LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099521.D
Acq On : 15 Oct 2017 18:46
Operator : SJ/JU
Sample : I5813-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** OK-03-101117

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-BF092317.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 | 5.057 | 503 | 505 | 517 | rBV | 23511 | 29353 | 5.43% | 0.553% |
| 2 | 5.463 | 571 | 574 | 596 | rBB | 182148 | 207717 | 38.43% | 3.914% |
| 3 | 6.475 | 743 | 746 | 759 | rBV | 186361 | 206855 | 38.27% | 3.897% |
| 4 | 6.616 | 766 | 770 | 780 | rVB | 256056 | 223380 | 41.33% | 4.209% |
| 5 | 6.845 | 805 | 809 | 819 | rBB | 505486 | 446927 | 82.69% | 8.421% |
| 6 | 6.998 | 832 | 835 | 846 | rBB | 211605 | 175413 | 32.45% | 3.305% |
| 7 | 7.404 | 901 | 904 | 916 | rBV | 105409 | 112883 | 20.88% | 2.127% |
| 8 | 8.122 | 1023 | 1026 | 1033 | rBV | 583477 | 540500 | 100.00% | 10.184% |
| 9 | 8.680 | 1119 | 1121 | 1128 | rBB | 9739 | 10101 | 1.87% | 0.190% |
| 10 | 9.198 | 1205 | 1209 | 1216 | rBV | 246233 | 203864 | 37.72% | 3.841% |
| 11 | 9.592 | 1269 | 1276 | 1282 | rBV | 27983 | 26541 | 4.91% | 0.500% |
| 12 | 9.880 | 1321 | 1325 | 1333 | rVB | 561641 | 471743 | 87.28% | 8.888% |
| 13 | 10.298 | 1394 | 1396 | 1398 | rVB | 10516 | 7540 | 1.40% | 0.142% |
| 14 | 10.516 | 1429 | 1433 | 1439 | rBV5 | 6441 | 11740 | 2.17% | 0.221% |
| 15 | 10.592 | 1443 | 1446 | 1451 | rVB | 43458 | 37504 | 6.94% | 0.707% |
| 16 | 10.669 | 1456 | 1459 | 1463 | rBV | 83165 | 73416 | 13.58% | 1.383% |
| 17 | 10.769 | 1474 | 1476 | 1478 | rBV | 18094 | 19379 | 3.59% | 0.365% |
| 18 | 11.092 | 1528 | 1531 | 1533 | rBV4 | 5042 | 6224 | 1.15% | 0.117% |
| 19 | 11.216 | 1547 | 1552 | 1555 | rBV | 23367 | 25123 | 4.65% | 0.473% |
| 20 | 11.245 | 1555 | 1557 | 1560 | rVV2 | 17227 | 14911 | 2.76% | 0.281% |
| 21 | 11.369 | 1574 | 1578 | 1581 | rBV | 497227 | 411565 | 76.15% | 7.755% |
| 22 | 11.392 | 1581 | 1582 | 1585 | rVB | 16164 | 9902 | 1.83% | 0.187% |
| 23 | 11.469 | 1592 | 1595 | 1596 | rBV3 | 6989 | 7115 | 1.32% | 0.134% |
| 24 | 11.527 | 1602 | 1605 | 1608 | rBV5 | 8161 | 10667 | 1.97% | 0.201% |
| 25 | 11.598 | 1614 | 1617 | 1620 | rBV4 | 11089 | 10523 | 1.95% | 0.198% |
| 26 | 11.645 | 1621 | 1625 | 1628 | rVB | 37385 | 32171 | 5.95% | 0.606% |
| 27 | 11.704 | 1631 | 1635 | 1639 | rVV5 | 12731 | 15525 | 2.87% | 0.293% |
| 28 | 11.745 | 1639 | 1642 | 1644 | rVB4 | 6353 | 7411 | 1.37% | 0.140% |
| 29 | 11.786 | 1644 | 1649 | 1650 | rBV5 | 8087 | 10316 | 1.91% | 0.194% |
| 30 | 11.874 | 1661 | 1664 | 1665 | rBV2 | 9903 | 11128 | 2.06% | 0.210% |
| 31 | 11.980 | 1680 | 1682 | 1684 | rBV | 8909 | 7086 | 1.31% | 0.134% |
| 32 | 12.051 | 1692 | 1694 | 1697 | rBV | 40325 | 31266 | 5.78% | 0.589% |
| 33 | 12.298 | 1734 | 1736 | 1740 | rVB4 | 9644 | 8962 | 1.66% | 0.169% |
| 34 | 12.345 | 1740 | 1744 | 1746 | rBV5 | 10217 | 13701 | 2.53% | 0.258% |

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099521.D
Acq On : 15 Oct 2017 18:46
Operator : SJ/JU
Sample : I5813-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** OK-03-101117

