LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

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-BF012519.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 | 5.475 | 572 | 576 | 595 | rBV | 306276 | 457357 | 3.61% | 0.945% |
| 2 | 6.487 | 745 | 748 | 764 | rBV | 339687 | 496521 | 3.92% | 1.026% |
| 3 | 6.616 | 766 | 770 | 776 | rVV | 494104 | 512774 | 4.05% | 1.060% |
| 4 | 6.834 | 804 | 807 | 814 | rBV | 674568 | 594081 | 4.69% | 1.228% |
| 5 | 6.992 | 829 | 834 | 841 | rBV | 451032 | 430085 | 3.39% | 0.889% |
| 6 | 7.398 | 900 | 903 | 906 | rBV | 253486 | 245248 | 1.94% | 0.507% |
| 7 | 7.428 | 906 | 908 | 912 | rVB | 169773 | 131132 | 1.03% | 0.271% |
| 8 | 8.098 | 1019 | 1022 | 1023 | rBV | 279243 | 239492 | 1.89% | 0.495% |
| 9 | 8.116 | 1023 | 1025 | 1031 | rVV | 751646 | 739002 | 5.83% | 1.528% |
| 10 | 8.175 | 1031 | 1035 | 1037 | rVB2 | 119185 | 135415 | 1.07% | 0.280% |
| 11 | 8.404 | 1070 | 1074 | 1081 | rBV4 | 98315 | 137768 | 1.09% | 0.285% |
| 12 | 8.704 | 1122 | 1125 | 1129 | rBV | 426252 | 350781 | 2.77% | 0.725% |
| 13 | 9.069 | 1183 | 1187 | 1191 | rBV3 | 93339 | 128736 | 1.02% | 0.266% |
| 14 | 9.192 | 1205 | 1208 | 1212 | rBV | 563162 | 521939 | 4.12% | 1.079% |
| 15 | 9.269 | 1217 | 1221 | 1224 | rBV | 514953 | 439376 | 3.47% | 0.908% |
| 16 | 9.586 | 1272 | 1275 | 1278 | rBV3 | 175346 | 221255 | 1.75% | 0.457% |
| 17 | 9.798 | 1308 | 1311 | 1314 | rVB | 540908 | 393581 | 3.11% | 0.814% |
| 18 | 9.875 | 1320 | 1324 | 1328 | rVB | 806227 | 684562 | 5.40% | 1.415% |
| 19 | 10.122 | 1362 | 1366 | 1370 | rBV5 | 119928 | 153702 | 1.21% | 0.318% |
| 20 | 10.298 | 1390 | 1396 | 1399 | rBV | 566120 | 506337 | 4.00% | 1.047% |
| 21 | 10.428 | 1411 | 1418 | 1427 | rBV | 49278 | 166287 | 1.31% | 0.344% |
| 22 | 10.516 | 1429 | 1433 | 1439 | rVB | 168609 | 247061 | 1.95% | 0.511% |
| 23 | 10.669 | 1456 | 1459 | 1469 | rBV | 276773 | 335166 | 2.65% | 0.693% |
| 24 | 10.769 | 1473 | 1476 | 1485 | rVB | 504856 | 564729 | 4.46% | 1.167% |
| 25 | 11.216 | 1549 | 1552 | 1555 | rBV | 403553 | 351235 | 2.77% | 0.726% |
| 26 | 11.245 | 1555 | 1557 | 1563 | rVB2 | 162478 | 195844 | 1.55% | 0.405% |
| 27 | 11.363 | 1574 | 1577 | 1580 | rBV | 779625 | 714283 | 5.64% | 1.476% |
| 28 | 11.386 | 1580 | 1581 | 1588 | rVB2 | 133580 | 146680 | 1.16% | 0.303% |
| 29 | 11.645 | 1622 | 1625 | 1627 | rBV | 379113 | 299888 | 2.37% | 0.620% |
| 30 | 11.751 | 1638 | 1643 | 1646 | rBV | 4407602 | 4012108 | 31.66% | 8.293% |
| 31 | 11.886 | 1663 | 1666 | 1673 | rVB3 | 147614 | 178485 | 1.41% | 0.369% |
| 32 | 12.051 | 1689 | 1694 | 1701 | rVB | 324203 | 326660 | 2.58% | 0.675% |
| 33 | 12.445 | 1754 | 1761 | 1762 | rBV | 8449888 | 11020865 | 86.98% | 22.780% |
| 34 | 12.469 | 1762 | 1765 | 1770 | rVV2 | 10185123 | 12670844 | 100.00% | 26.191% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 12.539 | 1774 | 1777 | 1780 | rVB | 2345317 | 1825404 | 14.41% | 3.773% |
| 36 | 12.598 | 1780 | 1787 | 1789 | rBV3 | 466337 | 827240 | 6.53% | 1.710% |
| 37 | 12.774 | 1813 | 1817 | 1820 | rBV | 422714 | 419372 | 3.31% | 0.867% |
| 38 | 12.816 | 1820 | 1824 | 1830 | rVB2 | 306256 | 389635 | 3.08% | 0.805% |
| 39 | 12.945 | 1843 | 1846 | 1849 | rVB | 607107 | 498866 | 3.94% | 1.031% |
| 40 | 13.098 | 1869 | 1872 | 1874 | rBV | 283139 | 296299 | 2.34% | 0.612% |
| 41 | 13.121 | 1874 | 1876 | 1881 | rVV4 | 199527 | 345878 | 2.73% | 0.715% |
| 42 | 13.169 | 1881 | 1884 | 1885 | rVV | 283106 | 253479 | 2.00% | 0.524% |
| 43 | 13.180 | 1885 | 1886 | 1890 | rVB | 302117 | 249851 | 1.97% | 0.516% |
| 44 | 13.263 | 1896 | 1900 | 1904 | rBV | 340185 | 347390 | 2.74% | 0.718% |
| 45 | 13.369 | 1915 | 1918 | 1922 | rBV3 | 179112 | 181804 | 1.43% | 0.376% |
| 46 | 13.510 | 1939 | 1942 | 1946 | rBV | 173624 | 149630 | 1.18% | 0.309% |
| 47 | 13.839 | 1995 | 1998 | 2001 | rBV | 176087 | 155348 | 1.23% | 0.321% |
| 48 | 13.927 | 2010 | 2013 | 2021 | rBV | 334853 | 348039 | 2.75% | 0.719% |
| 49 | 14.016 | 2024 | 2028 | 2031 | rBV | 744153 | 738087 | 5.83% | 1.526% |
| 50 | 14.151 | 2048 | 2051 | 2054 | rBV | 181357 | 179506 | 1.42% | 0.371% |
| 51 | 14.457 | 2099 | 2103 | 2106 | rBV2 | 253342 | 303245 | 2.39% | 0.627% |
| 52 | 14.545 | 2116 | 2118 | 2122 | rBV | 145979 | 145888 | 1.15% | 0.302% |
| 53 | 14.763 | 2152 | 2155 | 2158 | rBV | 194698 | 181920 | 1.44% | 0.376% |
| 54 | 14.880 | 2171 | 2175 | 2184 | rVB | 497575 | 756704 | 5.97% | 1.564% |
| 55 | 15.098 | 2209 | 2212 | 2221 | rVB | 257062 | 362444 | 2.86% | 0.749% |
| 56 | 15.498 | 2273 | 2280 | 2284 | rVB2 | 367476 | 673796 | 5.32% | 1.393% |

