LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112813.D
Acq On : 1 Mar 2019 21:20
Operator : JU/SJ
Sample : K1675-17 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-4-A-B

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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 | 5.345 | 550 | 554 | 568 | rBV | 692944 | 690907 | 46.61% | 4.796% |
| 2 | 6.363 | 724 | 727 | 742 | rBV | 735826 | 721605 | 48.68% | 5.009% |
| 3 | 6.504 | 748 | 751 | 755 | rBV | 819455 | 731723 | 49.36% | 5.079% |
| 4 | 6.745 | 788 | 792 | 801 | rBV | 1013964 | 918335 | 61.95% | 6.375% |
| 5 | 6.898 | 814 | 818 | 829 | rBV | 659197 | 566831 | 38.24% | 3.935% |
| 6 | 7.298 | 882 | 886 | 896 | rBV | 400690 | 400798 | 27.04% | 2.782% |
| 7 | 8.022 | 1005 | 1009 | 1033 | rBV | 1096243 | 1101691 | 74.32% | 7.647% |
| 8 | 9.098 | 1188 | 1192 | 1206 | rBV | 657314 | 645994 | 43.58% | 4.484% |
| 9 | 9.492 | 1256 | 1259 | 1265 | rBV | 30407 | 28049 | 1.89% | 0.195% |
| 10 | 9.663 | 1286 | 1288 | 1297 | rVB3 | 10917 | 18797 | 1.27% | 0.130% |
| 11 | 9.775 | 1303 | 1307 | 1319 | rBV | 977221 | 977538 | 65.94% | 6.786% |
| 12 | 10.551 | 1436 | 1439 | 1449 | rBV | 346307 | 378495 | 25.53% | 2.627% |
| 13 | 11.251 | 1554 | 1558 | 1560 | rBV | 1004633 | 951644 | 64.20% | 6.606% |
| 14 | 11.269 | 1560 | 1561 | 1567 | rVV | 174984 | 156751 | 10.57% | 1.088% |
| 15 | 11.322 | 1567 | 1570 | 1574 | rVB | 26479 | 28322 | 1.91% | 0.197% |
| 16 | 11.480 | 1592 | 1597 | 1600 | rBV2 | 15043 | 20831 | 1.41% | 0.145% |
| 17 | 11.751 | 1640 | 1643 | 1645 | rBV | 27634 | 22743 | 1.53% | 0.158% |
| 18 | 11.780 | 1645 | 1648 | 1653 | rVV | 85034 | 86798 | 5.86% | 0.603% |
| 19 | 11.863 | 1659 | 1662 | 1664 | rBV | 40050 | 42952 | 2.90% | 0.298% |
| 20 | 11.886 | 1664 | 1666 | 1671 | rVB | 21312 | 21503 | 1.45% | 0.149% |
| 21 | 12.045 | 1691 | 1693 | 1695 | rBV | 20382 | 19381 | 1.31% | 0.135% |
| 22 | 12.063 | 1695 | 1696 | 1703 | rVB2 | 27802 | 29448 | 1.99% | 0.204% |
| 23 | 12.298 | 1733 | 1736 | 1740 | rBV2 | 35093 | 38950 | 2.63% | 0.270% |
| 24 | 12.380 | 1747 | 1750 | 1756 | rVB2 | 28004 | 32610 | 2.20% | 0.226% |
| 25 | 12.457 | 1759 | 1763 | 1767 | rVV | 416893 | 385369 | 26.00% | 2.675% |
| 26 | 12.569 | 1780 | 1782 | 1784 | rBV2 | 22005 | 21603 | 1.46% | 0.150% |
| 27 | 12.680 | 1795 | 1801 | 1805 | rBV | 405424 | 413054 | 27.86% | 2.867% |
| 28 | 12.733 | 1808 | 1810 | 1816 | rVB2 | 17322 | 24627 | 1.66% | 0.171% |
| 29 | 12.804 | 1818 | 1822 | 1823 | rBV | 21339 | 20847 | 1.41% | 0.145% |
| 30 | 12.827 | 1823 | 1826 | 1832 | rVB | 805035 | 688740 | 46.46% | 4.781% |
| 31 | 12.904 | 1834 | 1839 | 1842 | rBV2 | 33522 | 48194 | 3.25% | 0.335% |
| 32 | 12.986 | 1846 | 1853 | 1854 | rBV6 | 28662 | 37918 | 2.56% | 0.263% |
| 33 | 13.010 | 1855 | 1857 | 1860 | rVB2 | 36304 | 35504 | 2.40% | 0.246% |
| 34 | 13.074 | 1866 | 1868 | 1871 | rBV | 20968 | 20458 | 1.38% | 0.142% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112813.D
Acq On : 1 Mar 2019 21:20
Operator : JU/SJ
Sample : K1675-17 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-4-A-B