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 12.421 | 1754 | 1757 | 1758 | rBV | 20814 | 21024 | 3.89% | 0.396% |
| 36 | 12.439 | 1758 | 1760 | 1765 | rVB2 | 61003 | 61835 | 11.44% | 1.165% |
| 37 | 12.539 | 1775 | 1777 | 1780 | rVB4 | 18659 | 17020 | 3.15% | 0.321% |
| 38 | 12.586 | 1782 | 1785 | 1788 | rBV | 22724 | 22718 | 4.20% | 0.428% |
| 39 | 12.680 | 1799 | 1801 | 1804 | rVB4 | 9635 | 7676 | 1.42% | 0.145% |
| 40 | 12.757 | 1812 | 1814 | 1817 | rVB4 | 14751 | 15472 | 2.86% | 0.292% |
| 41 | 12.810 | 1821 | 1823 | 1830 | rVV3 | 62080 | 70653 | 13.07% | 1.331% |
| 42 | 12.868 | 1830 | 1833 | 1835 | rVV3 | 15406 | 12746 | 2.36% | 0.240% |
| 43 | 12.921 | 1840 | 1842 | 1843 | rBV2 | 16750 | 11228 | 2.08% | 0.212% |
| 44 | 12.945 | 1843 | 1846 | 1850 | rVV | 198176 | 176529 | 32.66% | 3.326% |
| 45 | 13.168 | 1881 | 1884 | 1886 | rBV | 51490 | 46773 | 8.65% | 0.881% |
| 46 | 13.386 | 1919 | 1921 | 1924 | rVB3 | 23493 | 21889 | 4.05% | 0.412% |
| 47 | 13.510 | 1939 | 1942 | 1946 | rBV | 52048 | 47849 | 8.85% | 0.902% |
| 48 | 13.839 | 1995 | 1998 | 2001 | rBV | 62570 | 55329 | 10.24% | 1.042% |
| 49 | 14.010 | 2024 | 2027 | 2031 | rBV | 518823 | 499834 | 92.48% | 9.418% |
| 50 | 14.151 | 2049 | 2051 | 2054 | rBV | 51986 | 45409 | 8.40% | 0.856% |
| 51 | 14.457 | 2101 | 2103 | 2108 | rBV | 62034 | 53847 | 9.96% | 1.015% |
| 52 | 14.762 | 2152 | 2155 | 2159 | rBV | 56643 | 52663 | 9.74% | 0.992% |
| 53 | 15.098 | 2209 | 2212 | 2220 | rVB | 79627 | 113528 | 21.00% | 2.139% |
| 54 | 15.486 | 2272 | 2278 | 2282 | rBV | 378275 | 514955 | 95.27% | 9.703% |

