LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.057 | 501 | 505 | 514 | rBV | 437025 | 502473 | 14.77% | 1.425% |
| 2 | 5.469 | 571 | 575 | 596 | rBV | 2519855 | 2301874 | 67.67% | 6.527% |
| 3 | 6.092 | 677 | 681 | 688 | rBV3 | 28302 | 42091 | 1.24% | 0.119% |
| 4 | 6.381 | 726 | 730 | 736 | rBV4 | 43548 | 53430 | 1.57% | 0.151% |
| 5 | 6.487 | 743 | 748 | 757 | rBV | 2727974 | 2602143 | 76.50% | 7.378% |
| 6 | 6.622 | 767 | 771 | 774 | rBV | 3368522 | 2769839 | 81.43% | 7.853% |
| 7 | 6.681 | 778 | 781 | 784 | rBV | 98286 | 81973 | 2.41% | 0.232% |
| 8 | 6.851 | 806 | 810 | 817 | rVB | 966436 | 841413 | 24.74% | 2.386% |
| 9 | 7.010 | 831 | 837 | 840 | rBV | 2385080 | 2245270 | 66.00% | 6.366% |
| 10 | 7.122 | 851 | 856 | 859 | rVB4 | 37898 | 43692 | 1.28% | 0.124% |
| 11 | 7.245 | 871 | 877 | 879 | rBV3 | 30974 | 44812 | 1.32% | 0.127% |
| 12 | 7.416 | 902 | 906 | 909 | rBV | 1758175 | 1558171 | 45.81% | 4.418% |
| 13 | 7.445 | 909 | 911 | 915 | rVB | 100073 | 88931 | 2.61% | 0.252% |
| 14 | 8.116 | 1022 | 1025 | 1026 | rBV | 70447 | 65520 | 1.93% | 0.186% |
| 15 | 8.139 | 1026 | 1029 | 1035 | rVV | 1102387 | 1044496 | 30.71% | 2.961% |
| 16 | 8.192 | 1035 | 1038 | 1041 | rVB | 72485 | 69109 | 2.03% | 0.196% |
| 17 | 8.428 | 1074 | 1078 | 1083 | rBV5 | 46128 | 56685 | 1.67% | 0.161% |
| 18 | 8.557 | 1096 | 1100 | 1102 | rBV | 91783 | 91481 | 2.69% | 0.259% |
| 19 | 8.728 | 1126 | 1129 | 1133 | rBV2 | 58331 | 58371 | 1.72% | 0.165% |
| 20 | 8.822 | 1142 | 1145 | 1149 | rVB2 | 37647 | 40384 | 1.19% | 0.115% |
| 21 | 9.045 | 1180 | 1183 | 1187 | rVB3 | 30307 | 43108 | 1.27% | 0.122% |
| 22 | 9.092 | 1187 | 1191 | 1195 | rBV5 | 35568 | 44870 | 1.32% | 0.127% |
| 23 | 9.157 | 1199 | 1202 | 1207 | rVB | 125989 | 108577 | 3.19% | 0.308% |
| 24 | 9.216 | 1207 | 1212 | 1215 | rBV | 4031276 | 3384573 | 99.50% | 9.596% |
| 25 | 9.292 | 1222 | 1225 | 1228 | rBV | 96876 | 98968 | 2.91% | 0.281% |
| 26 | 9.327 | 1228 | 1231 | 1236 | rVV2 | 174709 | 161201 | 4.74% | 0.457% |
| 27 | 9.486 | 1254 | 1258 | 1262 | rBV4 | 42454 | 57204 | 1.68% | 0.162% |