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.116 | 1871 | 1875 | 1879 | rBV | 49749 | 54982 | 3.71% | 0.382% |
| 36 | 13.204 | 1888 | 1890 | 1893 | rVB | 28344 | 23888 | 1.61% | 0.166% |
| 37 | 13.239 | 1893 | 1896 | 1901 | rBV2 | 23925 | 26670 | 1.80% | 0.185% |
| 38 | 13.416 | 1923 | 1926 | 1931 | rBV6 | 15791 | 21473 | 1.45% | 0.149% |
| 39 | 13.516 | 1939 | 1943 | 1947 | rBV | 61141 | 66855 | 4.51% | 0.464% |
| 40 | 13.621 | 1957 | 1961 | 1965 | rBV2 | 56076 | 85446 | 5.76% | 0.593% |
| 41 | 13.657 | 1965 | 1967 | 1969 | rVV | 31039 | 23788 | 1.60% | 0.165% |
| 42 | 13.674 | 1969 | 1970 | 1972 | rBV | 23607 | 22193 | 1.50% | 0.154% |
| 43 | 13.716 | 1975 | 1977 | 1979 | rBV2 | 45126 | 43954 | 2.97% | 0.305% |
| 44 | 13.874 | 1999 | 2004 | 2007 | rBV2 | 1405896 | 1482408 | 100.00% | 10.290% |
| 45 | 13.898 | 2007 | 2008 | 2015 | rVB | 250312 | 185526 | 12.52% | 1.288% |
| 46 | 14.063 | 2033 | 2036 | 2038 | rVB2 | 32843 | 27333 | 1.84% | 0.190% |
| 47 | 14.263 | 2067 | 2070 | 2072 | rVV | 40011 | 37743 | 2.55% | 0.262% |
| 48 | 14.298 | 2073 | 2076 | 2079 | rVB2 | 36005 | 39090 | 2.64% | 0.271% |
| 49 | 14.663 | 2135 | 2138 | 2142 | rVB | 60835 | 71935 | 4.85% | 0.499% |
| 50 | 14.886 | 2172 | 2176 | 2179 | rBV | 195003 | 287207 | 19.37% | 1.994% |
| 51 | 14.980 | 2189 | 2192 | 2199 | rVB2 | 109516 | 134767 | 9.09% | 0.935% |
| 52 | 15.168 | 2221 | 2224 | 2230 | rVB | 108505 | 118053 | 7.96% | 0.819% |
| 53 | 15.221 | 2230 | 2233 | 2237 | rBV | 126319 | 137368 | 9.27% | 0.954% |
| 54 | 15.286 | 2239 | 2244 | 2247 | rVV | 725184 | 847134 | 57.15% | 5.880% |
| 55 | 15.339 | 2250 | 2253 | 2257 | rVB | 92371 | 115480 | 7.79% | 0.802% |
| 56 | 15.745 | 2319 | 2322 | 2326 | rVB2 | 86764 | 105228 | 7.10% | 0.730% |
| 57 | 16.215 | 2399 | 2402 | 2408 | rVB | 74753 | 118721 | 8.01% | 0.824% |

