LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

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-BF121918.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 | 5.128 | 513 | 517 | 522 | rBV | 192573 | 209750 | 2.10% | 0.306% |
| 2 | 5.545 | 584 | 588 | 592 | rVB | 2406452 | 2338759 | 23.38% | 3.407% |
| 3 | 6.551 | 751 | 759 | 764 | rBV | 2387379 | 2541892 | 25.41% | 3.703% |
| 4 | 6.681 | 777 | 781 | 785 | rBV | 2724175 | 2483556 | 24.83% | 3.618% |
| 5 | 6.904 | 816 | 819 | 826 | rBV | 971103 | 760201 | 7.60% | 1.107% |
| 6 | 7.063 | 842 | 846 | 849 | rBV | 2465816 | 1991997 | 19.92% | 2.902% |
| 7 | 7.463 | 909 | 914 | 917 | rBV | 1813756 | 1535475 | 15.35% | 2.237% |
| 8 | 8.186 | 1033 | 1037 | 1041 | rVB | 1048279 | 842097 | 8.42% | 1.227% |
| 9 | 9.257 | 1215 | 1219 | 1223 | rBV | 2994619 | 2563242 | 25.63% | 3.734% |
| 10 | 9.392 | 1239 | 1242 | 1246 | rBV | 136932 | 122561 | 1.23% | 0.179% |
| 11 | 9.651 | 1280 | 1286 | 1287 | rBV | 273919 | 276732 | 2.77% | 0.403% |
| 12 | 9.663 | 1287 | 1288 | 1291 | rVB | 444448 | 264106 | 2.64% | 0.385% |
| 13 | 9.939 | 1332 | 1335 | 1339 | rBV | 940230 | 867180 | 8.67% | 1.263% |
| 14 | 10.733 | 1465 | 1470 | 1473 | rBV | 1775189 | 1568619 | 15.68% | 2.285% |
| 15 | 10.969 | 1507 | 1510 | 1513 | rVB | 142904 | 117295 | 1.17% | 0.171% |
| 16 | 11.075 | 1525 | 1528 | 1535 | rBV2 | 153811 | 218760 | 2.19% | 0.319% |
| 17 | 11.380 | 1576 | 1580 | 1582 | rBV3 | 82449 | 113088 | 1.13% | 0.165% |
| 18 | 11.427 | 1585 | 1588 | 1591 | rVV | 1070147 | 891913 | 8.92% | 1.299% |
| 19 | 11.474 | 1594 | 1596 | 1601 | rVB2 | 260579 | 258680 | 2.59% | 0.377% |
| 20 | 11.645 | 1620 | 1625 | 1629 | rVB4 | 167795 | 208766 | 2.09% | 0.304% |
| 21 | 11.957 | 1674 | 1678 | 1685 | rVB2 | 347188 | 356381 | 3.56% | 0.519% |
| 22 | 12.127 | 1704 | 1707 | 1713 | rVB3 | 102401 | 123765 | 1.24% | 0.180% |
| 23 | 12.286 | 1731 | 1734 | 1737 | rBV | 126267 | 121557 | 1.22% | 0.177% |
| 24 | 12.469 | 1762 | 1765 | 1767 | rBV | 141056 | 136255 | 1.36% | 0.198% |
| 25 | 12.516 | 1770 | 1773 | 1775 | rVV | 265170 | 224043 | 2.24% | 0.326% |
| 26 | 12.557 | 1775 | 1780 | 1783 | rVV3 | 261325 | 320384 | 3.20% | 0.467% |
| 27 | 12.692 | 1800 | 1803 | 1805 | rBV | 270046 | 217122 | 2.17% | 0.316% |
| 28 | 12.739 | 1808 | 1811 | 1815 | rVB | 218014 | 190478 | 1.90% | 0.277% |
| 29 | 12.886 | 1833 | 1836 | 1845 | rBV | 152835 | 150070 | 1.50% | 0.219% |
| 30 | 13.010 | 1853 | 1857 | 1864 | rVB | 2613343 | 2524089 | 25.23% | 3.677% |
| 31 | 13.104 | 1871 | 1873 | 1876 | rBV | 150588 | 137047 | 1.37% | 0.200% |
| 32 | 13.216 | 1886 | 1892 | 1894 | rBV2 | 733866 | 1086088 | 10.86% | 1.582% |
| 33 | 13.245 | 1894 | 1897 | 1900 | rVB | 1270601 | 1098160 | 10.98% | 1.600% |
| 34 | 13.386 | 1918 | 1921 | 1924 | rBV | 550690 | 502265 | 5.02% | 0.732% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

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-BF121918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.421 | 1924 | 1927 | 1930 | rBV3 | 140382 | 135810 | 1.36% | 0.198% |
| 36 | 13.492 | 1936 | 1939 | 1942 | rBV2 | 264503 | 300800 | 3.01% | 0.438% |
| 37 | 13.586 | 1953 | 1955 | 1957 | rBV | 273879 | 255754 | 2.56% | 0.373% |
| 38 | 13.704 | 1972 | 1975 | 1979 | rBV2 | 480008 | 482259 | 4.82% | 0.702% |
| 39 | 13.751 | 1981 | 1983 | 1986 | rVB2 | 144880 | 107760 | 1.08% | 0.157% |
| 40 | 13.910 | 2005 | 2010 | 2017 | rBV2 | 5278742 | 8237331 | 82.35% | 11.999% |
| 41 | 14.033 | 2028 | 2031 | 2034 | rBV2 | 201542 | 181398 | 1.81% | 0.264% |
| 42 | 14.068 | 2034 | 2037 | 2040 | rVB | 918578 | 763020 | 7.63% | 1.111% |
| 43 | 14.098 | 2040 | 2042 | 2045 | rVB | 475256 | 425831 | 4.26% | 0.620% |
| 44 | 14.174 | 2052 | 2055 | 2058 | rBV | 189438 | 194476 | 1.94% | 0.283% |
| 45 | 14.227 | 2061 | 2064 | 2070 | rVB2 | 794162 | 1079374 | 10.79% | 1.572% |
| 46 | 14.315 | 2077 | 2079 | 2082 | rBV | 198158 | 201501 | 2.01% | 0.294% |
| 47 | 14.351 | 2082 | 2085 | 2089 | rVV | 641715 | 627282 | 6.27% | 0.914% |
| 48 | 14.545 | 2113 | 2118 | 2124 | rBV | 8055642 | 10002437 | 100.00% | 14.570% |
| 49 | 14.592 | 2124 | 2126 | 2131 | rVB | 412702 | 385872 | 3.86% | 0.562% |
| 50 | 14.663 | 2136 | 2138 | 2140 | rVV | 219289 | 159373 | 1.59% | 0.232% |
| 51 | 14.851 | 2166 | 2170 | 2179 | rVB2 | 672863 | 1091008 | 10.91% | 1.589% |
| 52 | 14.998 | 2191 | 2195 | 2199 | rVB | 866491 | 939135 | 9.39% | 1.368% |
| 53 | 15.204 | 2225 | 2230 | 2232 | rBV | 2405085 | 3330052 | 33.29% | 4.851% |
| 54 | 15.280 | 2240 | 2243 | 2249 | rVB | 636182 | 753830 | 7.54% | 1.098% |
| 55 | 15.368 | 2256 | 2258 | 2265 | rVB2 | 301297 | 349976 | 3.50% | 0.510% |
| 56 | 15.562 | 2287 | 2291 | 2293 | rBV | 438916 | 585028 | 5.85% | 0.852% |
| 57 | 15.586 | 2293 | 2295 | 2299 | rVB | 404537 | 470797 | 4.71% | 0.686% |
| 58 | 15.798 | 2326 | 2331 | 2334 | rBV | 1001456 | 1438617 | 14.38% | 2.096% |
| 59 | 16.039 | 2368 | 2372 | 2377 | rBV | 888726 | 1310301 | 13.10% | 1.909% |
| 60 | 16.086 | 2377 | 2380 | 2385 | rVB | 387790 | 502802 | 5.03% | 0.732% |
| 61 | 16.162 | 2389 | 2393 | 2398 | rVB | 602749 | 896288 | 8.96% | 1.306% |
| 62 | 16.215 | 2399 | 2402 | 2409 | rVB4 | 329299 | 522094 | 5.22% | 0.760% |
| 63 | 16.286 | 2411 | 2414 | 2417 | rBV2 | 284511 | 426921 | 4.27% | 0.622% |
| 64 | 16.862 | 2507 | 2512 | 2520 | rVB | 785202 | 1494858 | 14.94% | 2.177% |
| 65 | 17.368 | 2594 | 2598 | 2603 | rBV | 409855 | 826319 | 8.26% | 1.204% |
| 66 | 17.427 | 2604 | 2608 | 2622 | rVB3 | 678418 | 1469135 | 14.69% | 2.140% |
| 67 | 18.527 | 2791 | 2795 | 2806 | rVB3 | 578906 | 1341747 | 13.41% | 1.954% |

Sum of corrected areas: 68651559

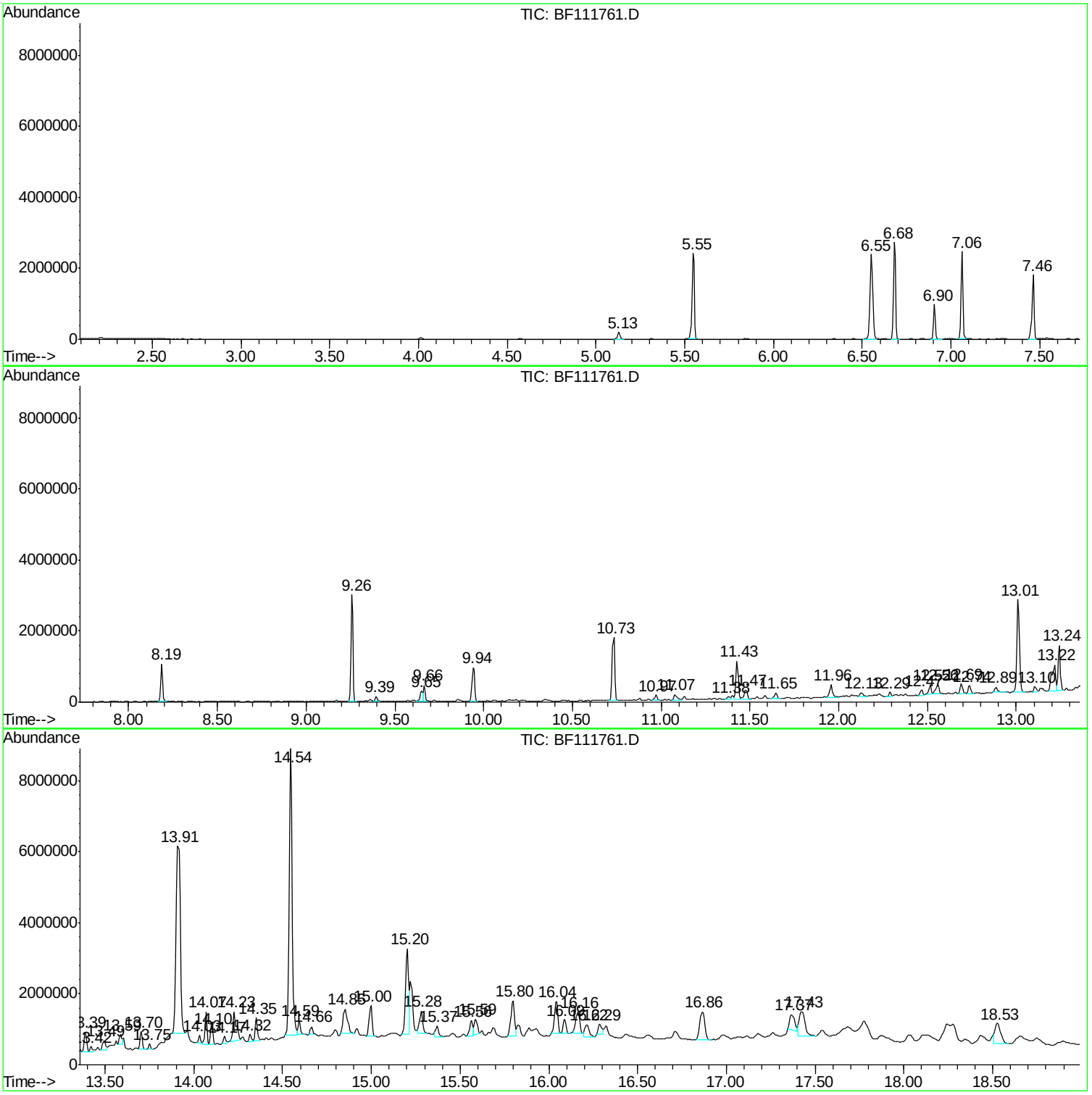
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