| 28 | 9.551 | 1267 | 1269 | 1275 | rVB3 | 57582 | 85512 | 2.51% | 0.242% |
| 29 | 9.610 | 1275 | 1279 | 1282 | rBV | 577774 | 544719 | 16.01% | 1.544% |
| 30 | 9.763 | 1302 | 1305 | 1308 | rBV3 | 46085 | 44432 | 1.31% | 0.126% |
| 31 | 9.804 | 1308 | 1312 | 1314 | rBV3 | 55583 | 65871 | 1.94% | 0.187% |
| 32 | 9.898 | 1320 | 1328 | 1332 | rBV | 1543814 | 1347716 | 39.62% | 3.821% |
| 33 | 9.927 | 1332 | 1333 | 1337 | rVB2 | 68882 | 59483 | 1.75% | 0.169% |
| 34 | 9.998 | 1343 | 1345 | 1350 | rVB2 | 55301 | 67330 | 1.98% | 0.191% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 10.057 | 1350 | 1355 | 1357 | rBV4 | 40453 | 65648 | 1.93% | 0.186% |
| 36 | 10.104 | 1357 | 1363 | 1367 | rVV3 | 63579 | 130514 | 3.84% | 0.370% |
| 37 | 10.145 | 1367 | 1370 | 1374 | rVB3 | 82378 | 100813 | 2.96% | 0.286% |
| 38 | 10.216 | 1379 | 1382 | 1384 | rBV | 70764 | 67774 | 1.99% | 0.192% |
| 39 | 10.304 | 1393 | 1397 | 1399 | rBV3 | 68618 | 82727 | 2.43% | 0.235% |
| 40 | 10.322 | 1399 | 1400 | 1403 | rVB | 61326 | 44948 | 1.32% | 0.127% |
| 41 | 10.451 | 1418 | 1422 | 1423 | rBV2 | 51562 | 59807 | 1.76% | 0.170% |
| 42 | 10.474 | 1423 | 1426 | 1432 | rVV4 | 76992 | 88016 | 2.59% | 0.250% |
| 43 | 10.545 | 1434 | 1438 | 1443 | rVB | 165926 | 203728 | 5.99% | 0.578% |
| 44 | 10.692 | 1460 | 1463 | 1474 | rVB | 2389041 | 2120843 | 62.35% | 6.013% |
| 45 | 10.810 | 1479 | 1483 | 1487 | rBV | 369357 | 378090 | 11.11% | 1.072% |
| 46 | 10.992 | 1511 | 1514 | 1518 | rBV5 | 39788 | 61219 | 1.80% | 0.174% |
| 47 | 11.027 | 1518 | 1520 | 1523 | rVB3 | 57945 | 46375 | 1.36% | 0.131% |
| 48 | 11.280 | 1559 | 1563 | 1569 | rVB2 | 213938 | 255144 | 7.50% | 0.723% |
| 49 | 11.392 | 1578 | 1582 | 1585 | rBV | 1563156 | 1370801 | 40.30% | 3.887% |
| 50 | 11.416 | 1585 | 1586 | 1590 | rVV | 280711 | 205110 | 6.03% | 0.582% |
| 51 | 11.469 | 1592 | 1595 | 1598 | rVV | 96767 | 111364 | 3.27% | 0.316% |
| 52 | 11.504 | 1598 | 1601 | 1603 | rVV3 | 36592 | 48782 | 1.43% | 0.138% |