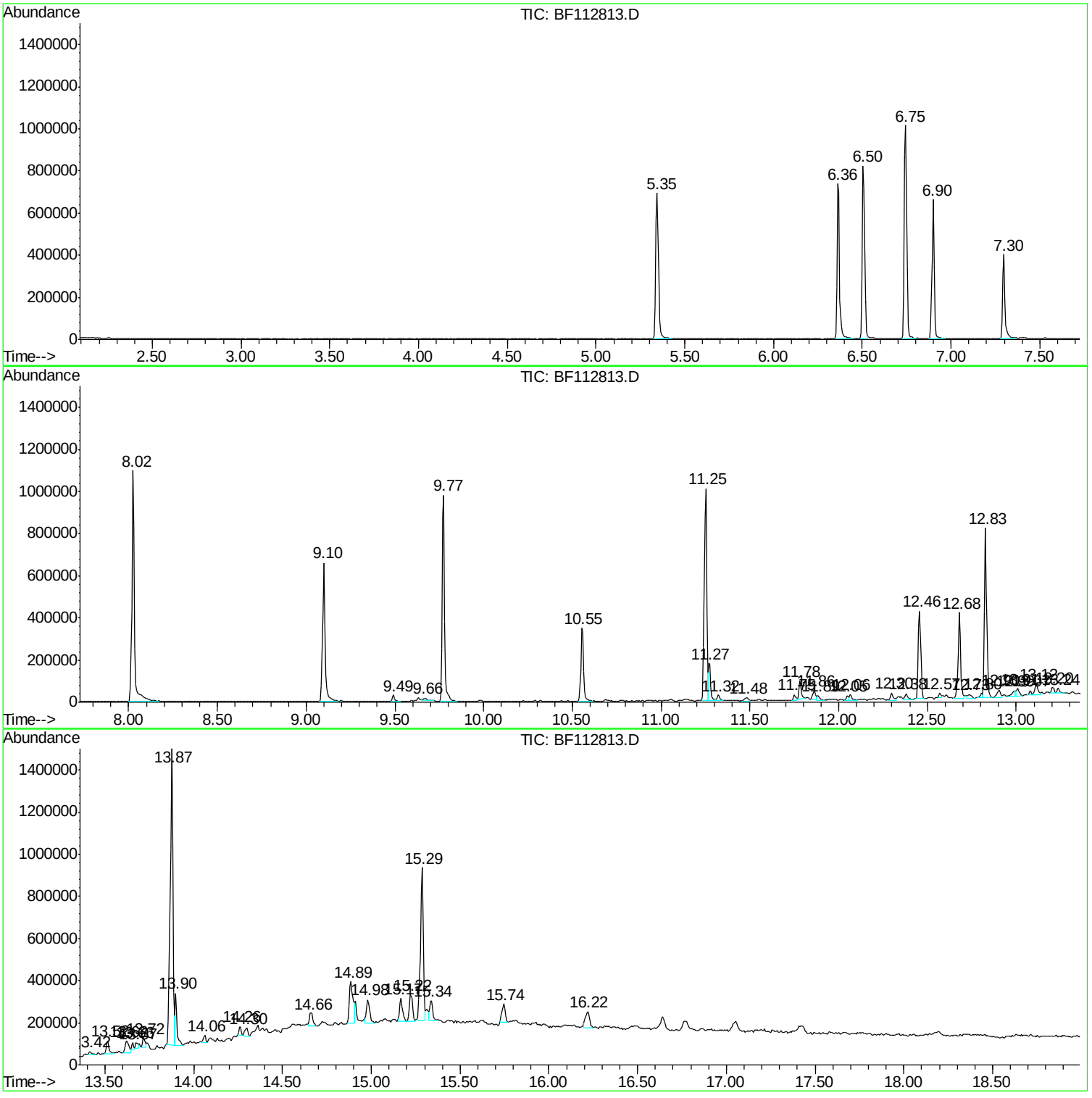
Sum of corrected areas: 14406252

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112813.D
Acq On : 1 Mar 2019 21:20
Operator : JU/SJ
Sample : K1675-17 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
Z-4-A-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112813.D
Acq On : 1 Mar 2019 21:20
Operator : JU/SJ
Sample : K1675-17 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-4-A-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

