LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DUP-X

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 | 3.530 | 168 | 170 | 178 | rBB | 9455 | 22742 | 1.18% | 0.135% |
| 2 | 4.410 | 243 | 247 | 261 | rVB | 579725 | 1168466 | 60.39% | 6.942% |
| 3 | 4.913 | 288 | 291 | 293 | rBV | 1320925 | 1738613 | 89.85% | 10.329% |
| 4 | 5.336 | 326 | 328 | 332 | rBB | 22525 | 21473 | 1.11% | 0.128% |
| 5 | 6.033 | 386 | 389 | 391 | rBV | 1434618 | 1875273 | 96.91% | 11.141% |
| 6 | 6.124 | 395 | 397 | 399 | rBV | 1887689 | 1661976 | 85.89% | 9.874% |
| 7 | 6.353 | 415 | 417 | 420 | rBV | 385906 | 355386 | 18.37% | 2.111% |
| 8 | 6.513 | 428 | 431 | 433 | rBV | 1548763 | 1343355 | 69.42% | 7.981% |
| 9 | 6.936 | 465 | 468 | 470 | rBV | 1159806 | 1141728 | 59.00% | 6.783% |
| 10 | 7.645 | 528 | 530 | 533 | rBV | 542578 | 457763 | 23.66% | 2.720% |
| 11 | 8.730 | 622 | 625 | 627 | rBV | 2149009 | 1935024 | 100.00% | 11.496% |
| 12 | 9.130 | 658 | 660 | 662 | rBV | 375172 | 329113 | 17.01% | 1.955% |
| 13 | 9.382 | 680 | 682 | 685 | rVB | 490049 | 462936 | 23.92% | 2.750% |
| 14 | 10.171 | 748 | 751 | 753 | rBV | 1100594 | 1107245 | 57.22% | 6.578% |
| 15 | 10.319 | 762 | 764 | 768 | rVB | 31270 | 34533 | 1.78% | 0.205% |
| 16 | 10.765 | 801 | 803 | 804 | rBV | 26616 | 23183 | 1.20% | 0.138% |
| 17 | 10.845 | 808 | 810 | 813 | rBV | 457925 | 467953 | 24.18% | 2.780% |
| 18 | 11.428 | 859 | 861 | 866 | rBV | 37235 | 48184 | 2.49% | 0.286% |
| 19 | 12.045 | 913 | 915 | 917 | rBV | 46601 | 39285 | 2.03% | 0.233% |
| 20 | 12.262 | 932 | 934 | 935 | rBV | 34821 | 34100 | 1.76% | 0.203% |
| 21 | 12.297 | 935 | 937 | 939 | rVB | 48050 | 58667 | 3.03% | 0.349% |
| 22 | 12.434 | 946 | 949 | 952 | rVB | 1602519 | 1524782 | 78.80% | 9.059% |
| 23 | 12.994 | 995 | 998 | 1000 | rBV | 43038 | 42179 | 2.18% | 0.251% |
| 24 | 13.359 | 1028 | 1030 | 1036 | rBV | 44872 | 95888 | 4.96% | 0.570% |
| 25 | 13.451 | 1036 | 1038 | 1043 | rVB | 353089 | 418209 | 21.61% | 2.485% |
| 26 | 13.680 | 1056 | 1058 | 1060 | rBV | 15709 | 20662 | 1.07% | 0.123% |
| 27 | 13.977 | 1082 | 1084 | 1087 | rBV | 23594 | 27763 | 1.43% | 0.165% |
| 28 | 14.434 | 1122 | 1124 | 1129 | rBV | 33459 | 52320 | 2.70% | 0.311% |
| 29 | 14.548 | 1133 | 1134 | 1136 | rVV | 27362 | 32634 | 1.69% | 0.194% |
| 30 | 14.674 | 1143 | 1145 | 1147 | rBV | 15893 | 22359 | 1.16% | 0.133% |
| 31 | 14.765 | 1151 | 1153 | 1155 | rBV | 206721 | 247384 | 12.78% | 1.470% |
| 32 | 15.154 | 1185 | 1187 | 1190 | rBV | 17627 | 21175 | 1.09% | 0.126% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DUP-X

