LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090815\
Data File : BF081533.D
Acq On : 8 Sep 2015 20:52
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-10

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 | 4.387 | 241 | 245 | 258 | rVB | 583686 | 1159812 | 58.59% | 6.764% |
| 2 | 4.890 | 287 | 289 | 292 | rBV | 1541003 | 1737184 | 87.76% | 10.131% |
| 3 | 6.022 | 385 | 388 | 390 | rBV | 1844647 | 1979518 | 100.00% | 11.544% |
| 4 | 6.113 | 394 | 396 | 399 | rVB | 1837974 | 1721752 | 86.98% | 10.041% |
| 5 | 6.342 | 414 | 416 | 419 | rVB | 377875 | 352361 | 17.80% | 2.055% |
| 6 | 6.502 | 428 | 430 | 432 | rBV | 1371669 | 1173904 | 59.30% | 6.846% |
| 7 | 6.924 | 464 | 467 | 469 | rBV | 1139565 | 1124172 | 56.79% | 6.556% |
| 8 | 7.633 | 527 | 529 | 532 | rBV | 519170 | 441425 | 22.30% | 2.574% |
| 9 | 8.719 | 621 | 624 | 626 | rBV | 2050127 | 1757638 | 88.79% | 10.250% |
| 10 | 9.119 | 657 | 659 | 662 | rBV | 360389 | 315768 | 15.95% | 1.841% |
| 11 | 9.370 | 679 | 681 | 683 | rVB | 476165 | 450326 | 22.75% | 2.626% |
| 12 | 10.159 | 747 | 750 | 752 | rBV | 1345341 | 1234924 | 62.39% | 7.202% |
| 13 | 10.308 | 761 | 763 | 767 | rBV | 34537 | 39447 | 1.99% | 0.230% |
| 14 | 10.753 | 795 | 802 | 803 | rBV | 30094 | 28857 | 1.46% | 0.168% |
| 15 | 10.833 | 807 | 809 | 813 | rBV | 352803 | 507853 | 25.66% | 2.962% |
| 16 | 11.416 | 858 | 860 | 861 | rBV | 83204 | 82252 | 4.16% | 0.480% |
| 17 | 11.439 | 861 | 862 | 866 | rVB | 28535 | 39167 | 1.98% | 0.228% |
| 18 | 12.034 | 911 | 914 | 916 | rBV | 183092 | 155744 | 7.87% | 0.908% |
| 19 | 12.251 | 931 | 933 | 936 | rBV | 142321 | 145475 | 7.35% | 0.848% |
| 20 | 12.422 | 946 | 948 | 951 | rBV | 1504644 | 1446782 | 73.09% | 8.437% |
| 21 | 12.594 | 958 | 963 | 964 | rBV2 | 14843 | 27084 | 1.37% | 0.158% |
| 22 | 12.685 | 970 | 971 | 975 | rVB2 | 21336 | 23262 | 1.18% | 0.136% |
| 23 | 13.028 | 995 | 1001 | 1002 | rBV2 | 10866 | 20410 | 1.03% | 0.119% |
| 24 | 13.348 | 1026 | 1029 | 1034 | rBV2 | 73223 | 122477 | 6.19% | 0.714% |
| 25 | 13.439 | 1034 | 1037 | 1042 | rVV | 299432 | 451791 | 22.82% | 2.635% |
| 26 | 13.668 | 1054 | 1057 | 1060 | rVB3 | 11604 | 20785 | 1.05% | 0.121% |
| 27 | 13.965 | 1080 | 1083 | 1088 | rVB3 | 14415 | 21179 | 1.07% | 0.124% |
| 28 | 14.422 | 1121 | 1123 | 1128 | rBV | 62088 | 109993 | 5.56% | 0.641% |
| 29 | 14.662 | 1142 | 1144 | 1146 | rVB | 33218 | 37541 | 1.90% | 0.219% |
| 30 | 14.708 | 1146 | 1148 | 1150 | rVB | 52237 | 57021 | 2.88% | 0.333% |
| 31 | 14.754 | 1150 | 1152 | 1154 | rBV | 292926 | 302079 | 15.26% | 1.762% |
| 32 | 15.817 | 1242 | 1245 | 1248 | rVB2 | 22452 | 34654 | 1.75% | 0.202% |
| 33 | 16.137 | 1270 | 1273 | 1276 | rBV | 13762 | 24809 | 1.25% | 0.145% |

LSC Area Percent Report

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Data File : BF081533.D
Acq On : 8 Sep 2015 20:52
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-10

