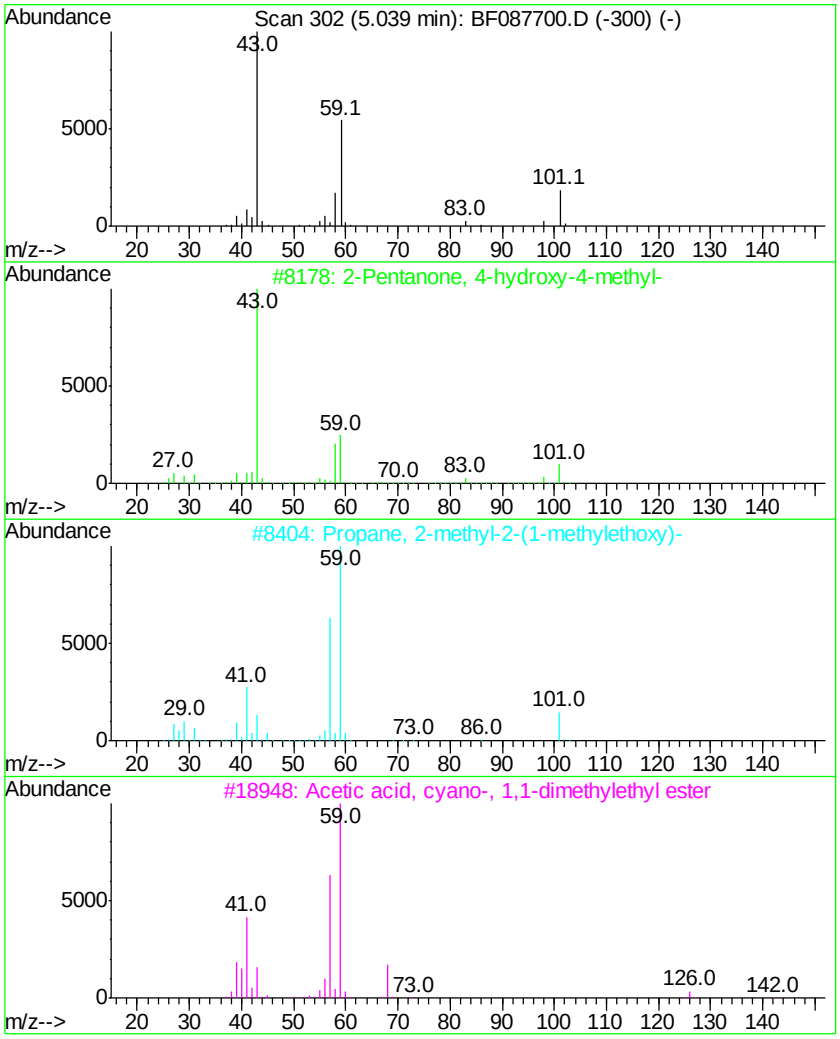
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

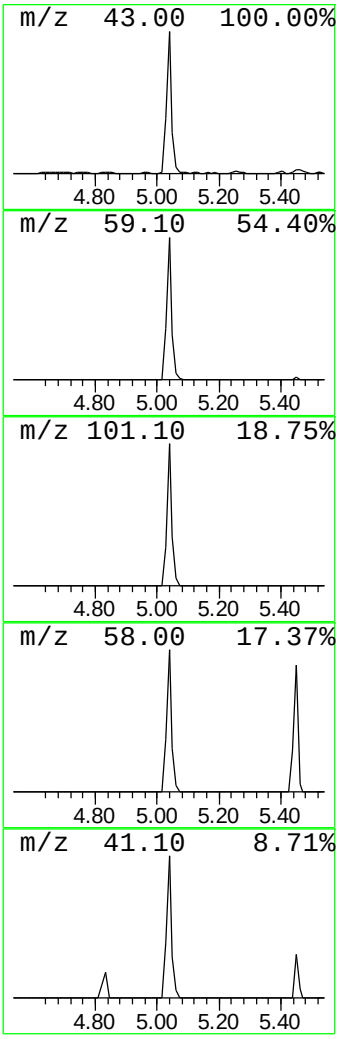
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.04 | 5.02 ng | 190303 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 33 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 4 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087700.D
Acq On : 5 Jun 2016 10:41
Operator : UM/SJ
Sample : H3312-04
Misc :
ALS Vial : 42 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