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

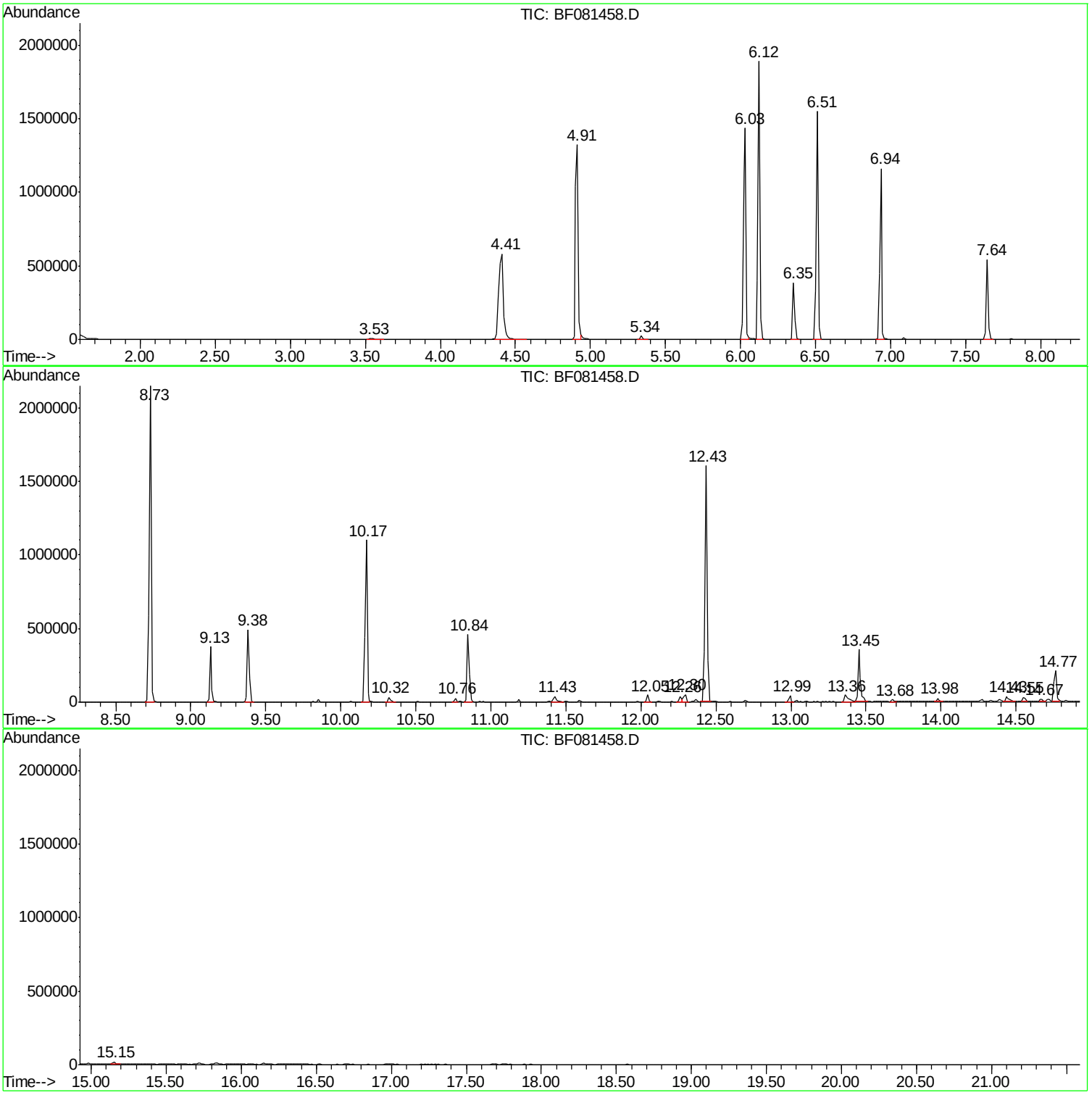
Sum of corrected areas: 16832353

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
DUP-X

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DUP-X

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

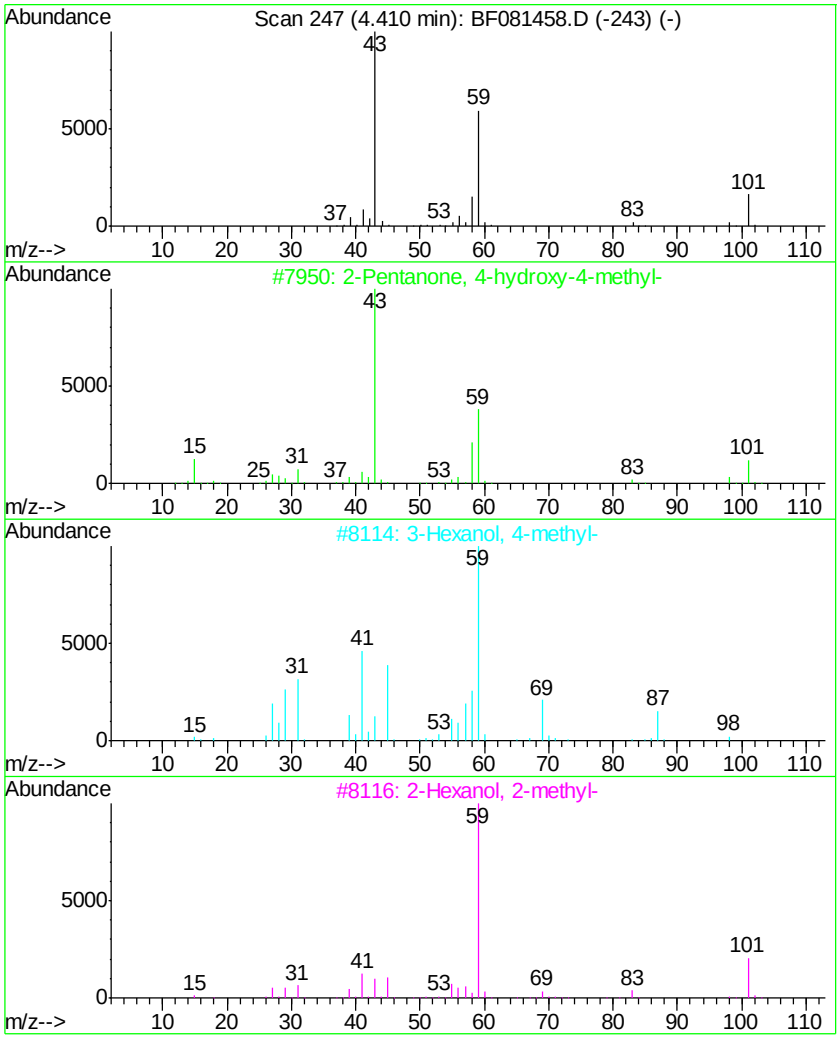
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