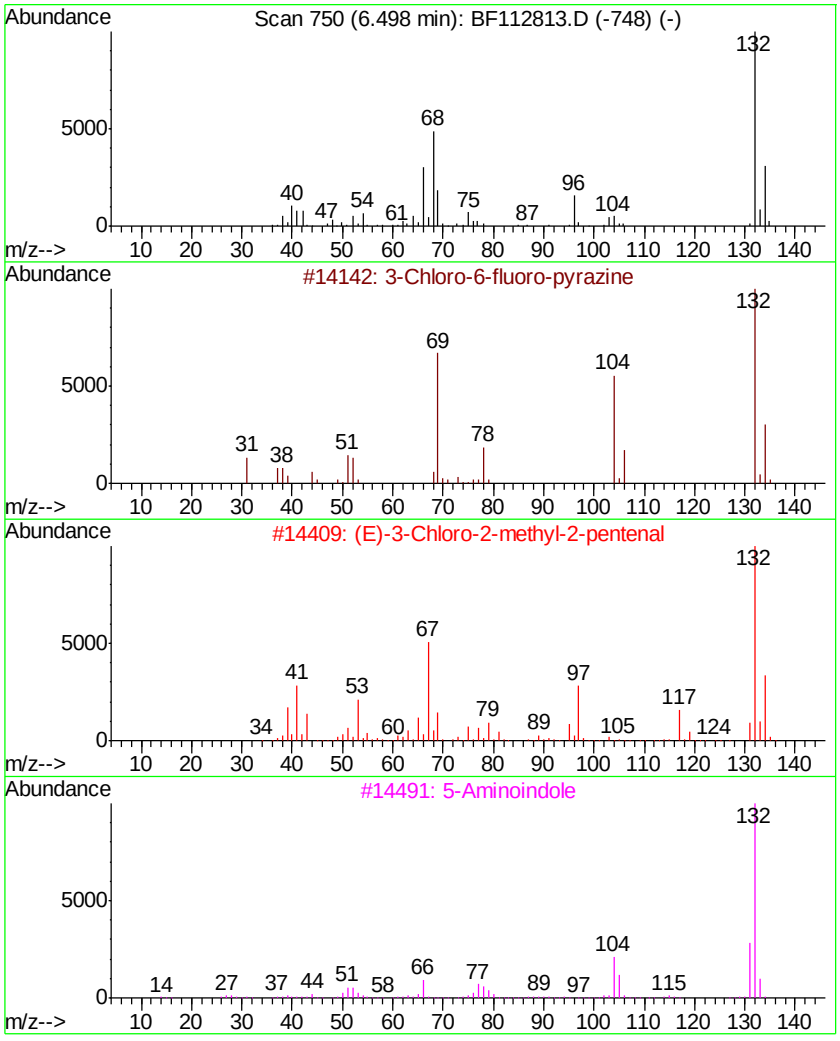
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

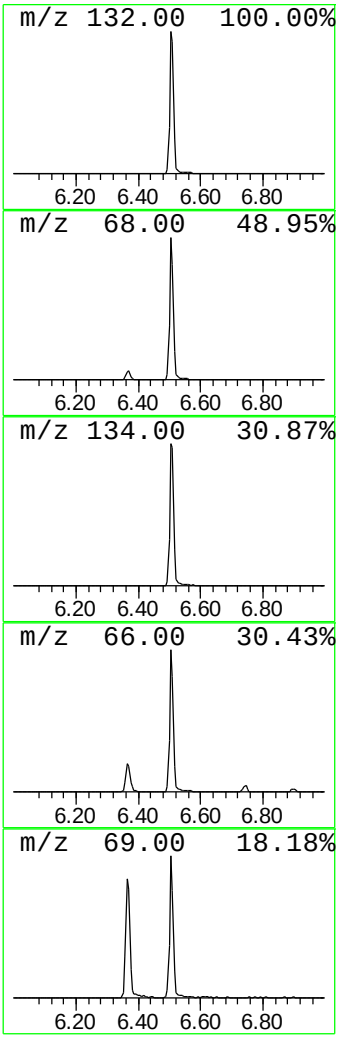
**********

Peak Number 1 unknown6.50 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.50 | 15.94 ng | 731723 | 1,4-Dichlorobenzene-d4 | 6.75 |

| 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 | 27 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | Amphetaminil | 250 | C17H18N2 | 017590-01-1 | 10 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112813.D
Acq On : 1 Mar 2019 21:20
Operator : JU/SJ
Sample : K1675-17 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-4-A-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

