LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

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-BF073019.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 | 3.869 | 298 | 303 | 323 | rBV | 312926 | 497749 | 35.90% | 3.472% |
| 2 | 5.463 | 571 | 574 | 604 | rBV | 229344 | 474802 | 34.24% | 3.312% |
| 3 | 6.475 | 743 | 746 | 766 | rBV | 301995 | 562382 | 40.56% | 3.923% |
| 4 | 6.610 | 766 | 769 | 788 | rVB | 530982 | 600638 | 43.32% | 4.189% |
| 5 | 6.834 | 804 | 807 | 826 | rVB | 770085 | 718831 | 51.84% | 5.014% |
| 6 | 6.993 | 830 | 834 | 849 | rBV | 407643 | 456232 | 32.90% | 3.182% |
| 7 | 7.404 | 901 | 904 | 926 | rBV | 174945 | 343110 | 24.74% | 2.393% |
| 8 | 8.116 | 1021 | 1025 | 1050 | rBV | 849472 | 992760 | 71.60% | 6.925% |
| 9 | 9.186 | 1204 | 1207 | 1218 | rBV | 615905 | 646160 | 46.60% | 4.507% |
| 10 | 9.263 | 1218 | 1220 | 1225 | rVB3 | 9886 | 15470 | 1.12% | 0.108% |
| 11 | 9.539 | 1262 | 1267 | 1270 | rBV5 | 11884 | 19273 | 1.39% | 0.134% |
| 12 | 9.592 | 1270 | 1276 | 1279 | rBV4 | 37132 | 51424 | 3.71% | 0.359% |
| 13 | 9.869 | 1319 | 1323 | 1339 | rVB | 1298983 | 1226110 | 88.42% | 8.552% |
| 14 | 10.122 | 1363 | 1366 | 1373 | rVB5 | 20875 | 31000 | 2.24% | 0.216% |
| 15 | 10.192 | 1375 | 1378 | 1381 | rBV4 | 12156 | 17230 | 1.24% | 0.120% |
| 16 | 10.233 | 1381 | 1385 | 1389 | rVB3 | 10330 | 14884 | 1.07% | 0.104% |
| 17 | 10.281 | 1389 | 1393 | 1396 | rBV4 | 13342 | 21383 | 1.54% | 0.149% |
| 18 | 10.516 | 1430 | 1433 | 1439 | rVB2 | 37164 | 46766 | 3.37% | 0.326% |
| 19 | 10.663 | 1455 | 1458 | 1468 | rBV | 284755 | 377285 | 27.21% | 2.632% |
| 20 | 10.781 | 1474 | 1478 | 1485 | rVB | 76188 | 77661 | 5.60% | 0.542% |
| 21 | 11.110 | 1531 | 1534 | 1540 | rVB7 | 9022 | 15223 | 1.10% | 0.106% |
| 22 | 11.245 | 1554 | 1557 | 1563 | rVB | 53653 | 55280 | 3.99% | 0.386% |
| 23 | 11.357 | 1572 | 1576 | 1592 | rBV | 1153215 | 1260268 | 90.89% | 8.790% |
| 24 | 11.880 | 1660 | 1665 | 1674 | rBV3 | 169126 | 290681 | 20.96% | 2.028% |
| 25 | 12.416 | 1753 | 1756 | 1760 | rBV4 | 10665 | 16180 | 1.17% | 0.113% |
| 26 | 12.527 | 1773 | 1775 | 1780 | rVB5 | 13318 | 15896 | 1.15% | 0.111% |
| 27 | 12.586 | 1781 | 1785 | 1792 | rBV4 | 16903 | 43989 | 3.17% | 0.307% |
| 28 | 12.663 | 1795 | 1798 | 1816 | rBV | 483444 | 830861 | 59.92% | 5.795% |
| 29 | 12.933 | 1838 | 1844 | 1855 | rVB | 740685 | 676978 | 48.82% | 4.722% |
| 30 | 13.116 | 1872 | 1875 | 1880 | rBV6 | 10954 | 17138 | 1.24% | 0.120% |
| 31 | 13.863 | 1999 | 2002 | 2003 | rBV3 | 20960 | 24025 | 1.73% | 0.168% |
| 32 | 13.998 | 2021 | 2025 | 2037 | rBV | 872881 | 974785 | 70.30% | 6.799% |
| 33 | 14.145 | 2047 | 2050 | 2053 | rBV | 49039 | 44224 | 3.19% | 0.308% |
| 34 | 14.451 | 2099 | 2102 | 2105 | rVB | 129444 | 117042 | 8.44% | 0.816% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

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-BF073019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 14.751 | 2150 | 2153 | 2157 | rBV | 251162 | 235624 | 16.99% | 1.643% |
| 36 | 14.821 | 2163 | 2165 | 2169 | rVB | 72425 | 74487 | 5.37% | 0.520% |
| 37 | 15.080 | 2205 | 2209 | 2216 | rVB | 347970 | 424022 | 30.58% | 2.958% |
| 38 | 15.463 | 2269 | 2274 | 2291 | rVB2 | 843043 | 1386619 | 100.00% | 9.672% |
| 39 | 15.880 | 2341 | 2345 | 2353 | rBV | 272748 | 398748 | 28.76% | 2.781% |
| 40 | 16.374 | 2425 | 2429 | 2435 | rVB | 144098 | 243593 | 17.57% | 1.699% |