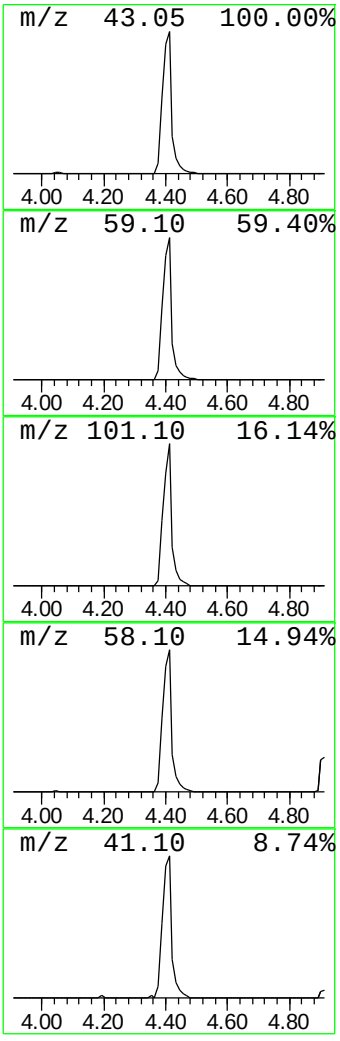
**********

Peak Number 1 unknown4.41 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.41 | 65.76 ng | 1168470 | 1,4-Dichlorobenzene-d4 | 6.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 40 |
| 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 | 23 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DUP-X

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

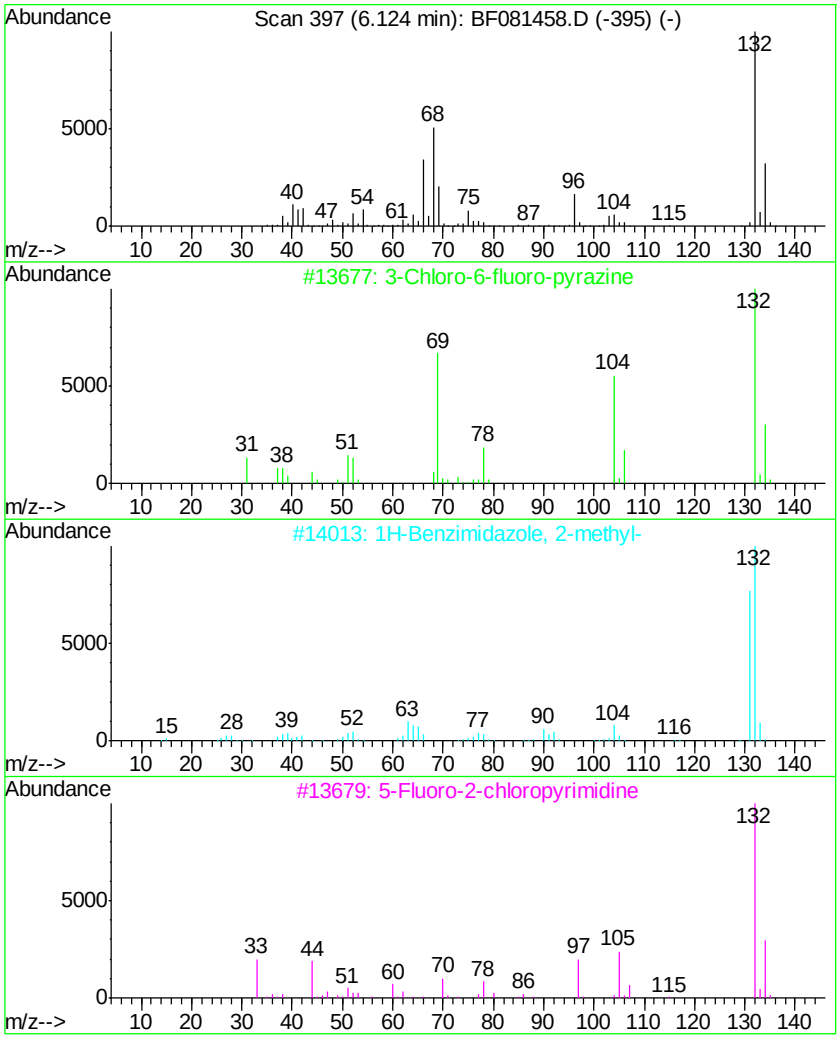
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