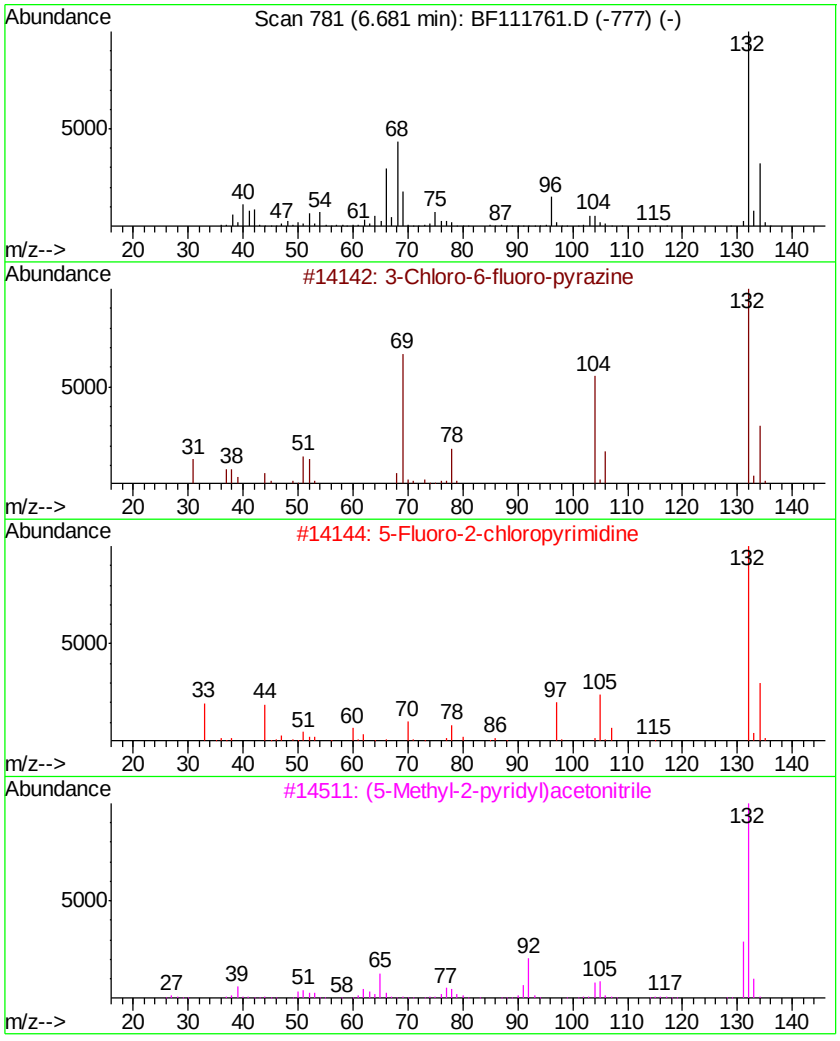
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

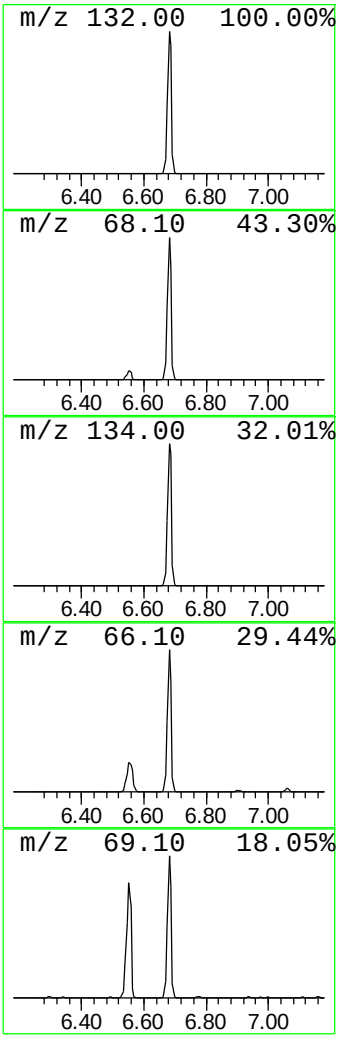
**********

Peak Number 1 unknown6.68 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.68 | 65.34 ng | 2483560 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 3 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 10 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

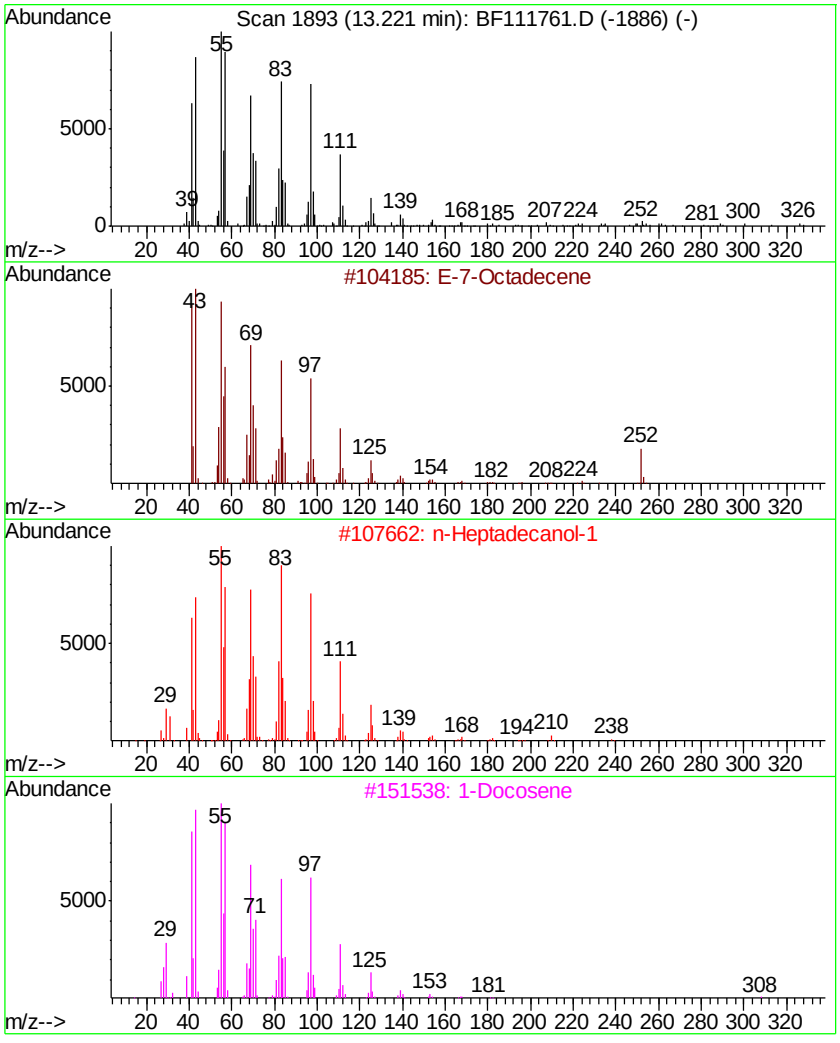
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

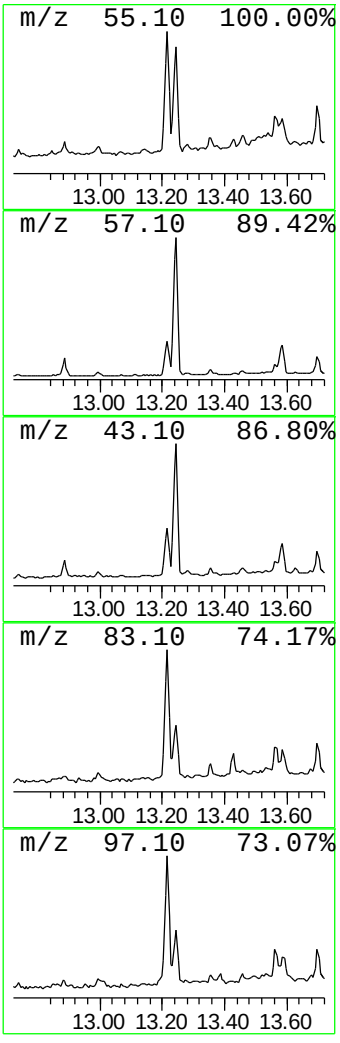
**********

Peak Number 3 E-7-Octadecene Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.22 | 28.47 ng | 1086090 | Chrysene-d12 | 14.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | E-7-Octadecene | 252 | C18H36 | 1000130-92-0 | 95 |
| 2 | n-Heptadecanol-1 | 256 | C17H36O | 001454-85-9 | 94 |
| 3 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 93 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 91 |
| 5 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 91 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

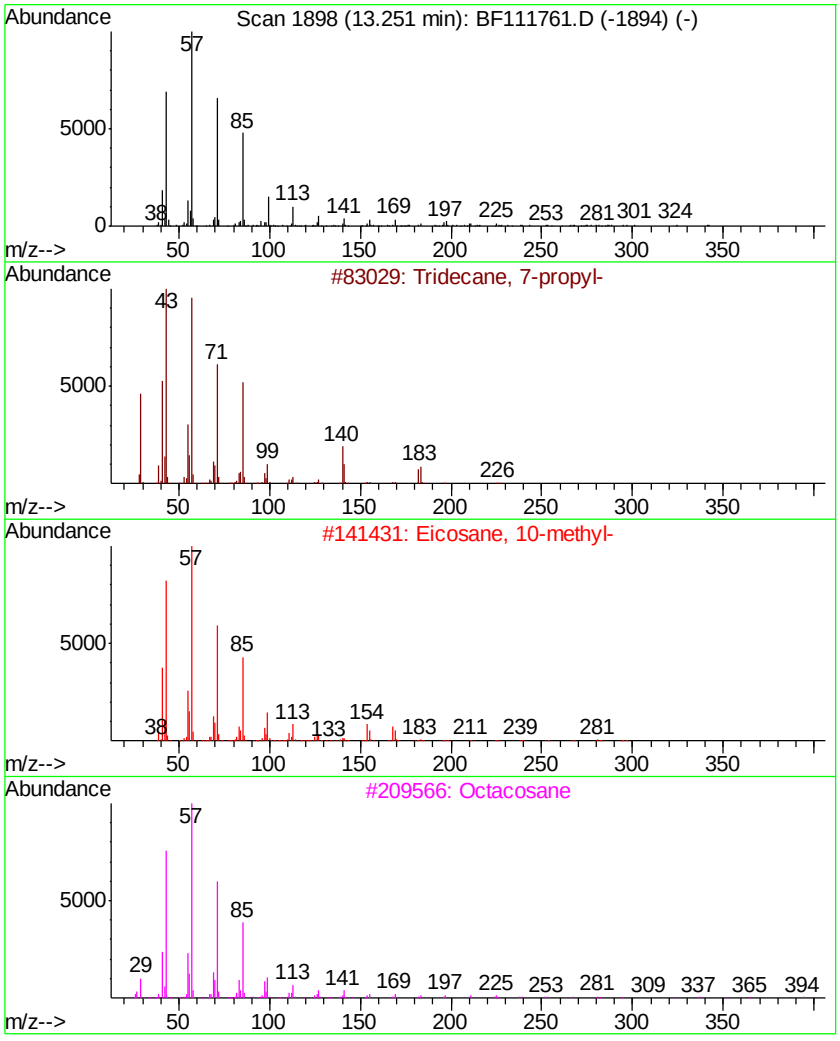
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

