LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020117\
Data File : BF092725.D
Acq On : 2 Feb 2017 2:09
Operator : SJ/MA
Sample : I1615-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-3

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-BF013017.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 | 5.127 | 264 | 266 | 269 | rBV | 1256881 | 1840778 | 45.43% | 5.213% |
| 2 | 5.562 | 301 | 304 | 306 | rBV | 3010612 | 3836001 | 94.67% | 10.863% |
| 3 | 6.213 | 359 | 361 | 363 | rBV | 398130 | 341628 | 8.43% | 0.967% |
| 4 | 6.579 | 390 | 393 | 396 | rBV | 2678878 | 4052004 | 100.00% | 11.475% |
| 5 | 6.716 | 402 | 405 | 407 | rBV | 3767632 | 3733996 | 92.15% | 10.574% |
| 6 | 6.945 | 423 | 425 | 427 | rBV | 1159107 | 991380 | 24.47% | 2.808% |
| 7 | 7.105 | 436 | 439 | 441 | rBV | 2766651 | 2922622 | 72.13% | 8.277% |
| 8 | 7.505 | 471 | 474 | 477 | rBV | 1728250 | 2507669 | 61.89% | 7.102% |
| 9 | 8.236 | 535 | 538 | 540 | rBV | 1351967 | 1302766 | 32.15% | 3.689% |
| 10 | 9.310 | 629 | 632 | 635 | rBV | 3360085 | 3596623 | 88.76% | 10.185% |
| 11 | 9.631 | 657 | 660 | 661 | rBV | 95926 | 100839 | 2.49% | 0.286% |
| 12 | 9.711 | 664 | 667 | 669 | rBV | 339151 | 314066 | 7.75% | 0.889% |
| 13 | 9.996 | 690 | 692 | 694 | rVB | 1576057 | 1402571 | 34.61% | 3.972% |
| 14 | 10.419 | 725 | 729 | 731 | rVB | 99760 | 105120 | 2.59% | 0.298% |
| 15 | 10.648 | 746 | 749 | 752 | rBV | 28728 | 53080 | 1.31% | 0.150% |
| 16 | 10.785 | 758 | 761 | 764 | rBV | 1939629 | 1983102 | 48.94% | 5.616% |
| 17 | 10.899 | 769 | 771 | 774 | rBV | 99334 | 133320 | 3.29% | 0.378% |
| 18 | 11.345 | 808 | 810 | 811 | rBV | 101329 | 82776 | 2.04% | 0.234% |
| 19 | 11.482 | 820 | 822 | 825 | rBV | 1287584 | 1134379 | 28.00% | 3.212% |
| 20 | 12.888 | 942 | 945 | 946 | rBV | 61974 | 60587 | 1.50% | 0.172% |
| 21 | 12.922 | 946 | 948 | 950 | rVB | 42689 | 40660 | 1.00% | 0.115% |
| 22 | 13.071 | 958 | 961 | 963 | rBV | 3005872 | 2850949 | 70.36% | 8.074% |
| 23 | 13.585 | 1005 | 1006 | 1008 | rVB | 47526 | 44489 | 1.10% | 0.126% |
| 24 | 14.122 | 1050 | 1053 | 1055 | rBV | 777677 | 853670 | 21.07% | 2.418% |
| 25 | 14.774 | 1108 | 1110 | 1115 | rBV | 104304 | 126606 | 3.12% | 0.359% |
| 26 | 15.585 | 1178 | 1181 | 1187 | rBV | 587217 | 788404 | 19.46% | 2.233% |
| 27 | 16.043 | 1217 | 1221 | 1224 | rBV | 28110 | 47994 | 1.18% | 0.136% |
| 28 | 16.557 | 1261 | 1266 | 1272 | rBV2 | 23049 | 63607 | 1.57% | 0.180% |