| 53 | 11.563 | 1607 | 1611 | 1613 | rVV4 | 34991 | 46202 | 1.36% | 0.131% |
| 54 | 11.627 | 1620 | 1622 | 1626 | rVB | 75967 | 70190 | 2.06% | 0.199% |
| 55 | 11.916 | 1665 | 1671 | 1678 | rBV3 | 195441 | 314927 | 9.26% | 0.893% |
| 56 | 12.010 | 1684 | 1687 | 1689 | rBV3 | 60883 | 62991 | 1.85% | 0.179% |
| 57 | 12.086 | 1697 | 1700 | 1705 | rBV3 | 45338 | 56024 | 1.65% | 0.159% |
| 58 | 12.368 | 1745 | 1748 | 1751 | rBV2 | 59529 | 57402 | 1.69% | 0.163% |
| 59 | 12.433 | 1756 | 1759 | 1764 | rBV2 | 121993 | 200340 | 5.89% | 0.568% |
| 60 | 12.474 | 1764 | 1766 | 1770 | rVB4 | 81570 | 75595 | 2.22% | 0.214% |
| 61 | 12.610 | 1786 | 1789 | 1796 | rBV | 318415 | 523644 | 15.39% | 1.485% |
| 62 | 12.704 | 1803 | 1805 | 1813 | rBV7 | 52030 | 77465 | 2.28% | 0.220% |
| 63 | 12.792 | 1818 | 1820 | 1823 | rVB3 | 43931 | 39530 | 1.16% | 0.112% |
| 64 | 12.845 | 1823 | 1829 | 1835 | rBV2 | 243260 | 354696 | 10.43% | 1.006% |
| 65 | 12.898 | 1836 | 1838 | 1841 | rVB3 | 53769 | 49571 | 1.46% | 0.141% |
| 66 | 12.980 | 1848 | 1852 | 1856 | rVB | 3617381 | 3401679 | 100.00% | 9.645% |
| 67 | 13.204 | 1887 | 1890 | 1893 | rBV | 88073 | 71710 | 2.11% | 0.203% |
| 68 | 13.239 | 1894 | 1896 | 1900 | rVB3 | 41647 | 42472 | 1.25% | 0.120% |
| 69 | 13.551 | 1946 | 1949 | 1952 | rVB2 | 88165 | 85654 | 2.52% | 0.243% |
| 70 | 13.874 | 2001 | 2004 | 2012 | rVB2 | 269558 | 336287 | 9.89% | 0.953% |
| 71 | 14.045 | 2029 | 2033 | 2037 | rBV | 1067274 | 1053733 | 30.98% | 2.988% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 14.198 | 2056 | 2059 | 2063 | rVB | 108004 | 98730 | 2.90% | 0.280% |
| 73 | 14.504 | 2108 | 2111 | 2113 | rBV | 137125 | 137932 | 4.05% | 0.391% |
| 74 | 14.809 | 2160 | 2163 | 2168 | rVB | 155525 | 159855 | 4.70% | 0.453% |
| 75 | 15.151 | 2218 | 2221 | 2227 | rVB | 156117 | 184112 | 5.41% | 0.522% |
| 76 | 15.539 | 2282 | 2287 | 2296 | rVB | 927168 | 1306771 | 38.42% | 3.705% |
| 77 | 15.980 | 2358 | 2362 | 2368 | rBV2 | 121344 | 172077 | 5.06% | 0.488% |
| 78 | 16.498 | 2446 | 2450 | 2458 | rVB | 80745 | 132570 | 3.90% | 0.376% |