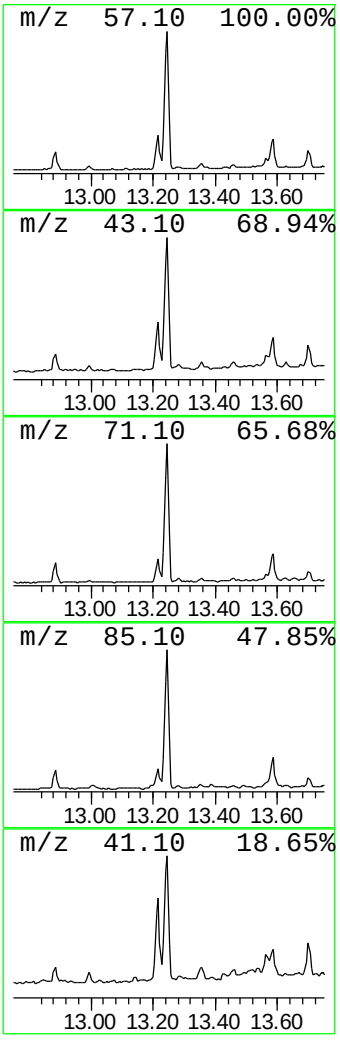
**********

Peak Number 4 Tridecane, 7-propyl- Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.25 | 28.78 ng | 1098160 | Chrysene-d12 | 14.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecane, 7-propyl- | 226 | C16H34 | 055045-09-5 | 93 |
| 2 | Eicosane, 10-methyl- | 296 | C21H44 | 054833-23-7 | 91 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 4 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 90 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

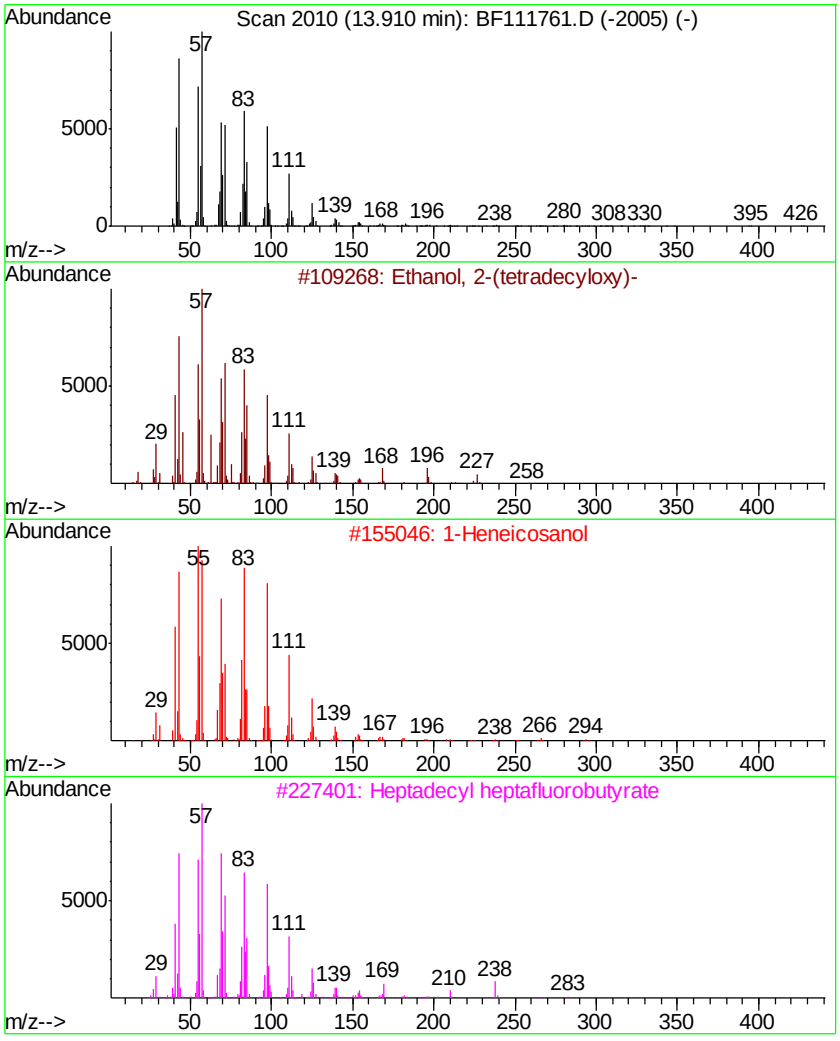
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

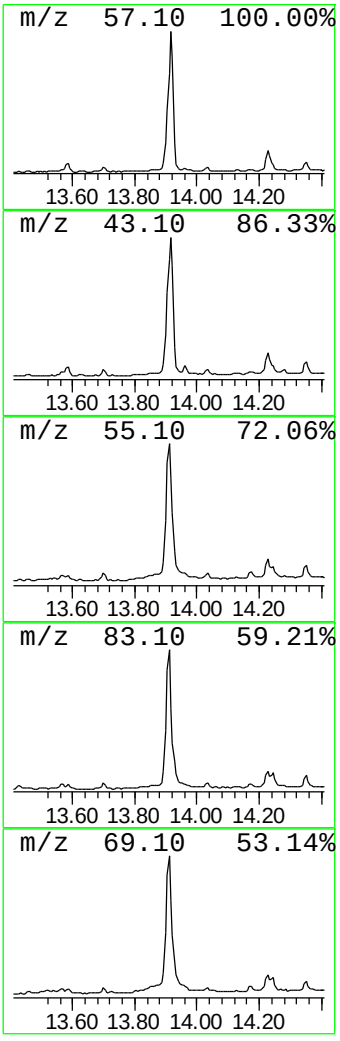
**********

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.91 | 215.91 ng | 8237330 | Chrysene-d12 | 14.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 93 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 3 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 91 |
| 4 | 1-Hexadecanesulfonyl chloride | 324 | C16H33ClO2S | 038775-38-1 | 91 |
| 5 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 91 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

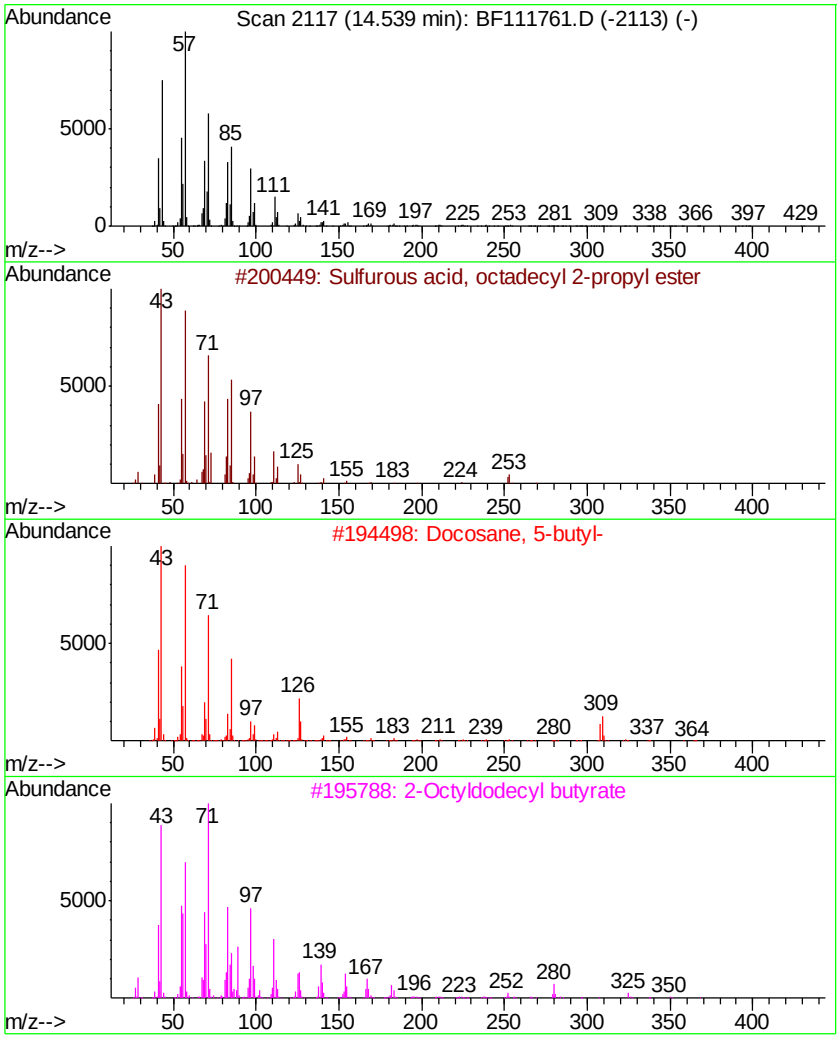
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

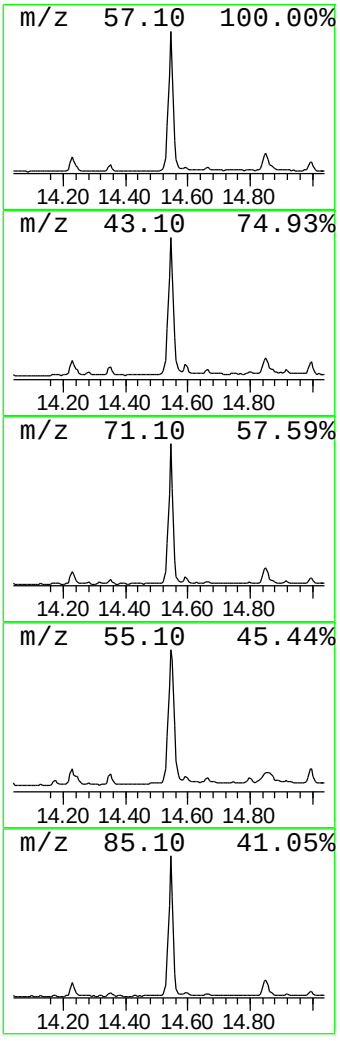
**********

Peak Number 7 Sulfurous acid, octadecyl 2... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.54 | 262.18 ng | 10002400 | Chrysene-d12 | 14.07 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfurous acid, octadecyl 2-prop... | 376 | C21H44O3S | 1000309-12-7 | 87 |
| 2 | Docosane, 5-butyl- | 366 | C26H54 | 055282-16-1 | 81 |
| 3 | 2-Octyldodecyl butyrate | 368 | C24H48O2 | 1000368-55-2 | 70 |
| 4 | Nonadecane | 268 | C19H40 | 000629-92-5 | 68 |
| 5 | Tetradecane | 198 | C14H30 | 000629-59-4 | 68 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