Sum of corrected areas: 35311686

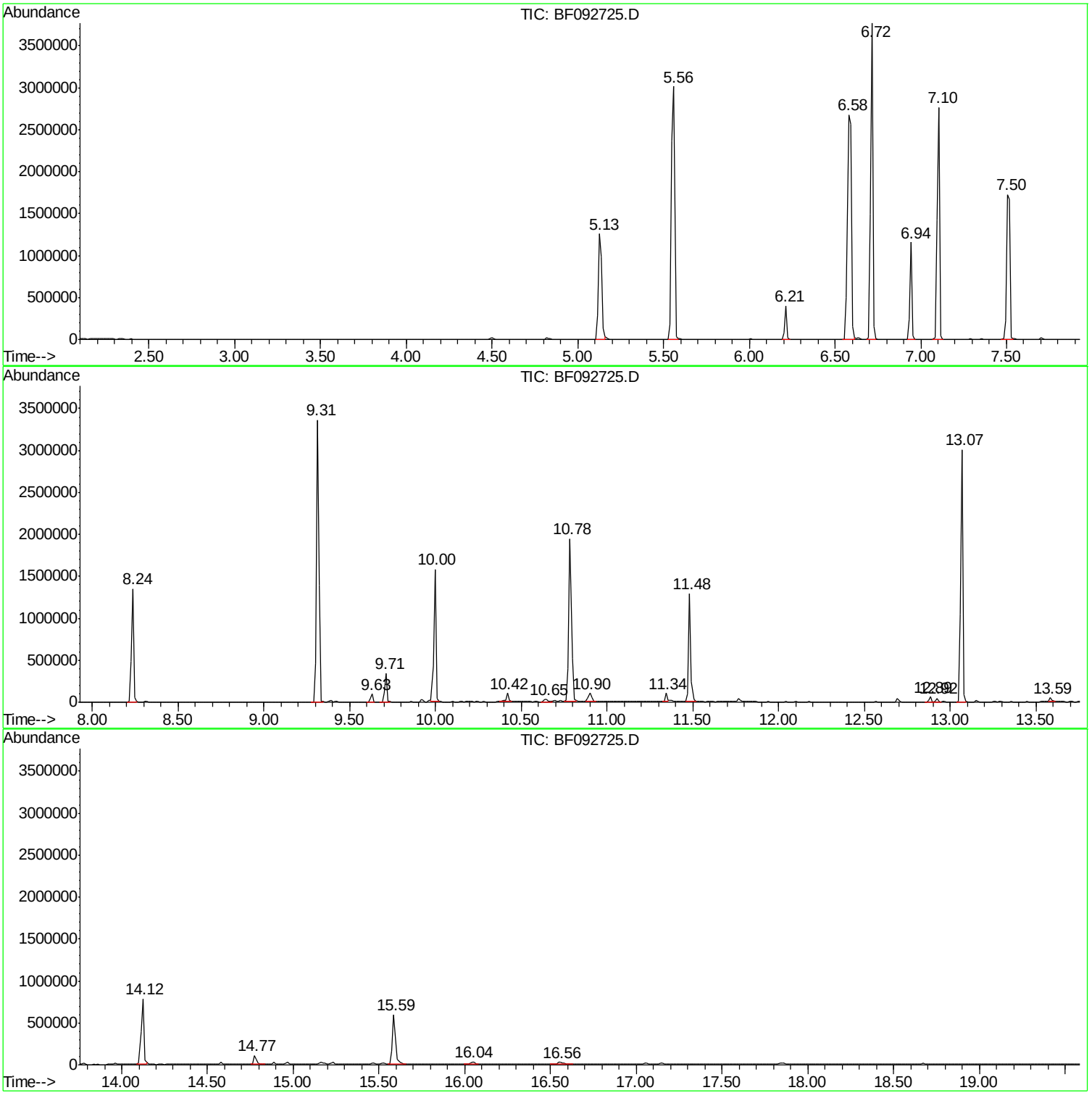
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020117\
Data File : BF092725.D
Acq On : 2 Feb 2017 2:09
Operator : SJ/MA
Sample : I1615-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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\BF020117\
Data File : BF092725.D
Acq On : 2 Feb 2017 2:09
Operator : SJ/MA
Sample : I1615-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