Sum of corrected areas: 35269584

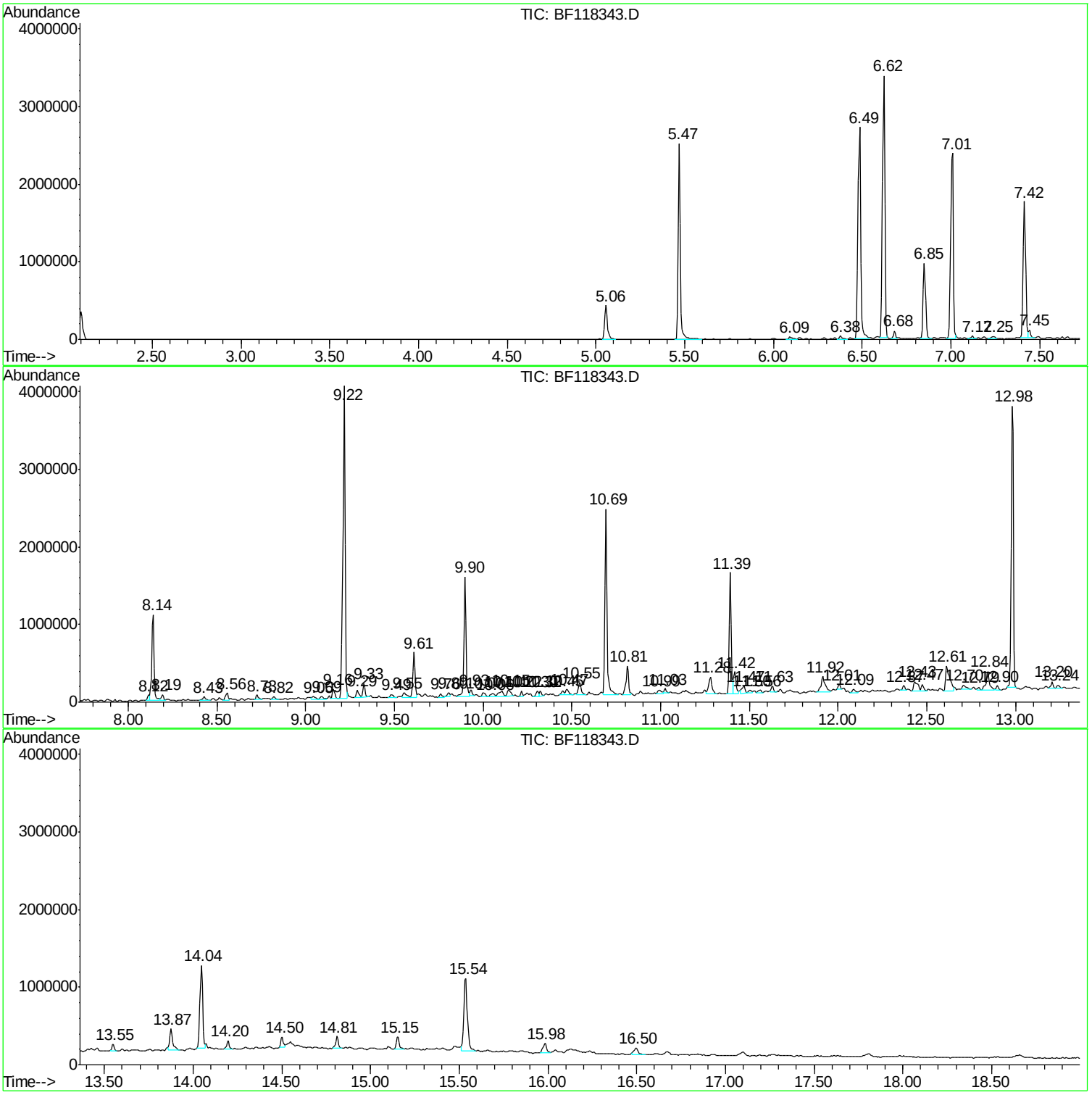
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