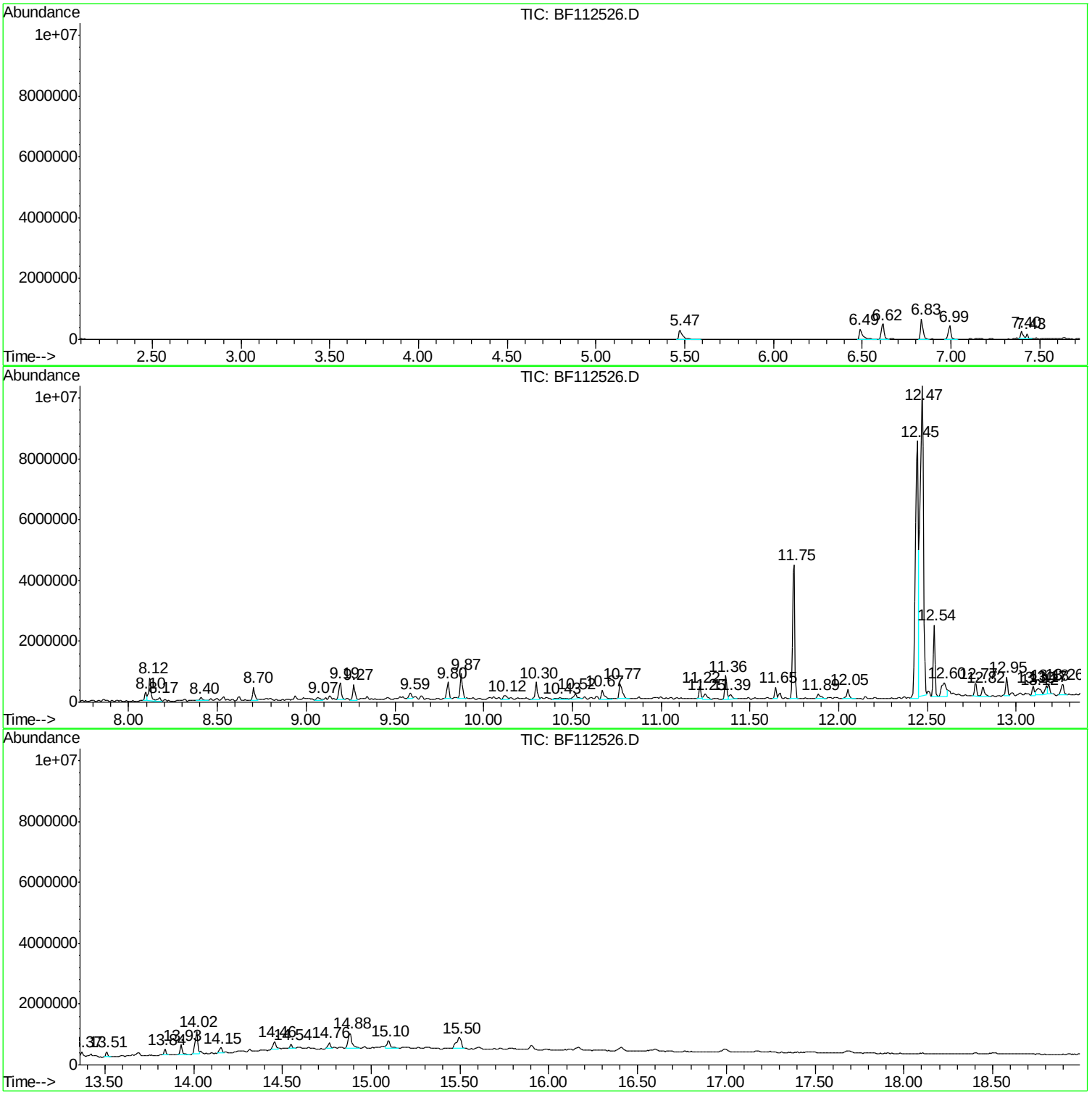
Sum of corrected areas: 48379104

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

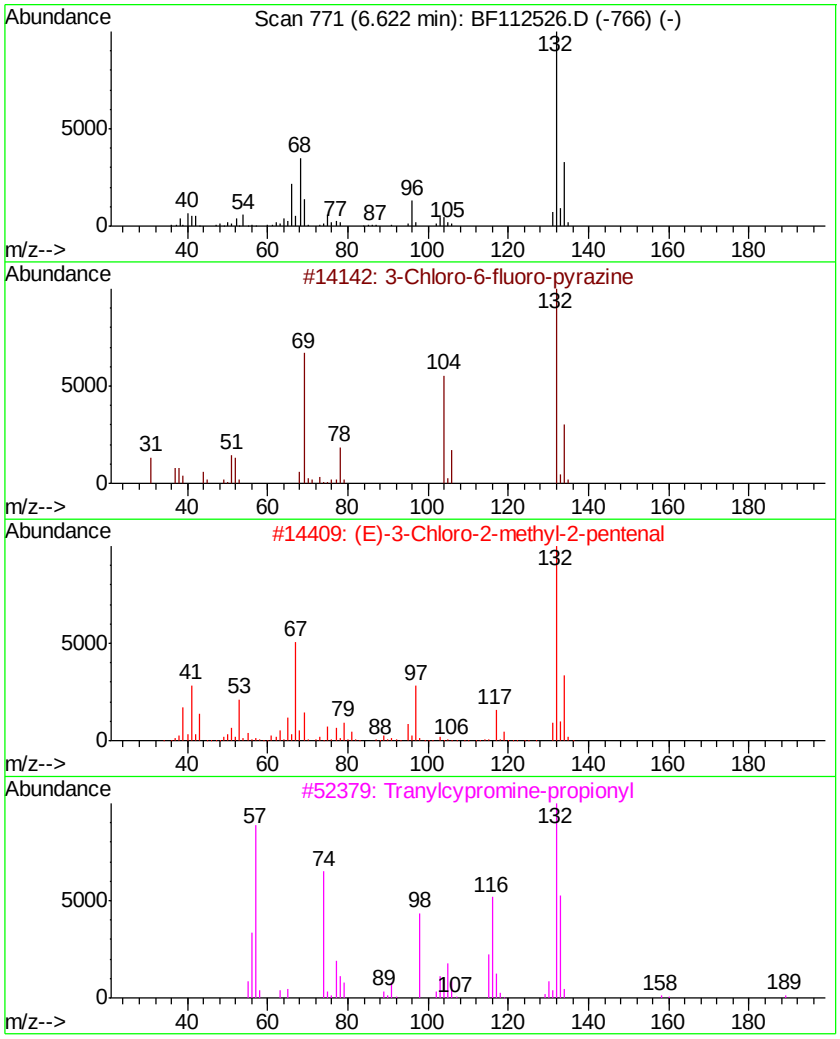
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

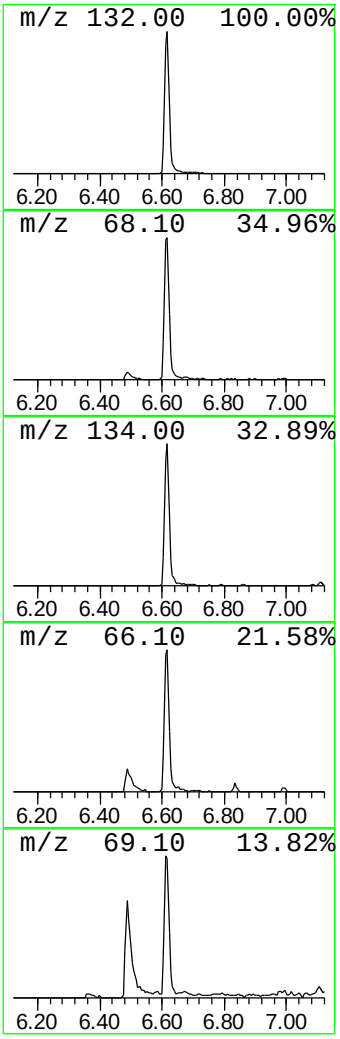
**********

Peak Number 1 unknown6.62 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.62 | 17.26 ng | 512774 | 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 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 16 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 16 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

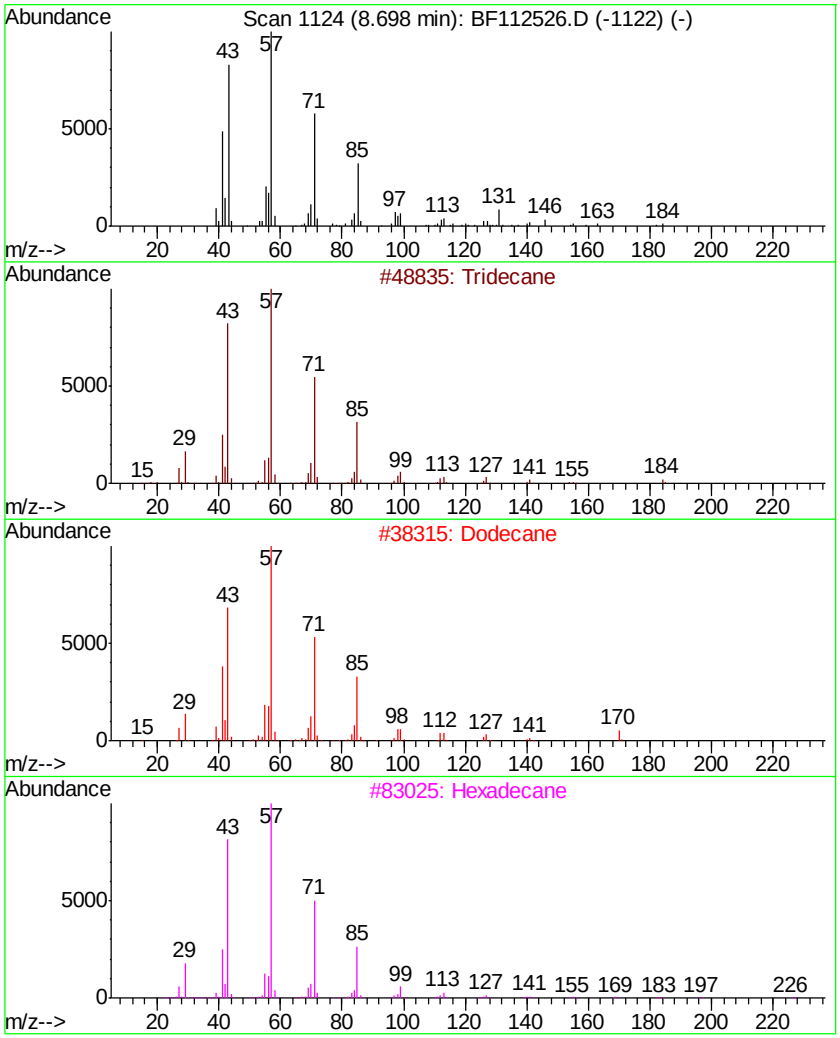
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

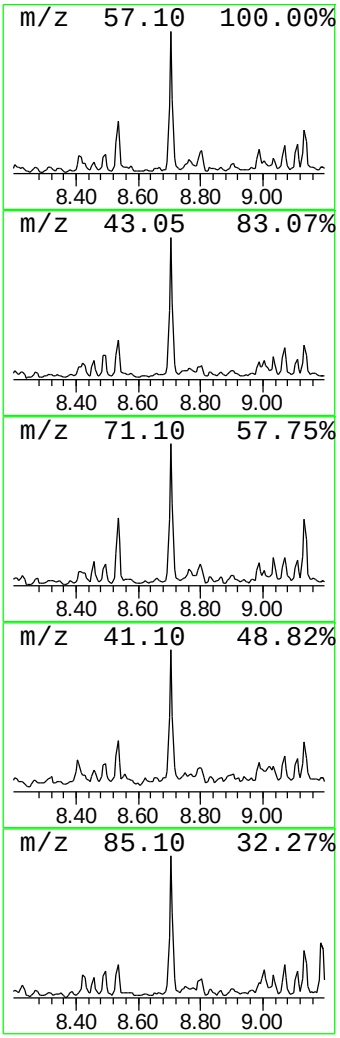
**********

Peak Number 3 Tridecane Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.70 | 9.49 ng | 350781 | Naphthalene-d8 | 8.12 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecane | 184 | C13H28 | 000629-50-5 | 87 |
| 2 | Dodecane | 170 | C12H26 | 000112-40-3 | 80 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 80 |
| 4 | Tetradecane | 198 | C14H30 | 000629-59-4 | 80 |
| 5 | Undecane, 2,3-dimethyl- | 184 | C13H28 | 017312-77-5 | 80 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

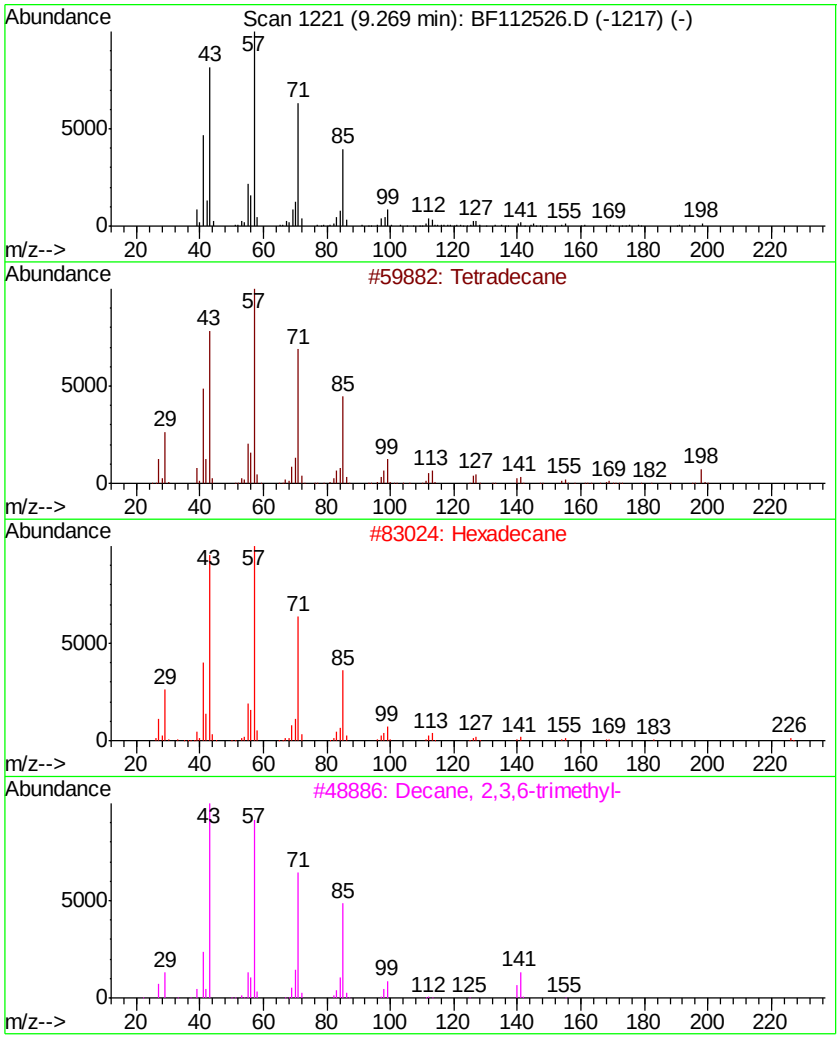
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