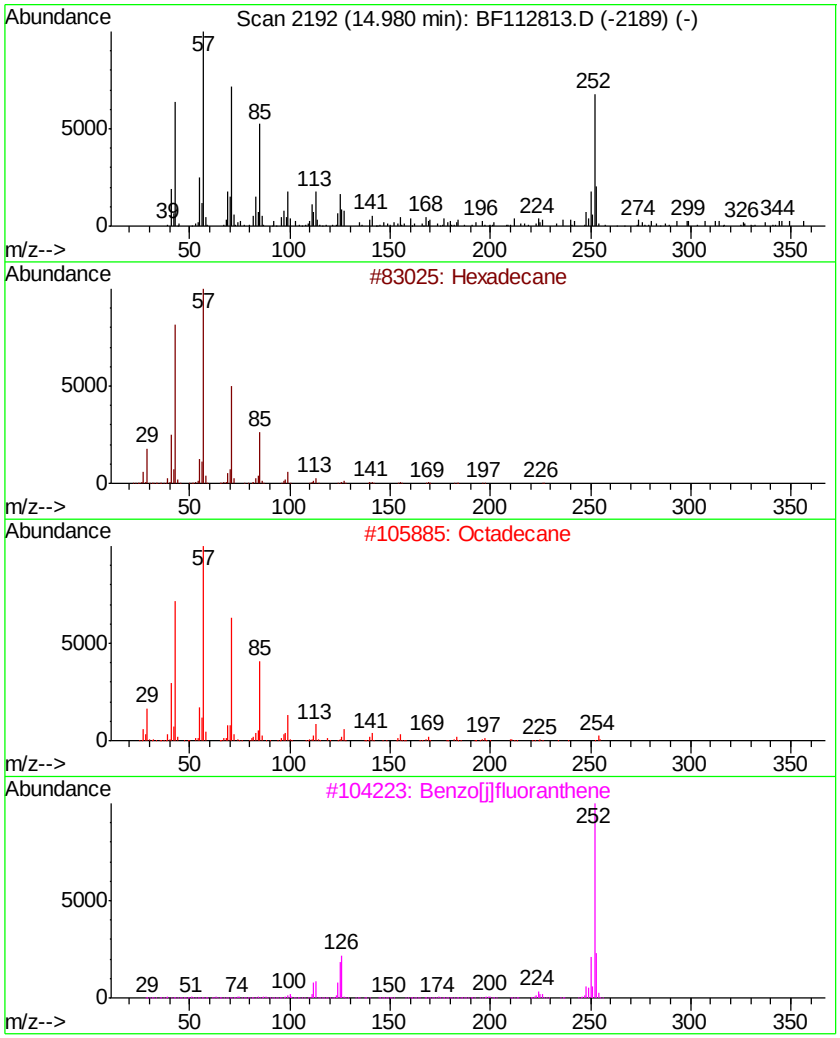
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

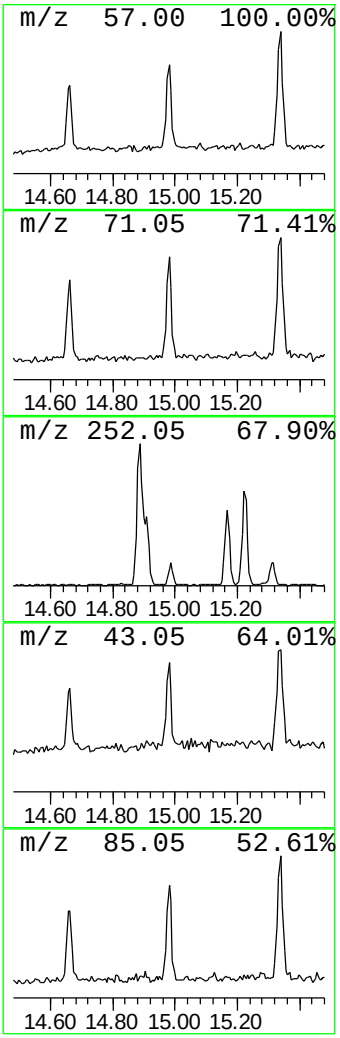
**********

Peak Number 3 Hexadecane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.98 | 3.18 ng | 134767 | Perylene-d12 | 15.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 89 |
| 2 | Octadecane | 254 | C18H38 | 000593-45-3 | 64 |
| 3 | Benzo[j]fluoranthene | 252 | C20H12 | 000205-82-3 | 55 |
| 4 | Hexadecane, 7,9-dimethyl- | 254 | C18H38 | 021164-95-4 | 51 |
| 5 | Benz[e]acephenanthrylene | 252 | C20H12 | 000205-99-2 | 49 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112813.D
Acq On : 1 Mar 2019 21:20
Operator : JU/SJ
Sample : K1675-17 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-4-A-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