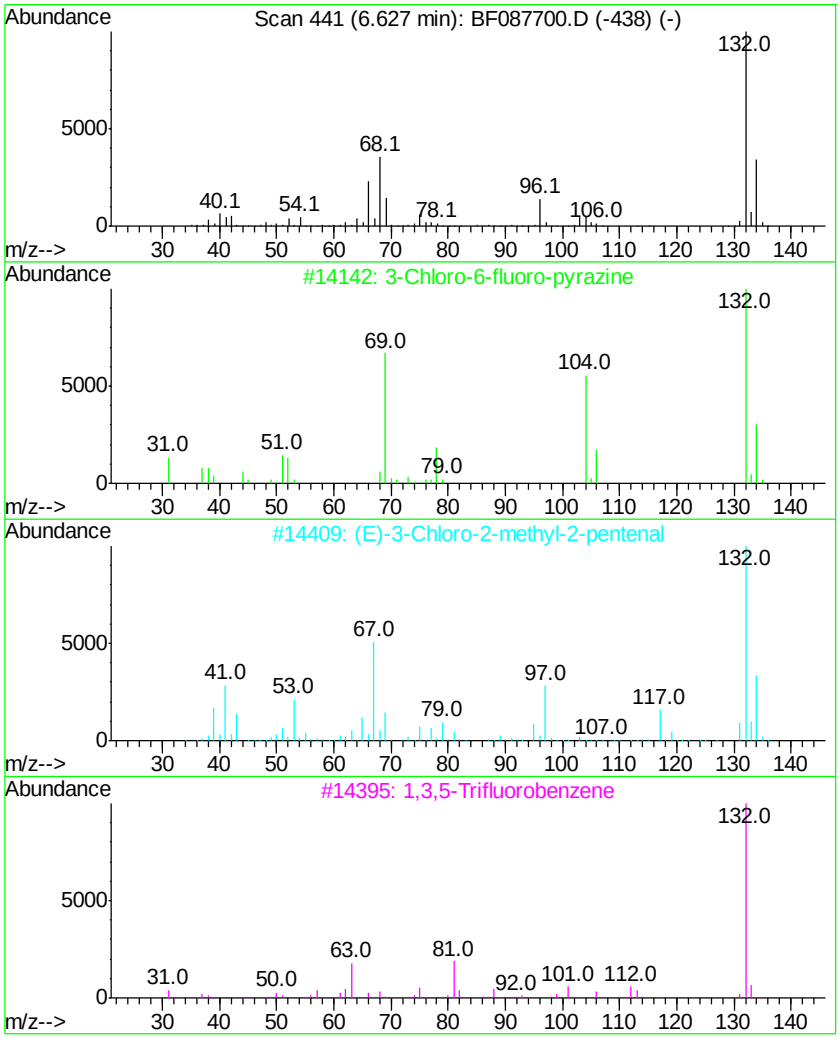
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