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

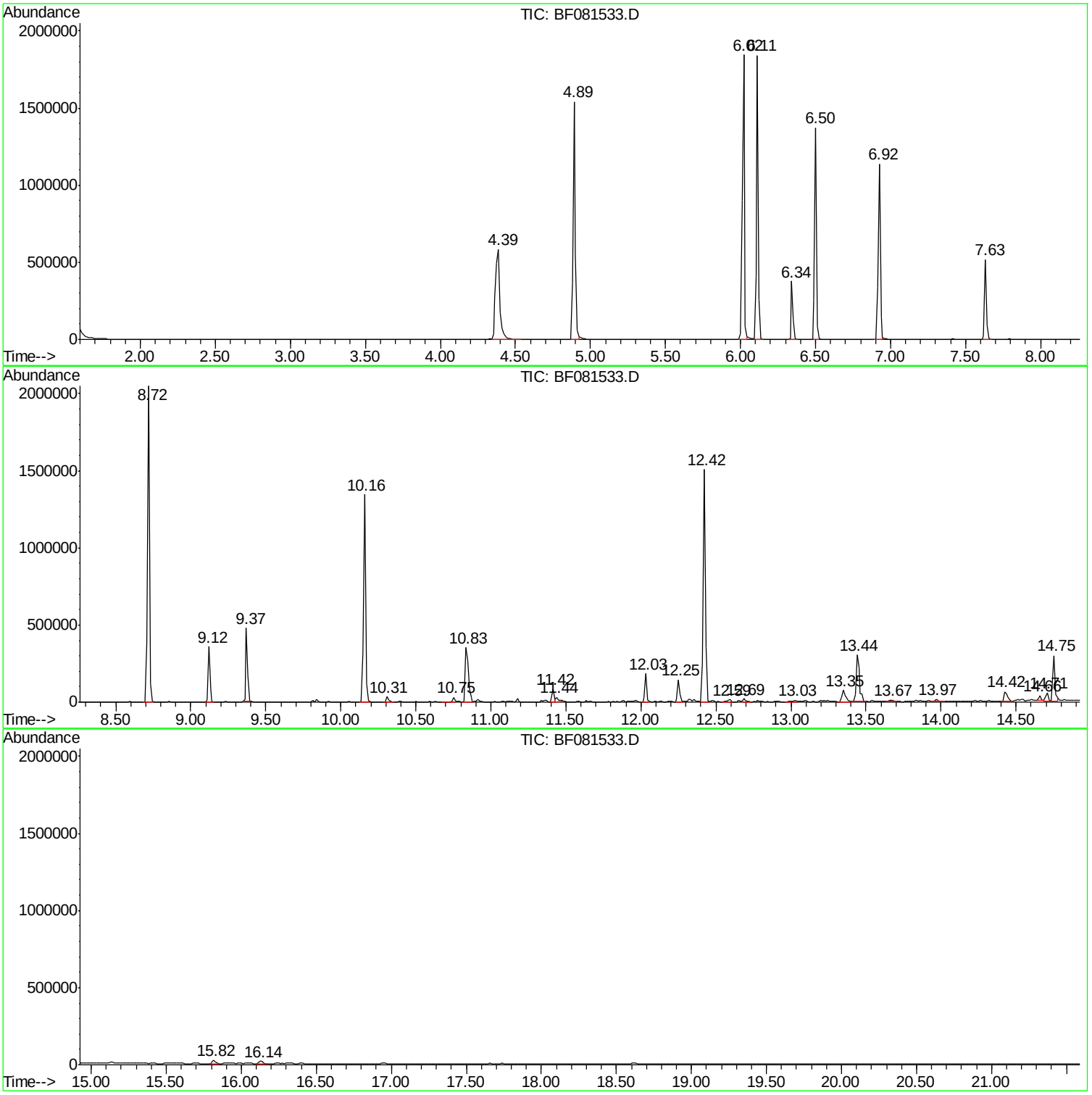
Sum of corrected areas: 17147446

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090815\
Data File : BF081533.D
Acq On : 8 Sep 2015 20:52
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-10

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\BF090815\
Data File : BF081533.D
Acq On : 8 Sep 2015 20:52
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-10