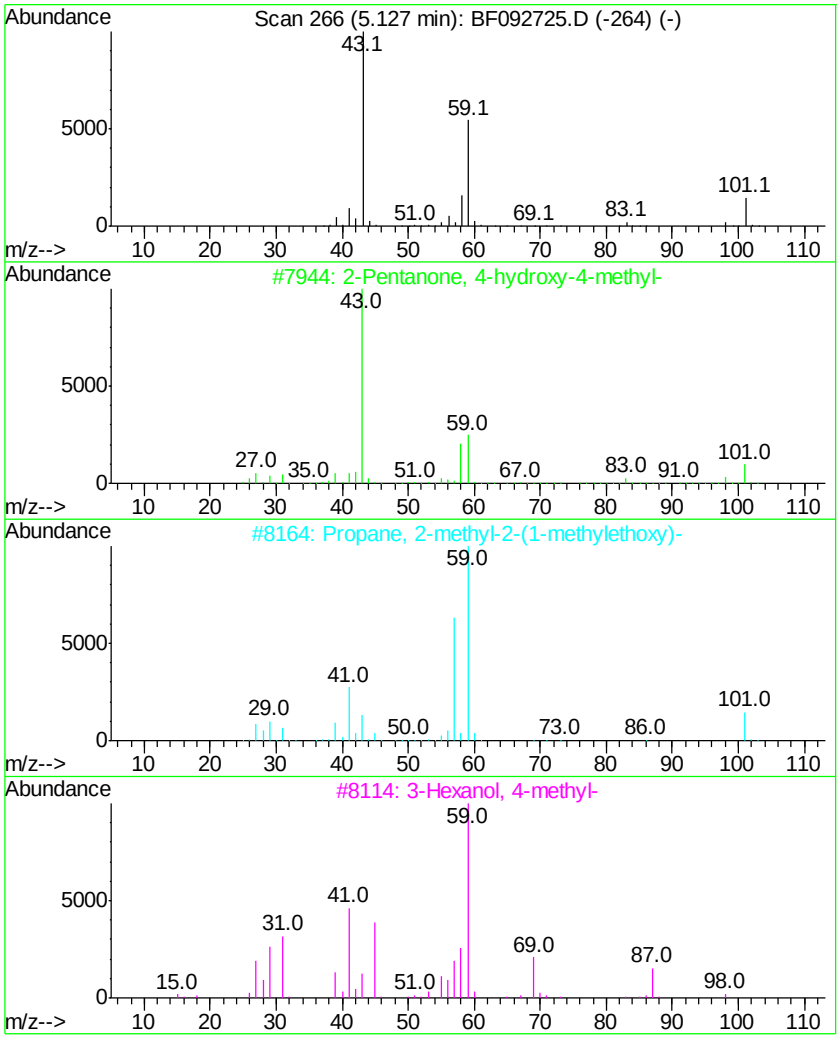
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

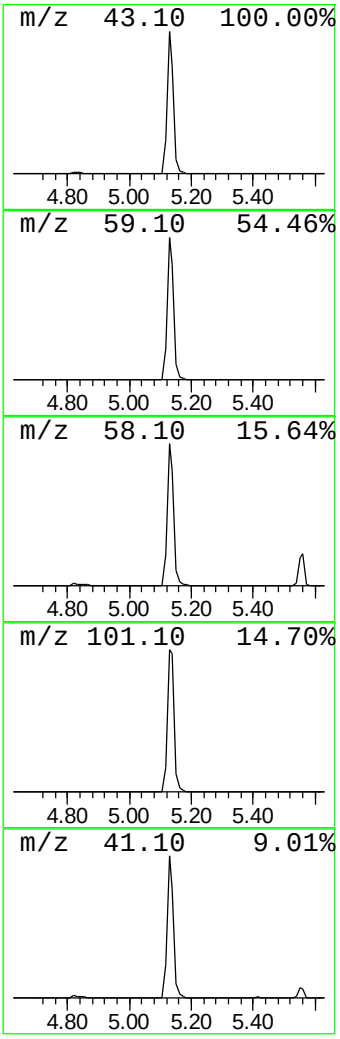
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.13 | 37.14 ng | 1840780 | 1,4-Dichlorobenzene-d4 | 6.94 |

| 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 | 42 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 4 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 32 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020117\
Data File : BF092725.D
Acq On : 2 Feb 2017 2:09
Operator : SJ/MA
Sample : I1615-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