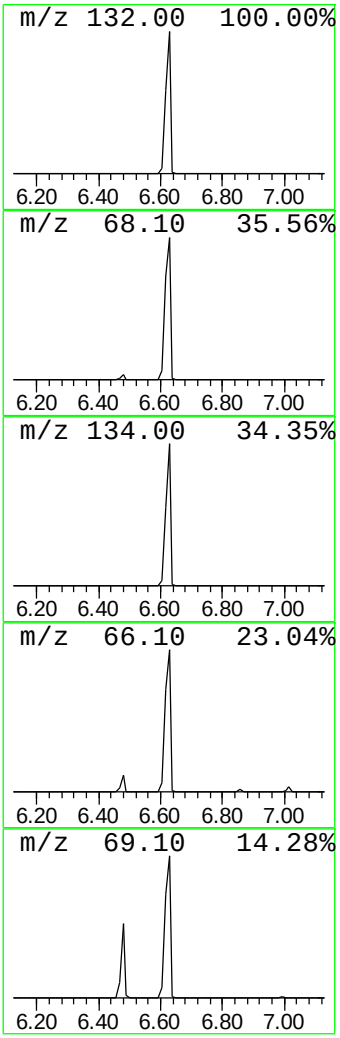
**********

Peak Number 4 unknown6.63 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.63 | 75.09 ng | 2847390 | 1,4-Dichlorobenzene-d4 | 6.86 |

| 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 | 12 |
| 3 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |
| 4 | Xenon | 132 | Xe | 007440-63-3 | 9 |
| 5 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087700.D
Acq On : 5 Jun 2016 10:41
Operator : UM/SJ
Sample : H3312-04
Misc :
ALS Vial : 42 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

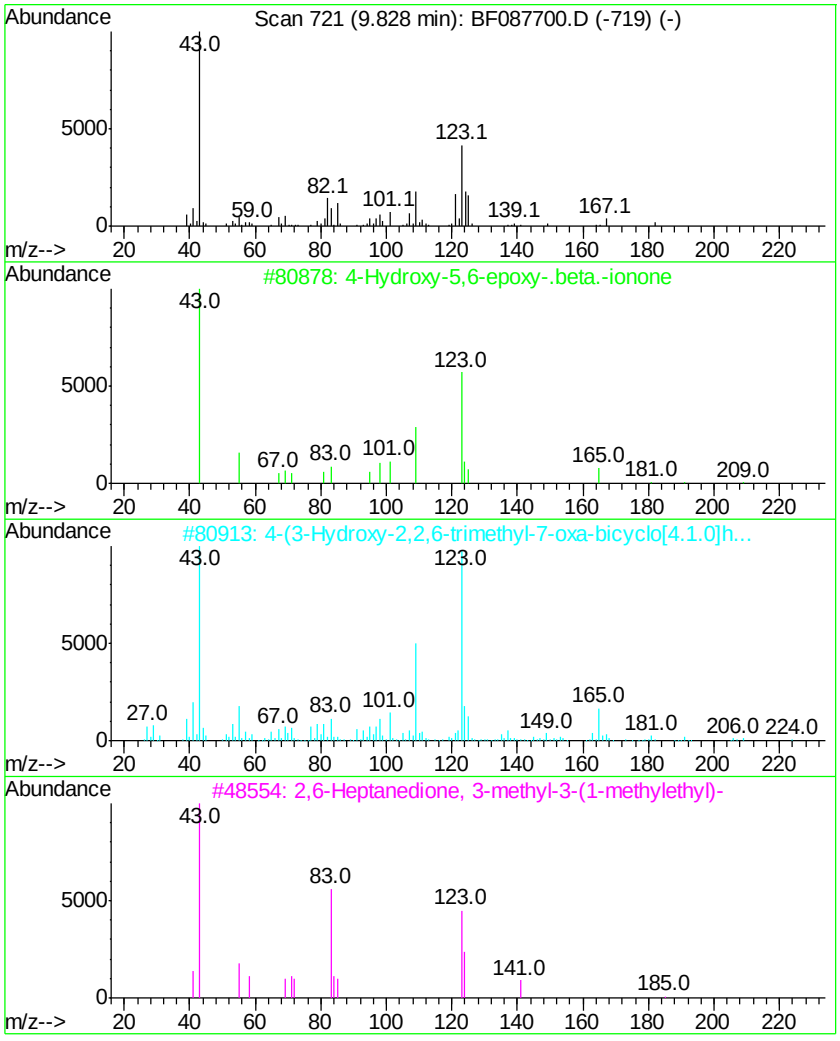
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