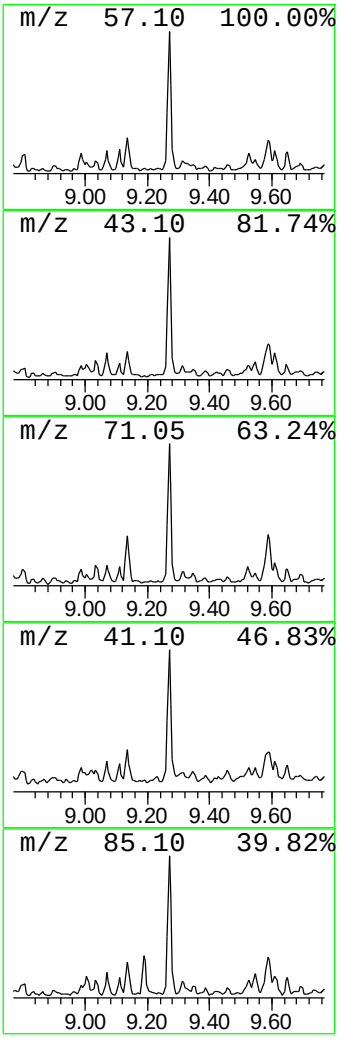
**********

Peak Number 4 Tetradecane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.27 | 12.84 ng | 439376 | Acenaphthene-d10 | 9.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecane | 198 | C14H30 | 000629-59-4 | 97 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 87 |
| 3 | Decane, 2,3,6-trimethyl- | 184 | C13H28 | 062238-12-4 | 86 |
| 4 | Tridecane | 184 | C13H28 | 000629-50-5 | 86 |
| 5 | Tridecane, 7-propyl- | 226 | C16H34 | 055045-09-5 | 86 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

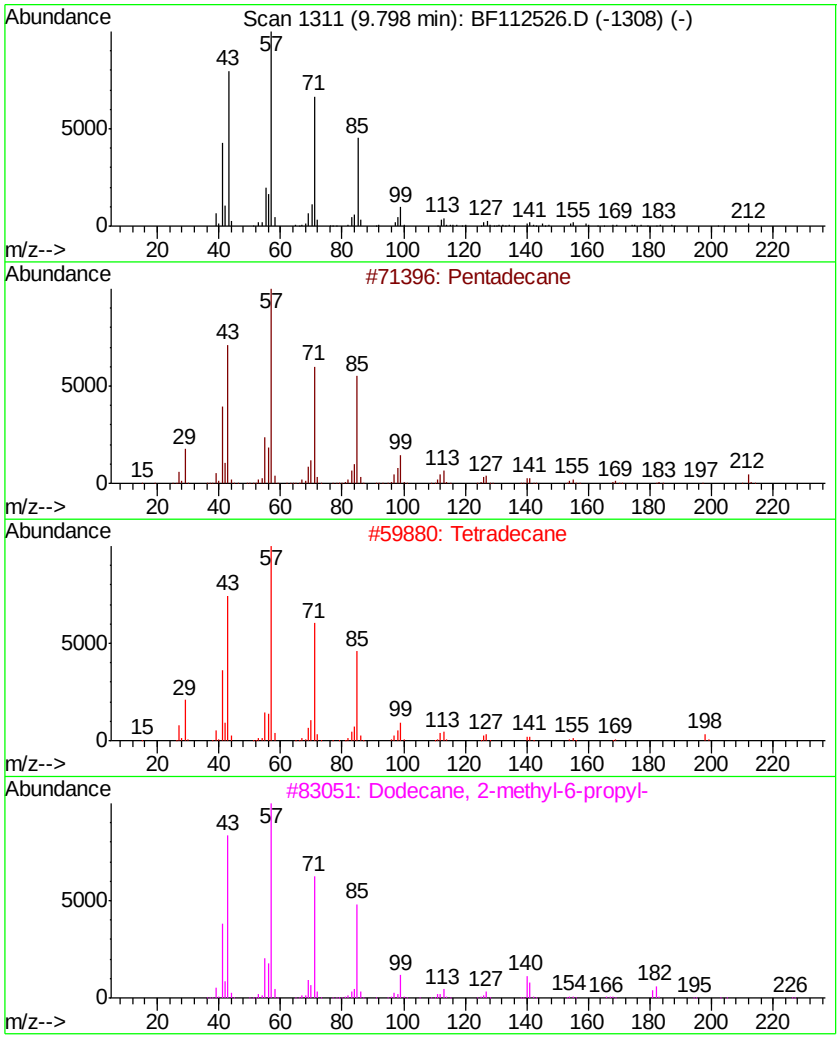
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

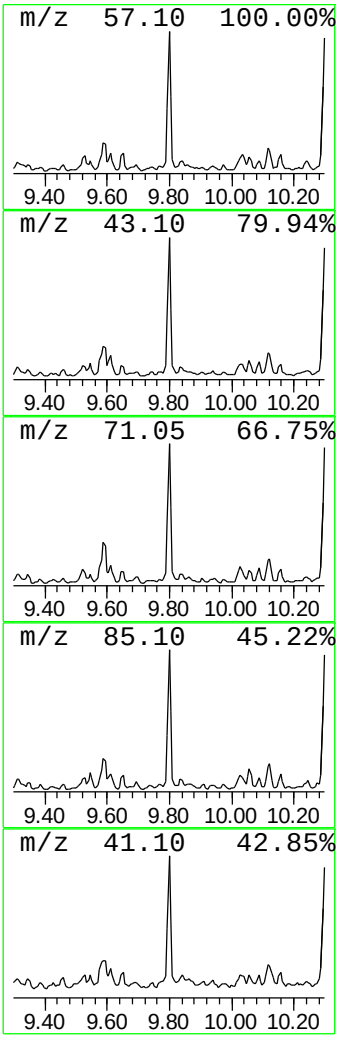
**********

Peak Number 5 Pentadecane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.80 | 11.50 ng | 393581 | Acenaphthene-d10 | 9.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecane | 212 | C15H32 | 000629-62-9 | 93 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 91 |
| 3 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 86 |
| 4 | Tridecane | 184 | C13H28 | 000629-50-5 | 80 |
| 5 | Hexadecane | 226 | C16H34 | 000544-76-3 | 80 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

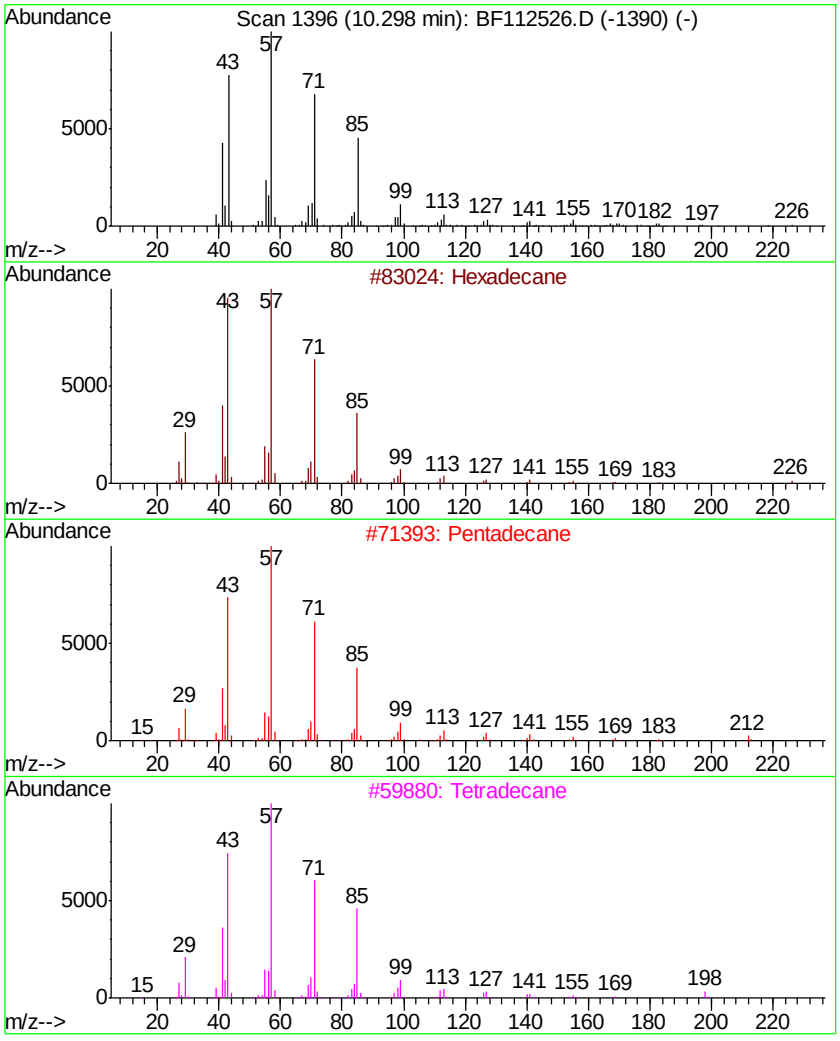
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

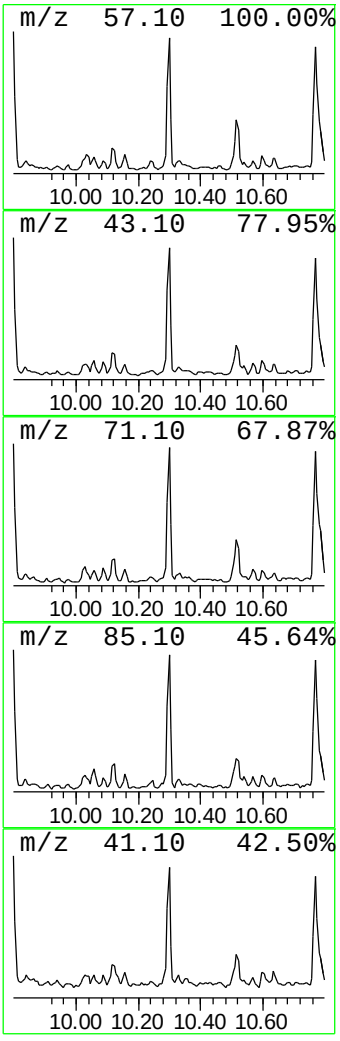
**********

Peak Number 6 Hexadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.30 | 14.79 ng | 506337 | Acenaphthene-d10 | 9.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 96 |
| 2 | Pentadecane | 212 | C15H32 | 000629-62-9 | 91 |
| 3 | Tetradecane | 198 | C14H30 | 000629-59-4 | 91 |
| 4 | Nonadecane | 268 | C19H40 | 000629-92-5 | 91 |
| 5 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