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

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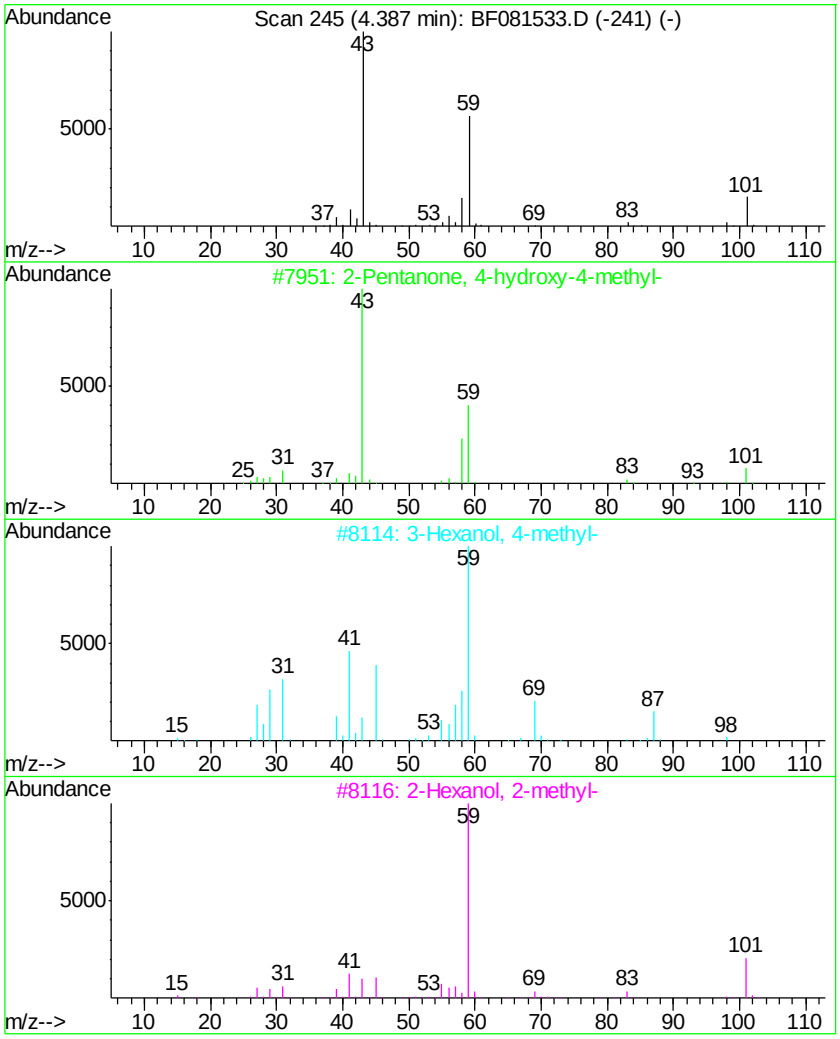
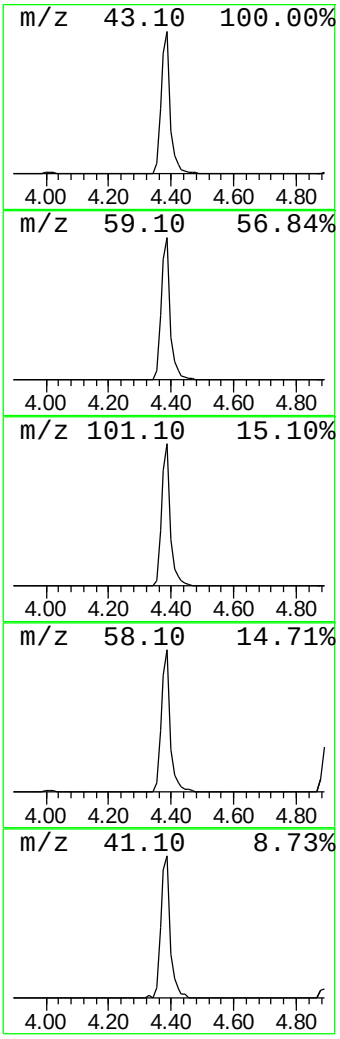
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.39 | 65.83 ng | 1159810 | 1,4-Dichlorobenzene-d4 | 6.34 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090815\
Data File : BF081533.D
Acq On : 8 Sep 2015 20:52
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-10