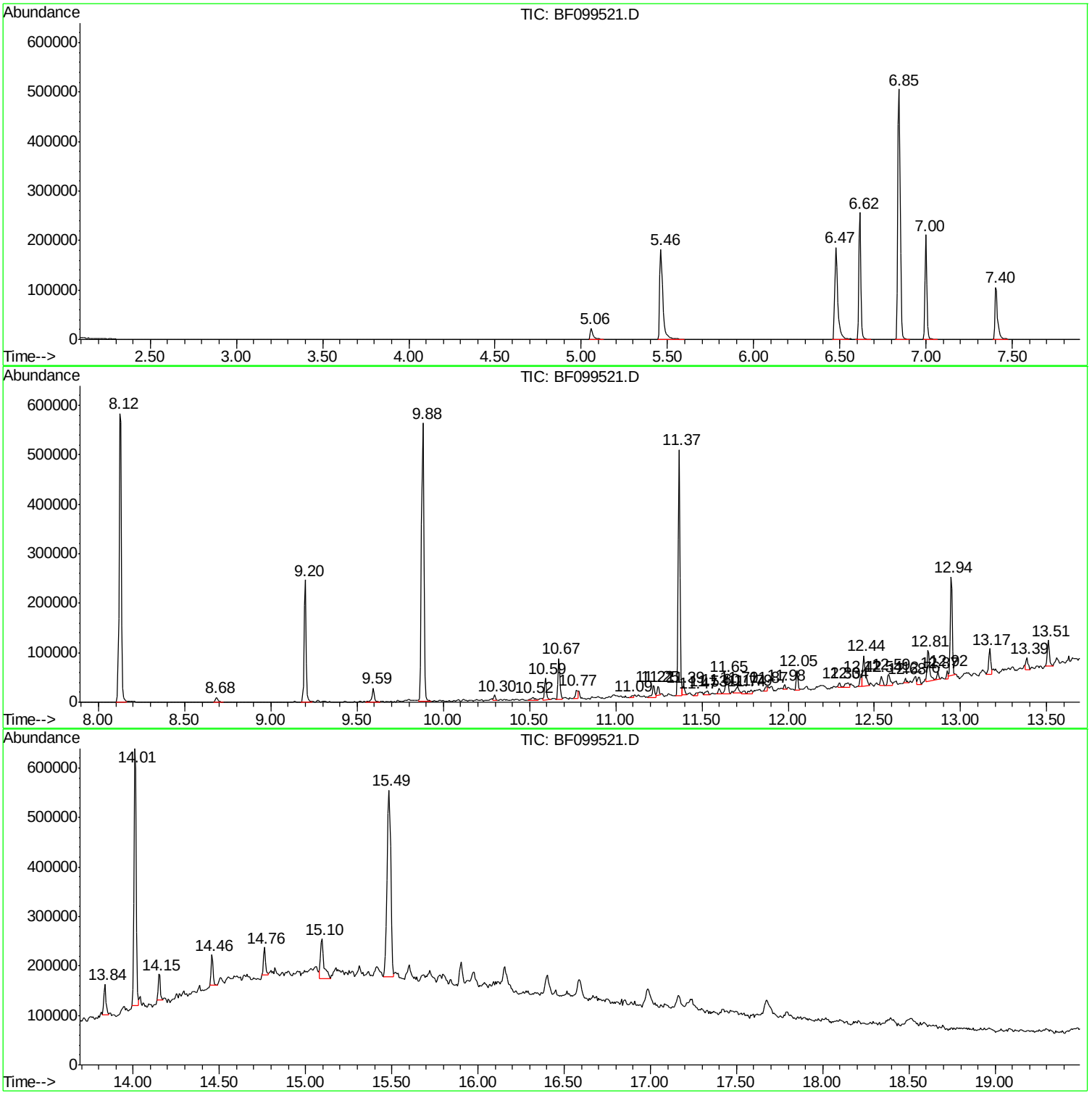
Sum of corrected areas: 5307429

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099521.D
Acq On : 15 Oct 2017 18:46
Operator : SJ/JU
Sample : I5813-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
OK-03-101117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099521.D
Acq On : 15 Oct 2017 18:46
Operator : SJ/JU
Sample : I5813-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** OK-03-101117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

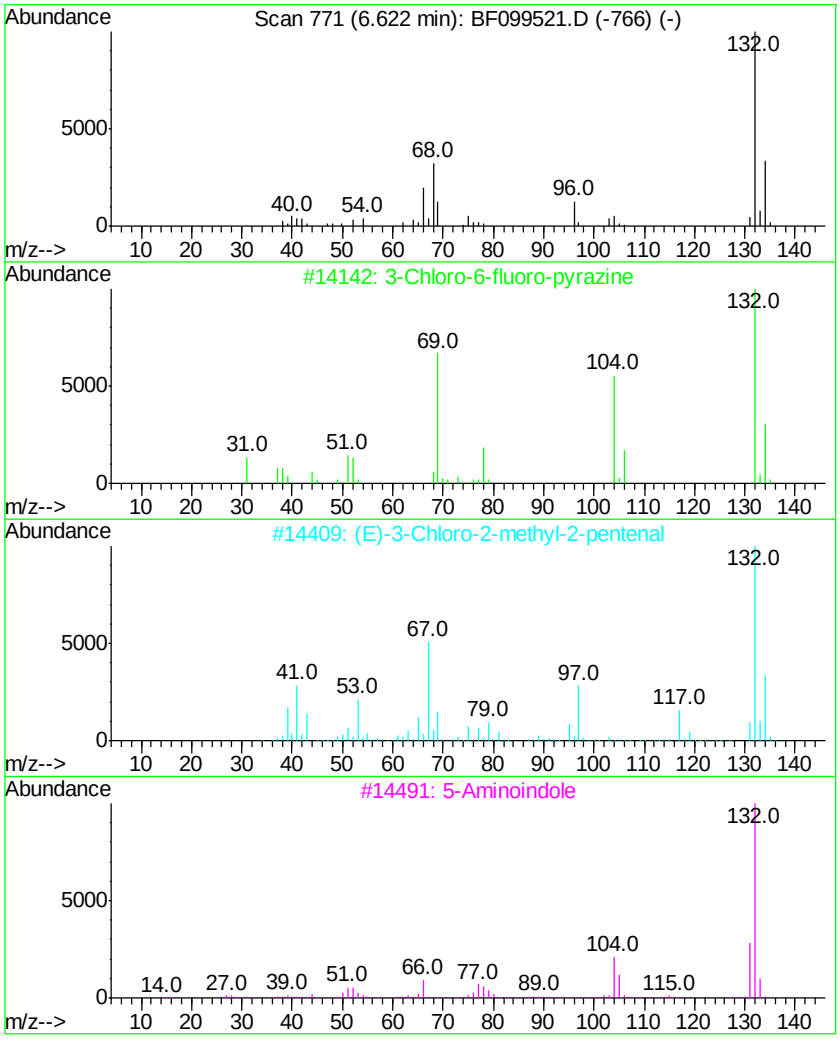
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