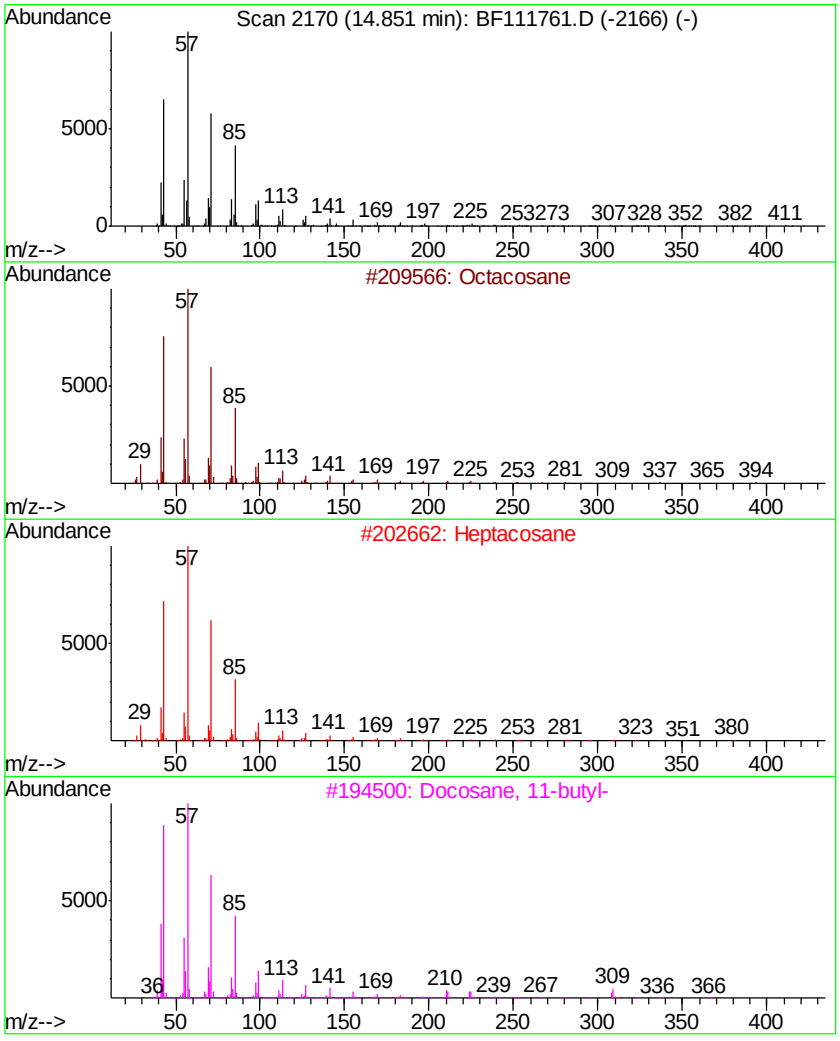
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

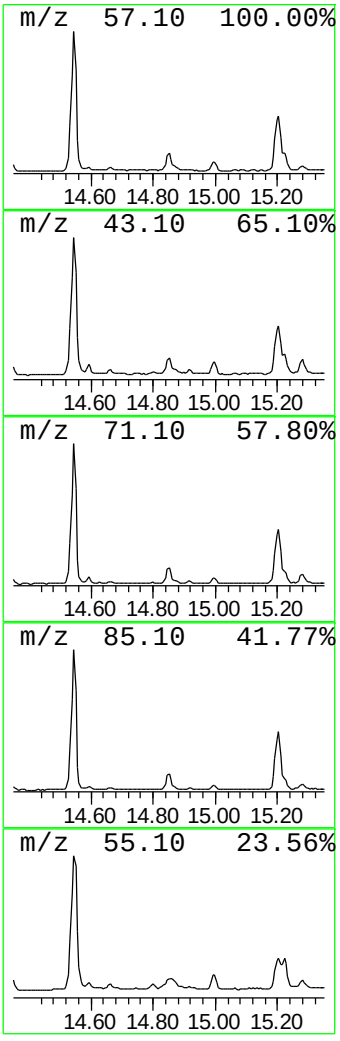
**********

Peak Number 8 Octacosane Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.85 | 37.30 ng | 1091010 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 98 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 96 |
| 3 | Docosane, 11-butyl- | 366 | C26H54 | 013475-76-8 | 91 |
| 4 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |
| 5 | Tricosane | 324 | C23H48 | 000638-67-5 | 91 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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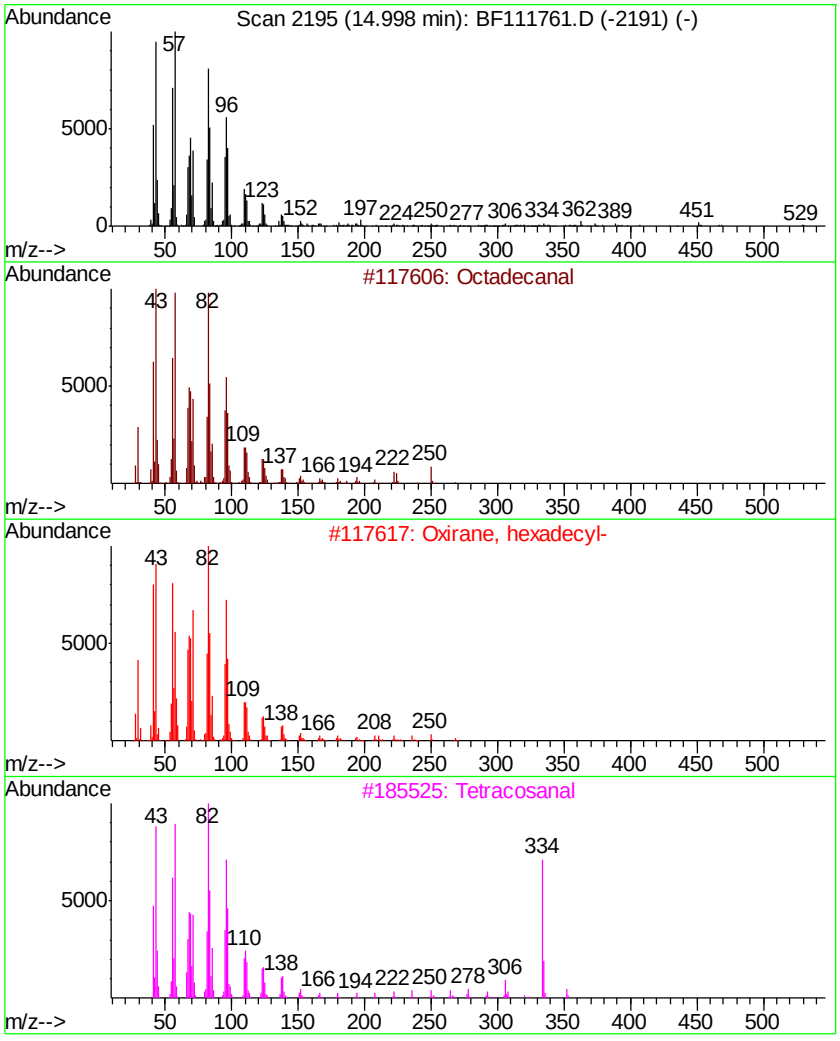
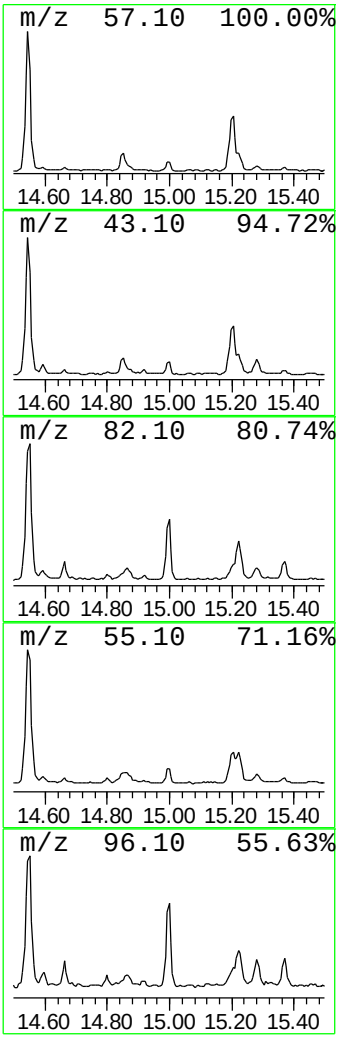
Peak Number 9 Octadecanal Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.00 | 32.11 ng | 939135 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanal | 268 | C18H36O | 000638-66-4 | 93 |
| 2 | Oxirane, hexadecyl- | 268 | C18H36O | 007390-81-0 | 91 |
| 3 | Tetracosanal | 352 | C24H48O | 057866-08-7 | 91 |
| 4 | Hexadecanal | 240 | C16H32O | 000629-80-1 | 91 |
| 5 | Z-13-Octadecen-1-yl acetate | 310 | C20H38O2 | 060037-58-3 | 86 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

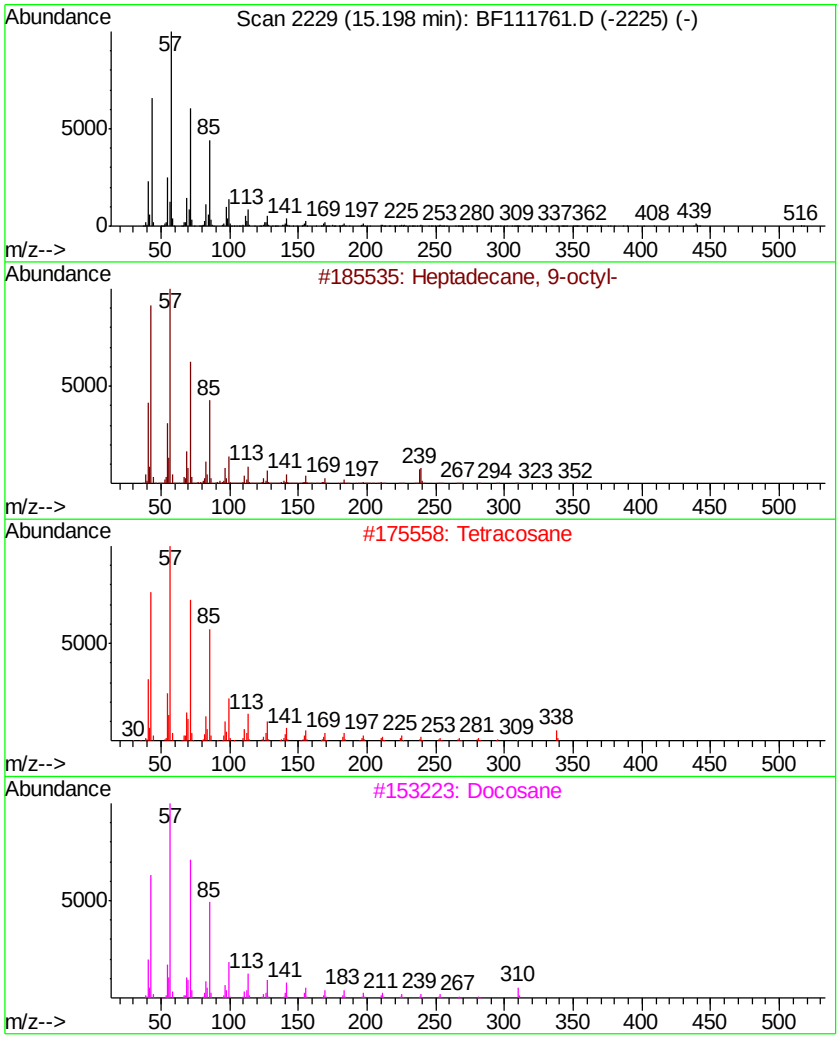
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