Sum of corrected areas: 14336813

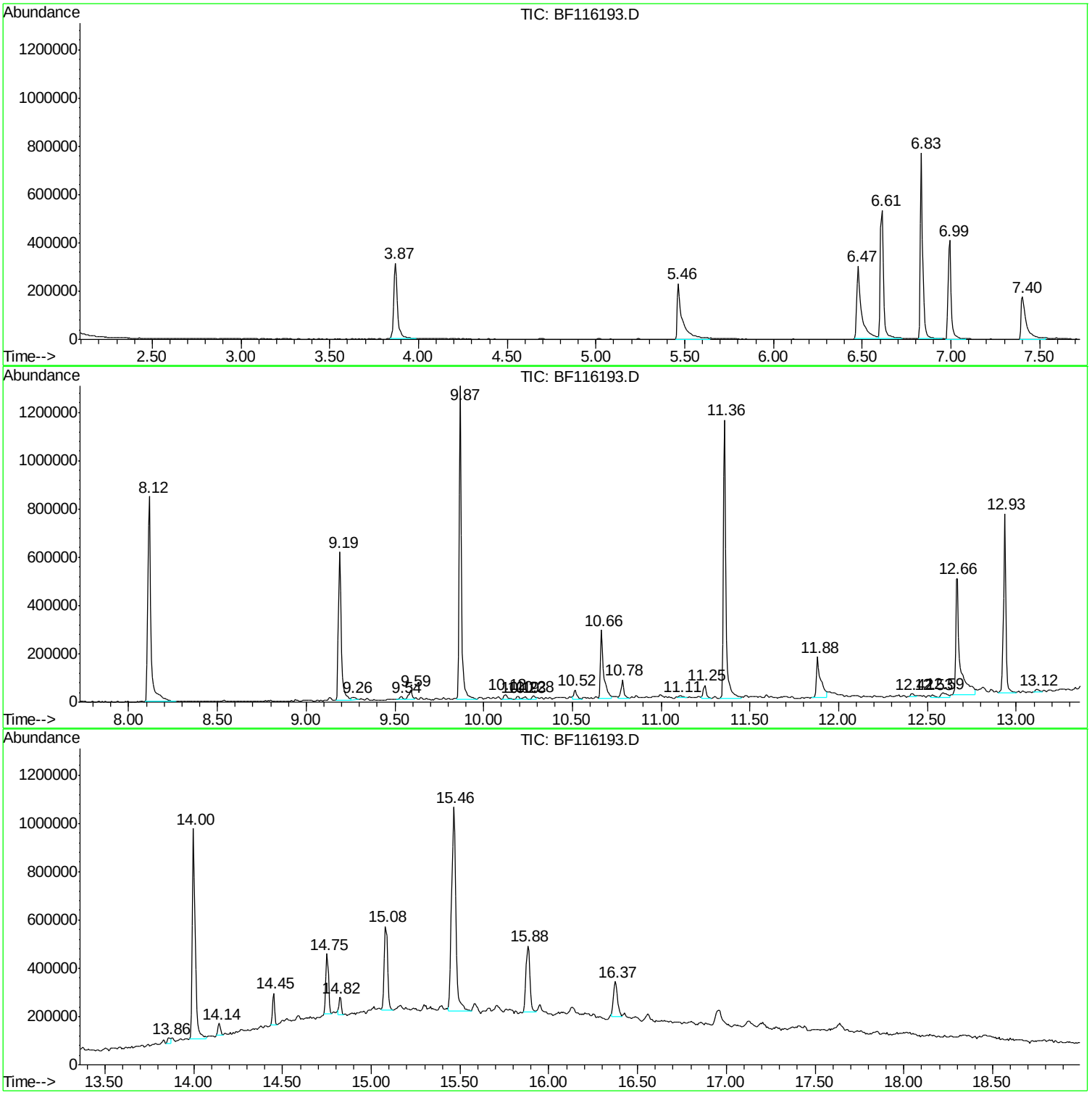
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

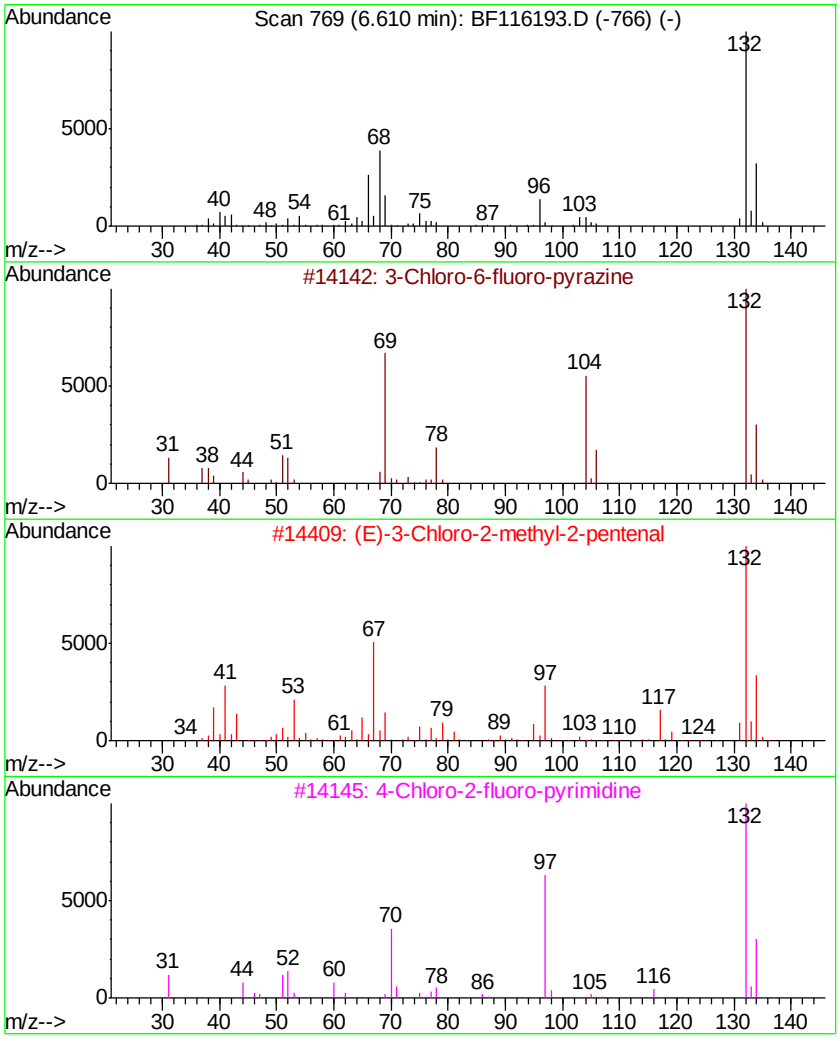
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