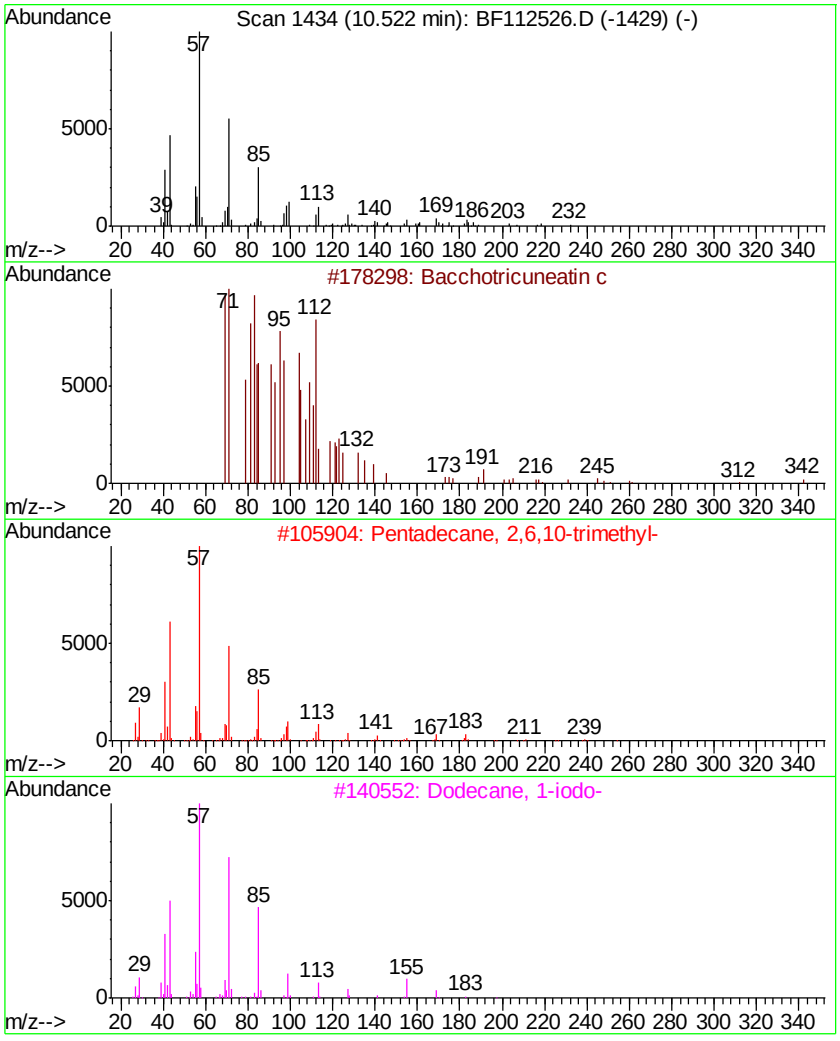
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

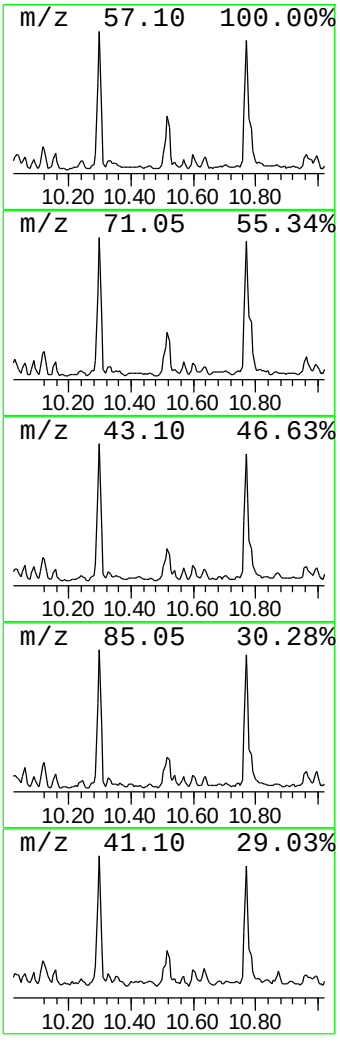
**********

Peak Number 7 Bacchotricuneatin c Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.52 | 7.22 ng | 247061 | Acenaphthene-d10 | 9.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bacchotricuneatin c | 342 | C20H22O5 | 066563-30-2 | 96 |
| 2 | Pentadecane, 2,6,10-trimethyl- | 254 | C18H38 | 003892-00-0 | 86 |
| 3 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 72 |
| 4 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 72 |
| 5 | Undecane, 2,6-dimethyl- | 184 | C13H28 | 017301-23-4 | 68 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

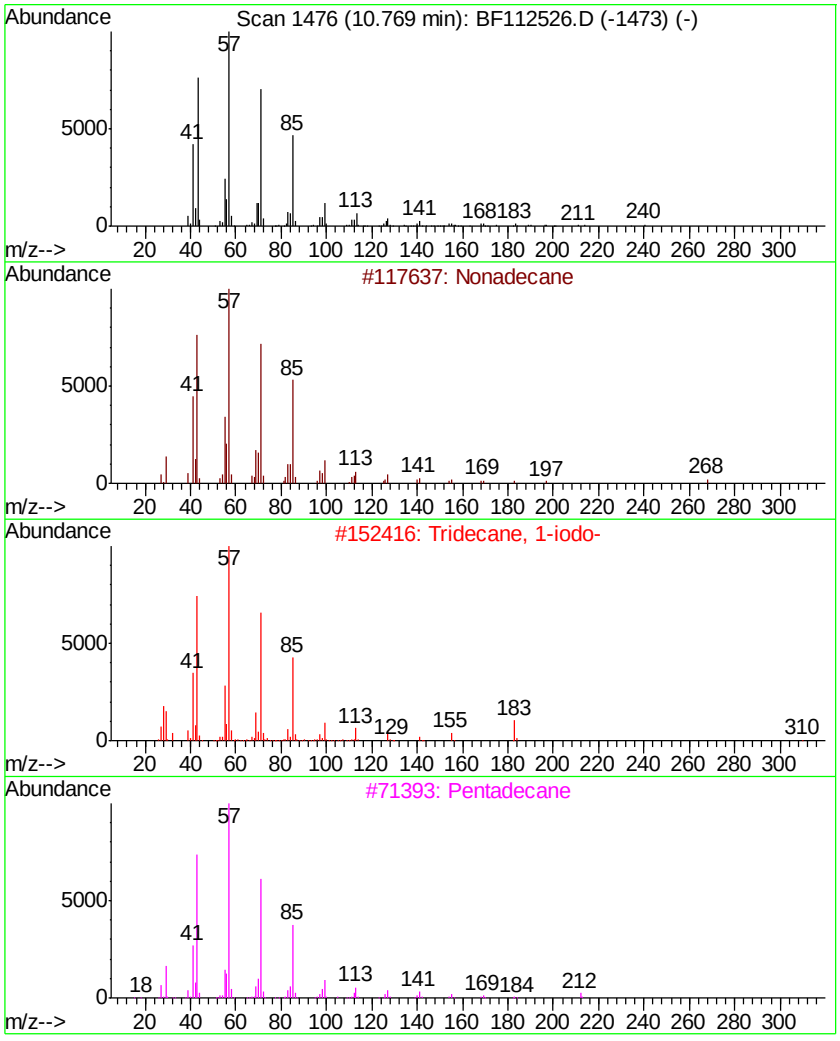
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

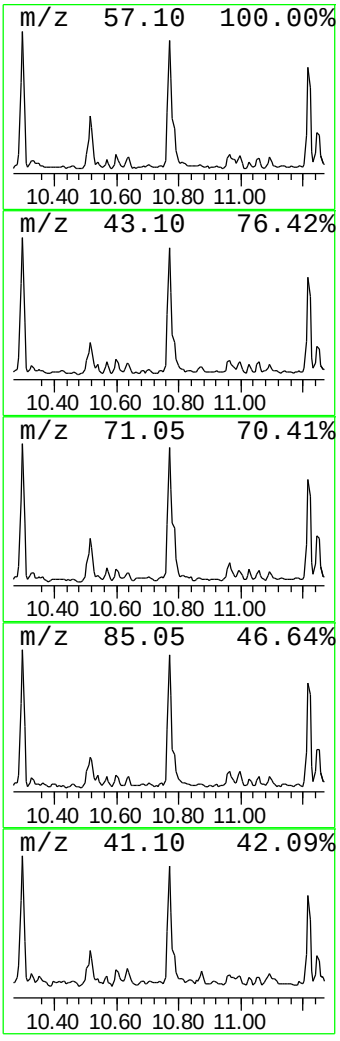
**********

Peak Number 8 Nonadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.77 | 15.81 ng | 564729 | Phenanthrene-d10 | 11.36 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Nonadecane | 268 | C19H40 | 000629-92-5 | 91 |
| 2 | Tridecane, 1-iodo- | 310 | C13H27I | 035599-77-0 | 91 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 91 |
| 4 | Octadecane | 254 | C18H38 | 000593-45-3 | 90 |
| 5 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