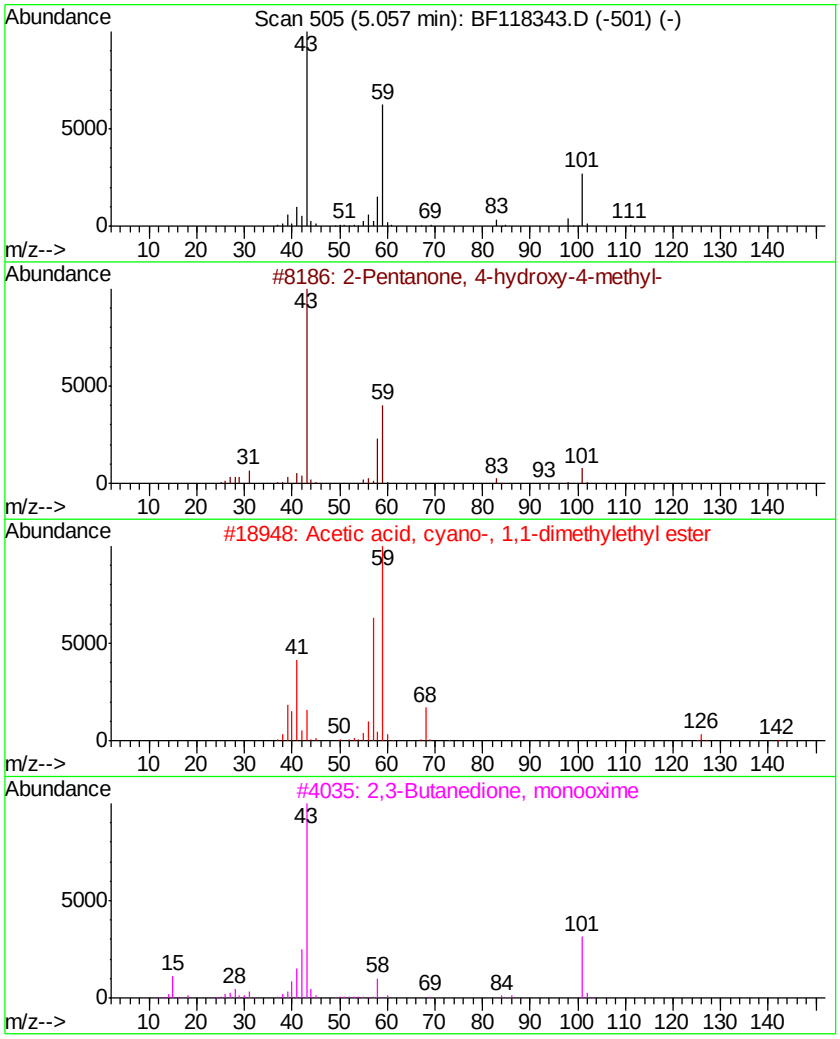
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

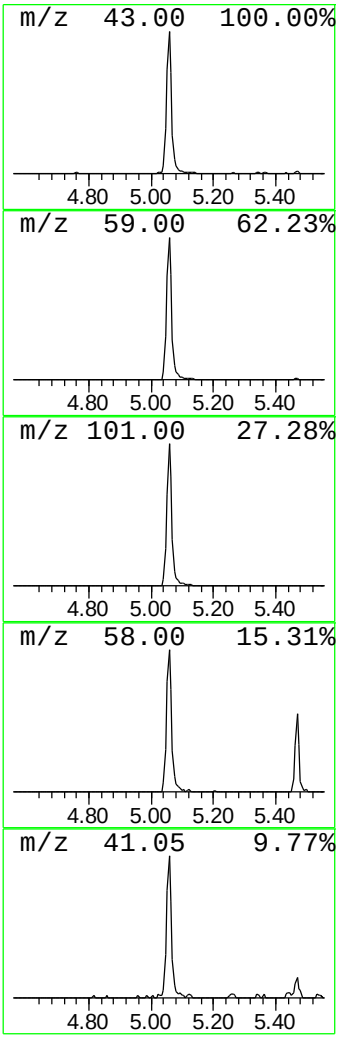
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.06 | 11.94 ng | 502473 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 17 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