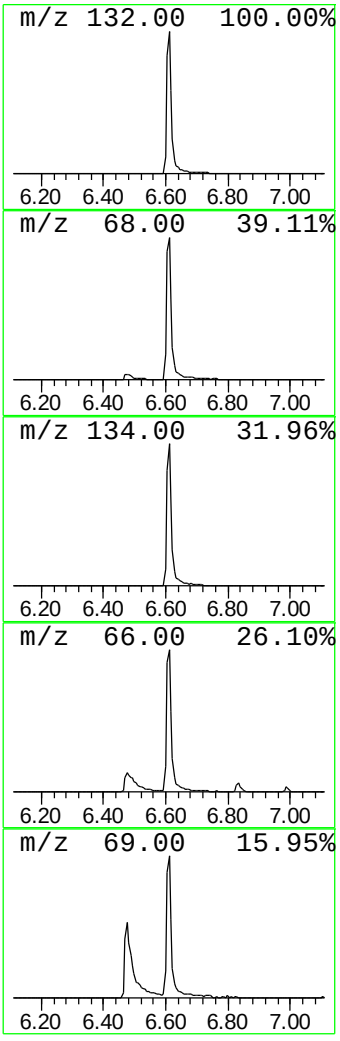
**********

Peak Number 2 unknown6.61 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.61 | 16.71 ng | 600638 | 1,4-Dichlorobenzene-d4 | 6.83 |

| 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 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 4 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |
| 5 | Xenon | 132 | Xe | 007440-63-3 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

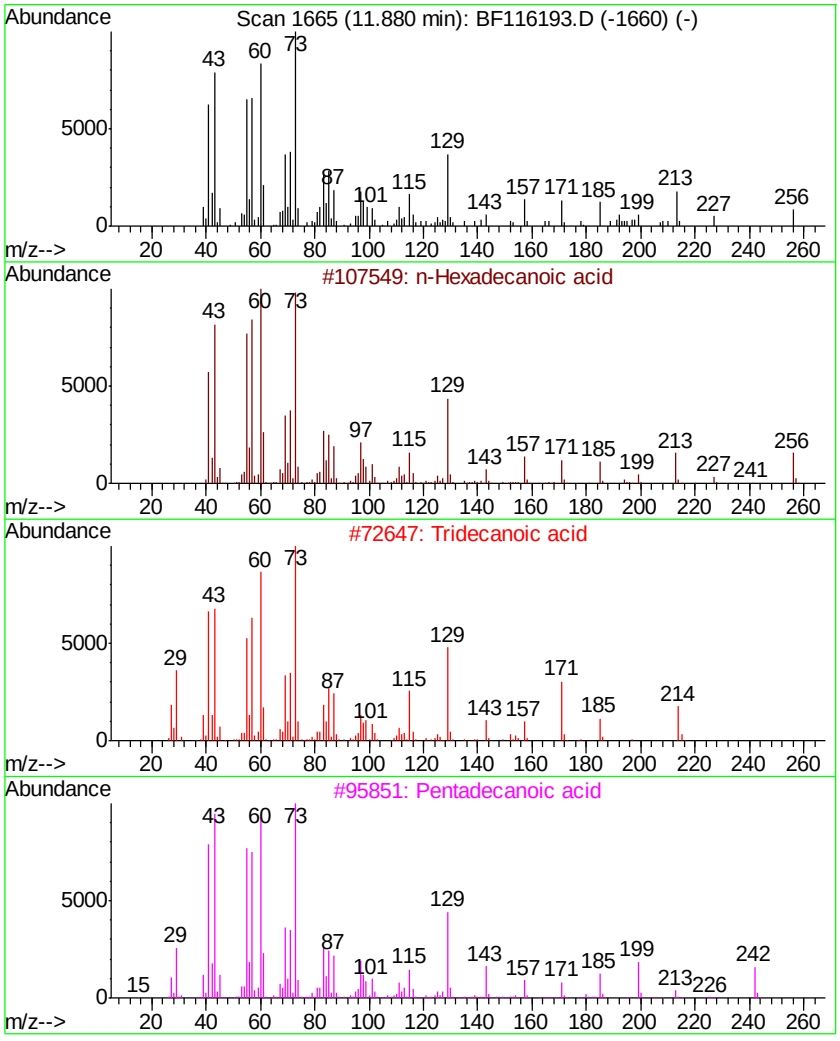
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