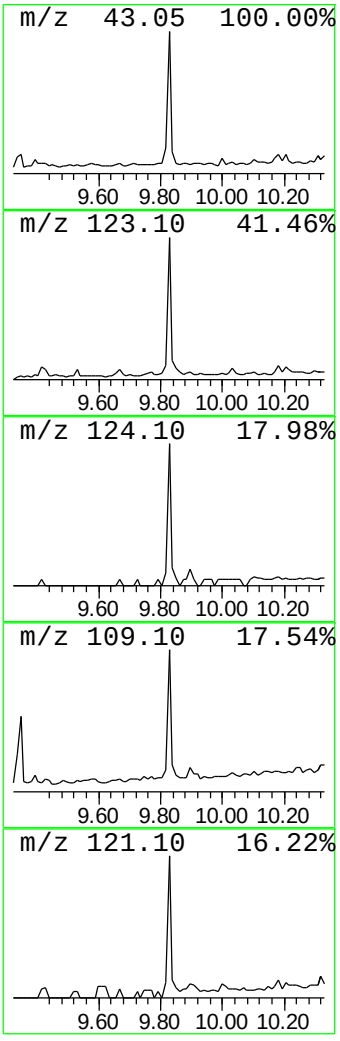
**********

Peak Number 6 unknown9.83 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.83 | 2.70 ng | 148643 | Acenaphthene-d10 | 9.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Hydroxy-5,6-epoxy-.beta.-ionone | 224 | C13H20O3 | 1000108-78-1 | 47 |
| 2 | 4-(3-Hydroxy-2,2,6-trimethyl-7-o... | 224 | C13H20O3 | 1000190-36-6 | 40 |
| 3 | 2,6-Heptanedione, 3-methyl-3-(1-... | 184 | C11H20O2 | 063922-59-8 | 9 |
| 4 | L-Mannitol, 1-deoxy-, cyclic 3,4... | 284 | C12H22B2O6 | 074779-69-4 | 9 |
| 5 | 3-Buten-2-one, 4-(2,5,5-trimethy... | 222 | C13H18O3 | 080114-19-8 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087700.D
Acq On : 5 Jun 2016 10:41
Operator : UM/SJ
Sample : H3312-04
Misc :
ALS Vial : 42 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

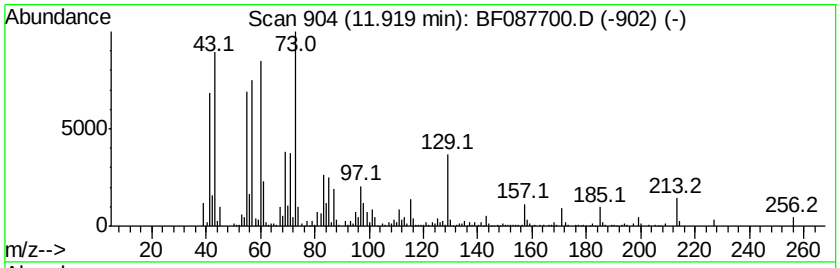
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

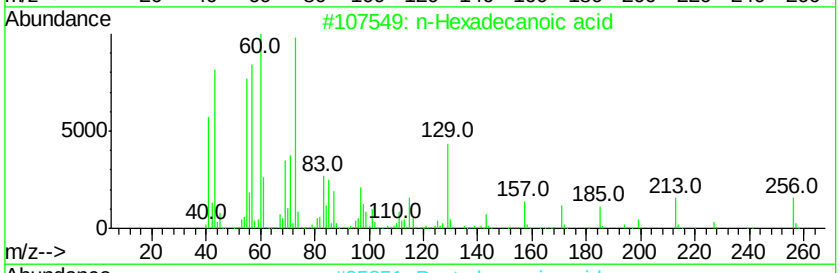
**********

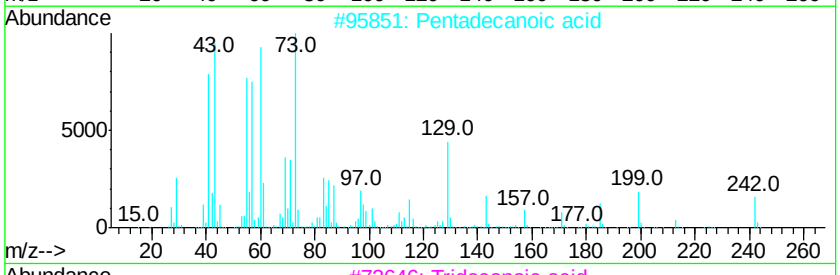
Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