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

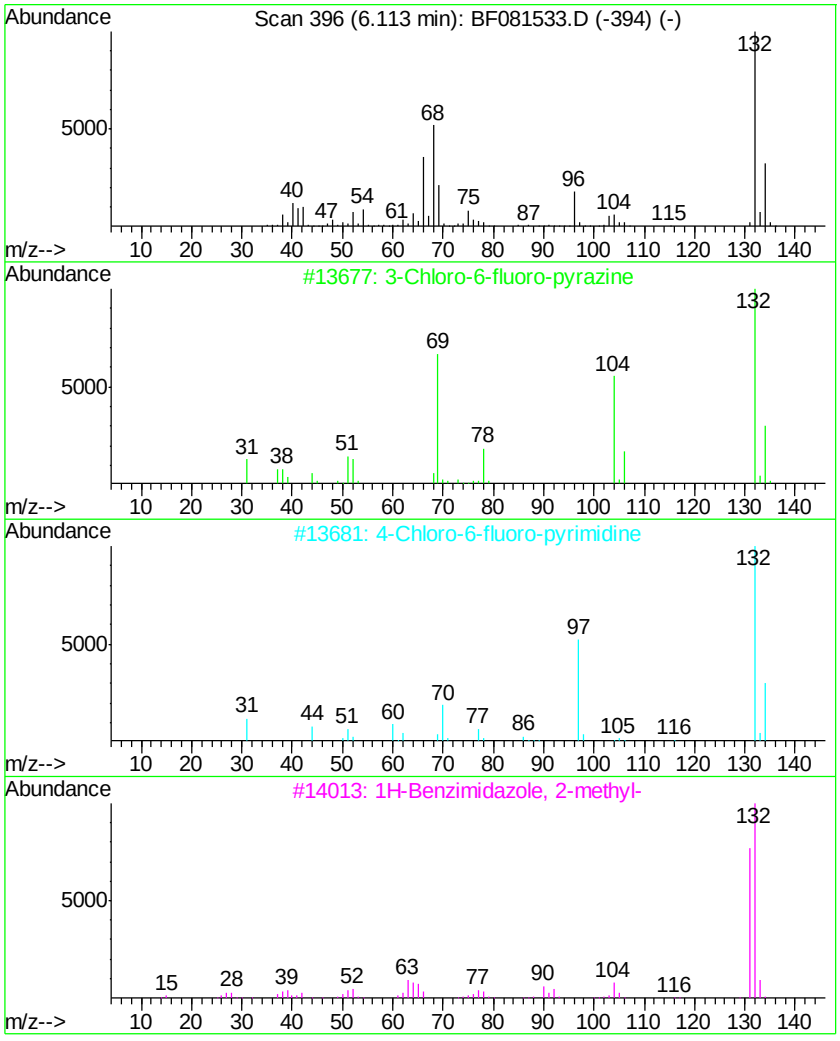
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

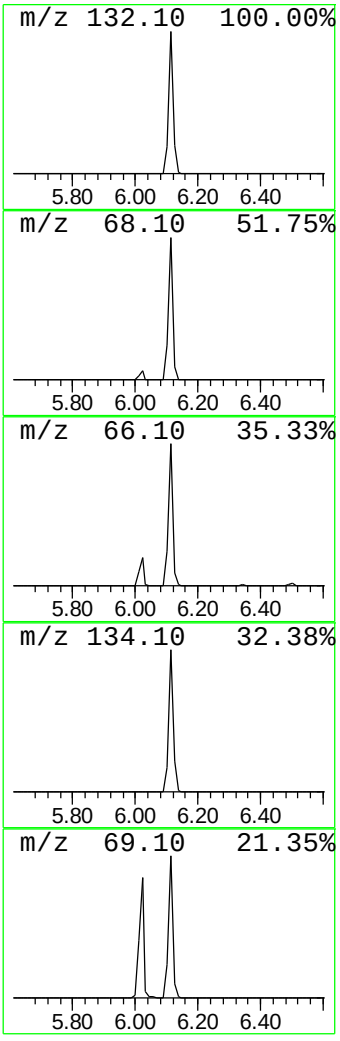
**********

Peak Number 2 unknown6.11 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.11 | 97.73 ng | 1721750 | 1,4-Dichlorobenzene-d4 | 6.34 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 5 | (5-METHYL-2-PYRIDYL)ACETONITRILE | 132 | C8H8N2 | 1000241-93-9 | 10 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090815\
Data File : BF081533.D
Acq On : 8 Sep 2015 20:52
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-10