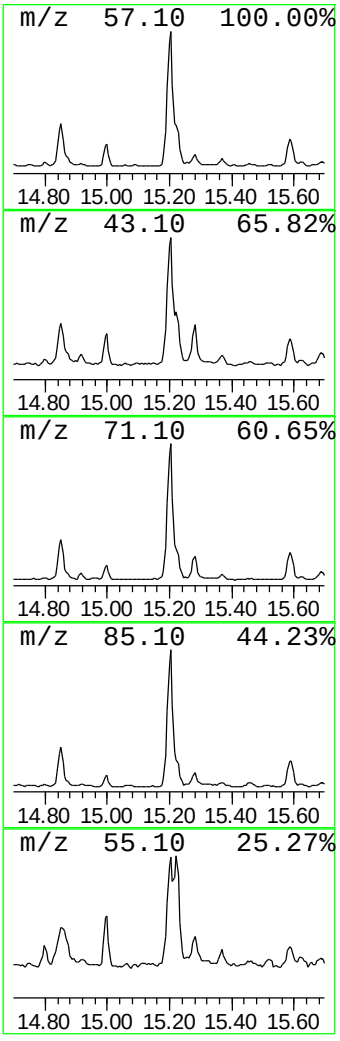
**********

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.20 | 113.84 ng | 3330050 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 97 |
| 2 | Tetracosane | 338 | C24H50 | 000646-31-1 | 97 |
| 3 | Docosane | 310 | C22H46 | 000629-97-0 | 96 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 95 |
| 5 | Octadecane, 5,14-dibutyl- | 366 | C26H54 | 055282-13-8 | 93 |



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Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

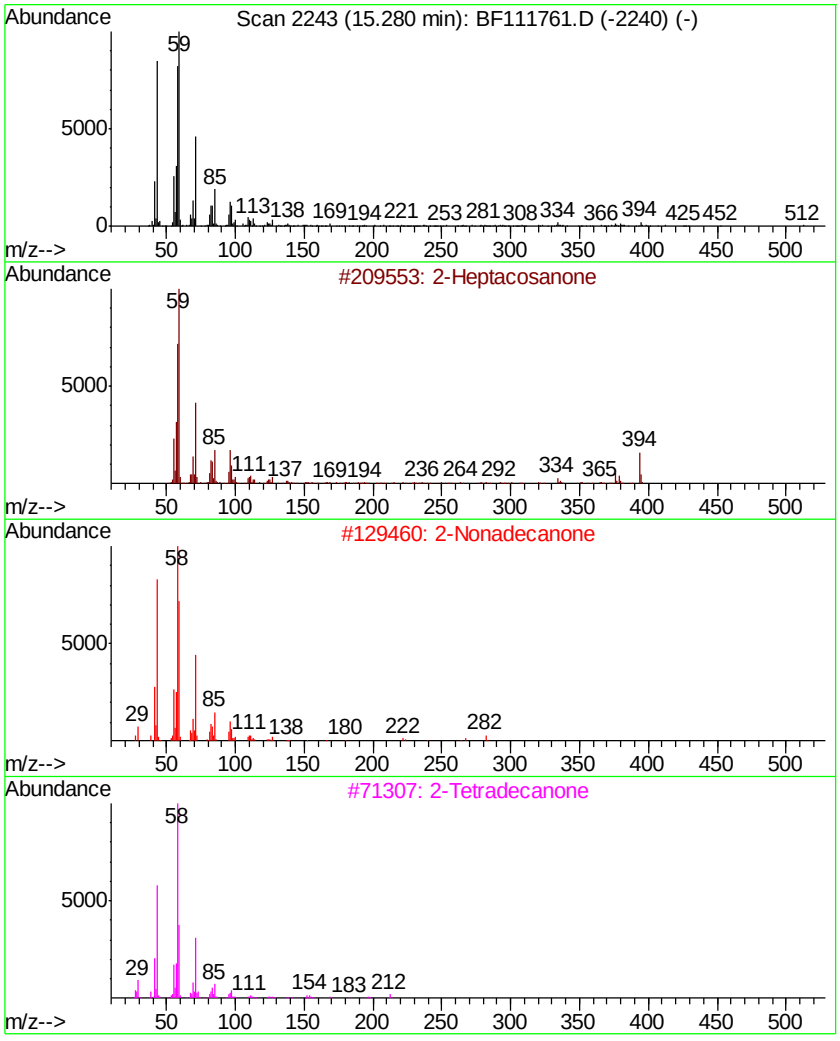
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

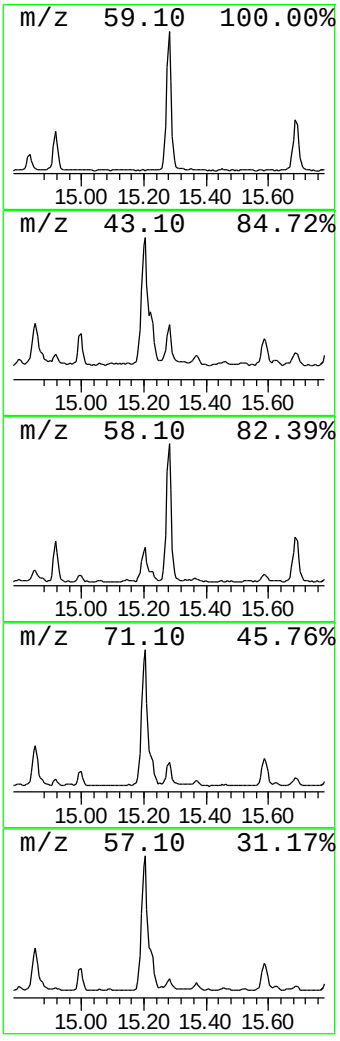
**********

Peak Number 11 2-Heptacosanone Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.28 | 25.77 ng | 753830 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Heptacosanone | 394 | C27H54O | 007796-19-2 | 97 |
| 2 | 2-Nonadecanone | 282 | C19H38O | 000629-66-3 | 72 |
| 3 | 2-Tetradecanone | 212 | C14H28O | 002345-27-9 | 50 |
| 4 | 2-Pentadecanone | 226 | C15H30O | 002345-28-0 | 50 |
| 5 | trans-2,3-Epoxynonane | 142 | C9H18O | 056820-01-0 | 43 |



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Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

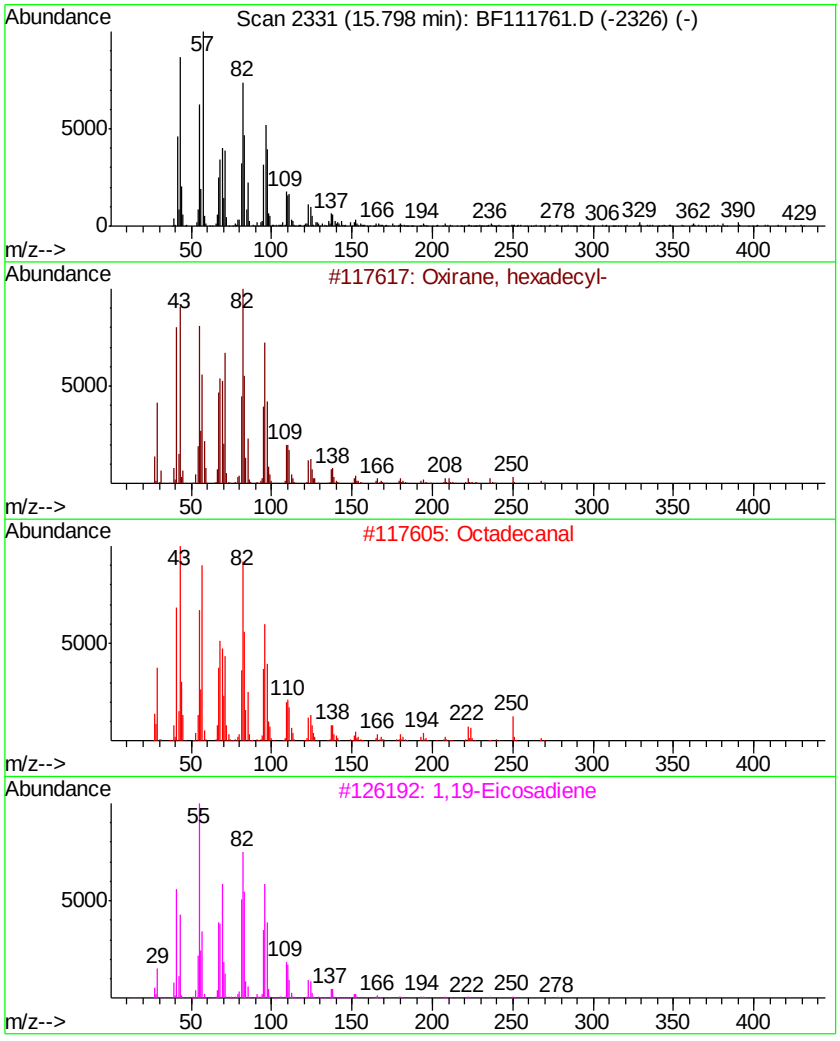
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

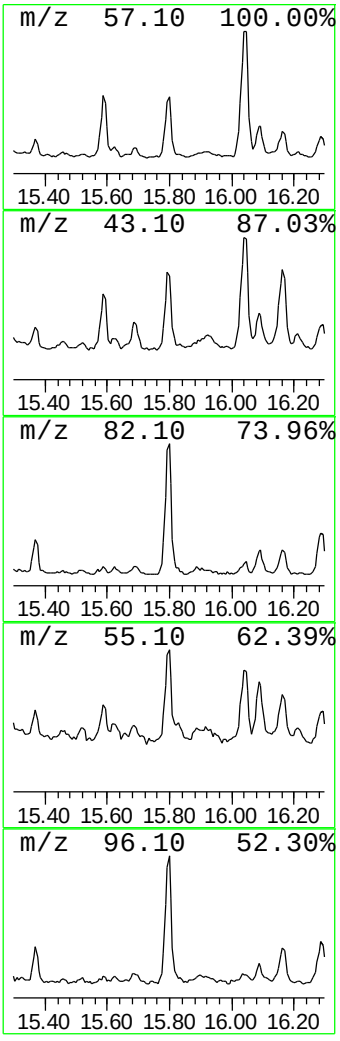
**********

Peak Number 12 Oxirane, hexadecyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.80 | 49.18 ng | 1438620 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxirane, hexadecyl- | 268 | C18H36O | 007390-81-0 | 91 |
| 2 | Octadecanal | 268 | C18H36O | 000638-66-4 | 91 |
| 3 | 1,19-Eicosadiene | 278 | C20H38 | 014811-95-1 | 90 |
| 4 | Hexadecanal | 240 | C16H32O | 000629-80-1 | 87 |
| 5 | Oxirane, heptadecyl- | 282 | C19H38O | 067860-04-2 | 83 |