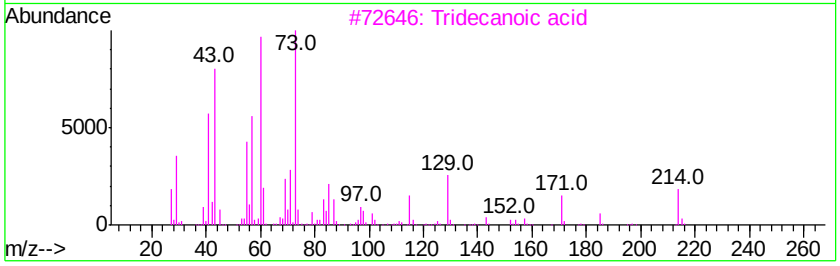
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.92 | 6.14 ng | 336372 | Phenanthrene-d10 | 11.38 |

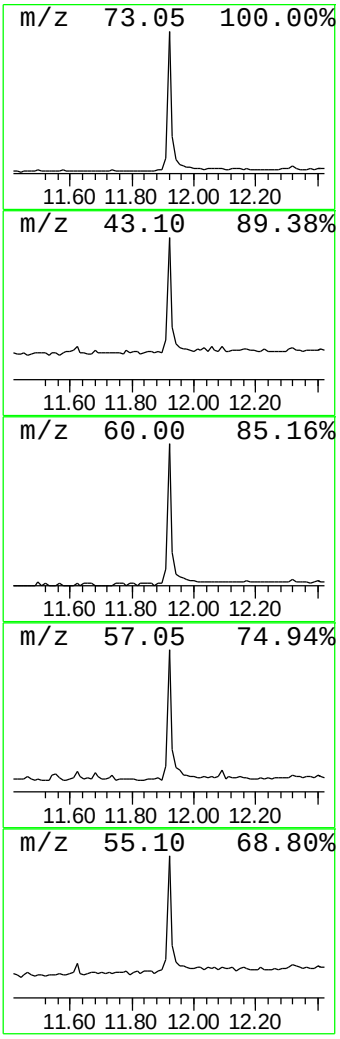
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 81 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 5 | Nonanoic acid | 158 | C9H18O2 | 000112-05-0 | 43 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087700.D
Acq On : 5 Jun 2016 10:41
Operator : UM/SJ
Sample : H3312-04
Misc :
ALS Vial : 42 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