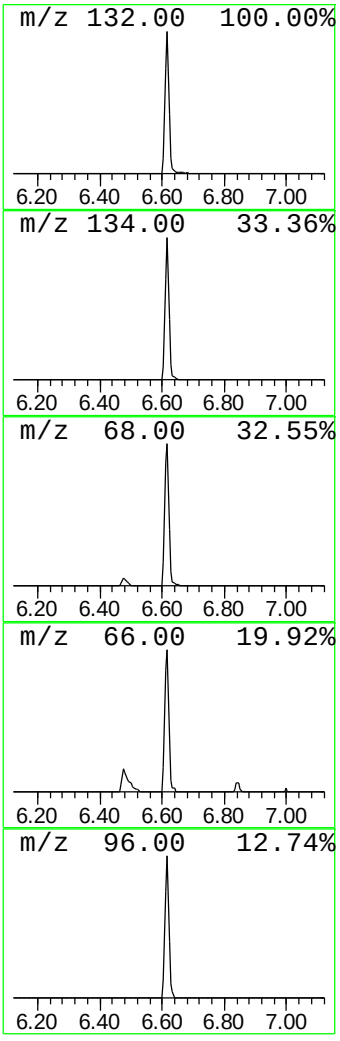
**********

Peak Number 1 unknown6.62 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.62 | 10.00 ng | 223380 | 1,4-Dichlorobenzene-d4 | 6.85 |

| 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 | 17 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 9 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099521.D
Acq On : 15 Oct 2017 18:46
Operator : SJ/JU
Sample : I5813-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** OK-03-101117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

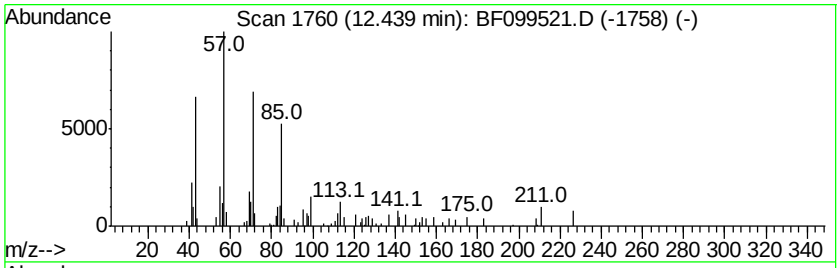
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

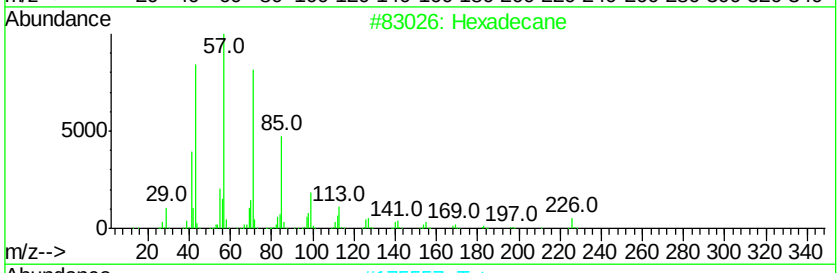
**********

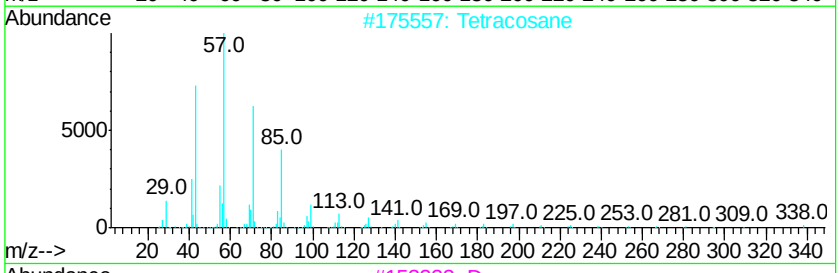
Peak Number 3 Hexadecane Concentration Rank 4

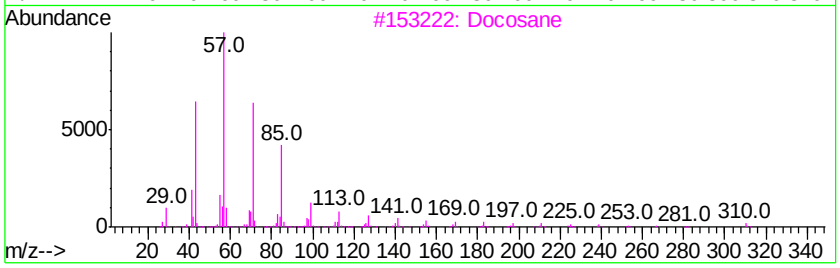
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.44 | 3.00 ng | 61835 | Phenanthrene-d10 | 11.37 |

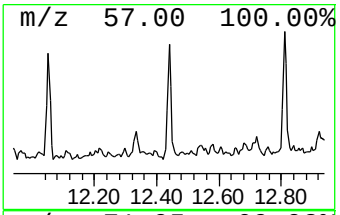
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 96 |
| 2 | Tetracosane | 338 | C24H50 | 000646-31-1 | 83 |
| 3 | Docosane | 310 | C22H46 | 000629-97-0 | 80 |
| 4 | Octadecane | 254 | C18H38 | 000593-45-3 | 80 |
| 5 | Heptadecane | 240 | C17H36 | 000629-78-7 | 74 |