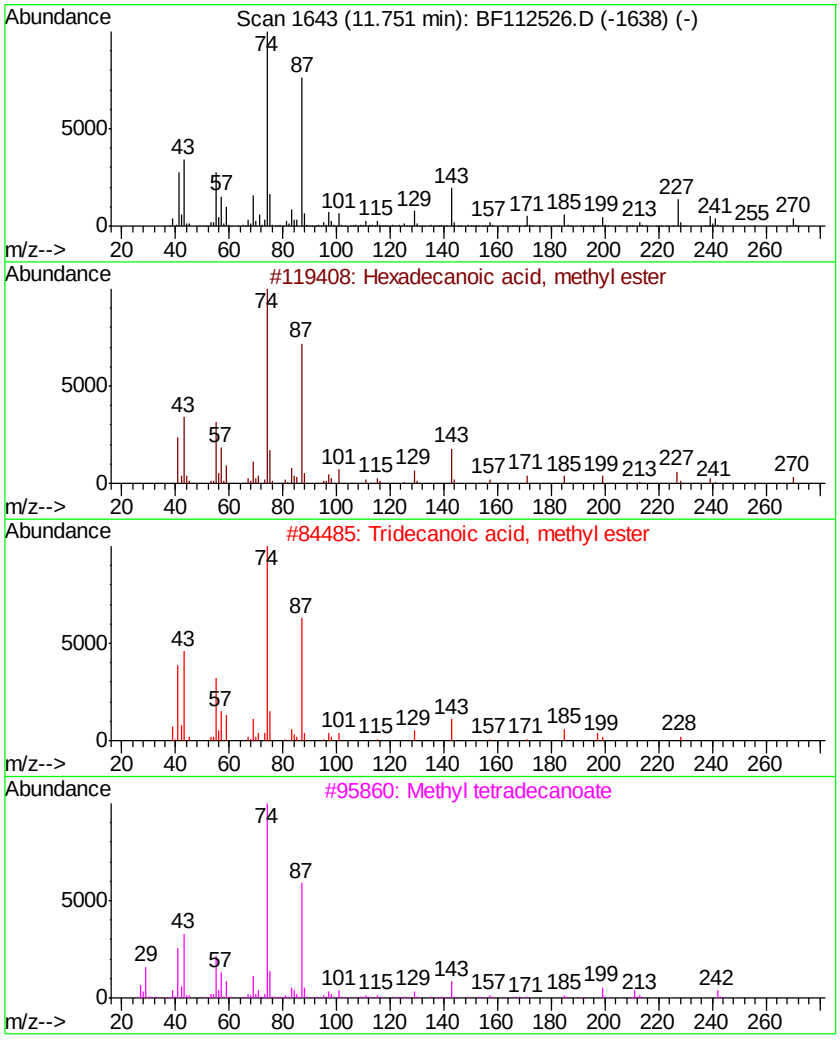
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

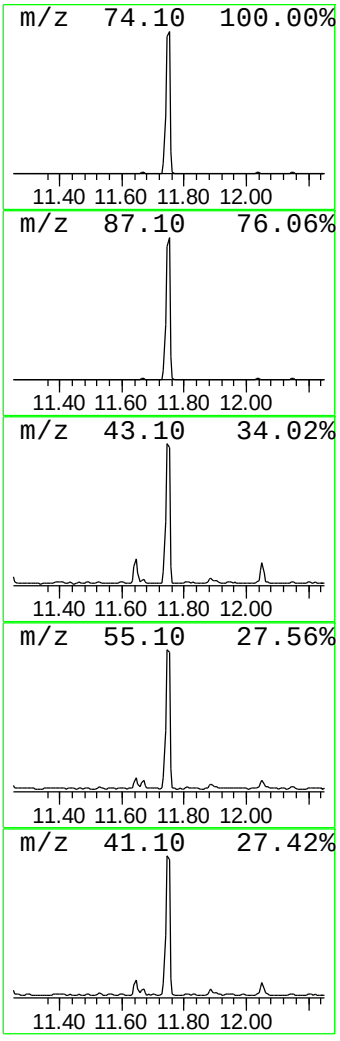
**********

Peak Number 11 Hexadecanoic acid, methyl e... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.75 | 112.34 ng | 4012110 | Phenanthrene-d10 | 11.36 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 98 |
| 2 | Tridecanoic acid, methyl ester | 228 | C14H28O2 | 001731-88-0 | 91 |
| 3 | Methyl tetradecanoate | 242 | C15H30O2 | 000124-10-7 | 81 |
| 4 | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 80 |
| 5 | Methyl 11-methyl-dodecanoate | 228 | C14H28O2 | 1000336-45-1 | 80 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

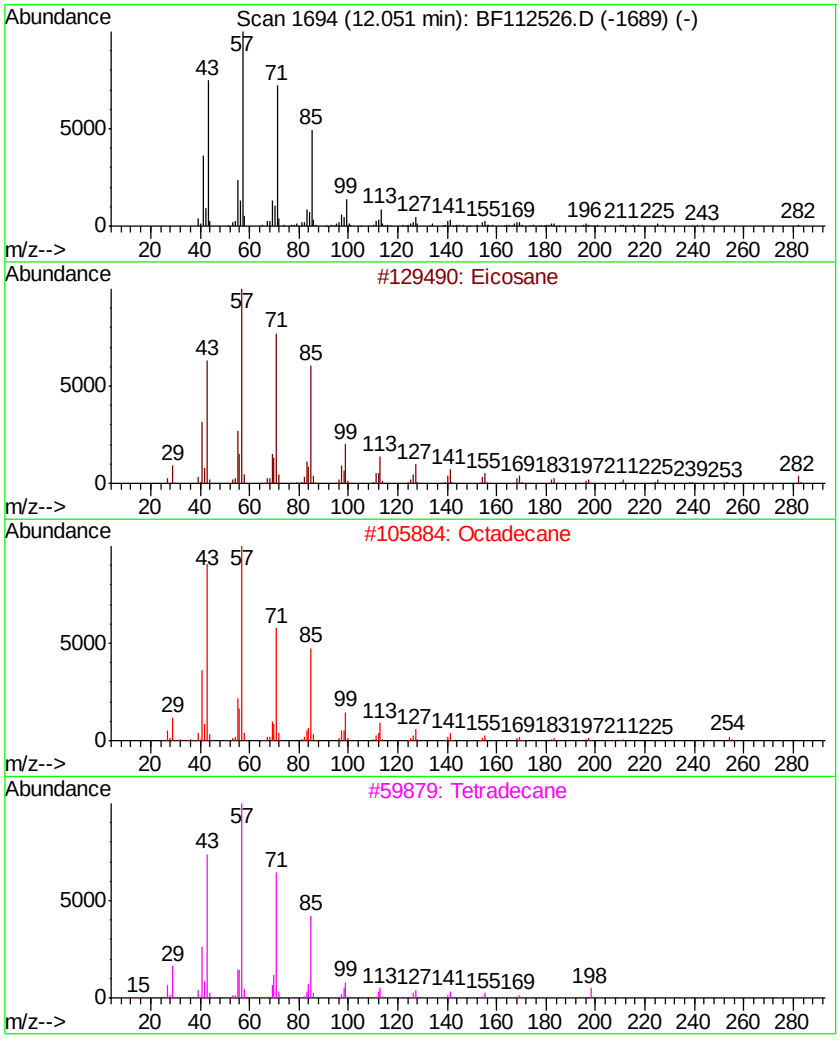
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

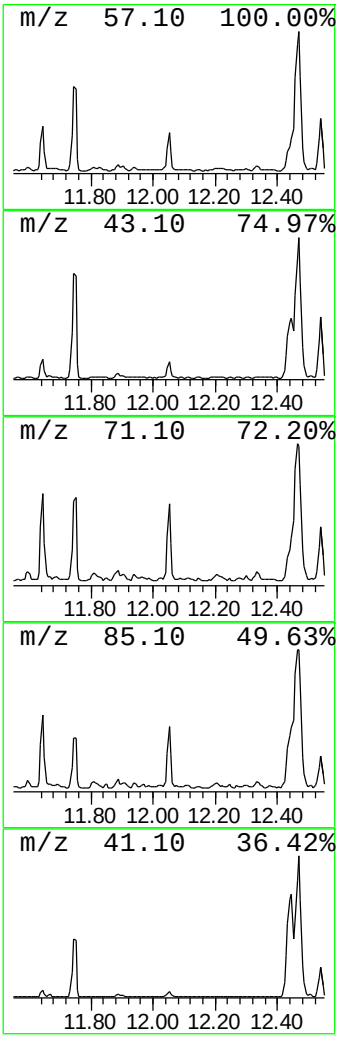
**********

Peak Number 12 Eicosane Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.05 | 9.15 ng | 326660 | Phenanthrene-d10 | 11.36 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 96 |
| 2 | Octadecane | 254 | C18H38 | 000593-45-3 | 91 |
| 3 | Tetradecane | 198 | C14H30 | 000629-59-4 | 91 |
| 4 | Pentadecane | 212 | C15H32 | 000629-62-9 | 91 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

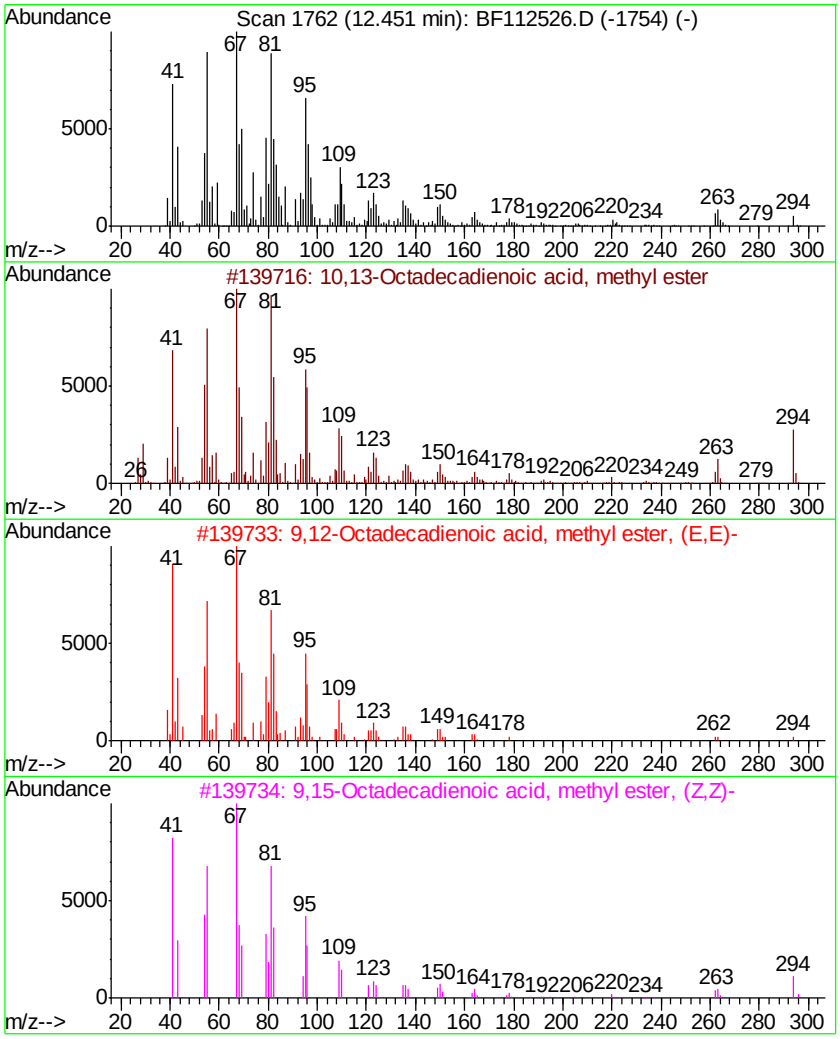
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