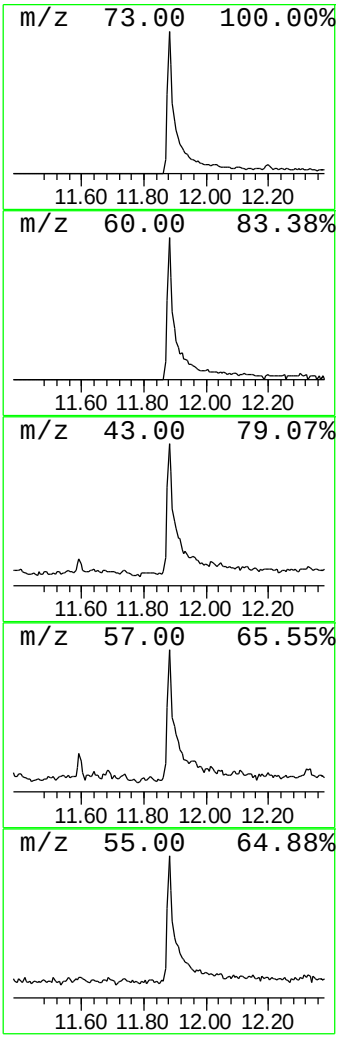
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.88 | 4.61 ng | 290681 | Phenanthrene-d10 | 11.36 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 96 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 5 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 59 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

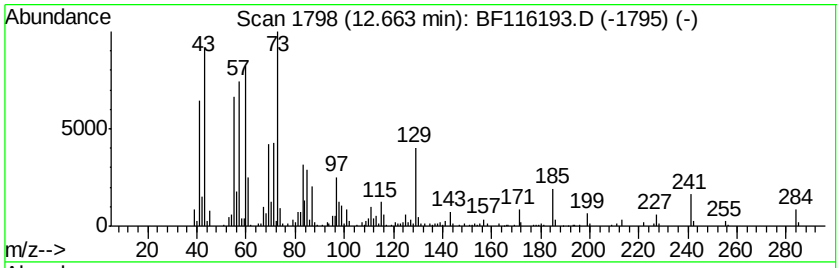
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

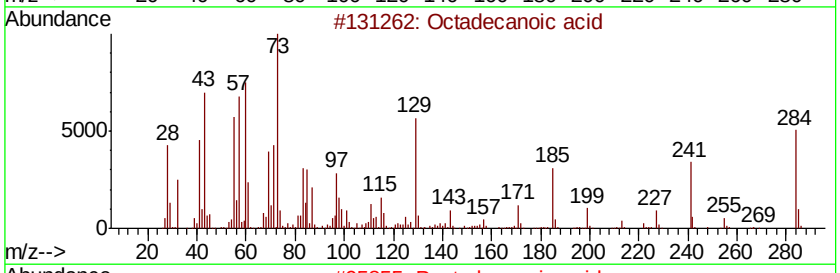
**********

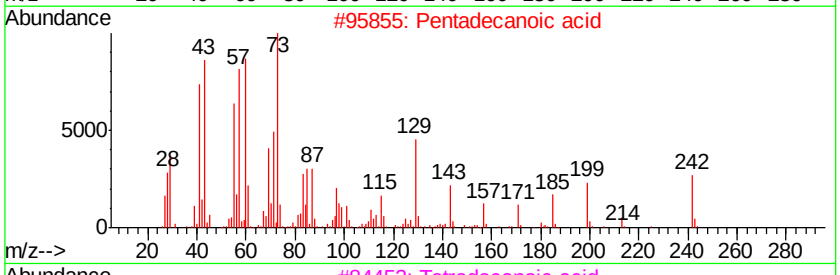
Peak Number 5 Octadecanoic acid Concentration Rank 3

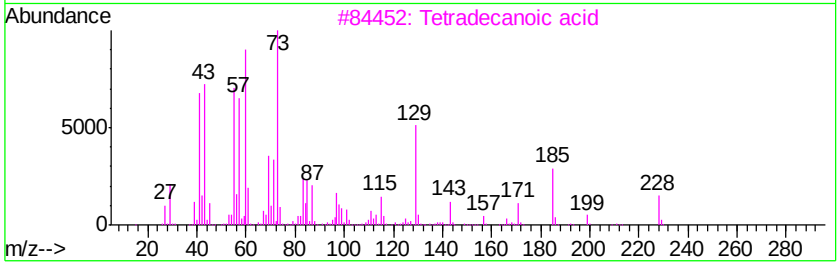
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.66 | 13.19 ng | 830861 | Phenanthrene-d10 | 11.36 |

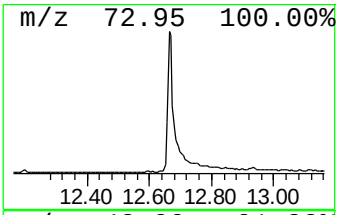
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 90 |
| 4 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 87 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 76 |