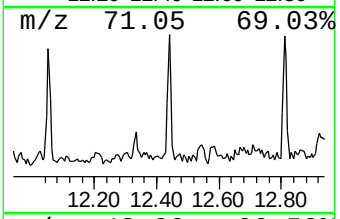


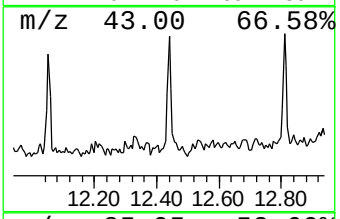



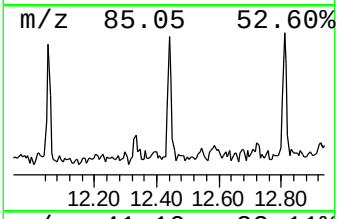



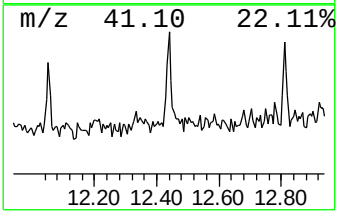



Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099521.D
Acq On : 15 Oct 2017 18:46
Operator : SJ/JU
Sample : I5813-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** OK-03-101117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

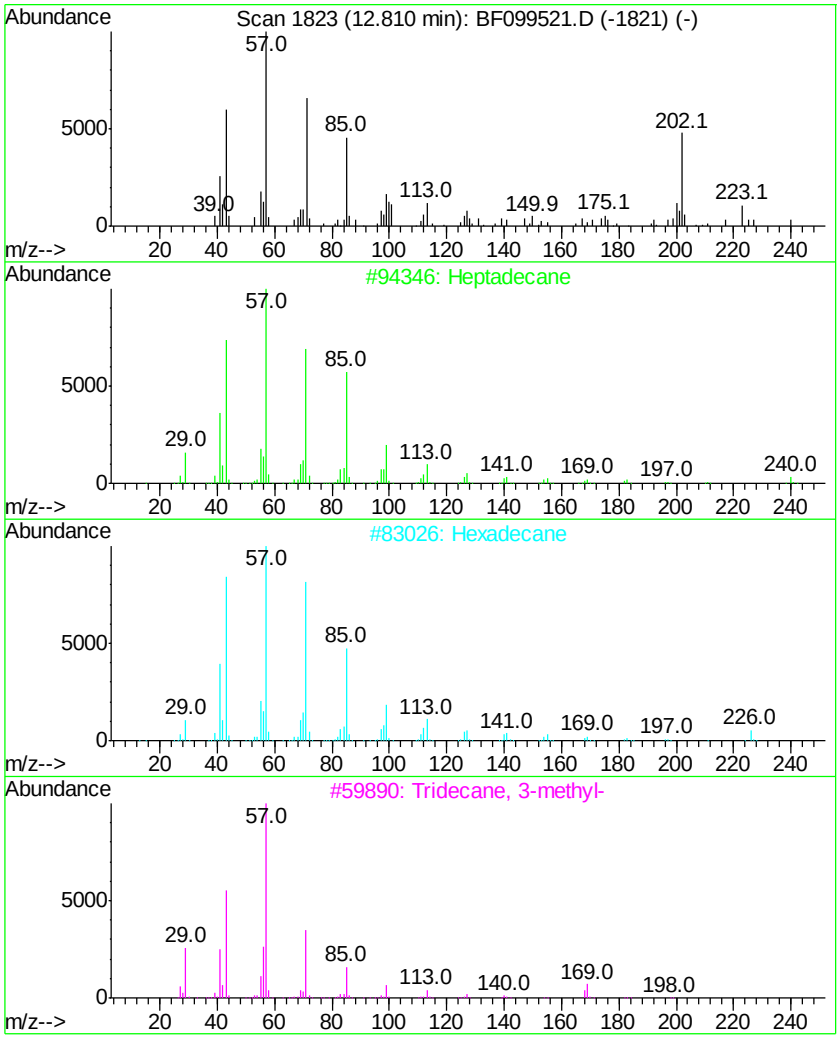
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

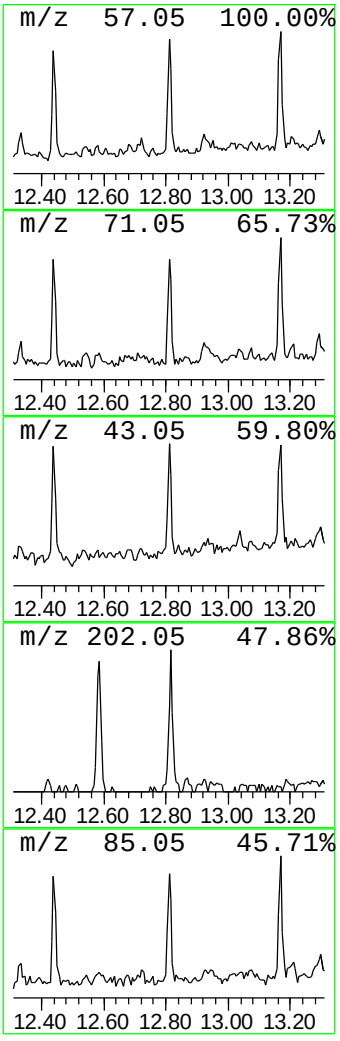
**********

Peak Number 4 Heptadecane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.81 | 2.83 ng | 70653 | Chrysene-d12 | 14.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 49 |
| 3 | Tridecane, 3-methyl- | 198 | C14H30 | 006418-41-3 | 46 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 46 |
| 5 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 46 |



# Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099521.D
Acq On : 15 Oct 2017 18:46
Operator : SJ/JU
Sample : I5813-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** OK-03-101117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

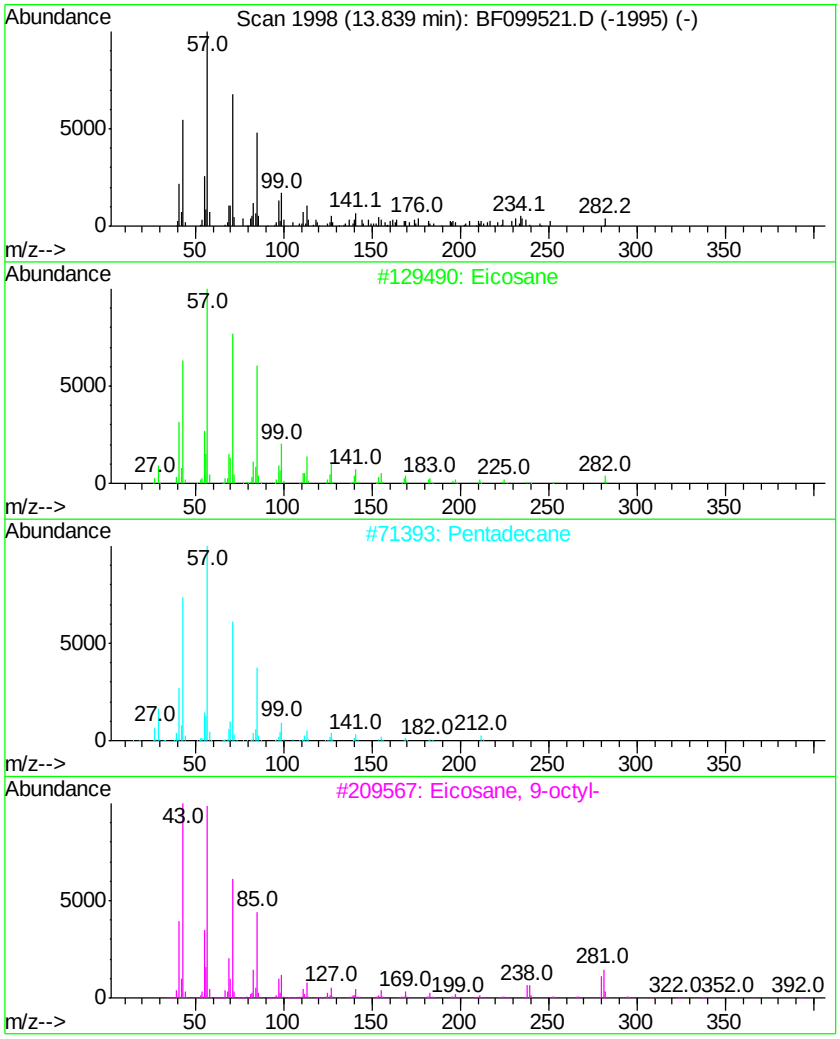
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

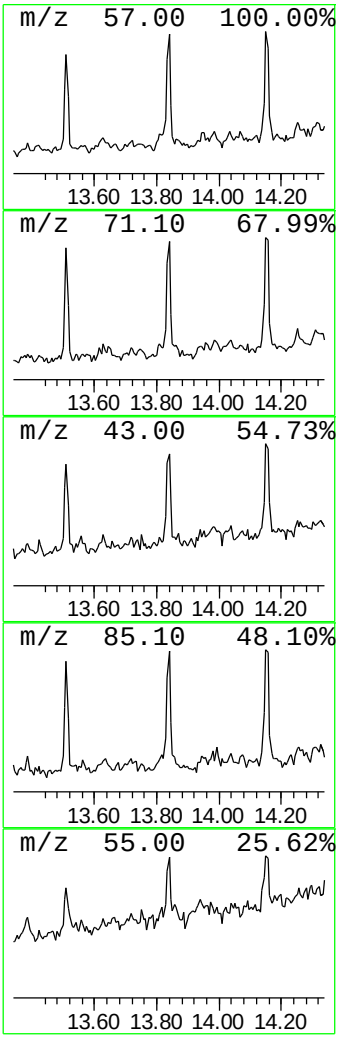
**********

Peak Number 5 Eicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.84 | 2.21 ng | 55329 | Chrysene-d12 | 14.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 2 | Pentadecane | 212 | C15H32 | 000629-62-9 | 90 |
| 3 | Eicosane, 9-octyl- | 394 | C28H58 | 013475-77-9 | 86 |
| 4 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 83 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 80 |



# Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099521.D
Acq On : 15 Oct 2017 18:46
Operator : SJ/JU
Sample : I5813-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** OK-03-101117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