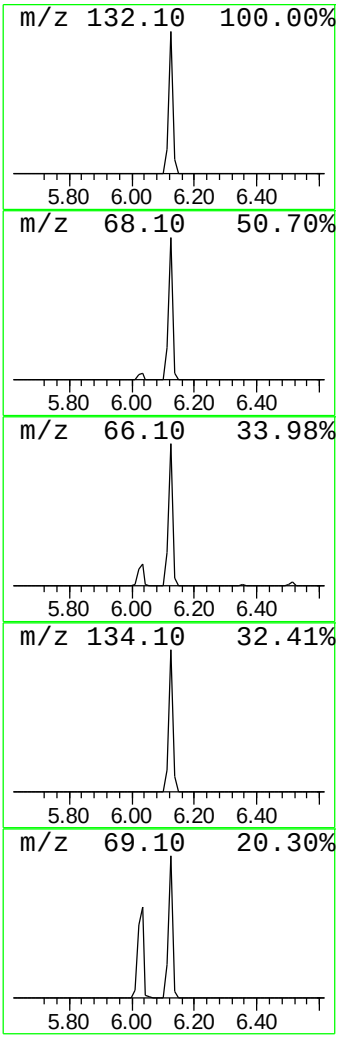
**********

Peak Number 2 unknown6.12 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.12 | 93.53 ng | 1661980 | 1,4-Dichlorobenzene-d4 | 6.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 4 | (5-METHYL-2-PYRIDYL)ACETONITRILE | 132 | C8H8N2 | 1000241-93-9 | 10 |
| 5 | 2-Cyclohexen-1-one | 96 | C6H8O | 000930-68-7 | 10 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DUP-X

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

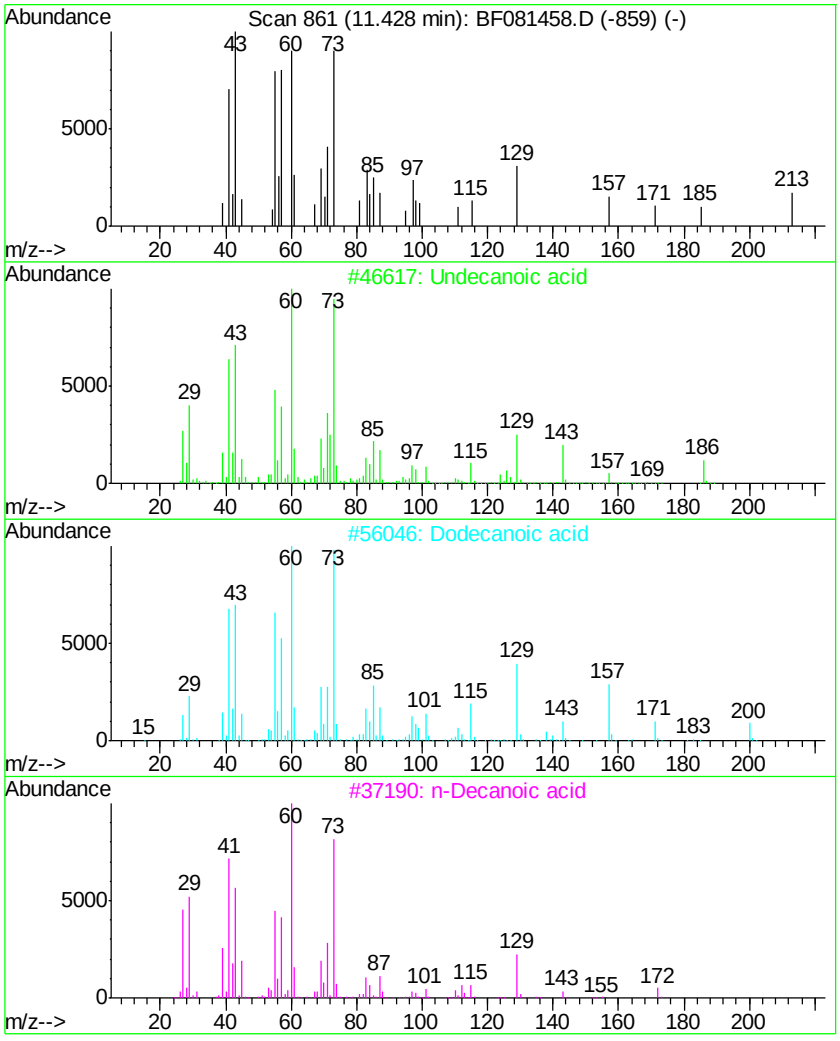
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