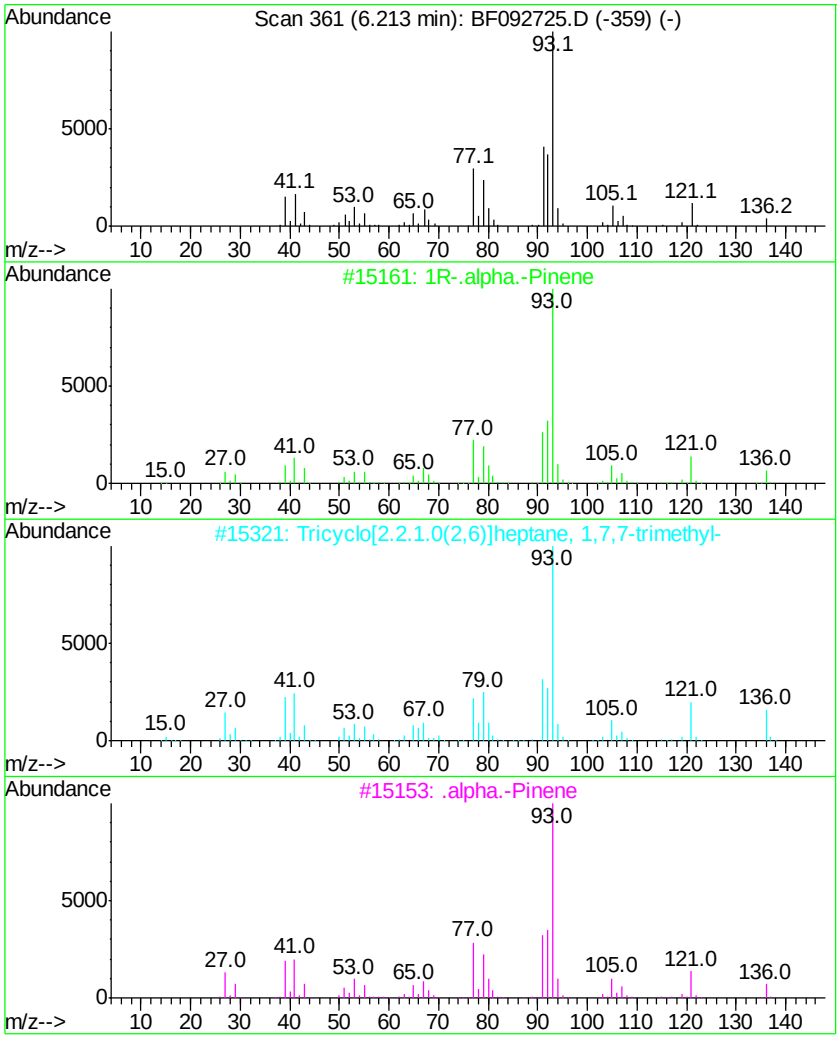
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