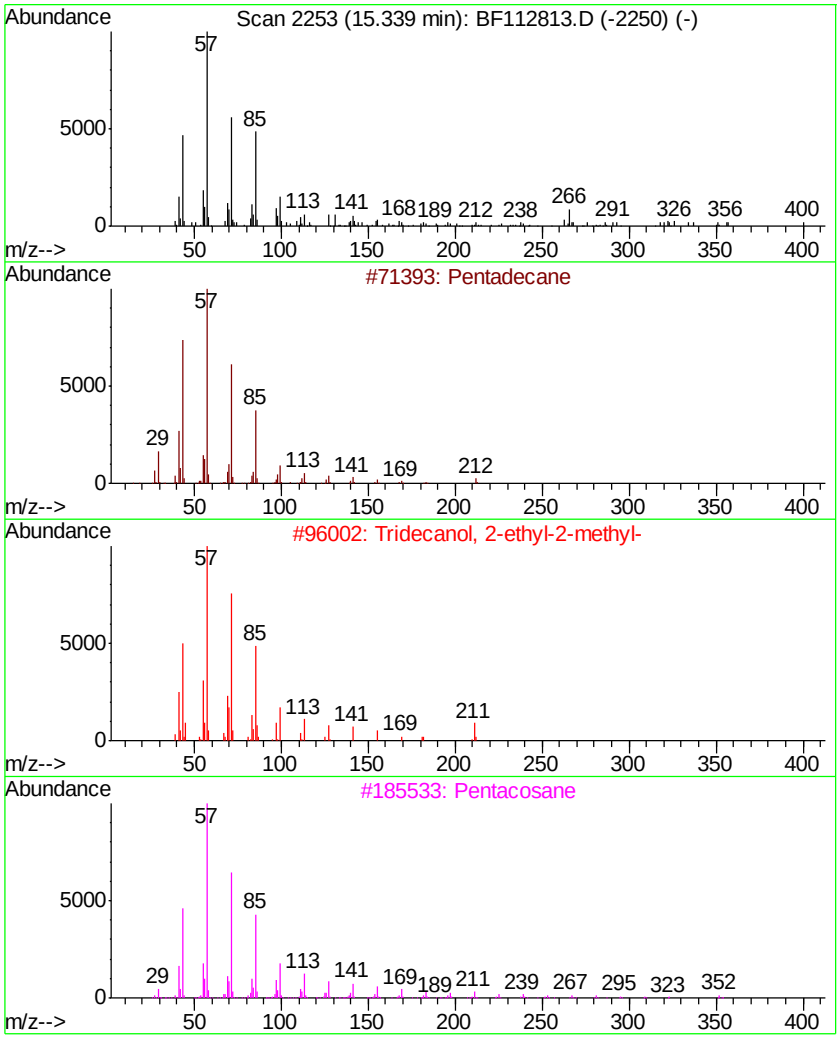
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

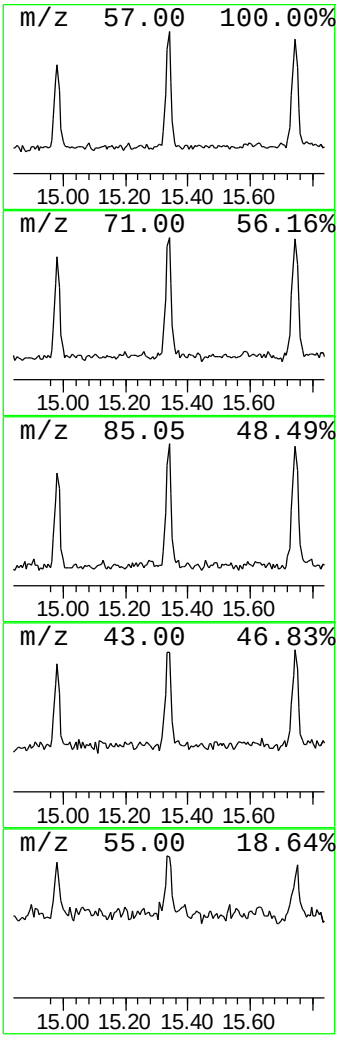
**********

Peak Number 5 Pentadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.34 | 2.73 ng | 115480 | Perylene-d12 | 15.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecane | 212 | C15H32 | 000629-62-9 | 93 |
| 2 | Tridecanol, 2-ethyl-2-methyl- | 242 | C16H34O | 1000115-66-1 | 80 |
| 3 | Pentacosane | 352 | C25H52 | 000629-99-2 | 80 |
| 4 | Nonadecane | 268 | C19H40 | 000629-92-5 | 80 |
| 5 | 6,6-Diethylhoctadecane | 310 | C22H46 | 1000360-41-8 | 72 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112813.D
Acq On : 1 Mar 2019 21:20
Operator : JU/SJ
Sample : K1675-17 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-4-A-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