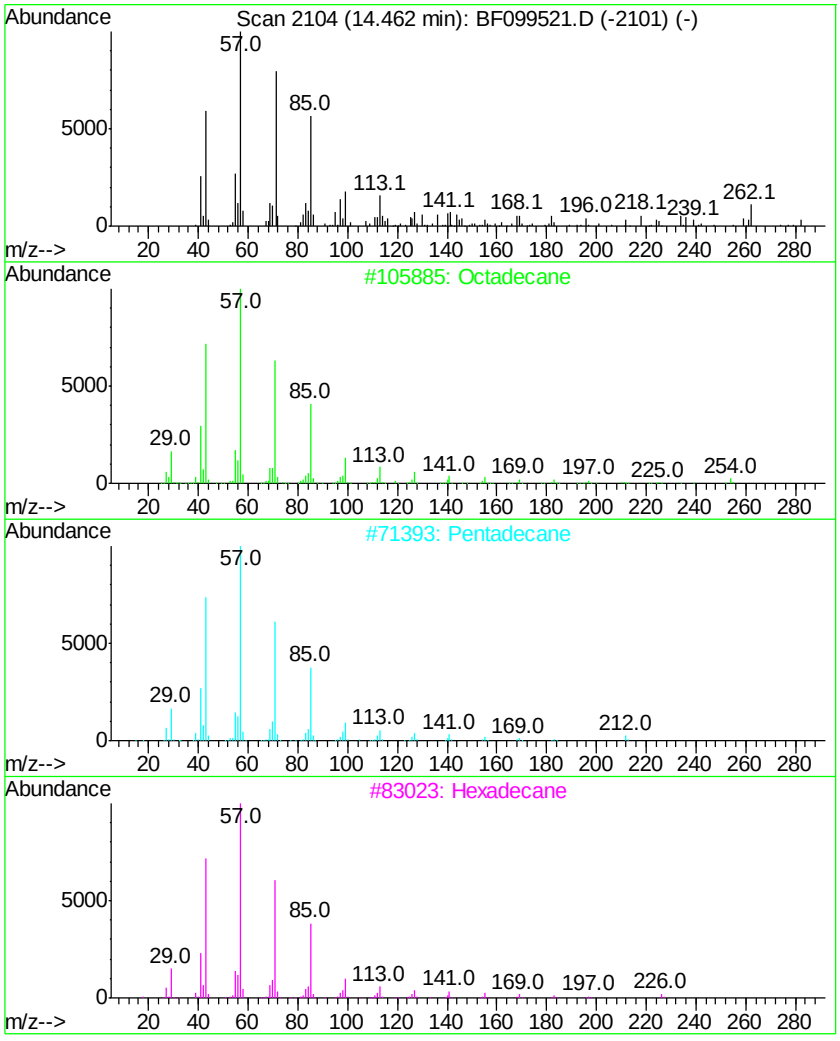
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

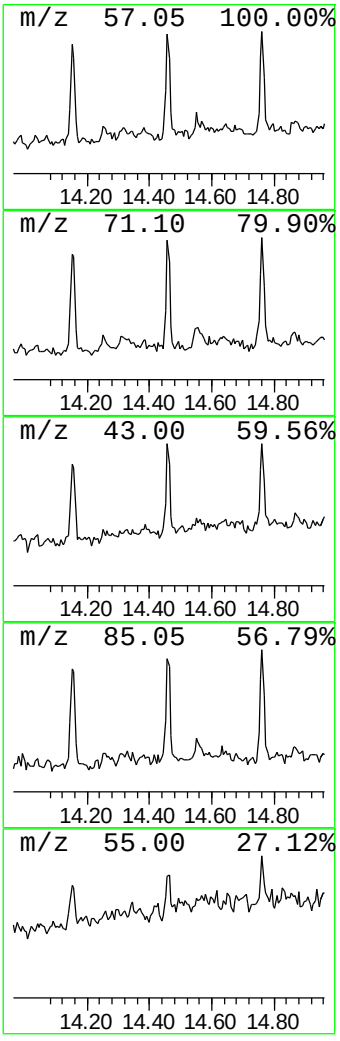
**********

Peak Number 6 Octadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.46 | 2.15 ng | 53847 | Chrysene-d12 | 14.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecane | 254 | C18H38 | 000593-45-3 | 93 |
| 2 | Pentadecane | 212 | C15H32 | 000629-62-9 | 93 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 87 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 80 |
| 5 | Eicosane | 282 | C20H42 | 000112-95-8 | 80 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099521.D
Acq On : 15 Oct 2017 18:46
Operator : SJ/JU
Sample : I5813-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** OK-03-101117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