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Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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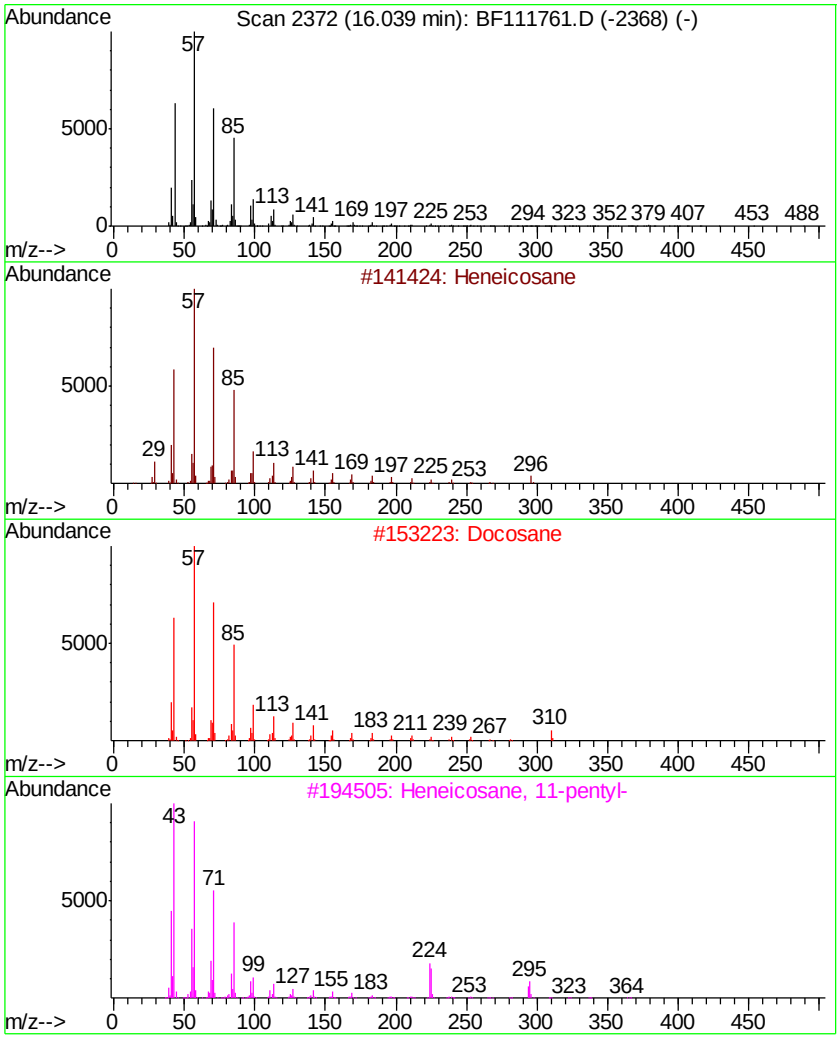
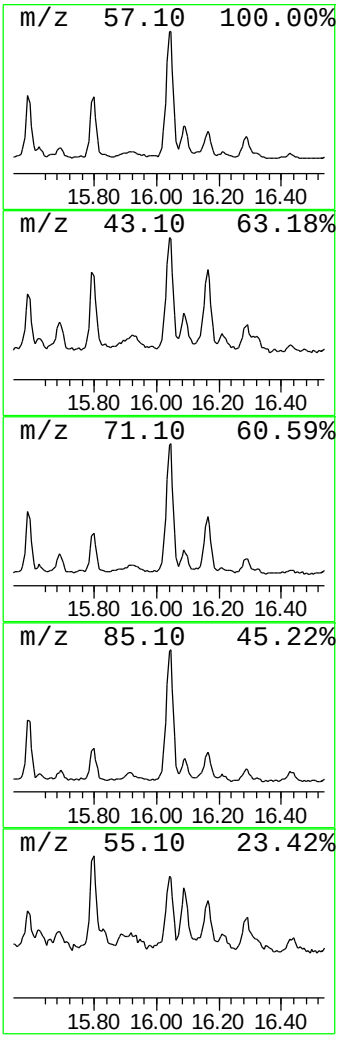
Peak Number 13 Heneicosane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.04 | 44.79 ng | 1310300 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 97 |
| 2 | Docosane | 310 | C22H46 | 000629-97-0 | 96 |
| 3 | Heneicosane, 11-pentyl- | 366 | C26H54 | 014739-72-1 | 94 |
| 4 | Tricosane | 324 | C23H48 | 000638-67-5 | 93 |
| 5 | Octadecane, 5,14-dibutyl- | 366 | C26H54 | 055282-13-8 | 93 |



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Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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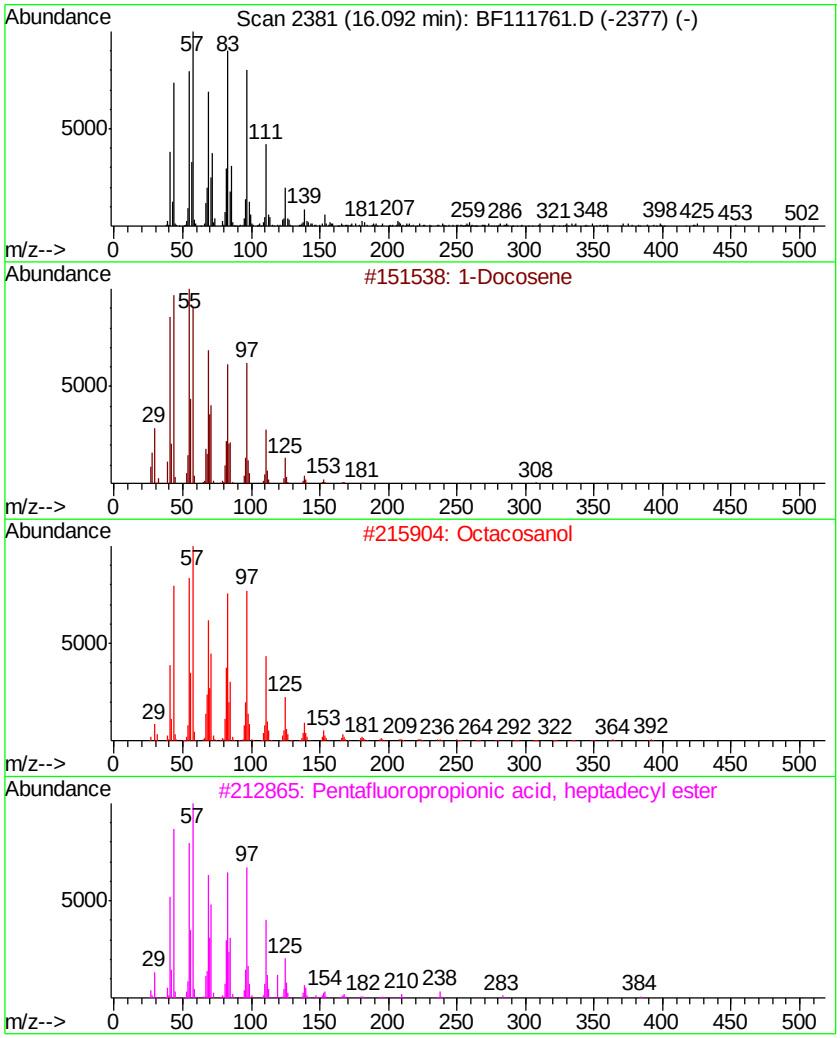
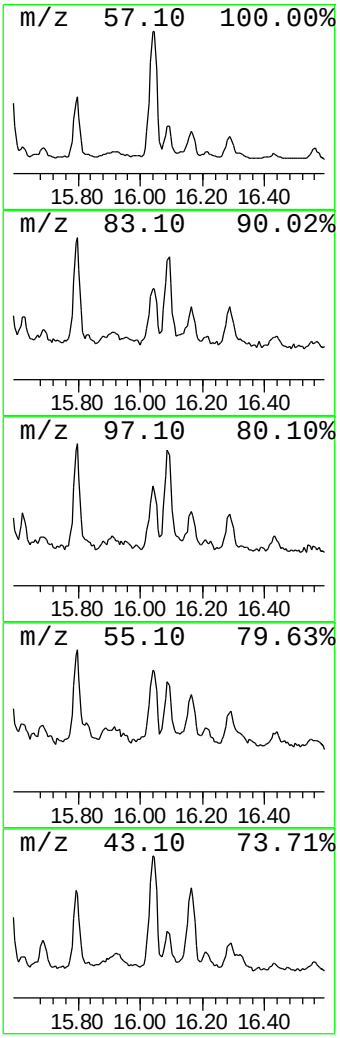
Peak Number 14 1-Docosene Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.09 | 17.19 ng | 502802 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 91 |
| 2 | Octacosanol | 410 | C28H58O | 000557-61-9 | 91 |
| 3 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 83 |
| 4 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 80 |
| 5 | Cyclotetracosane | 336 | C24H48 | 000297-03-0 | 68 |



Library Search Compound Report

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Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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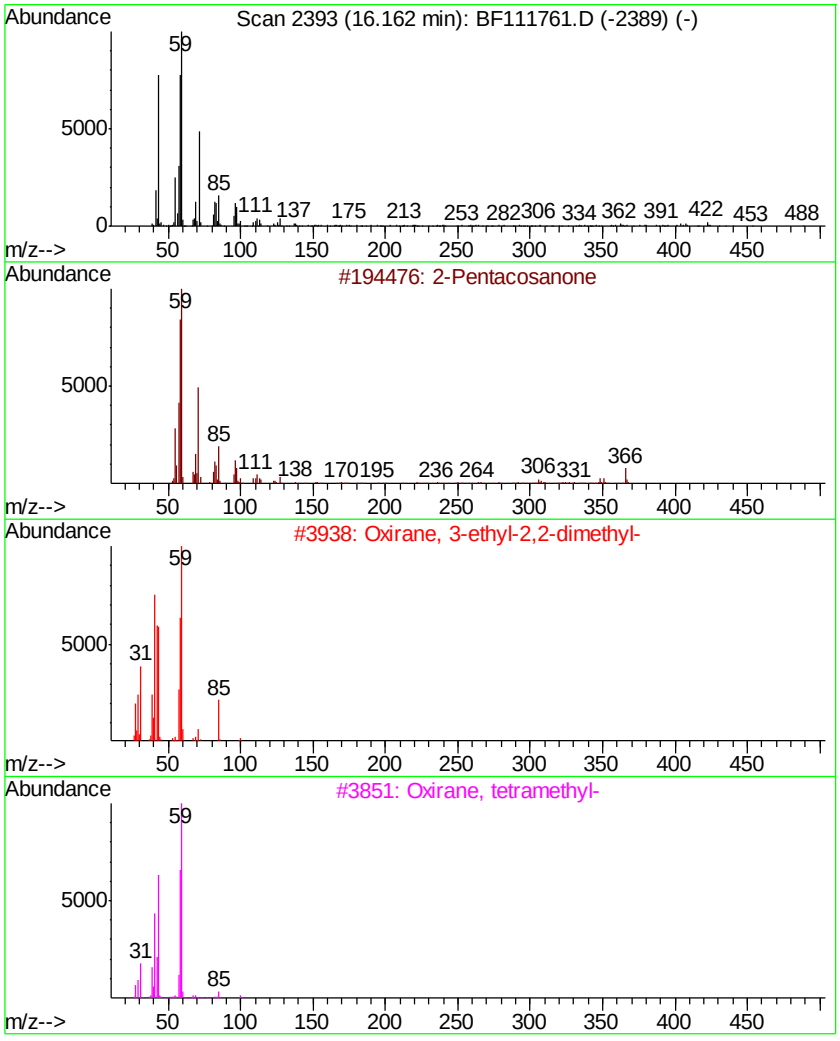
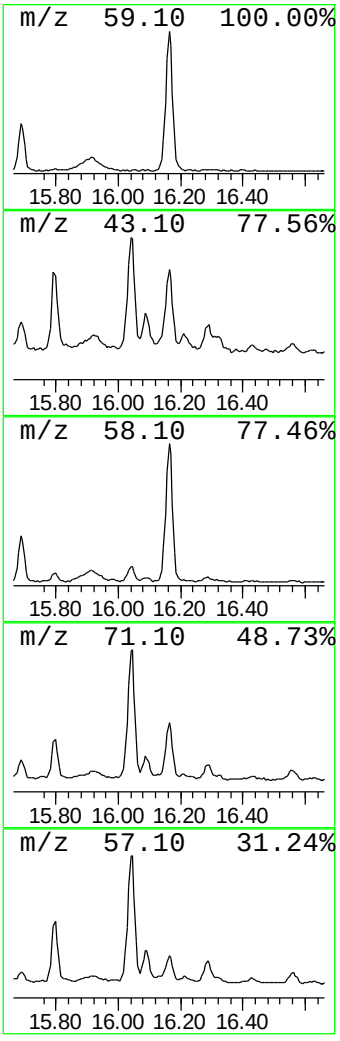
Peak Number 15 2-Pentacosanone Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.16 | 30.64 ng | 896288 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentacosanone | 366 | C25H50O | 075207-54-4 | 90 |
| 2 | Oxirane, 3-ethyl-2,2-dimethyl- | 100 | C6H12O | 001192-22-9 | 52 |
| 3 | Oxirane, tetramethyl- | 100 | C6H12O | 005076-20-0 | 50 |
| 4 | 2-Heptadecanone | 254 | C17H34O | 002922-51-2 | 50 |
| 5 | 2-Hexadecanone | 240 | C16H32O | 018787-63-8 | 47 |