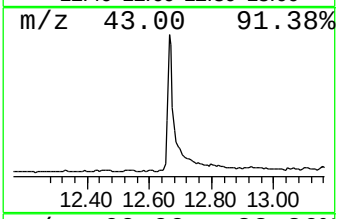


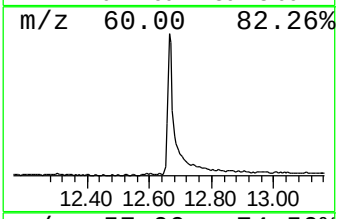



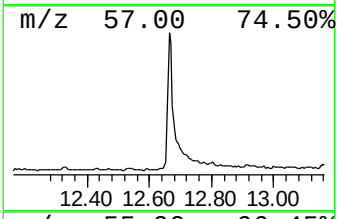



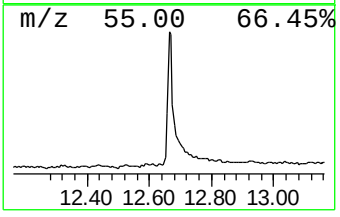



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

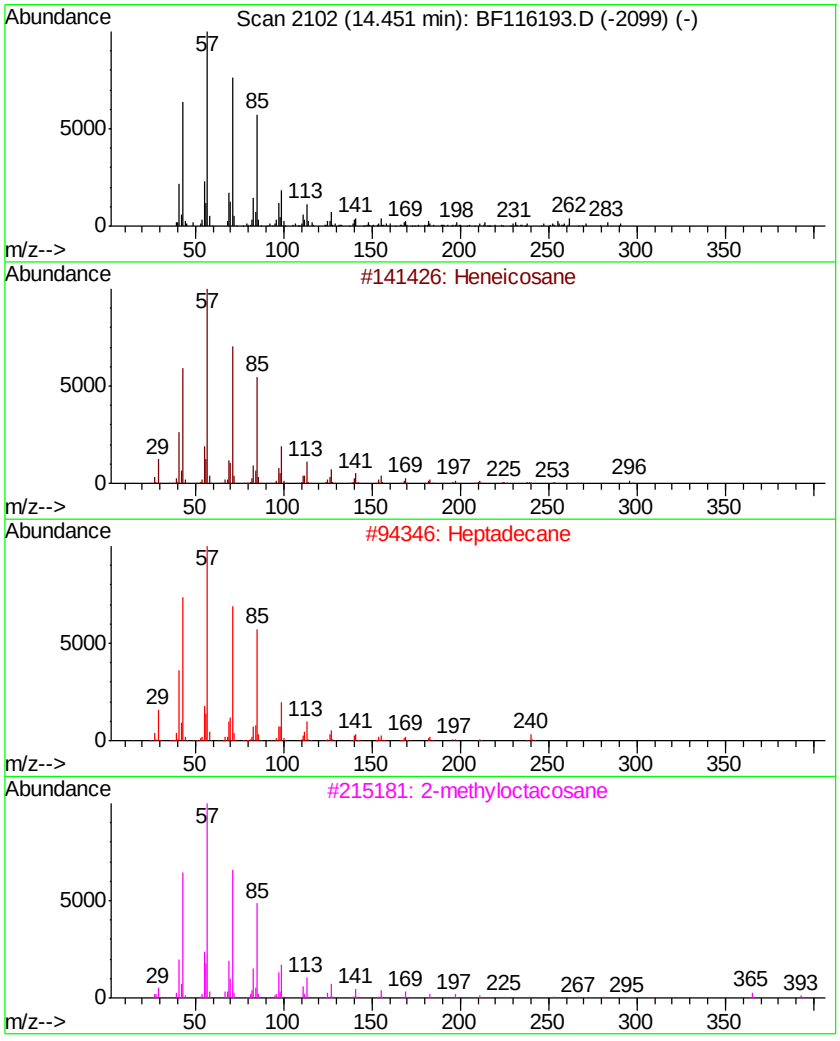
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

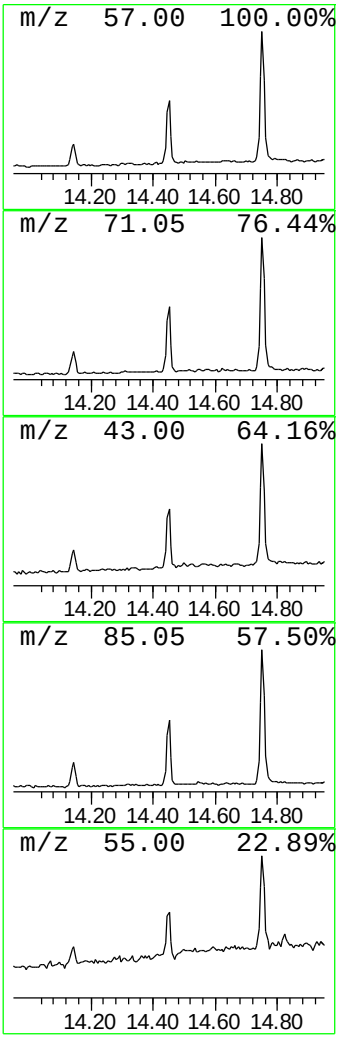
**********

Peak Number 6 Heneicosane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.45 | 2.40 ng | 117042 | Chrysene-d12 | 14.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |
| 3 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 87 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |
| 5 | Eicosane | 282 | C20H42 | 000112-95-8 | 87 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

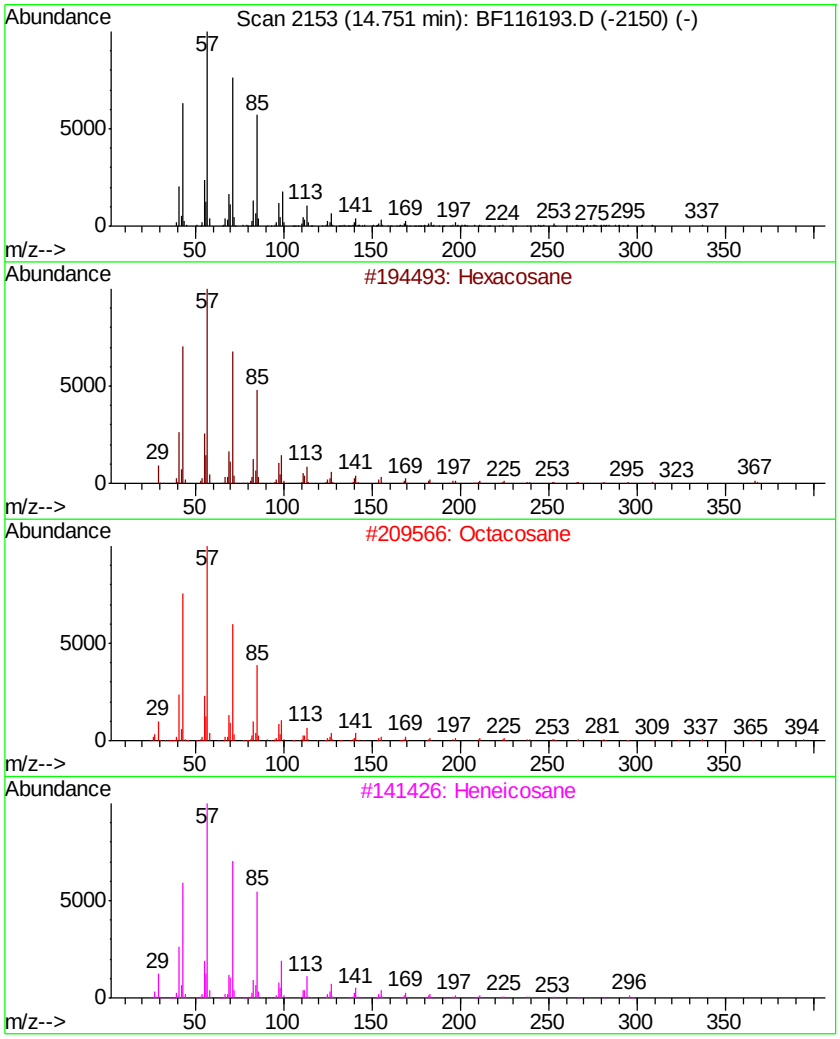
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