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

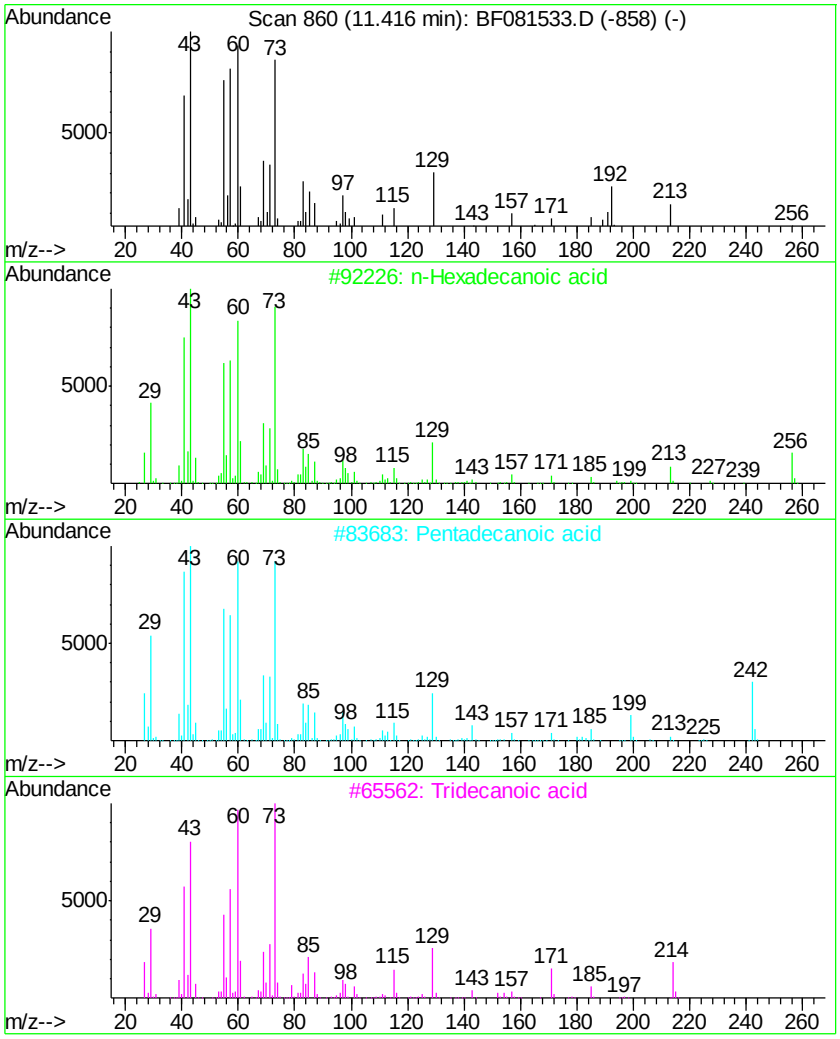
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

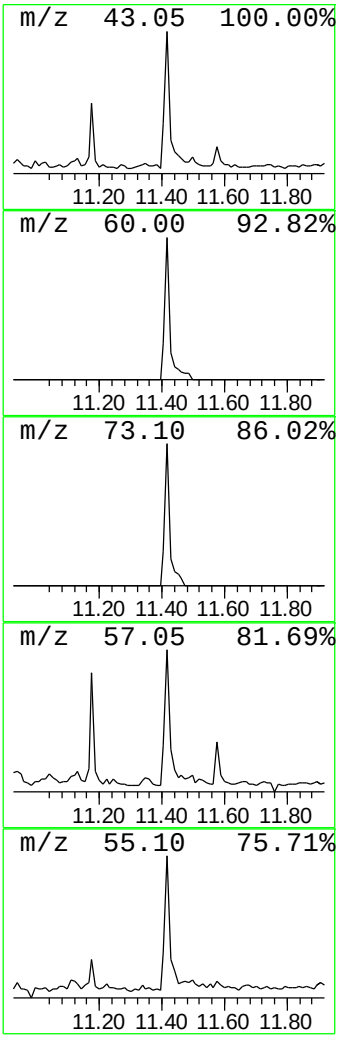
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.42 | 3.24 ng | 82252 | Phenanthrene-d10 | 10.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 83 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 68 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 62 |
| 4 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 59 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 53 |



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Data File : BF081533.D
Acq On : 8 Sep 2015 20:52
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-10