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Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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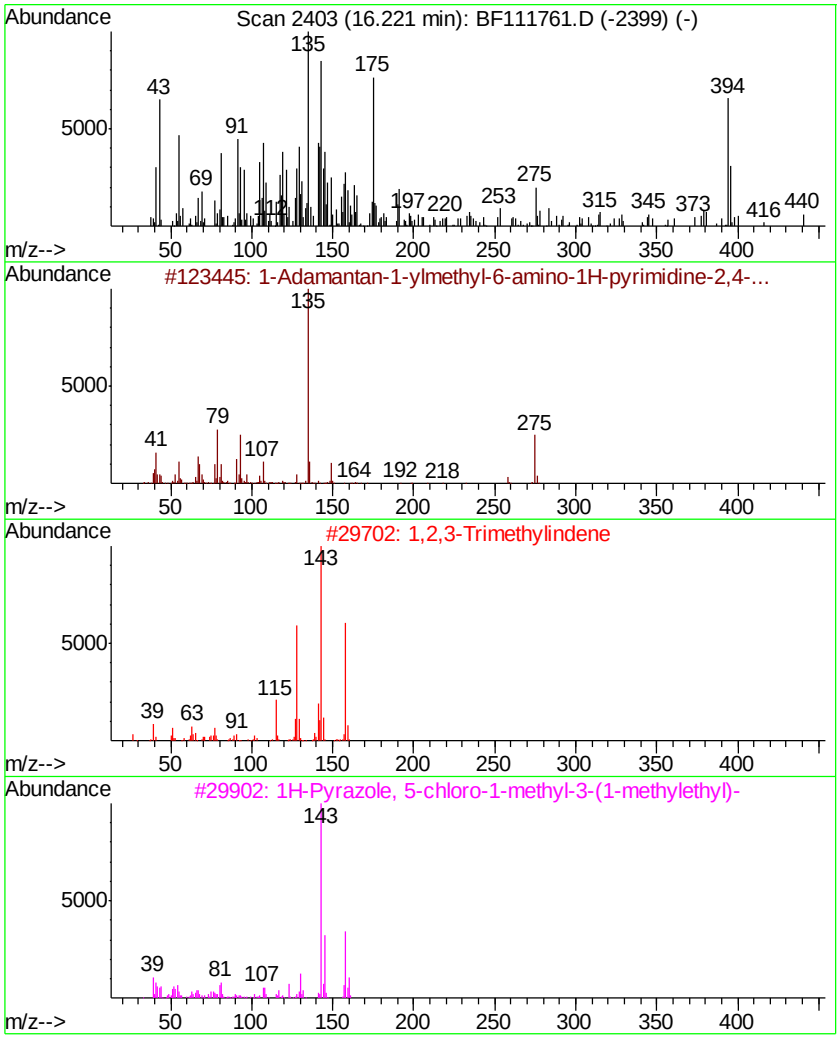
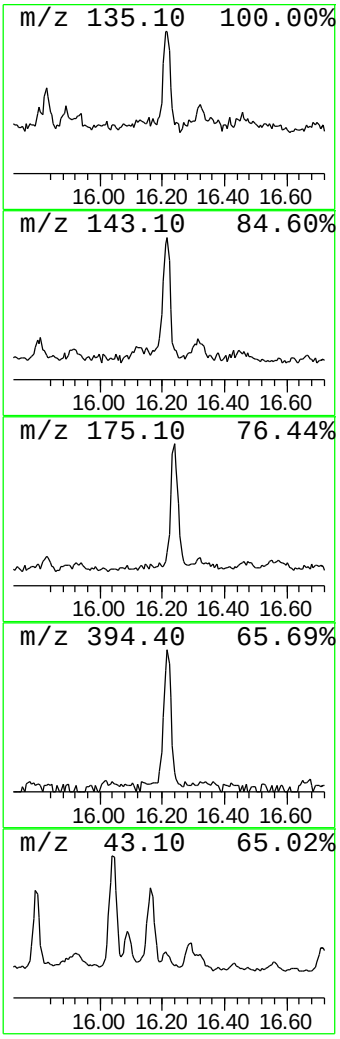
Peak Number 16 unknown16.22 Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.22 | 17.85 ng | 522094 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Adamantan-1-ylmethyl-6-amino-1... | 275 | C15H21N3O2 | 1000297-13-5 | 25 |
| 2 | 1,2,3-Trimethylindene | 158 | C12H14 | 004773-83-5 | 14 |
| 3 | 1H-Pyrazole, 5-chloro-1-methyl-3... | 158 | C7H11ClN2 | 1000319-90-4 | 11 |
| 4 | Quinoline, 6-methyl- | 143 | C10H9N | 000091-62-3 | 10 |
| 5 | 3-t-Butyl-6,6,7,7-tetracyano-2-o... | 313 | C15H15N5O3 | 1000192-86-4 | 10 |



Library Search Compound Report

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Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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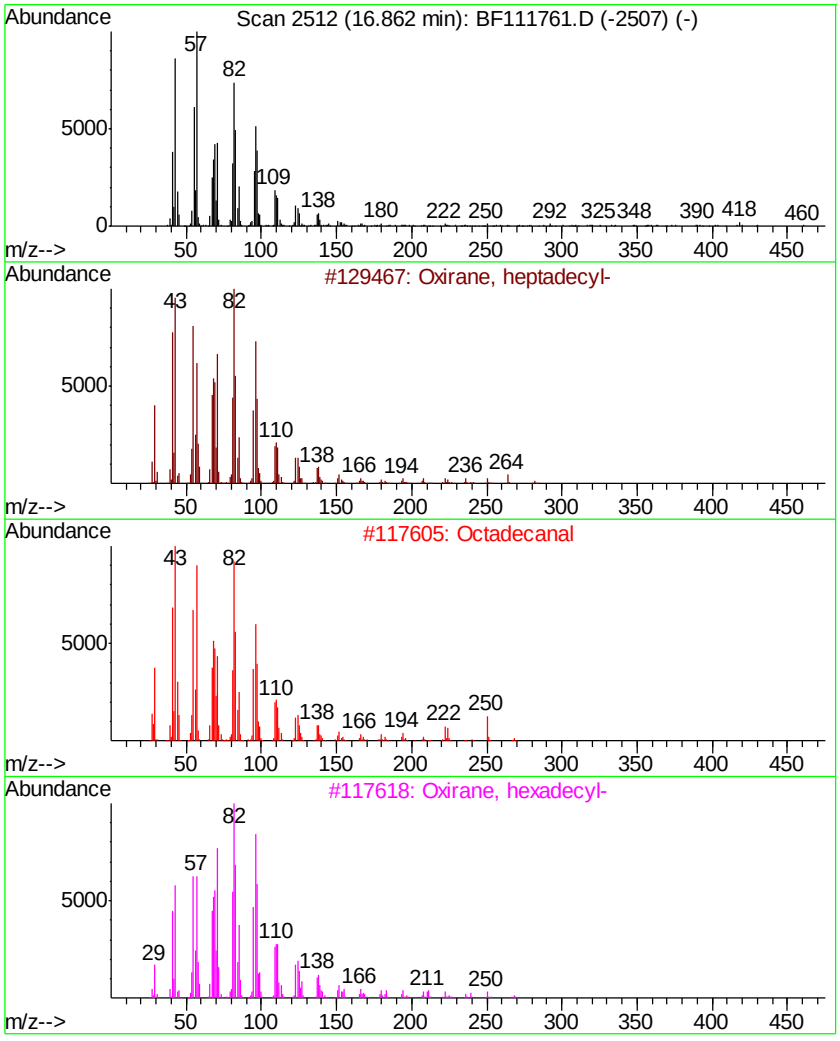
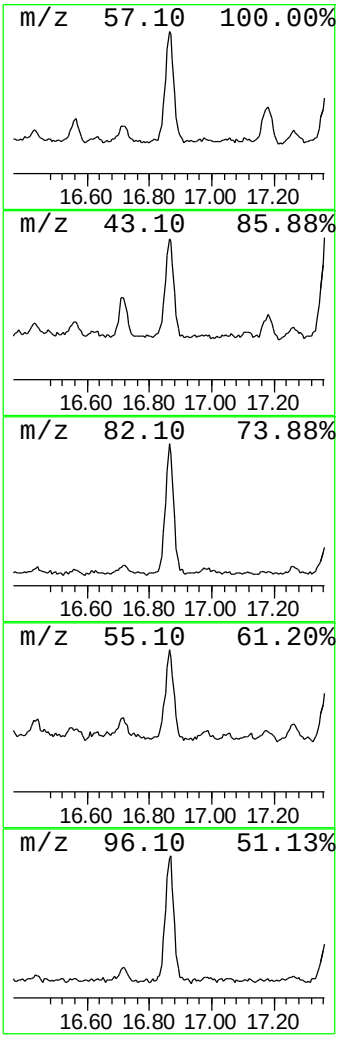
Peak Number 17 Oxirane, heptadecyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.86 | 51.10 ng | 1494860 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxirane, heptadecyl- | 282 | C19H38O | 067860-04-2 | 91 |
| 2 | Octadecanal | 268 | C18H36O | 000638-66-4 | 91 |
| 3 | Oxirane, hexadecyl- | 268 | C18H36O | 007390-81-0 | 91 |
| 4 | (Z)-14-Tricosenyl formate | 366 | C24H46O2 | 077899-10-6 | 90 |
| 5 | 17-Octadecenal | 266 | C18H34O | 056554-86-0 | 87 |



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Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