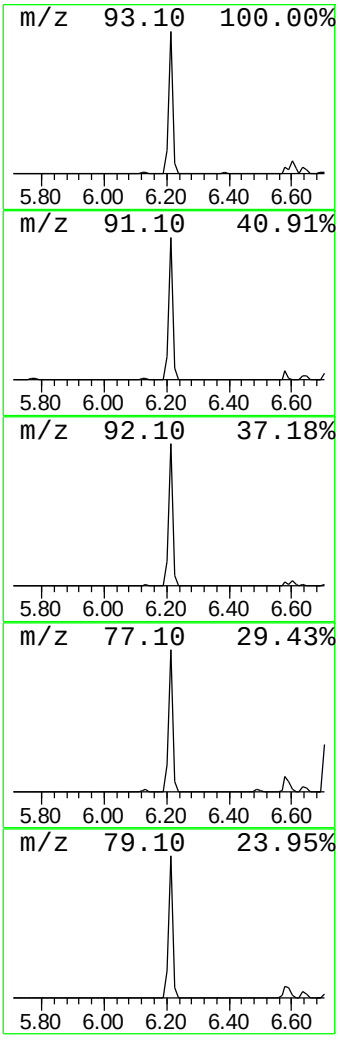
**********

Peak Number 2 1R-.alpha.-Pinene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.21 | 6.89 ng | 341628 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1R-.alpha.-Pinene | 136 | C10H16 | 007785-70-8 | 94 |
| 2 | Tricyclo[2.2.1.0(2,6)]heptane, 1... | 136 | C10H16 | 000508-32-7 | 91 |
| 3 | .alpha.-Pinene | 136 | C10H16 | 000080-56-8 | 91 |
| 4 | Bicyclo[3.1.1]hept-2-ene, 3,6,6-... | 136 | C10H16 | 004889-83-2 | 91 |
| 5 | Cyclohexene, 4-methylene-1-(1-me... | 136 | C10H16 | 000099-84-3 | 87 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020117\
Data File : BF092725.D
Acq On : 2 Feb 2017 2:09
Operator : SJ/MA
Sample : I1615-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

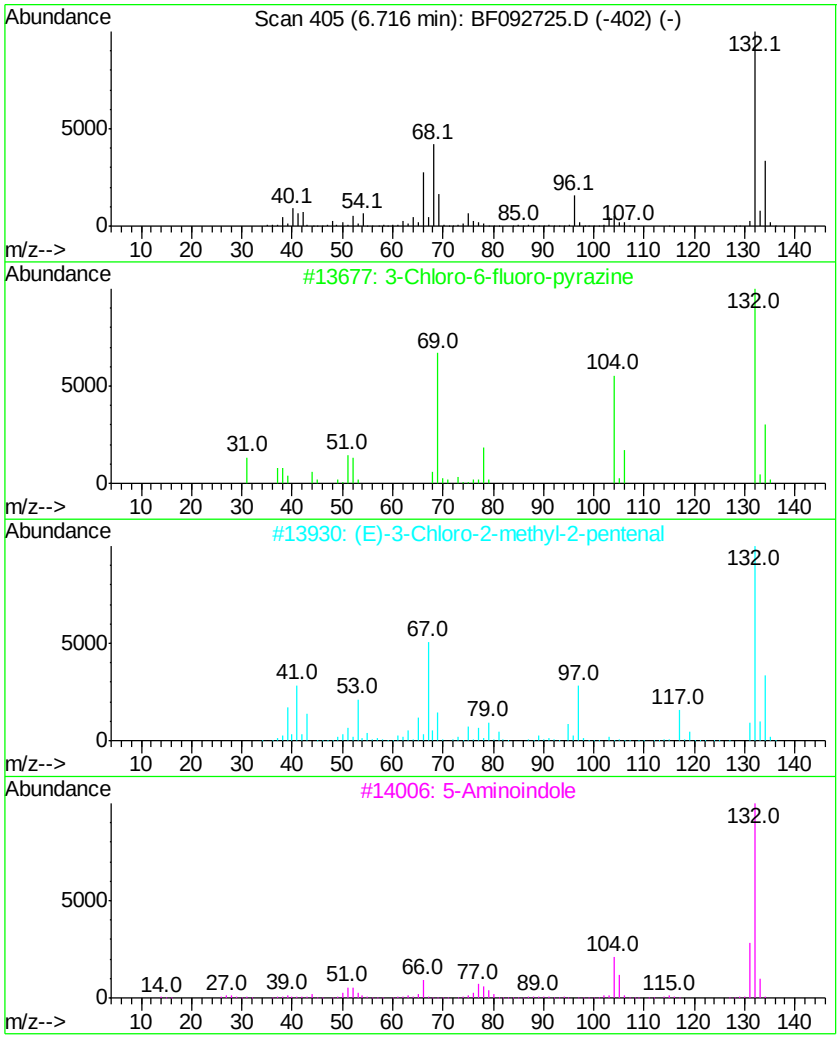
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