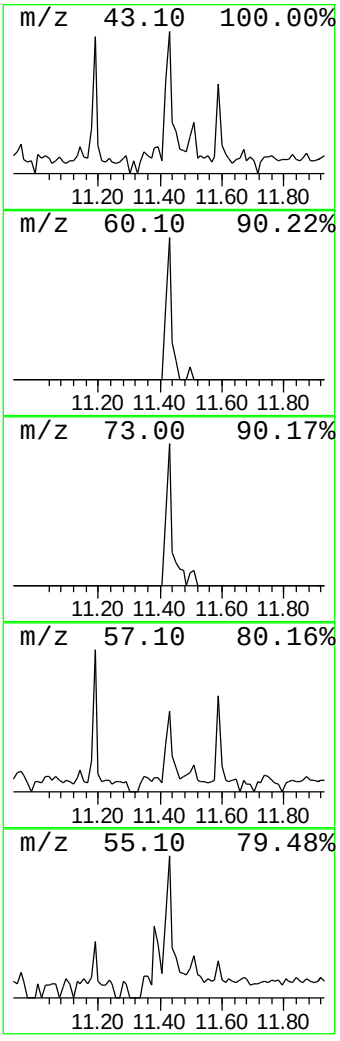
**********

Peak Number 4 Undecanoic acid Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.43 | 2.06 ng | 48184 | Phenanthrene-d10 | 10.84 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 59 |
| 2 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 53 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |
| 4 | Butyraldehyde, semicarbazone | 129 | C5H11N3O | 013183-21-6 | 50 |
| 5 | .alpha.-D-Glucopyranoside, O-.al... | 504 | C18H32O16 | 000597-12-6 | 38 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DUP-X

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

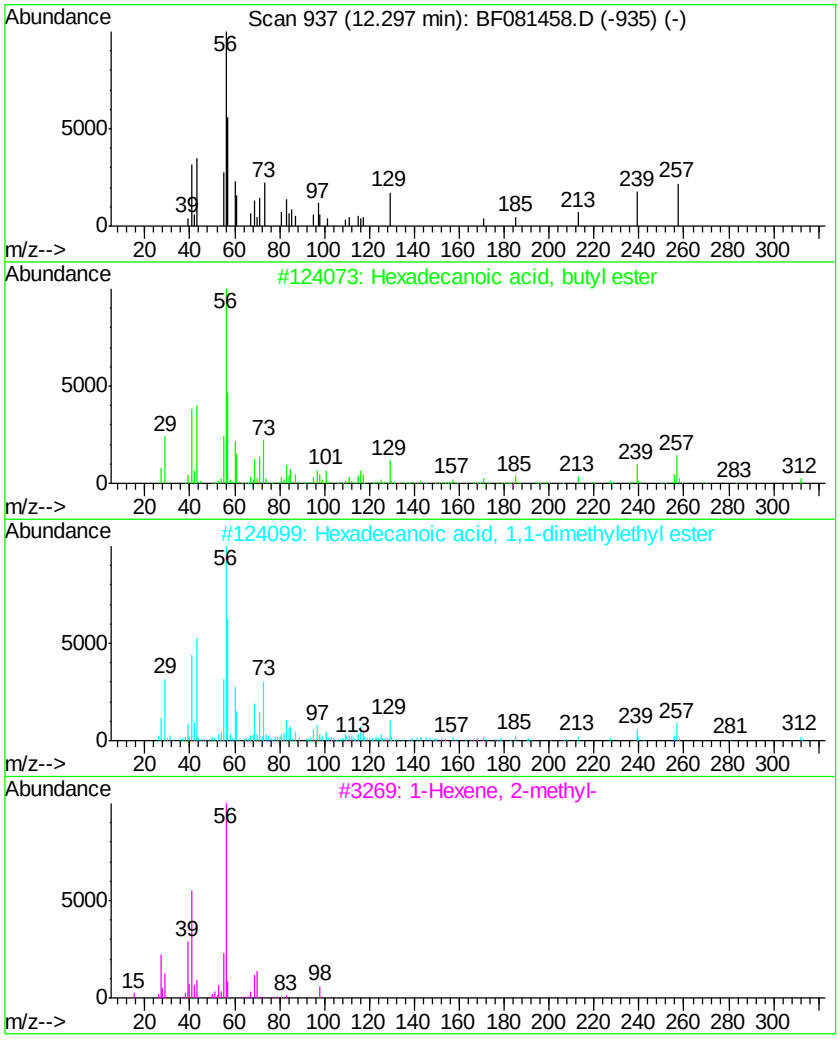
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

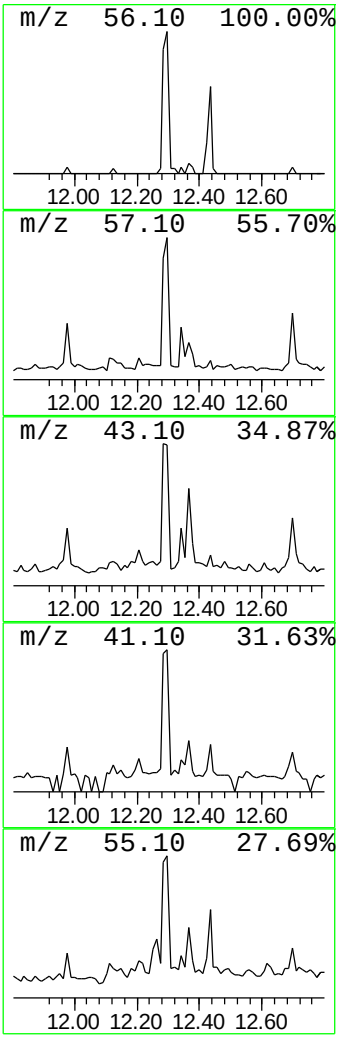
**********

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.30 | 2.81 ng | 58667 | Chrysene-d12 | 13.45 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 86 |
| 2 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 43 |
| 3 | 1-Hexene, 2-methyl- | 98 | C7H14 | 006094-02-6 | 27 |
| 4 | Cyclobutane, 1-hexyl-2,3-dimethyl- | 168 | C12H24 | 055170-84-8 | 25 |
| 5 | Pentadecane, 8-methylene- | 224 | C16H32 | 055668-09-2 | 25 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DUP-X