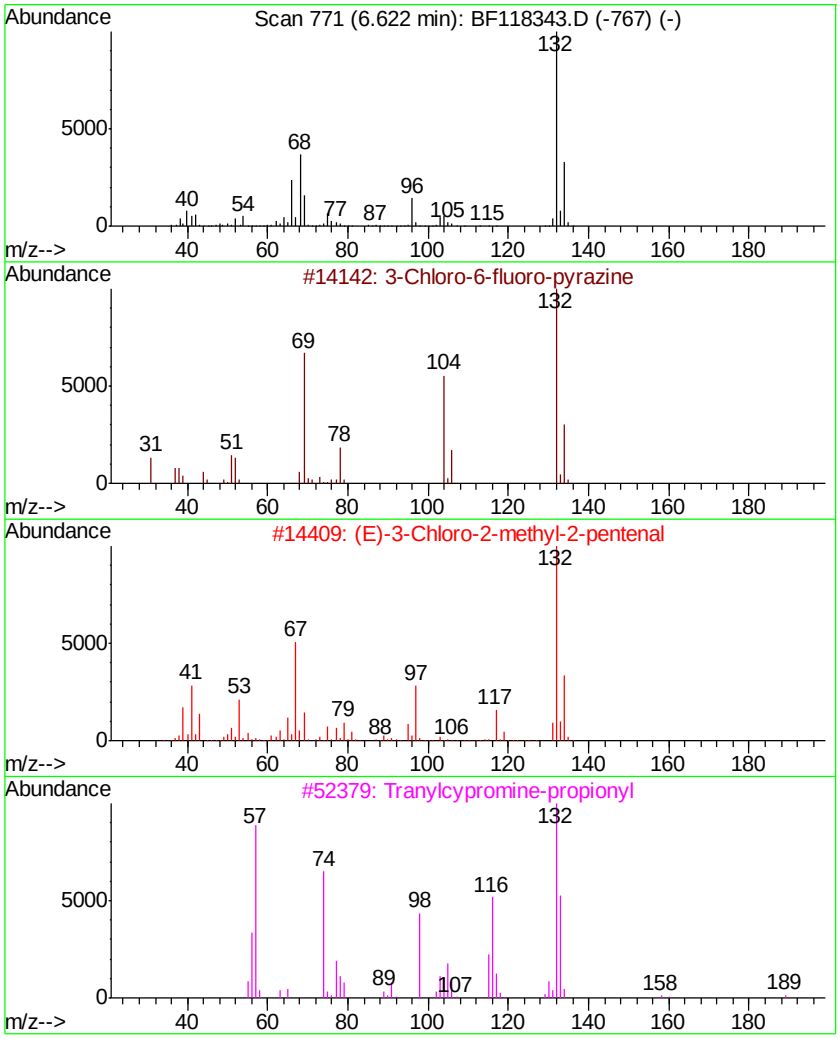
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

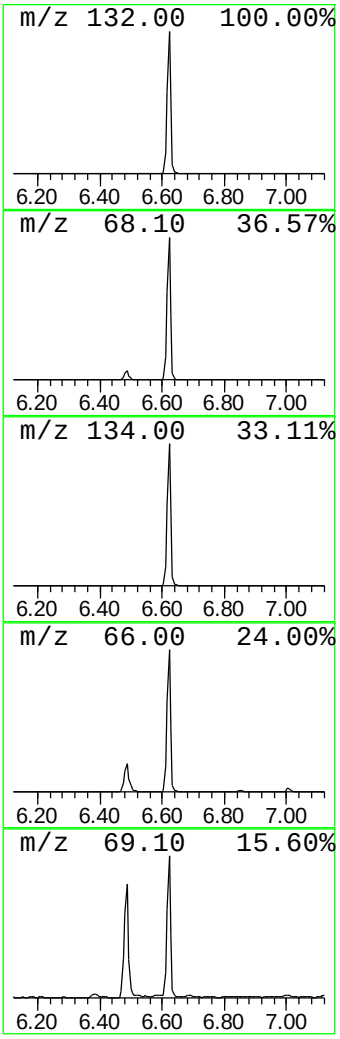
**********

Peak Number 2 unknown6.62 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.62 | 65.84 ng | 2769840 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 16 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | Cyclopropanamine, 1-phenyl- | 133 | C9H11N | 1000351-26-2 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