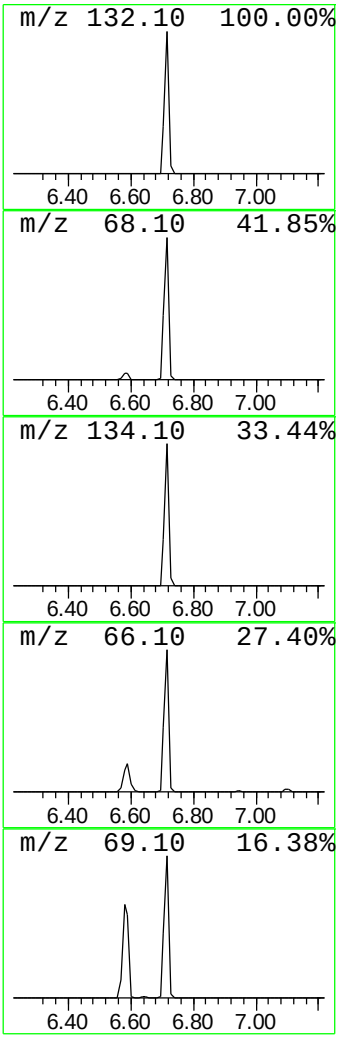
**********

Peak Number 3 unknown6.72 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.72 | 75.33 ng | 3734000 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020117\
Data File : BF092725.D
Acq On : 2 Feb 2017 2:09
Operator : SJ/MA
Sample : I1615-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

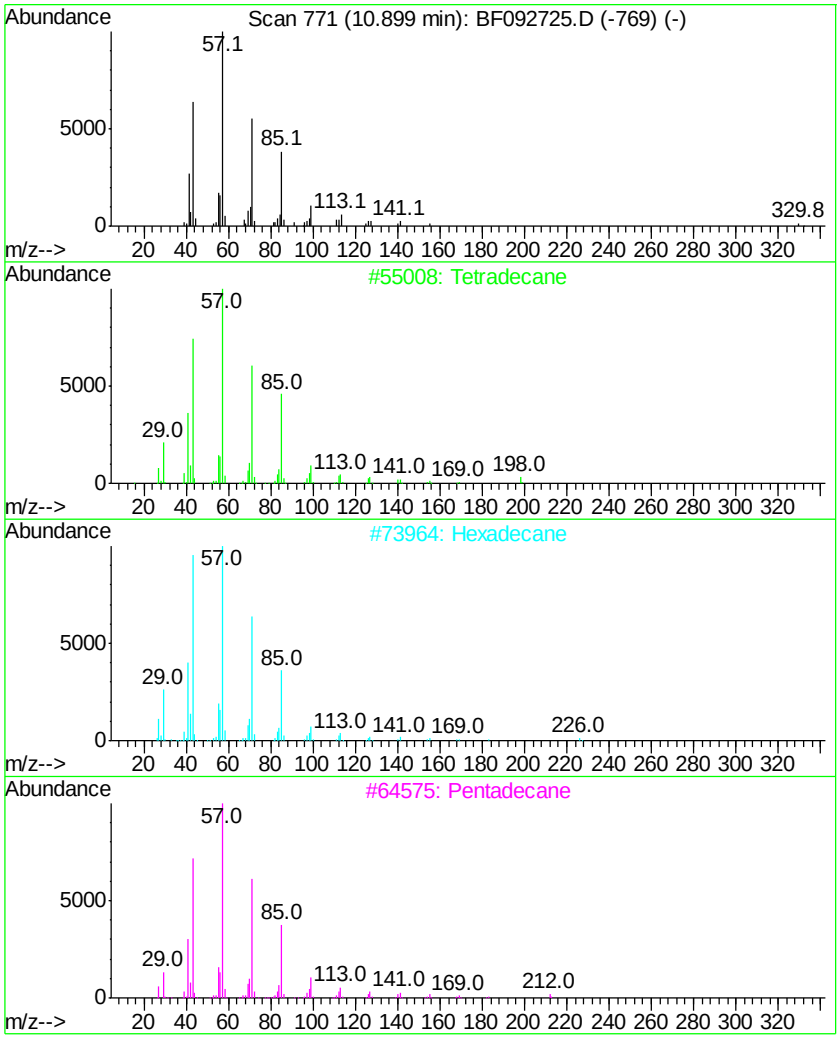
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