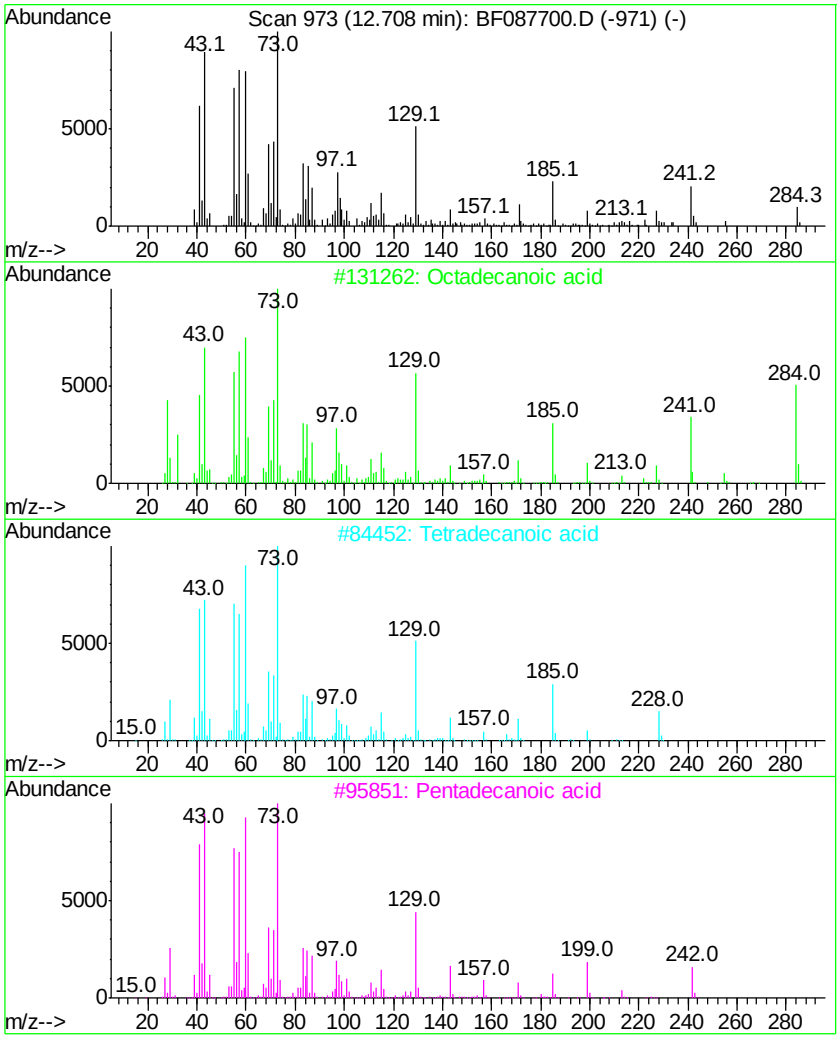
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

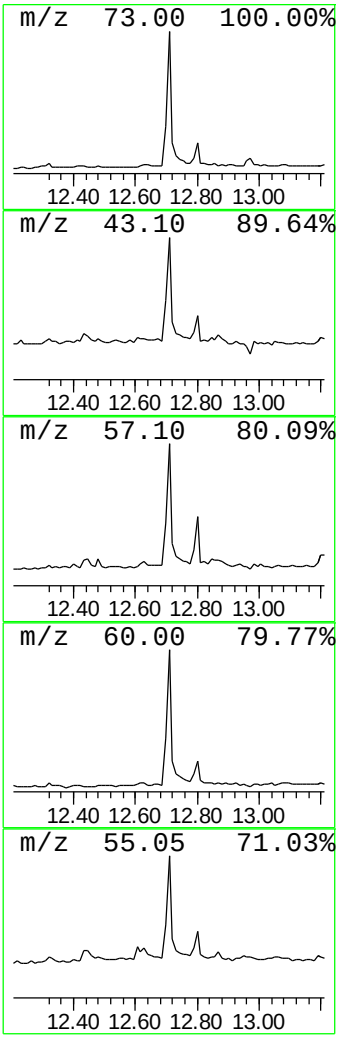
**********

Peak Number 8 Octadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.71 | 5.99 ng | 250386 | Chrysene-d12 | 14.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 91 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 4 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 87 |
| 5 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 74 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087700.D
Acq On : 5 Jun 2016 10:41
Operator : UM/SJ
Sample : H3312-04
Misc :
ALS Vial : 42 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SW1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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... | 5.04 | 5.0 | ng | 190303 | 1 | 6.86 | 758398 | 20.0 |
| unknown6.63 | 6.63 | 75.1 | ng | 2847390 | 1 | 6.86 | 758398 | 20.0 |
| unknown9.83 | 9.83 | 2.7 | ng | 148643 | 3 | 9.90 | 1102310 | 20.0 |
| n-Hexadecanoic acid | 11.92 | 6.1 | ng | 336372 | 4 | 11.38 | 1095420 | 20.0 |
| Octadecanoic acid | 12.71 | 6.0 | ng | 250386 | 5 | 14.01 | 835723 | 20.0 |