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

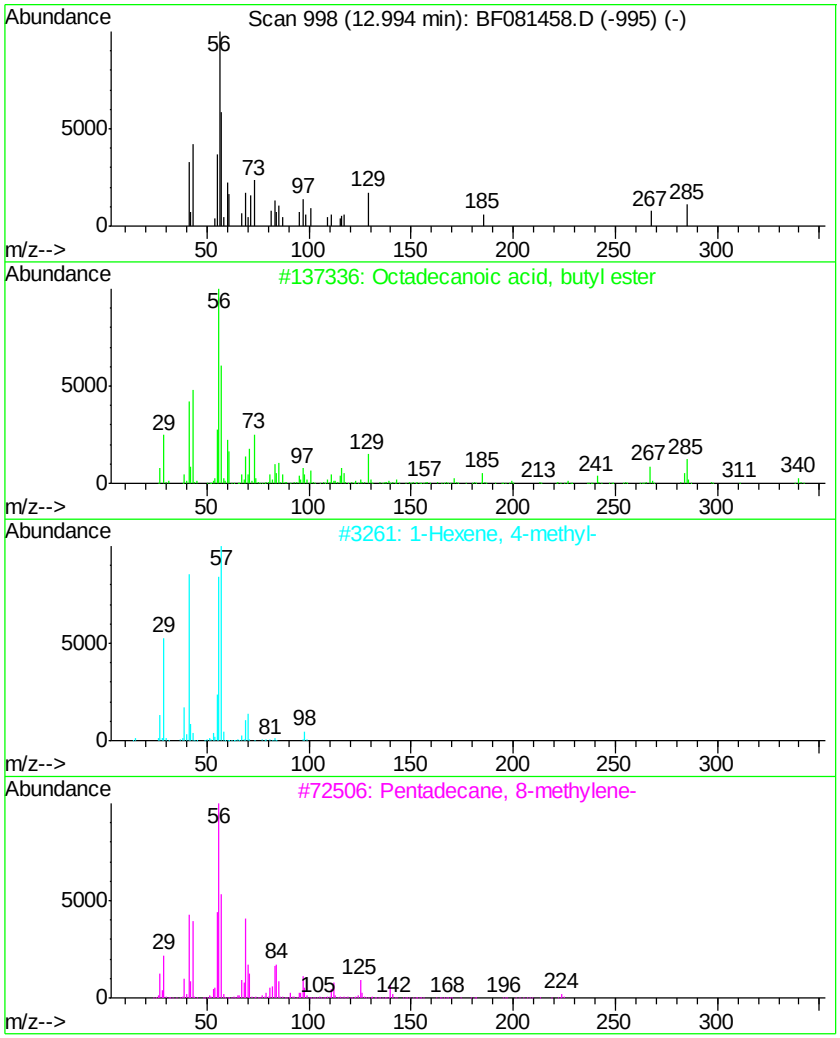
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

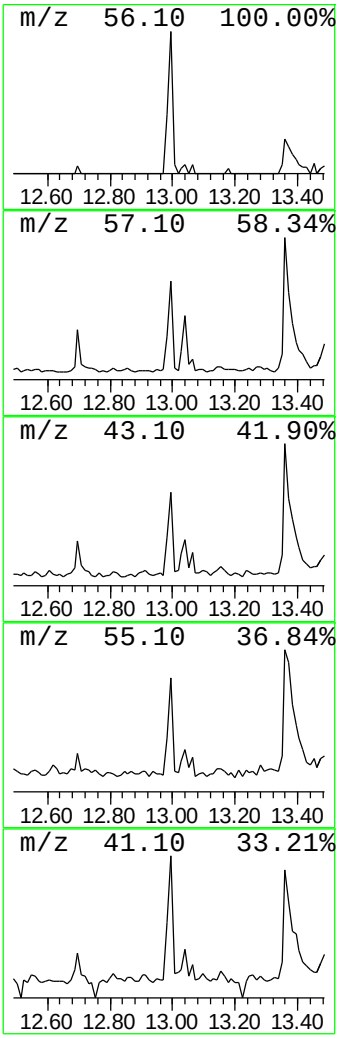
**********

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.99 | 2.02 ng | 42179 | Chrysene-d12 | 13.45 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid, butyl ester | 340 | C22H44O2 | 000123-95-5 | 90 |
| 2 | 1-Hexene, 4-methyl- | 98 | C7H14 | 003769-23-1 | 38 |
| 3 | Pentadecane, 8-methylene- | 224 | C16H32 | 055668-09-2 | 37 |
| 4 | 1-Pentene, 2,4-dimethyl- | 98 | C7H14 | 002213-32-3 | 35 |
| 5 | Cyclobutane, 1-hexyl-2,3-dimethyl- | 168 | C12H24 | 055170-84-8 | 32 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DUP-X