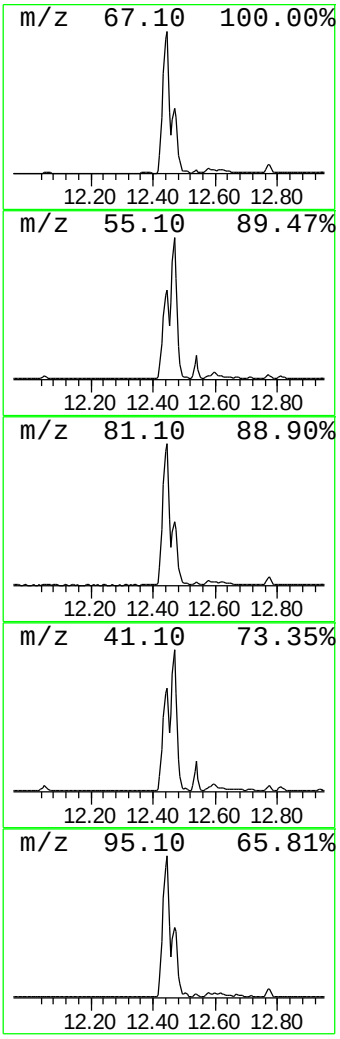
**********

Peak Number 13 10,13-Octadecadienoic acid,... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.45 | 308.59 ng | 11020900 | Phenanthrene-d10 | 11.36 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 10,13-Octadecadienoic acid, meth... | 294 | C19H34O2 | 056554-62-2 | 99 |
| 2 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4 | 99 |
| 3 | 9,15-Octadecadienoic acid, methy... | 294 | C19H34O2 | 017309-05-6 | 99 |
| 4 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002462-85-3 | 99 |
| 5 | 8,11-Octadecadienoic acid, methy... | 294 | C19H34O2 | 056599-58-7 | 99 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

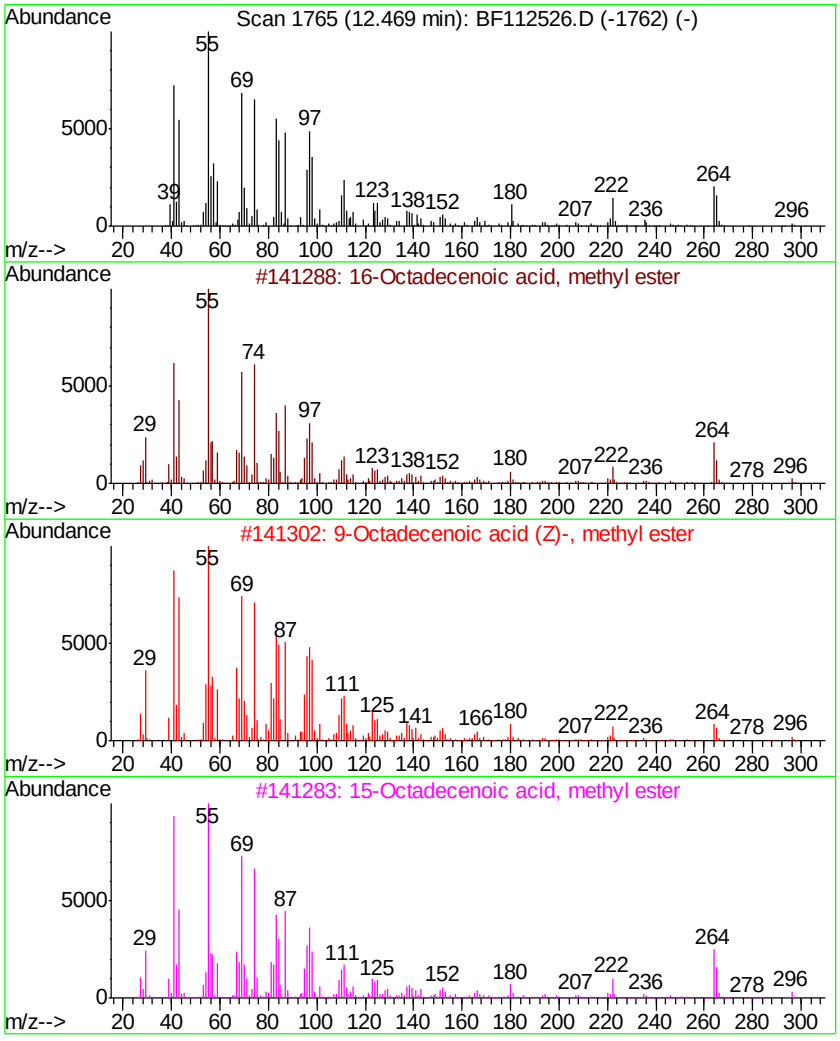
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

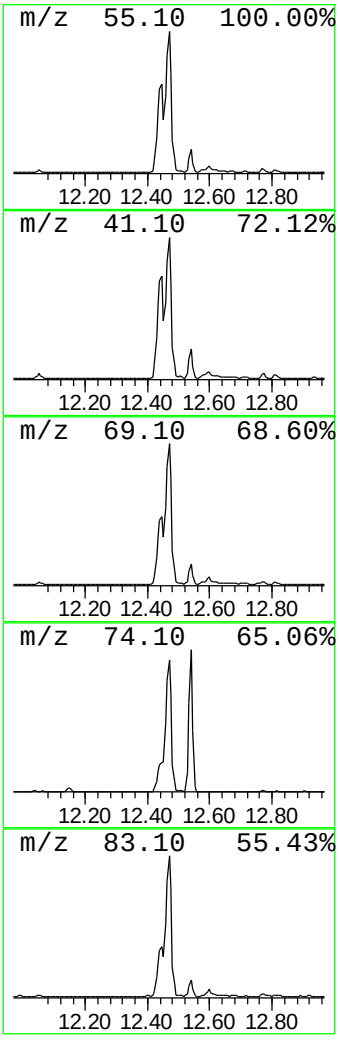
**********

Peak Number 14 16-Octadecenoic acid, methy... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.47 | 354.79 ng | 12670800 | Phenanthrene-d10 | 11.36 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 16-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-49-5 | 99 |
| 2 | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 98 |
| 3 | 15-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 004764-72-1 | 94 |
| 4 | 10-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 013481-95-3 | 94 |
| 5 | 13-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-47-3 | 93 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

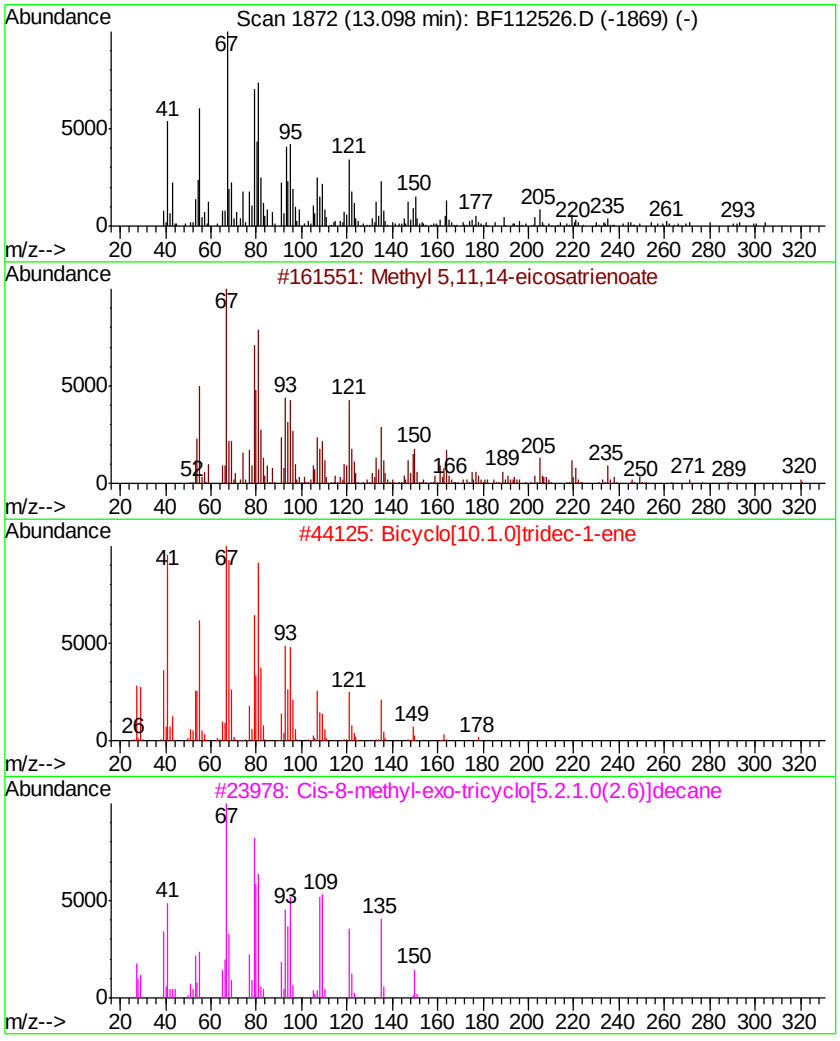
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

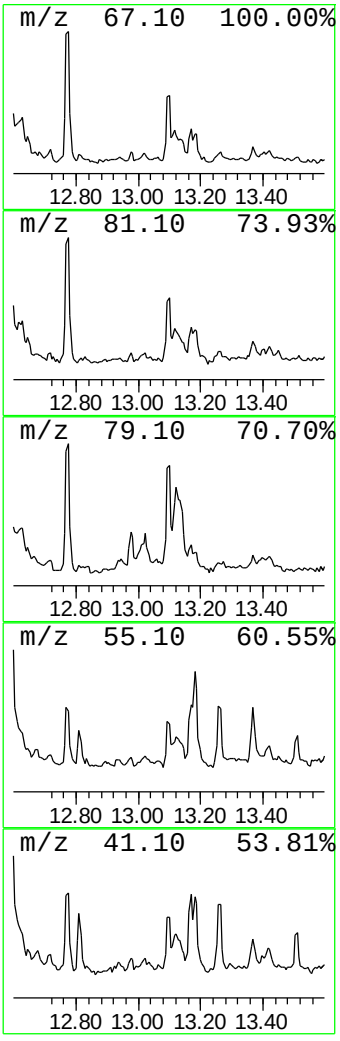
**********

Peak Number 15 Methyl 5,11,14-eicosatrienoate Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.10 | 8.03 ng | 296299 | Chrysene-d12 | 14.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl 5,11,14-eicosatrienoate | 320 | C21H36O2 | 1000336-40-2 | 94 |
| 2 | Bicyclo[10.1.0]tridec-1-ene | 178 | C13H22 | 054766-91-5 | 86 |
| 3 | Cis-8-methyl-exo-tricyclo[5.2.1.... | 150 | C11H18 | 1000215-29-3 | 60 |
| 4 | Methyl 7,11,14-eicosatrienoate | 320 | C21H36O2 | 1000336-40-3 | 58 |
| 5 | Methyl 9,12-heptadecadienoate | 280 | C18H32O2 | 1000336-36-2 | 52 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