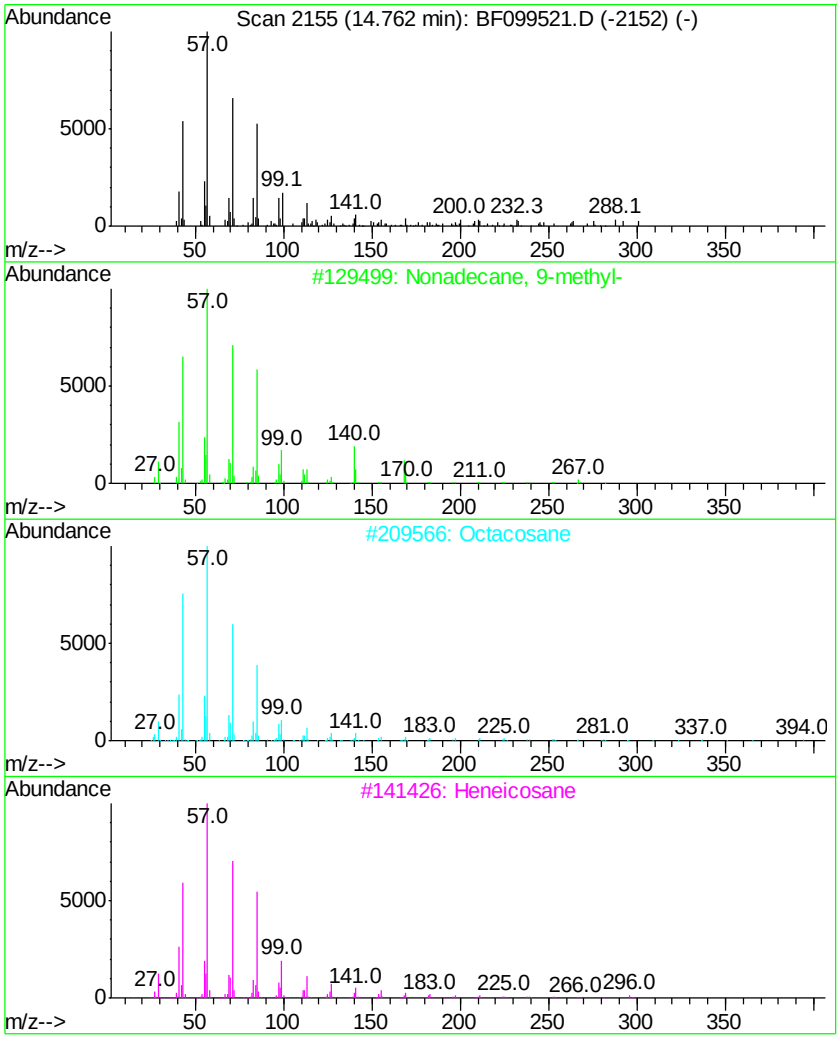
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

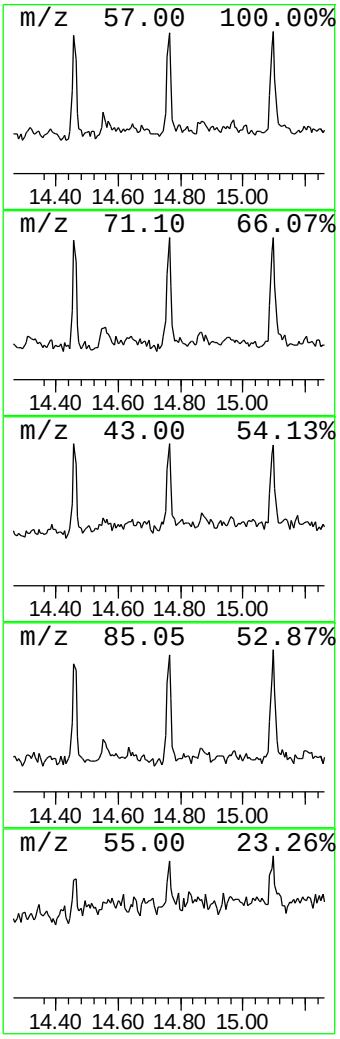
**********

Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.76 | 2.05 ng | 52663 | Perylene-d12 | 15.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Nonadecane, 9-methyl- | 282 | C20H42 | 013287-24-6 | 90 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 4 | Hexadecane, 1-iodo- | 352 | C16H33I | 000544-77-4 | 86 |
| 5 | Docosane | 310 | C22H46 | 000629-97-0 | 86 |



Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF101517\
Data File : BF099521.D
Acq On : 15 Oct 2017 18:46
Operator : SJ/JU
Sample : I5813-01 10X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** OK-03-101117

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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 |
| unknown6.62 | 6.62 | 10.0 | ng | 223380 | 1 | 6.85 | 446927 | 20.0 |
| Hexadecane | 12.44 | 3.0 | ng | 61835 | 4 | 11.37 | 411565 | 20.0 |
| Heptadecane | 12.81 | 2.8 | ng | 70653 | 5 | 14.01 | 499834 | 20.0 |
| Eicosane | 13.84 | 2.2 | ng | 55329 | 5 | 14.01 | 499834 | 20.0 |
| Octadecane | 14.46 | 2.1 | ng | 53847 | 5 | 14.01 | 499834 | 20.0 |
| Nonadecane, 9-met... | 14.76 | 2.0 | ng | 52663 | 6 | 15.49 | 514955 | 20.0 |