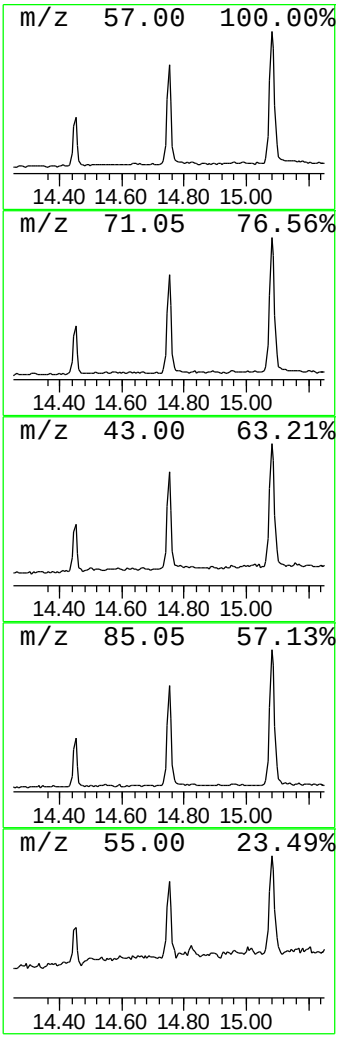
**********

Peak Number 7 Hexacosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.75 | 3.40 ng | 235624 | Perylene-d12 | 15.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 2 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 91 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

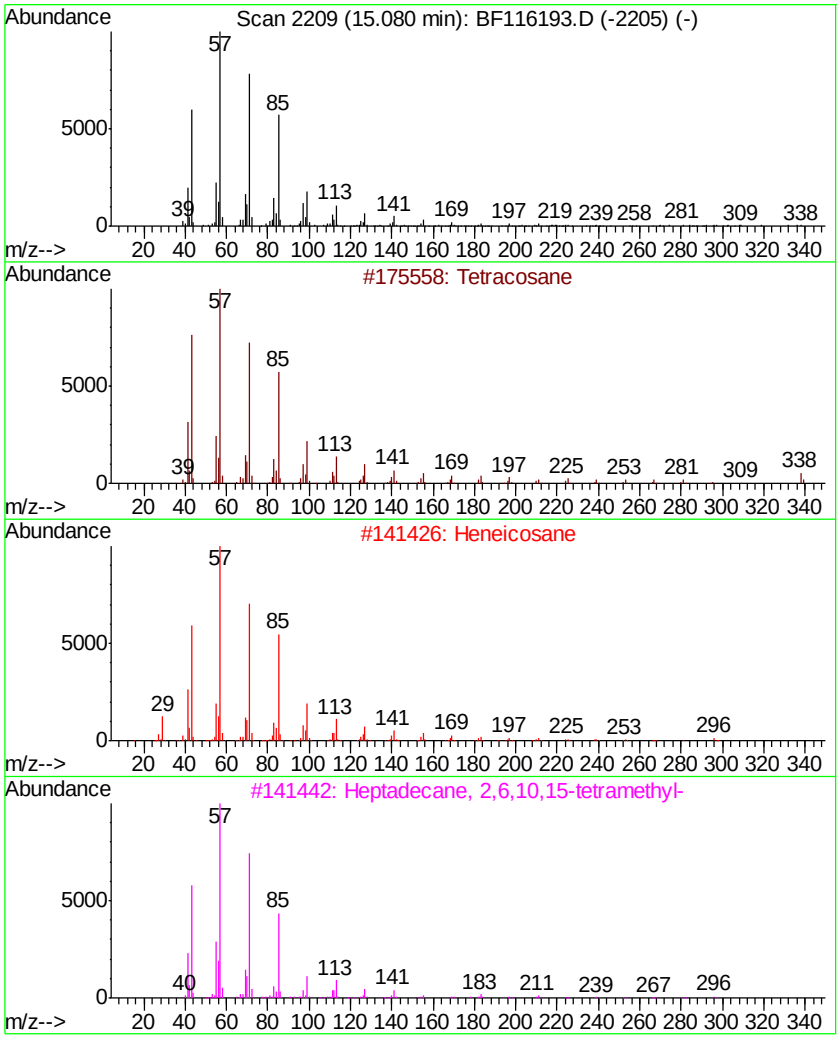
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