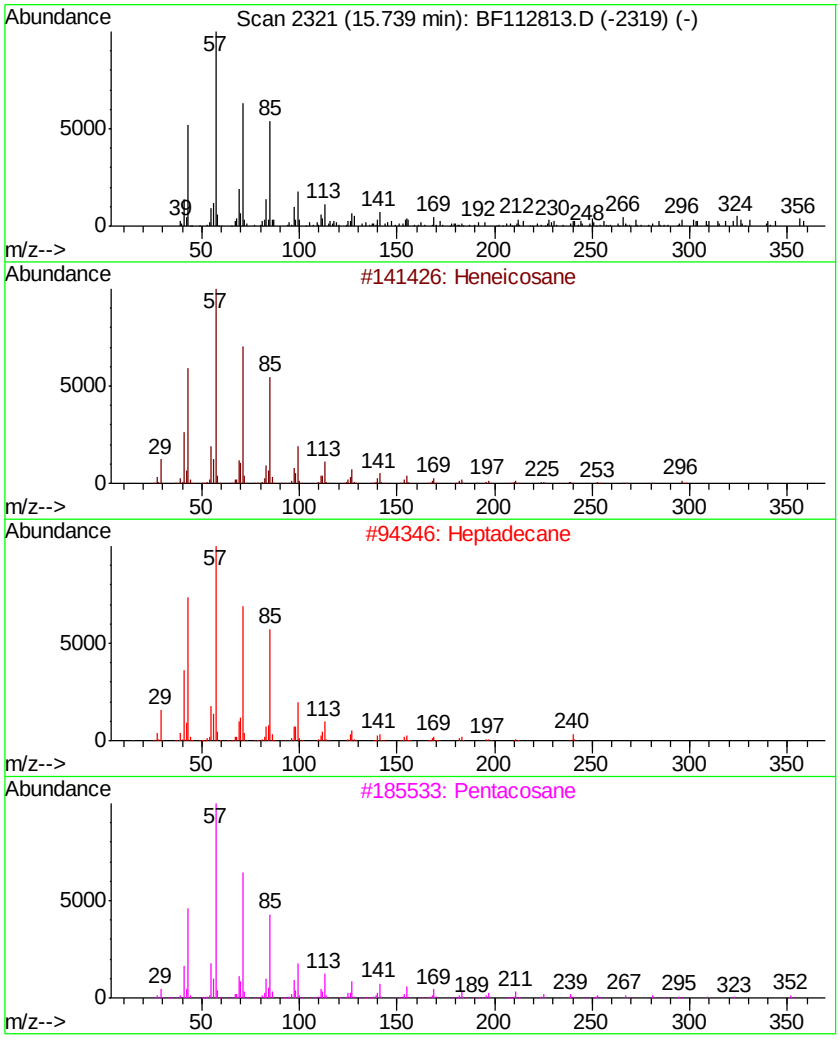
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

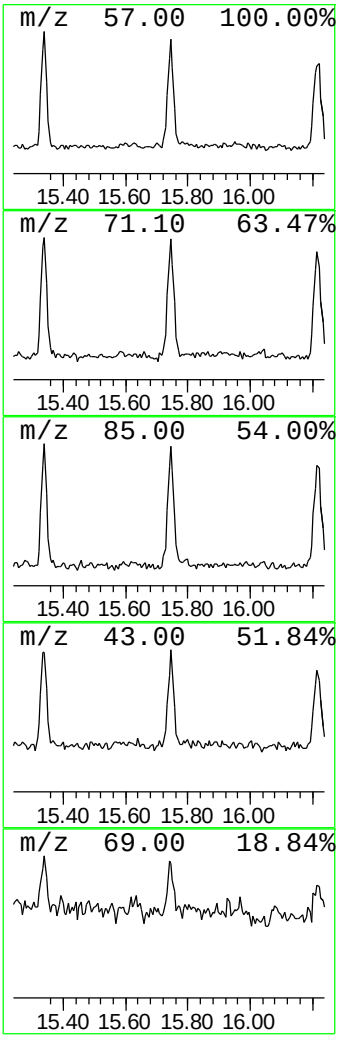
**********

Peak Number 6 Heneicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.74 | 2.48 ng | 105228 | Perylene-d12 | 15.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |
| 3 | Pentacosane | 352 | C25H52 | 000629-99-2 | 86 |
| 4 | Tricosane | 324 | C23H48 | 000638-67-5 | 81 |
| 5 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 58 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030119\
Data File : BF112813.D
Acq On : 1 Mar 2019 21:20
Operator : JU/SJ
Sample : K1675-17 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-4-A-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