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

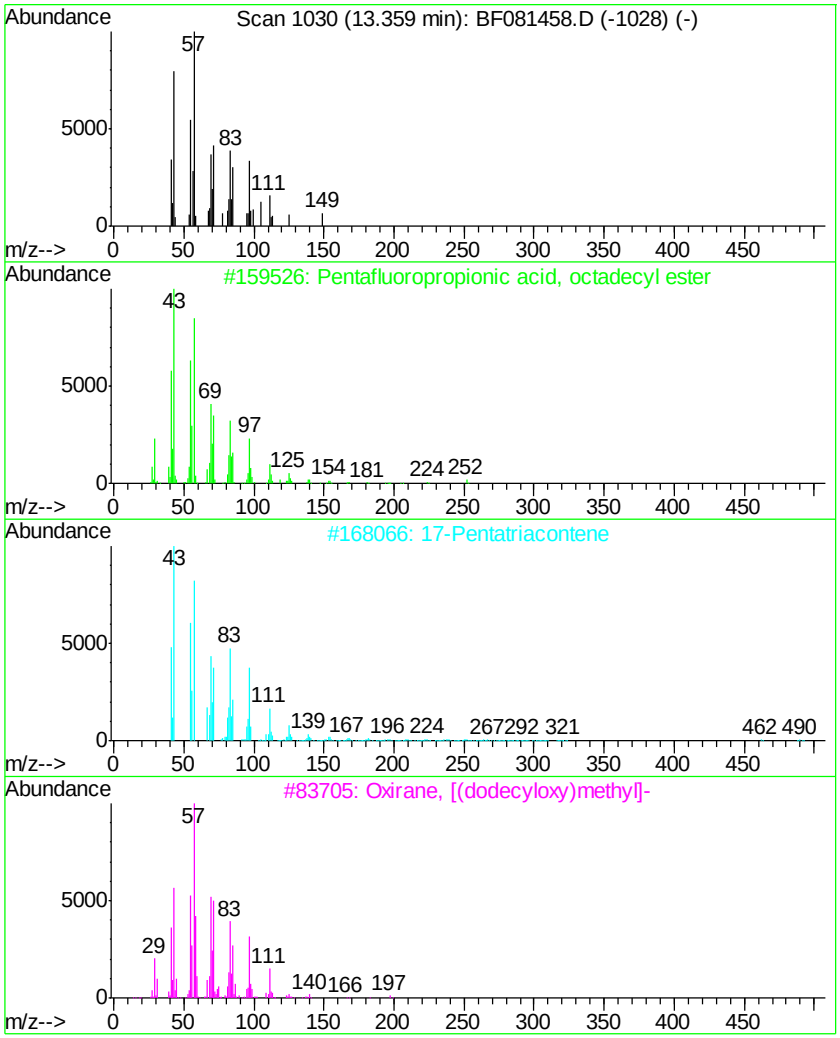
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

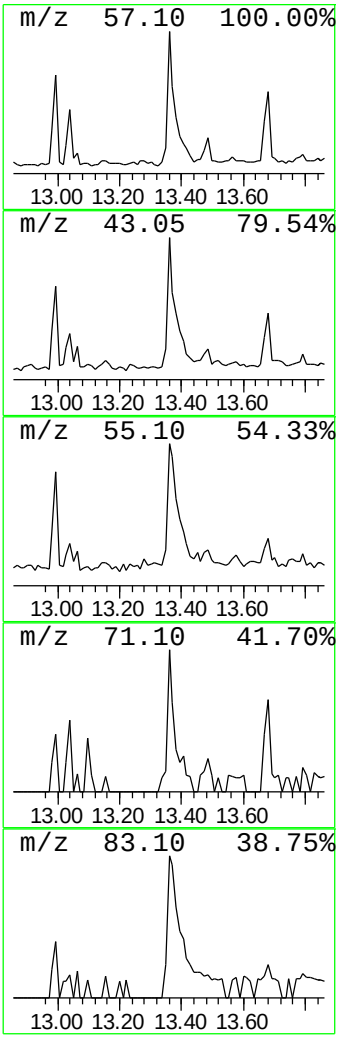
**********

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.36 | 4.59 ng | 95888 | Chrysene-d12 | 13.45 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2 | 1000280-07-7 | 87 |
| 2 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 83 |
| 3 | Oxirane, [(dodecyloxy)methyl]- | 242 | C15H30O2 | 002461-18-9 | 83 |
| 4 | Oxirane, [(hexadecyloxy)methyl]- | 298 | C19H38O2 | 015965-99-8 | 72 |
| 5 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 68 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DUP-X