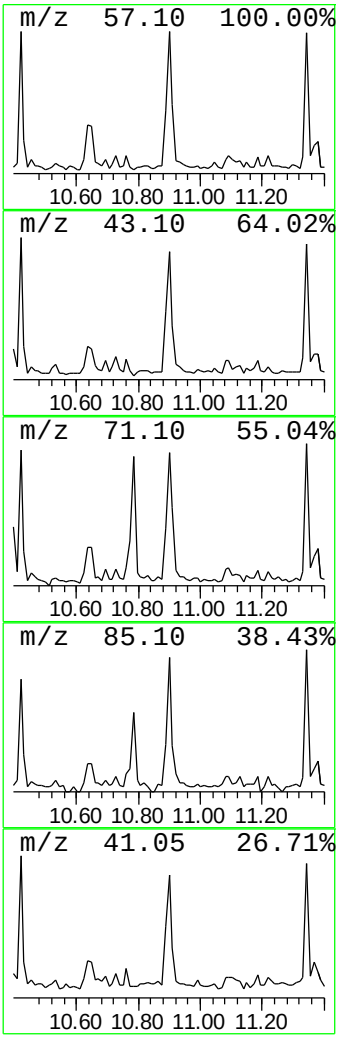
**********

Peak Number 5 Tetradecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.90 | 2.35 ng | 133320 | Phenanthrene-d10 | 11.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecane | 198 | C14H30 | 000629-59-4 | 91 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 90 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |
| 5 | Tridecane | 184 | C13H28 | 000629-50-5 | 90 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020117\
Data File : BF092725.D
Acq On : 2 Feb 2017 2:09
Operator : SJ/MA
Sample : I1615-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

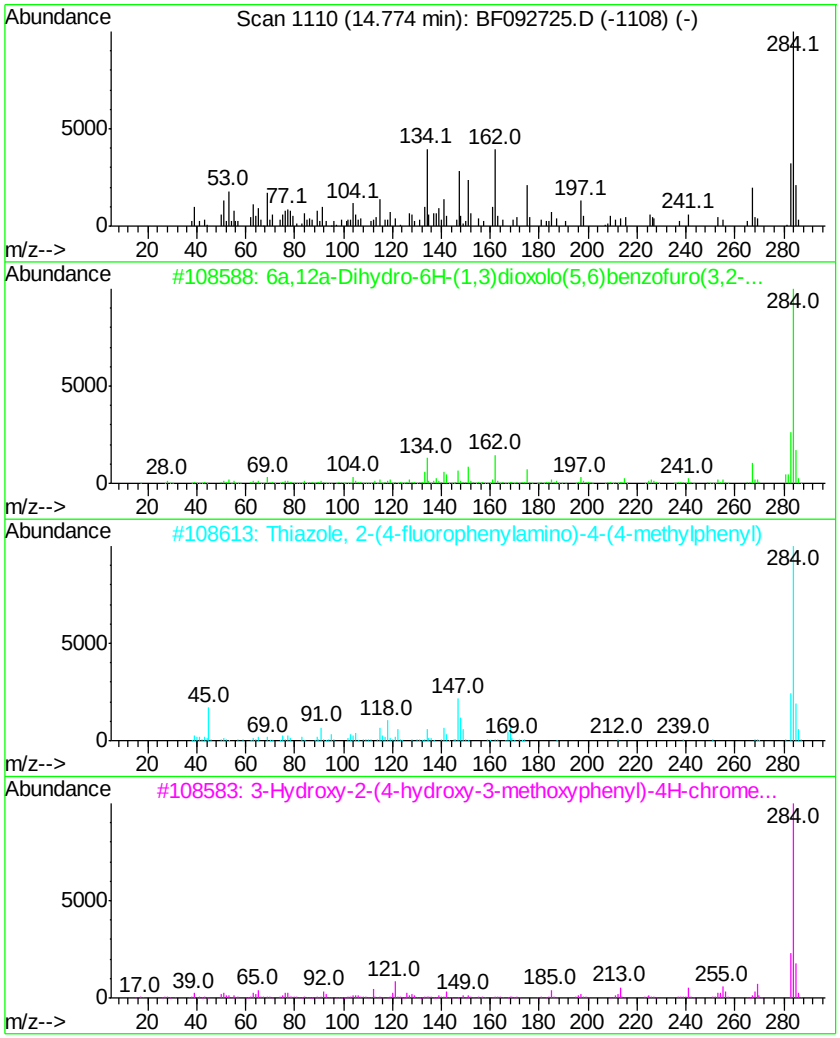
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