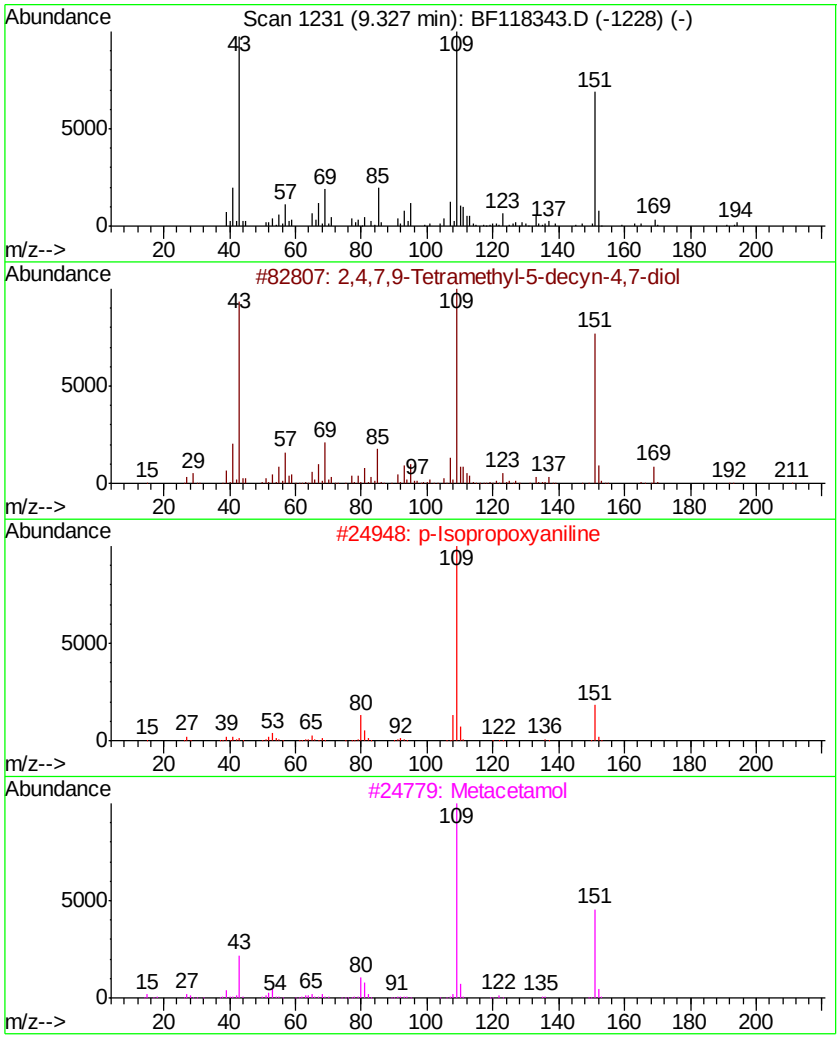
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

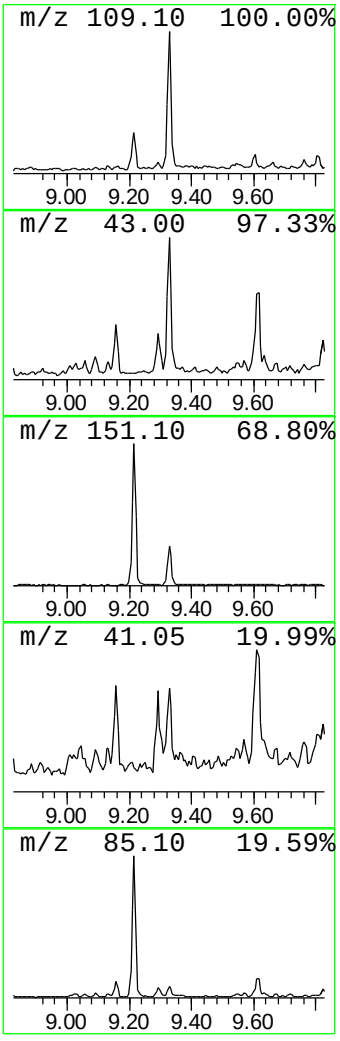
**********

Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.33 | 2.39 ng | 161201 | Acenaphthene-d10 | 9.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,7,9-Tetramethyl-5-decyn-4,7-... | 226 | C14H26O2 | 000126-86-3 | 87 |
| 2 | p-Isopropoxyaniline | 151 | C9H13NO | 007664-66-6 | 53 |
| 3 | Metacetamol | 151 | C8H9NO2 | 000621-42-1 | 53 |
| 4 | m-Isopropoxyaniline | 151 | C9H13NO | 041406-00-2 | 53 |
| 5 | Diacetamate | 193 | C10H11NO3 | 002623-33-8 | 53 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