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

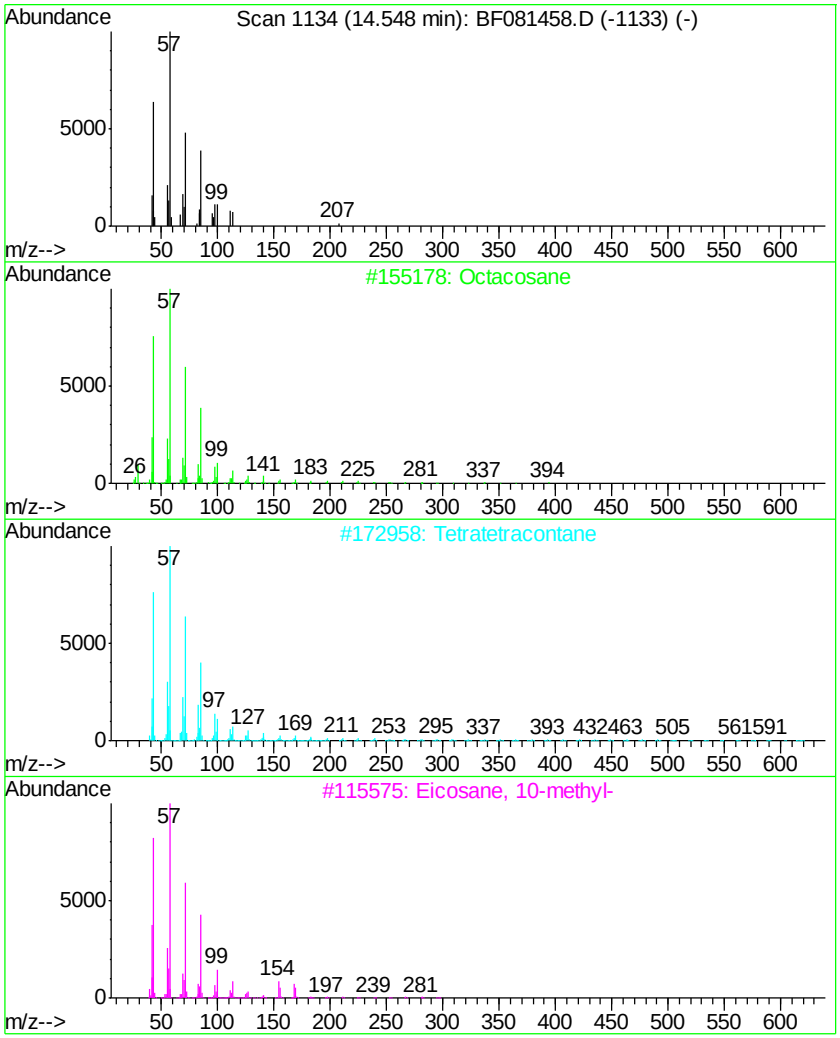
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

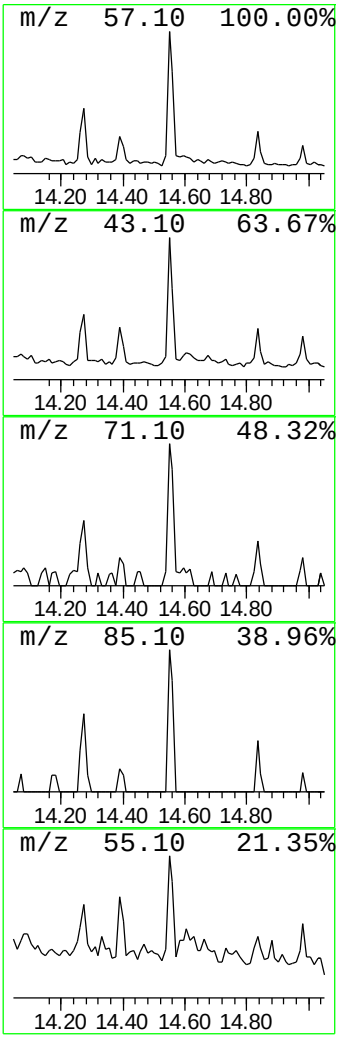
**********

Peak Number 9 Octacosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.55 | 2.64 ng | 32634 | Perylene-d12 | 14.77 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 86 |
| 2 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 86 |
| 3 | Eicosane, 10-methyl- | 296 | C21H44 | 054833-23-7 | 86 |
| 4 | Heptacosane | 380 | C27H56 | 000593-49-7 | 80 |
| 5 | 10-Methylnonadecane | 282 | C20H42 | 056862-62-5 | 80 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081458.D
Acq On : 5 Sep 2015 11:43
Operator : UM/IZ
Sample : G3511-21
Misc :
ALS Vial : 37 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** DUP-X

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 |
| unknown4.41 | 4.41 | 65.8 | ng | 1168470 | 1 | 6.35 | 355386 | 20.0 |
| unknown6.12 | 6.12 | 93.5 | ng | 1661980 | 1 | 6.35 | 355386 | 20.0 |
| Undecanoic acid | 11.43 | 2.1 | ng | 48184 | 4 | 10.84 | 467953 | 20.0 |
| Hexadecanoic acid... | 12.30 | 2.8 | ng | 58667 | 5 | 13.45 | 418209 | 20.0 |
| Octadecanoic acid... | 12.99 | 2.0 | ng | 42179 | 5 | 13.45 | 418209 | 20.0 |
| Pentafluoropropio... | 13.36 | 4.6 | ng | 95888 | 5 | 13.45 | 418209 | 20.0 |
| Octacosane | 14.55 | 2.6 | ng | 32634 | 6 | 14.77 | 247384 | 20.0 |