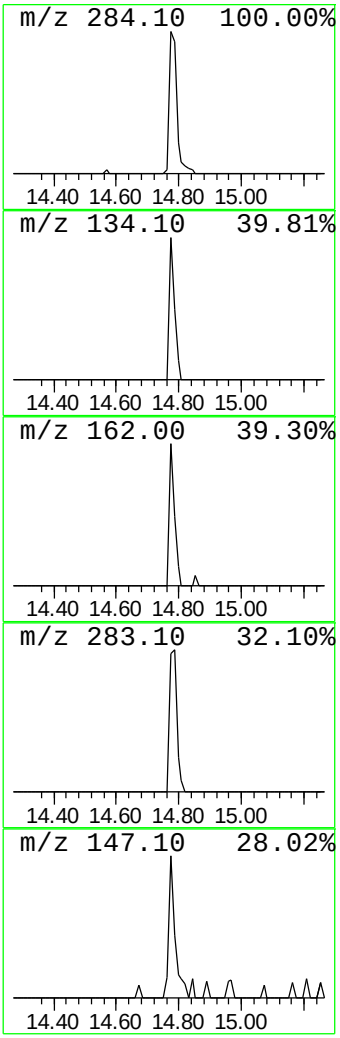
**********

Peak Number 6 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.77 | 2.97 ng | 126606 | Chrysene-d12 | 14.12 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6a,12a-Dihydro-6H-(1,3)dioxolo(5... | 284 | C16H12O5 | 022091-18-5 | 94 |
| 2 | Thiazole, 2-(4-fluorophenylamino... | 284 | C16H13FN2S | 340801-58-3 | 43 |
| 3 | 3-Hydroxy-2-(4-hydroxy-3-methoxy... | 284 | C16H12O5 | 159184-95-9 | 41 |
| 4 | Methanethione, bis[4-(dimethylam... | 284 | C17H20N2S | 001226-46-6 | 38 |
| 5 | 6H-Benzofuro[3,2-c][1]benzopyran... | 284 | C17H16O4 | 000606-91-7 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020117\
Data File : BF092725.D
Acq On : 2 Feb 2017 2:09
Operator : SJ/MA
Sample : I1615-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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... | 5.13 | 37.1 | ng | 1840780 | 1 | 6.94 | 991380 | 20.0 |
| 1R-.alpha.-Pinene | 6.21 | 6.9 | ng | 341628 | 1 | 6.94 | 991380 | 20.0 |
| unknown6.72 | 6.72 | 75.3 | ng | 3734000 | 1 | 6.94 | 991380 | 20.0 |
| Tetradecane | 10.90 | 2.4 | ng | 133320 | 4 | 11.48 | 1134380 | 20.0 |
| 6a,12a-Dihydro-6H... | 14.77 | 3.0 | ng | 126606 | 5 | 14.12 | 853670 | 20.0 |