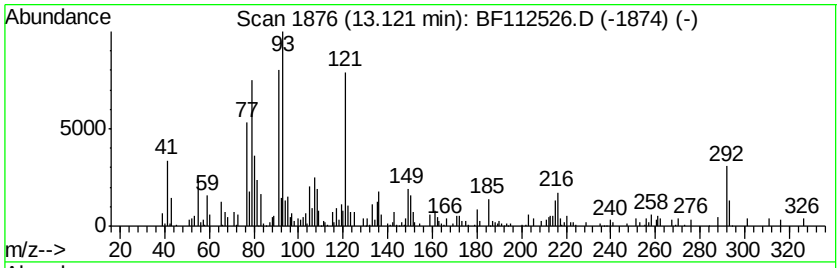
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

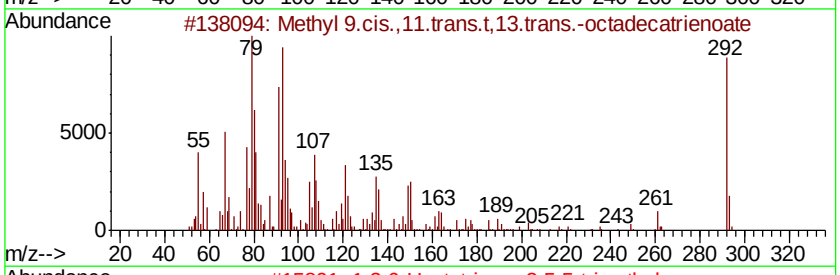
**********

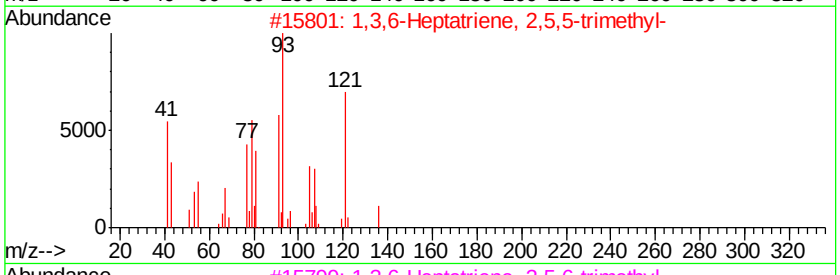
Peak Number 16 Methyl 9.cis.,11.trans.t,13... Concentration Rank 15

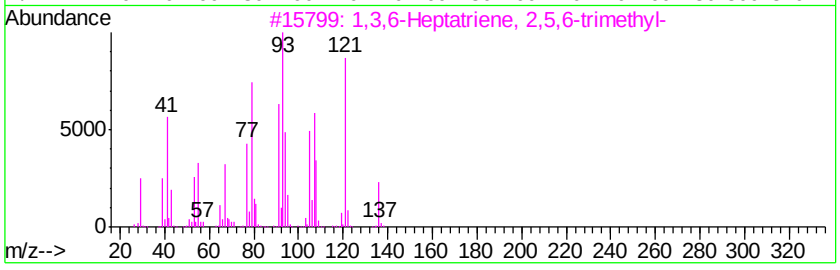
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.12 | 9.37 ng | 345878 | Chrysene-d12 | 14.02 |

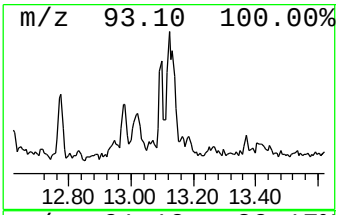
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl 9.cis.,11.trans.t,13.tran... | 292 | C19H32O2 | 1000336-42-6 | 78 |
| 2 | 1,3,6-Heptatriene, 2,5,5-trimethyl- | 136 | C10H16 | 029548-02-5 | 68 |
| 3 | 1,3,6-Heptatriene, 2,5,6-trimethyl- | 136 | C10H16 | 042123-66-0 | 58 |
| 4 | Bicyclo[2.2.1]heptane, 2,2-dimet... | 136 | C10H16 | 005794-04-7 | 49 |
| 5 | Camphene | 136 | C10H16 | 000079-92-5 | 49 |

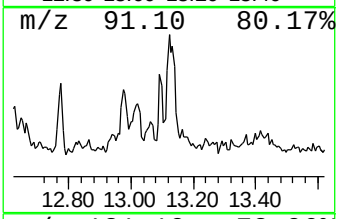


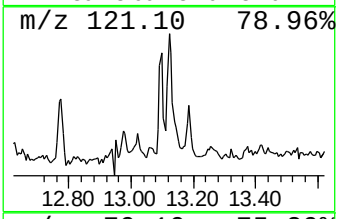



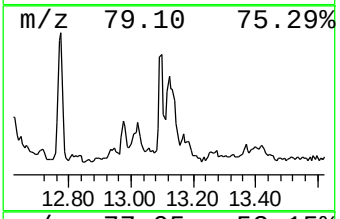



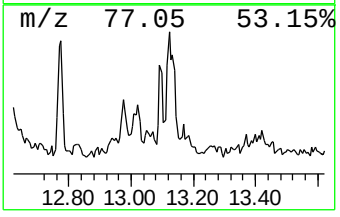



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

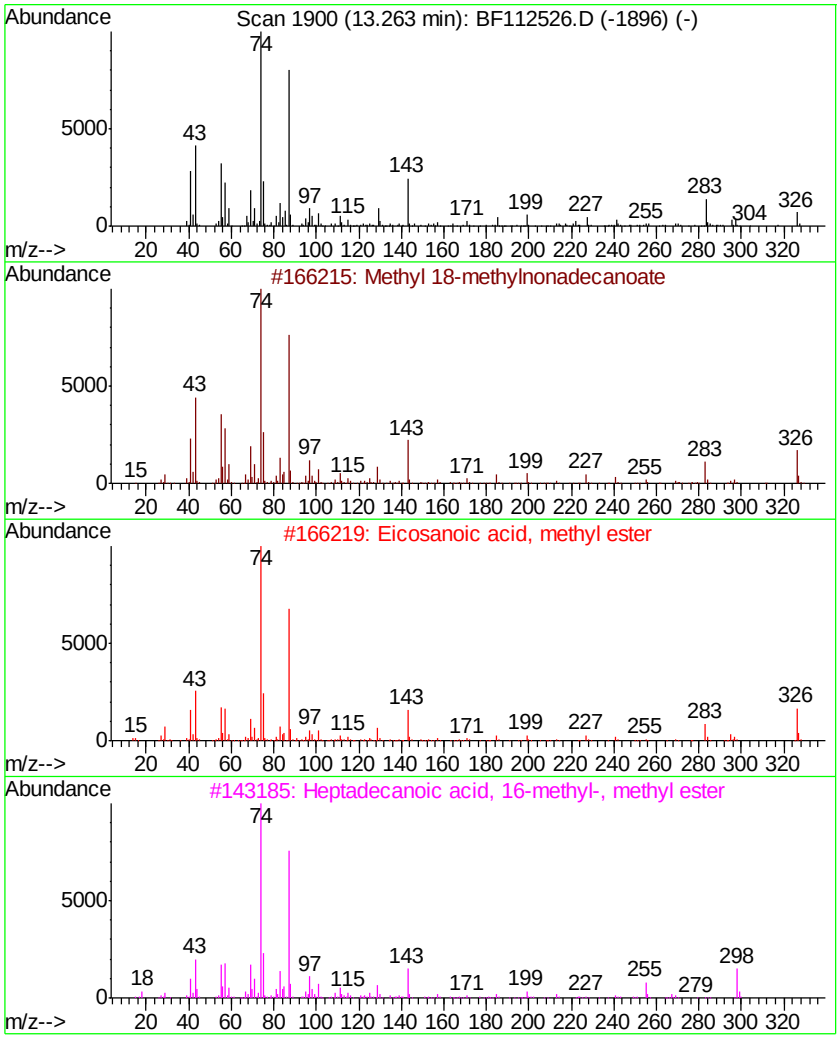
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

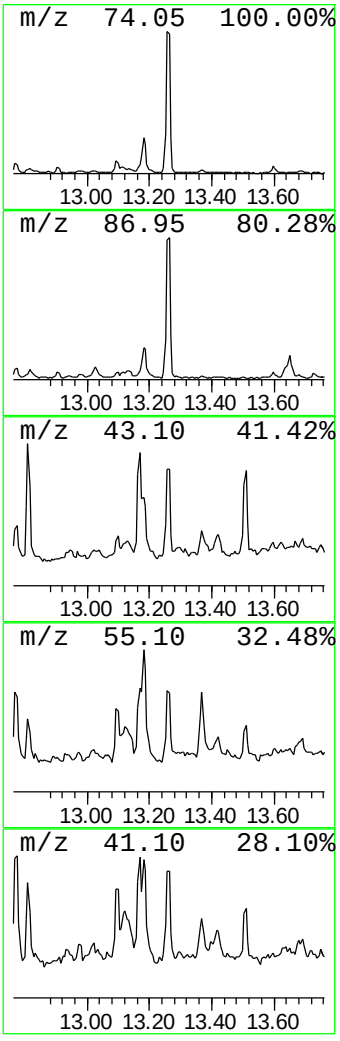
**********

Peak Number 17 Methyl 18-methylnonadecanoate Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.26 | 9.41 ng | 347390 | Chrysene-d12 | 14.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl 18-methylnonadecanoate | 326 | C21H42O2 | 1000352-20-6 | 98 |
| 2 | Eicosanoic acid, methyl ester | 326 | C21H42O2 | 001120-28-1 | 97 |
| 3 | Heptadecanoic acid, 16-methyl-, ... | 298 | C19H38O2 | 005129-61-3 | 95 |
| 4 | Hexadecanoic acid, 15-methyl-, m... | 284 | C18H36O2 | 006929-04-0 | 91 |
| 5 | Hexadecanoic acid, 14-methyl-, m... | 284 | C18H36O2 | 002490-49-5 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