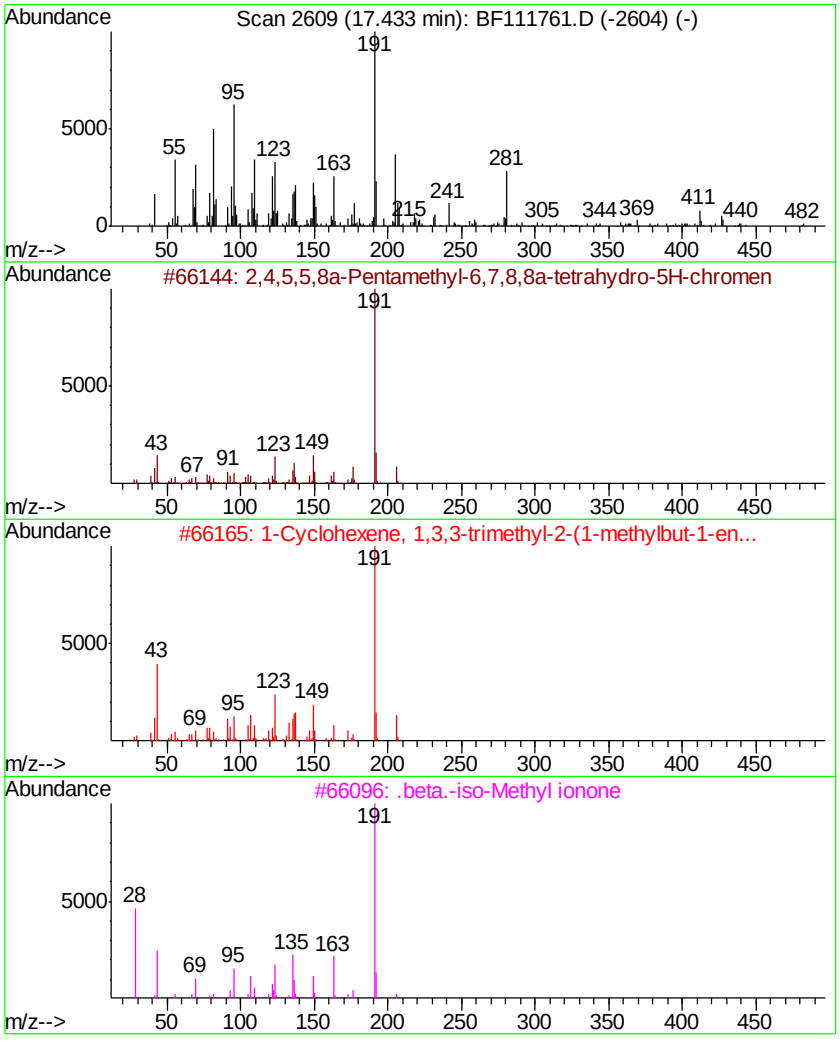
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

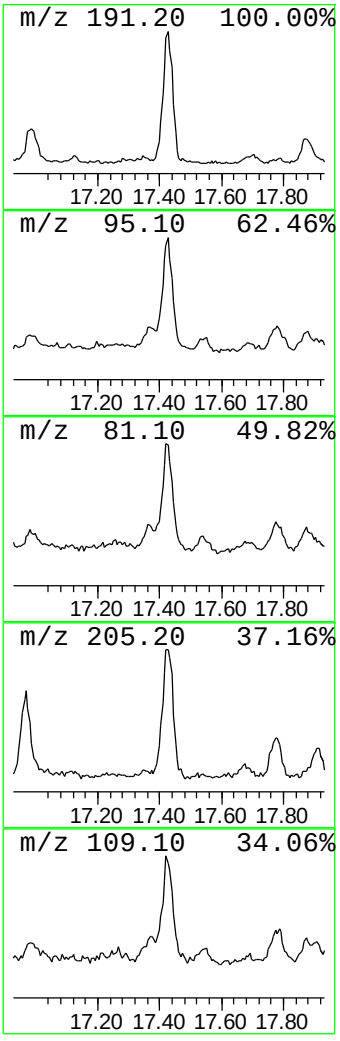
**********

Peak Number 19 2,4,5,5,8a-Pentamethyl-6,7,... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.43 | 50.22 ng | 1469140 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,5,5,8a-Pentamethyl-6,7,8,8a-... | 206 | C14H22O | 1000195-40-9 | 55 |
| 2 | 1-Cyclohexene, 1,3,3-trimethyl-2... | 206 | C14H22O | 1000197-08-4 | 49 |
| 3 | .beta.-iso-Methyl ionone | 206 | C14H22O | 1000285-40-2 | 47 |
| 4 | 2'-Fluoro-6'-(trifluoromethyl)-a... | 206 | C9H6F4O | 174013-29-7 | 38 |
| 5 | 2-(2-((2-Chloro-6-fluorobenzyl)s... | 334 | C17H16ClFN2S | 1000298-18-2 | 35 |



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Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

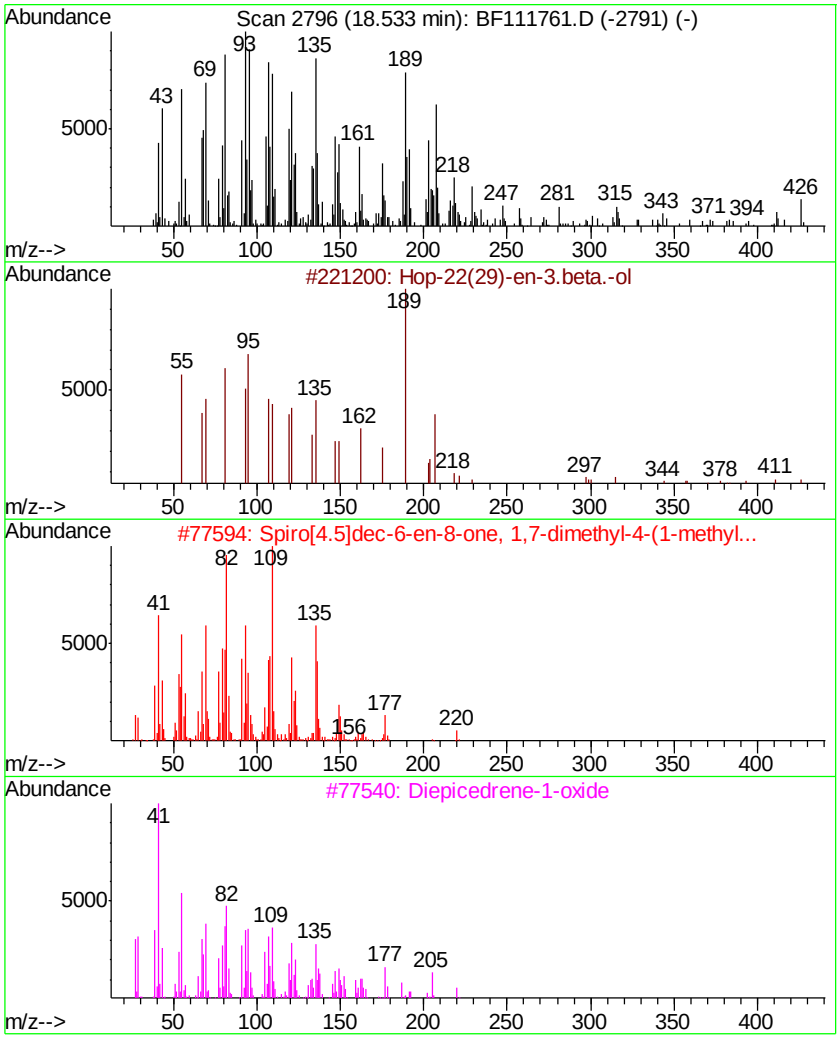
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

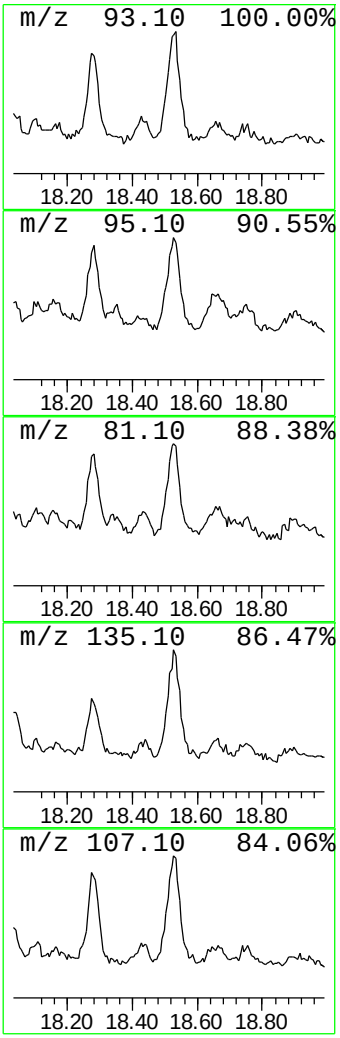
**********

Peak Number 20 Hop-22(29)-en-3.beta.-ol Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.53 | 45.87 ng | 1341750 | Perylene-d12 | 15.56 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hop-22(29)-en-3.beta.-ol | 426 | C30H50O | 058801-23-3 | 78 |
| 2 | Spiro[4.5]dec-6-en-8-one, 1,7-di... | 220 | C15H24O | 039510-36-6 | 56 |
| 3 | Diepicedrene-1-oxide | 220 | C15H24O | 1000156-11-0 | 55 |
| 4 | Guaia-9,11-diene | 204 | C15H24 | 1000374-19-8 | 53 |
| 5 | 1-Isopropenyl-3-propenylcyclopen... | 150 | C11H18 | 1000192-81-2 | 47 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122718\
Data File : BF111761.D
Acq On : 27 Dec 2018 14:43
Operator : JU/SJ
Sample : J6446-16
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS022-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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 |
| unknown6.68 | 6.68 | 65.3 | ng | 2483560 | 1 | 6.90 | 760201 | 20.0 |
| E-7-Octadecene | 13.22 | 28.5 | ng | 1086090 | 5 | 14.07 | 763020 | 20.0 |
| Tridecane, 7-propyl- | 13.25 | 28.8 | ng | 1098160 | 5 | 14.07 | 763020 | 20.0 |
| Ethanol, 2-(tetra... | 13.91 | 215.9 | ng | 8237330 | 5 | 14.07 | 763020 | 20.0 |
| Sulfurous acid, o... | 14.54 | 262.2 | ng | 10002400 | 5 | 14.07 | 763020 | 20.0 |
| Octacosane | 14.85 | 37.3 | ng | 1091010 | 6 | 15.56 | 585028 | 20.0 |
| Octadecanal | 15.00 | 32.1 | ng | 939135 | 6 | 15.56 | 585028 | 20.0 |
| Heptadecane, 9-oc... | 15.20 | 113.8 | ng | 3330050 | 6 | 15.56 | 585028 | 20.0 |
| 2-Heptacosanone | 15.28 | 25.8 | ng | 753830 | 6 | 15.56 | 585028 | 20.0 |
| Oxirane, hexadecyl- | 15.80 | 49.2 | ng | 1438620 | 6 | 15.56 | 585028 | 20.0 |
| Heneicosane | 16.04 | 44.8 | ng | 1310300 | 6 | 15.56 | 585028 | 20.0 |
| 1-Docosene | 16.09 | 17.2 | ng | 502802 | 6 | 15.56 | 585028 | 20.0 |
| 2-Pentacosanone | 16.16 | 30.6 | ng | 896288 | 6 | 15.56 | 585028 | 20.0 |
| unknown16.22 | 16.22 | 17.9 | ng | 522094 | 6 | 15.56 | 585028 | 20.0 |
| Oxirane, heptadecyl- | 16.86 | 51.1 | ng | 1494860 | 6 | 15.56 | 585028 | 20.0 |
| 2,4,5,5,8a-Pentam... | 17.43 | 50.2 | ng | 1469140 | 6 | 15.56 | 585028 | 20.0 |
| Hop-22(29)-en-3.b... | 18.53 | 45.9 | ng | 1341750 | 6 | 15.56 | 585028 | 20.0 |