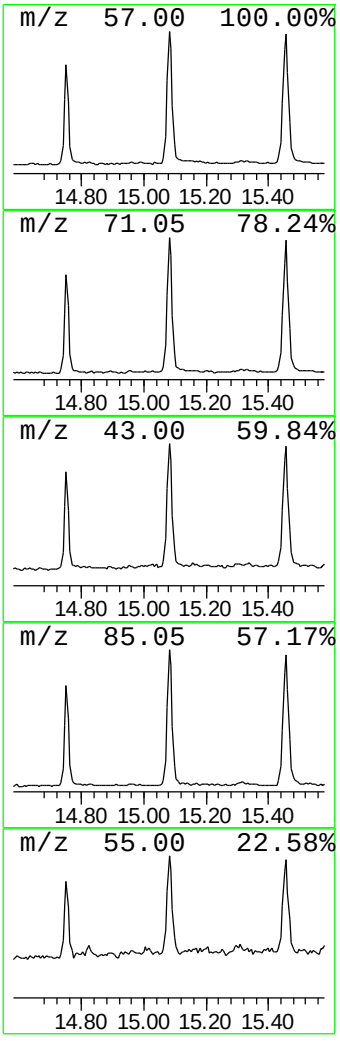
**********

Peak Number 8 Tetracosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.08 | 6.12 ng | 424022 | Perylene-d12 | 15.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 94 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 91 |
| 4 | Octadecane, 1-iodo- | 380 | C18H37I | 000629-93-6 | 86 |
| 5 | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54 | 055282-11-6 | 80 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

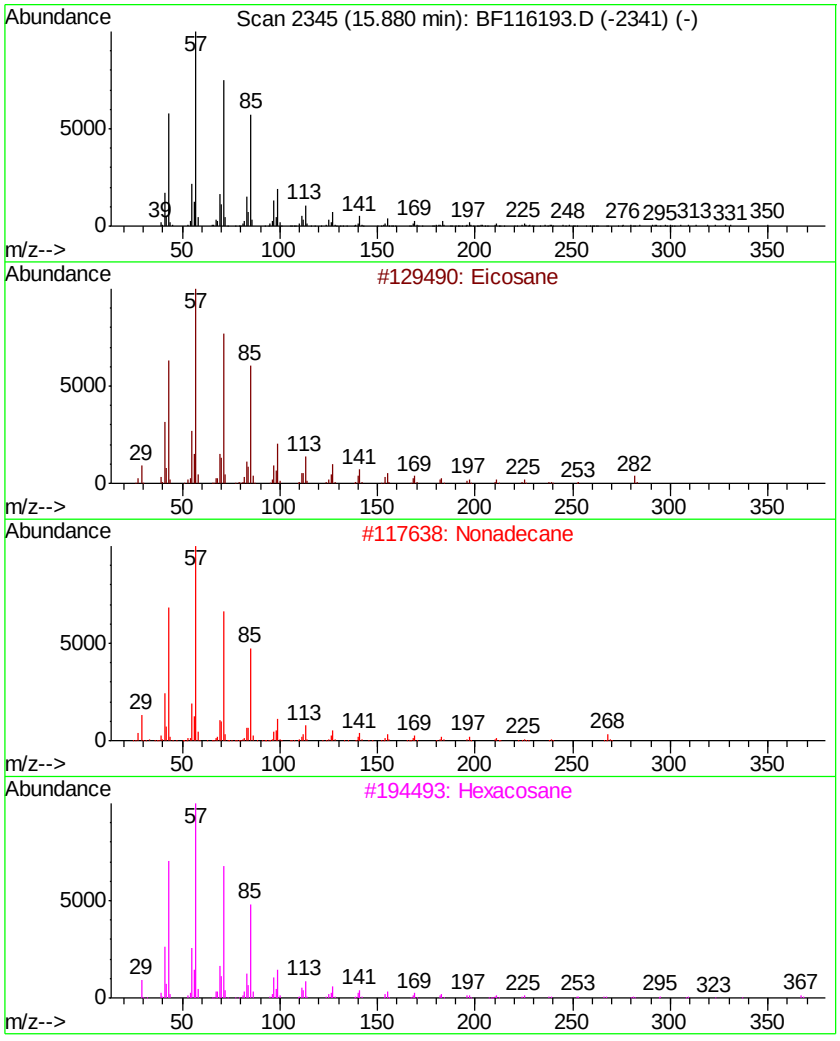
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

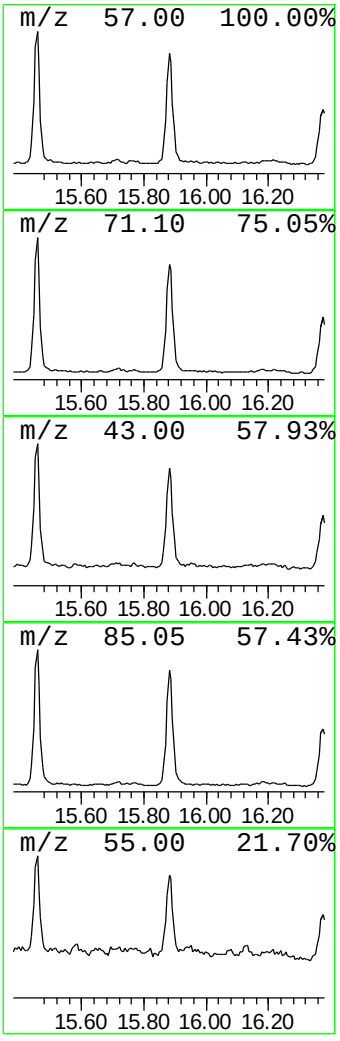
**********

Peak Number 9 Eicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.88 | 5.75 ng | 398748 | Perylene-d12 | 15.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 95 |
| 2 | Nonadecane | 268 | C19H40 | 000629-92-5 | 94 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 5 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