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

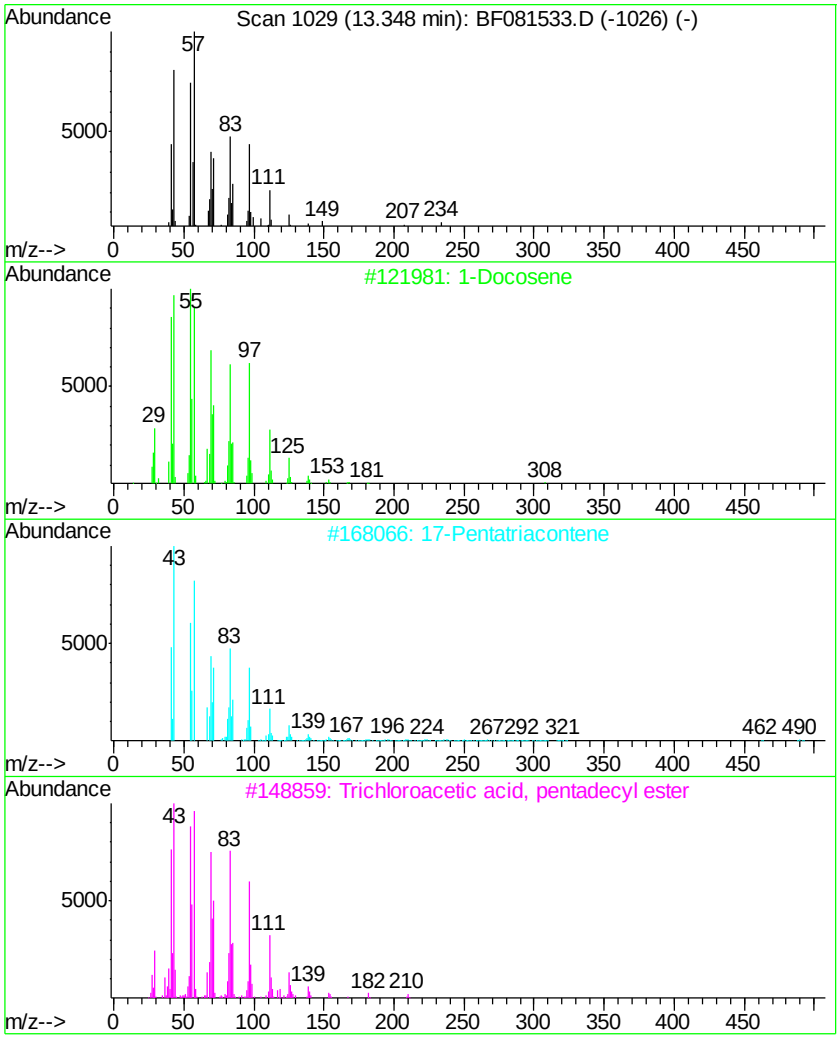
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

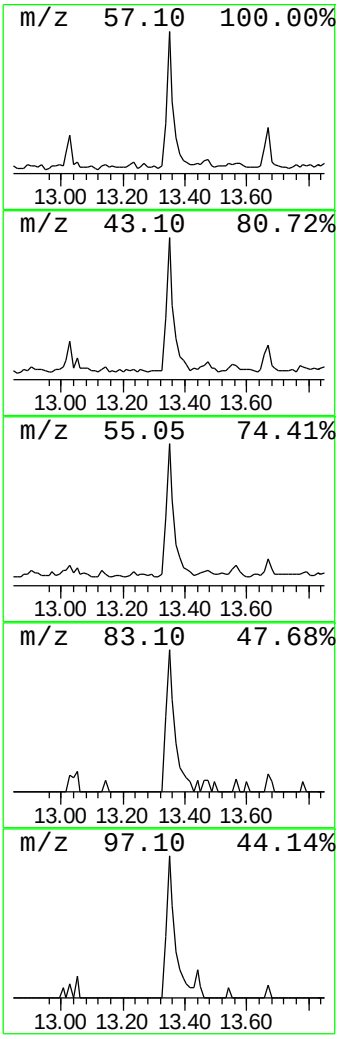
**********

Peak Number 5 1-Docosene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.35 | 5.42 ng | 122477 | Chrysene-d12 | 13.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 90 |
| 2 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 90 |
| 3 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 87 |
| 4 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 83 |
| 5 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 83 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090815\
Data File : BF081533.D
Acq On : 8 Sep 2015 20:52
Operator : UM/IZ
Sample : G3555-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-10

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... | 4.39 | 65.8 | ng | 1159810 | 1 | 6.34 | 352361 | 20.0 |
| unknown6.11 | 6.11 | 97.7 | ng | 1721750 | 1 | 6.34 | 352361 | 20.0 |
| n-Hexadecanoic acid | 11.42 | 3.2 | ng | 82252 | 4 | 10.83 | 507853 | 20.0 |
| 1-Docosene | 13.35 | 5.4 | ng | 122477 | 5 | 13.44 | 451791 | 20.0 |