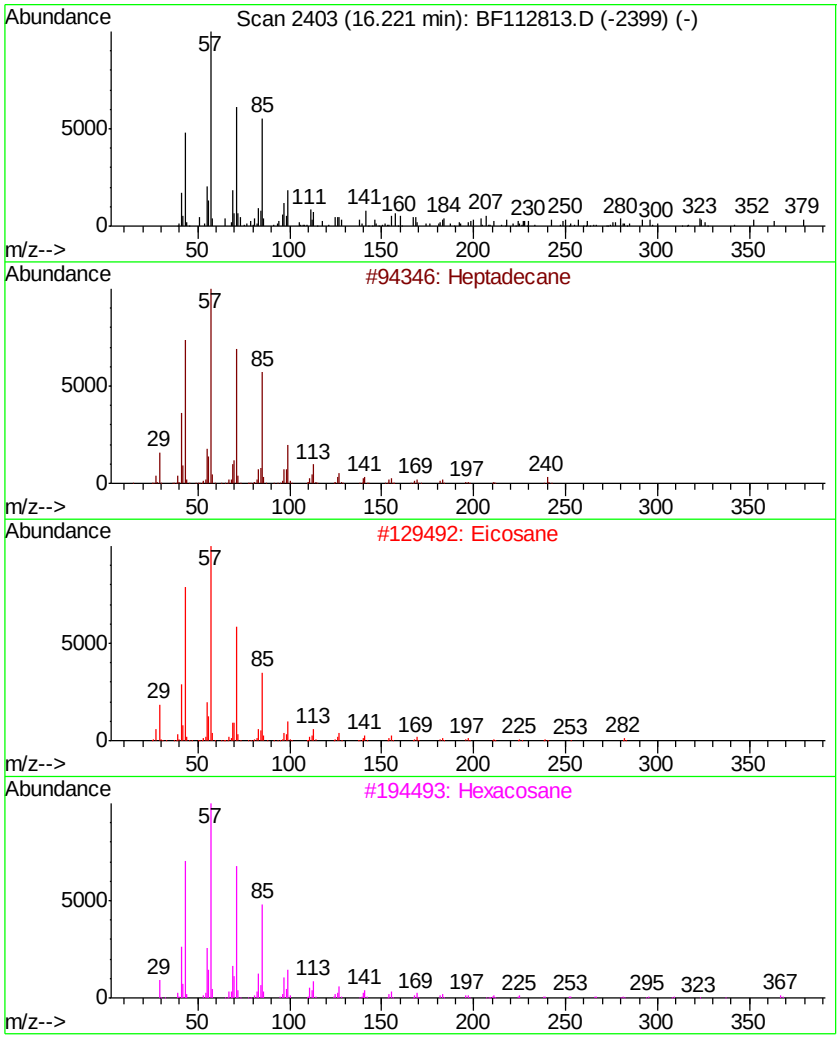
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

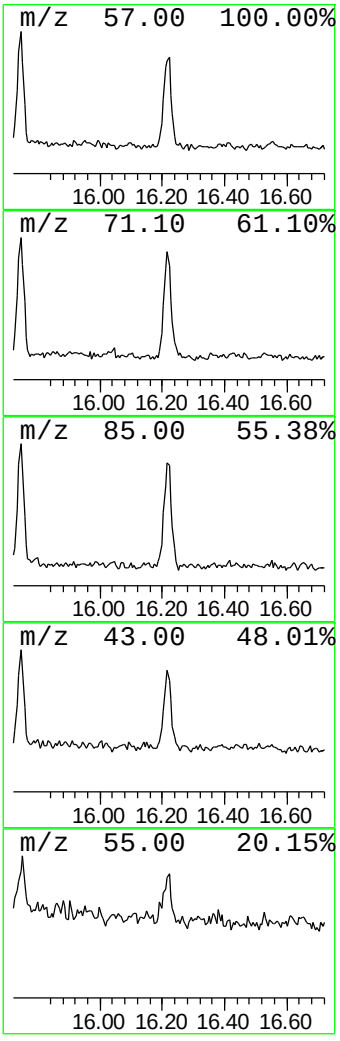
**********

Peak Number 7 Heptadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.22 | 2.80 ng | 118721 | Perylene-d12 | 15.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 93 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 76 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 72 |
| 4 | Tridecane, 2-methyl- | 198 | C14H30 | 001560-96-9 | 72 |
| 5 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 72 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030119\
Data File : BF112813.D
Acq On : 1 Mar 2019 21:20
Operator : JU/SJ
Sample : K1675-17 5X
Misc :
ALS Vial : 24 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** Z-4-A-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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 |
| unknown6.50 | 6.50 | 15.9 | ng | 731723 | 1 | 6.75 | 918335 | 20.0 |
| Hexadecane | 14.98 | 3.2 | ng | 134767 | 6 | 15.29 | 847134 | 20.0 |
| Pentadecane | 15.34 | 2.7 | ng | 115480 | 6 | 15.29 | 847134 | 20.0 |
| Heneicosane | 15.74 | 2.5 | ng | 105228 | 6 | 15.29 | 847134 | 20.0 |
| Heptadecane | 16.22 | 2.8 | ng | 118721 | 6 | 15.29 | 847134 | 20.0 |