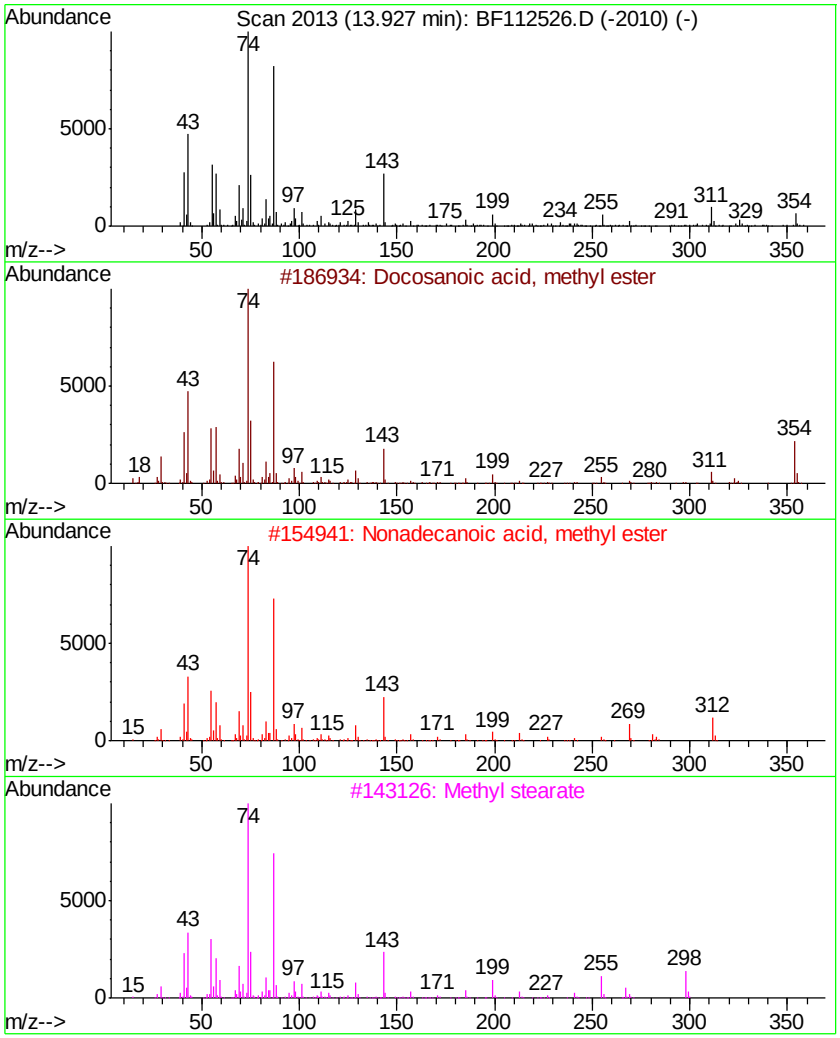
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

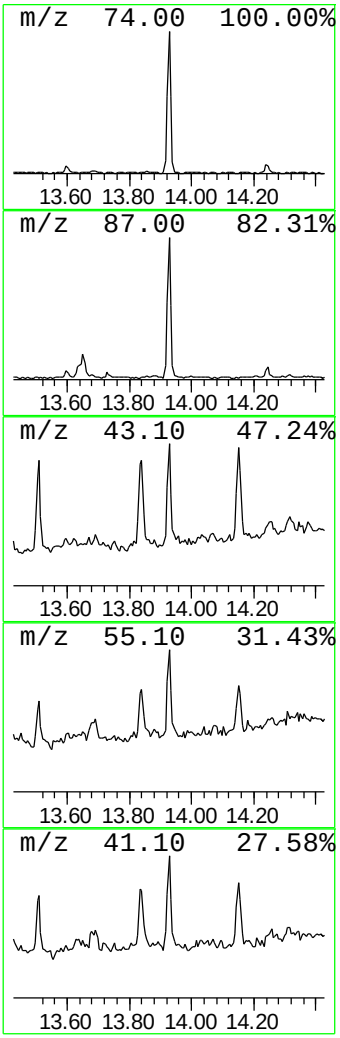
**********

Peak Number 18 Docosanoic acid, methyl ester Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.93 | 9.43 ng | 348039 | Chrysene-d12 | 14.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosanoic acid, methyl ester | 354 | C23H46O2 | 000929-77-1 | 95 |
| 2 | Nonadecanoic acid, methyl ester | 312 | C20H40O2 | 001731-94-8 | 90 |
| 3 | Methyl stearate | 298 | C19H38O2 | 000112-61-8 | 90 |
| 4 | Methyl 20-methyl-heneicosanoate | 354 | C23H46O2 | 1000336-47-4 | 86 |
| 5 | Heneicosanoic acid, methyl ester | 340 | C22H44O2 | 006064-90-0 | 86 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

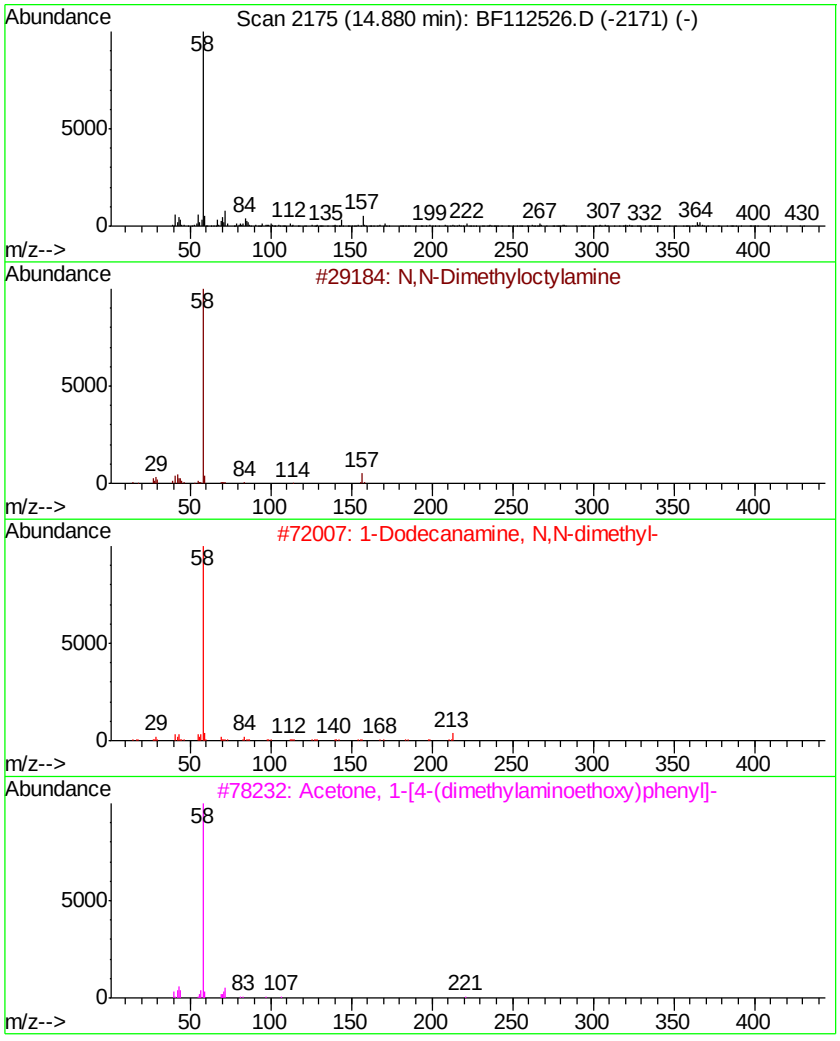
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

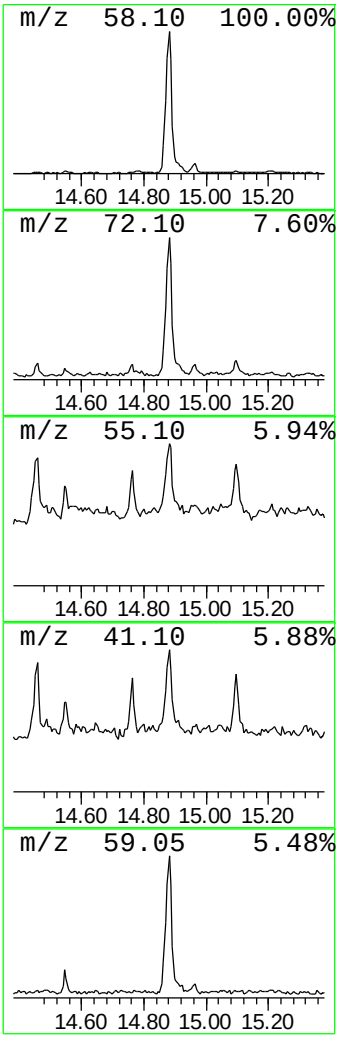
**********

Peak Number 20 N,N-Dimethyloctylamine Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.88 | 22.46 ng | 756704 | Perylene-d12 | 15.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | N,N-Dimethyloctylamine | 157 | C10H23N | 007378-99-6 | 72 |
| 2 | 1-Dodecanamine, N,N-dimethyl- | 213 | C14H31N | 000112-18-5 | 64 |
| 3 | Acetone, 1-[4-(dimethylaminoetho... | 221 | C13H19NO2 | 086608-11-9 | 64 |
| 4 | N,N-Dimethyl-2-cyclohexyloxyethy... | 171 | C10H21NO | 071126-60-8 | 64 |
| 5 | Tetradonium Bromide | 335 | C17H38BrN | 001119-97-7 | 64 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021219\
Data File : BF112526.D
Acq On : 13 Feb 2019 00:16
Operator : JU/SJ
Sample : K1343-19 5X
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-02-021119-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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 | 17.3 | ng | 512774 | 1 | 6.83 | 594081 | 20.0 |
| Tridecane | 8.70 | 9.5 | ng | 350781 | 2 | 8.12 | 739002 | 20.0 |
| Tetradecane | 9.27 | 12.8 | ng | 439376 | 3 | 9.87 | 684562 | 20.0 |
| Pentadecane | 9.80 | 11.5 | ng | 393581 | 3 | 9.87 | 684562 | 20.0 |
| Hexadecane | 10.30 | 14.8 | ng | 506337 | 3 | 9.87 | 684562 | 20.0 |
| Bacchotricuneatin c | 10.52 | 7.2 | ng | 247061 | 3 | 9.87 | 684562 | 20.0 |
| Nonadecane | 10.77 | 15.8 | ng | 564729 | 4 | 11.36 | 714283 | 20.0 |
| Hexadecanoic acid... | 11.75 | 112.3 | ng | 4012110 | 4 | 11.36 | 714283 | 20.0 |
| Eicosane | 12.05 | 9.2 | ng | 326660 | 4 | 11.36 | 714283 | 20.0 |
| 10,13-Octadecadie... | 12.45 | 308.6 | ng | 11020900 | 4 | 11.36 | 714283 | 20.0 |
| 16-Octadecenoic a... | 12.47 | 354.8 | ng | 12670800 | 4 | 11.36 | 714283 | 20.0 |
| Methyl 5,11,14-ei... | 13.10 | 8.0 | ng | 296299 | 5 | 14.02 | 738087 | 20.0 |
| Methyl 9.cis.,11.... | 13.12 | 9.4 | ng | 345878 | 5 | 14.02 | 738087 | 20.0 |
| Methyl 18-methyln... | 13.26 | 9.4 | ng | 347390 | 5 | 14.02 | 738087 | 20.0 |
| Docosanoic acid, ... | 13.93 | 9.4 | ng | 348039 | 5 | 14.02 | 738087 | 20.0 |
| N,N-Dimethyloctyl... | 14.88 | 22.5 | ng | 756704 | 6 | 15.50 | 673796 | 20.0 |