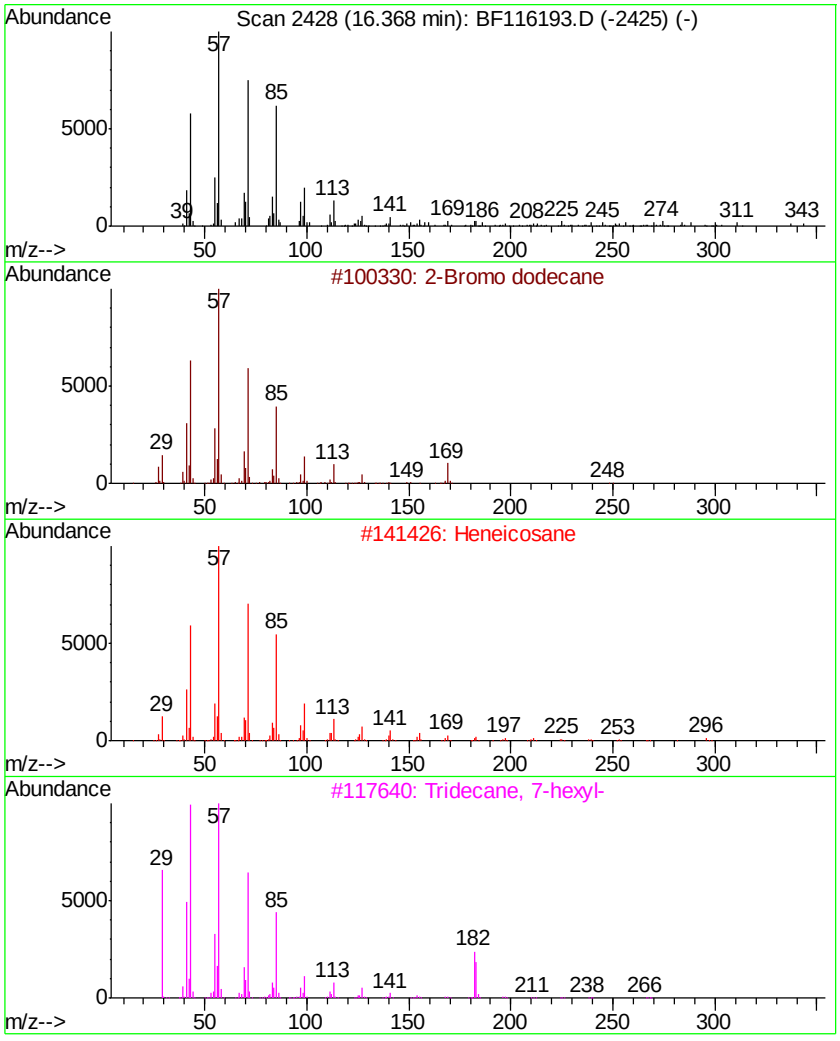
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

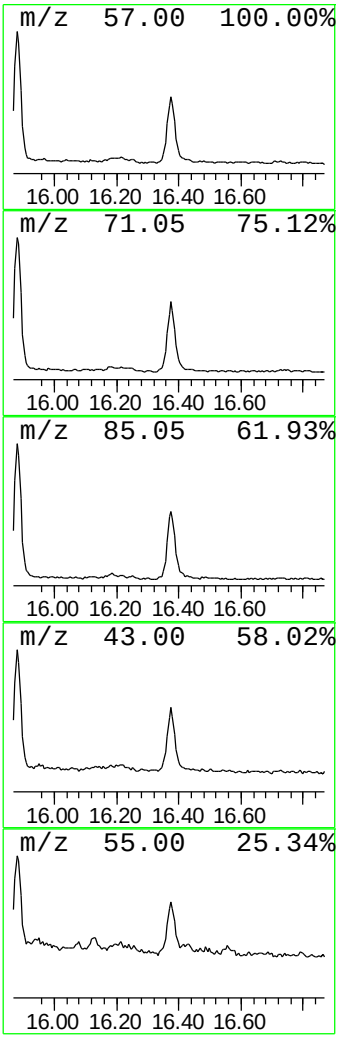
**********

Peak Number 10 2-Bromo dodecane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.37 | 3.51 ng | 243593 | Perylene-d12 | 15.47 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 93 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 3 | Tridecane, 7-hexyl- | 268 | C19H40 | 007225-66-3 | 90 |
| 4 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 90 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081219\
Data File : BF116193.D
Acq On : 12 Aug 2019 15:52
Operator : HP/JU
Sample : K3613-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AU-05-080719-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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 |
| unknown6.61 | 6.61 | 16.7 | ng | 600638 | 1 | 6.83 | 718831 | 20.0 |
| n-Hexadecanoic acid | 11.88 | 4.6 | ng | 290681 | 4 | 11.36 | 1260270 | 20.0 |
| Octadecanoic acid | 12.66 | 13.2 | ng | 830861 | 4 | 11.36 | 1260270 | 20.0 |
| Heneicosane | 14.45 | 2.4 | ng | 117042 | 5 | 14.00 | 974785 | 20.0 |
| Hexacosane | 14.75 | 3.4 | ng | 235624 | 6 | 15.47 | 1386620 | 20.0 |
| Tetracosane | 15.08 | 6.1 | ng | 424022 | 6 | 15.47 | 1386620 | 20.0 |
| Eicosane | 15.88 | 5.8 | ng | 398748 | 6 | 15.47 | 1386620 | 20.0 |
| 2-Bromo dodecane | 16.37 | 3.5 | ng | 243593 | 6 | 15.47 | 1386620 | 20.0 |