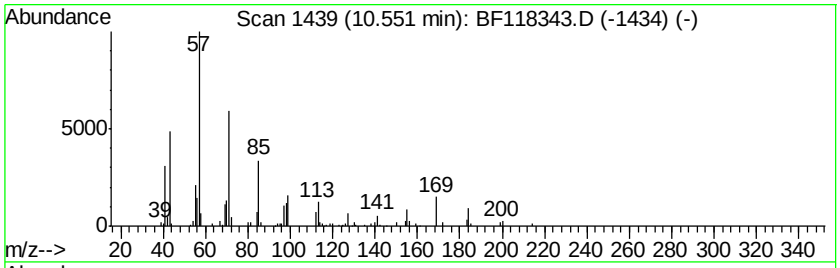
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

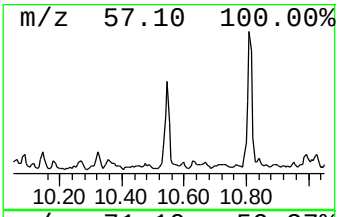
**********

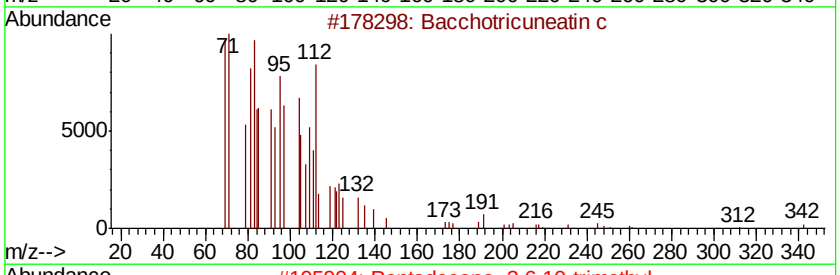
Peak Number 5 Bacchotricuneatin c Concentration Rank 8

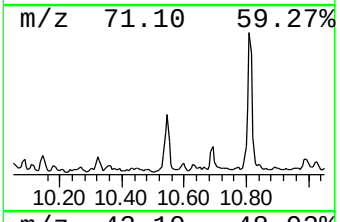
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.55 | 3.02 ng | 203728 | Acenaphthene-d10 | 9.90 |

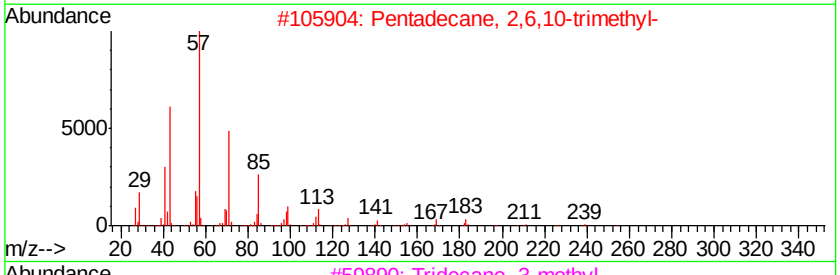
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bacchotricuneatin c | 342 | C20H22O5 | 066563-30-2 | 95 |
| 2 | Pentadecane, 2,6,10-trimethyl- | 254 | C18H38 | 003892-00-0 | 91 |
| 3 | Tridecane, 3-methyl- | 198 | C14H30 | 006418-41-3 | 80 |
| 4 | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42 | 000638-36-8 | 72 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 72 |

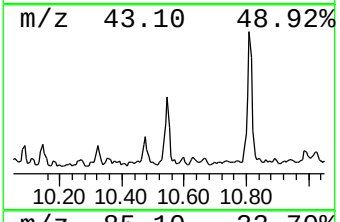


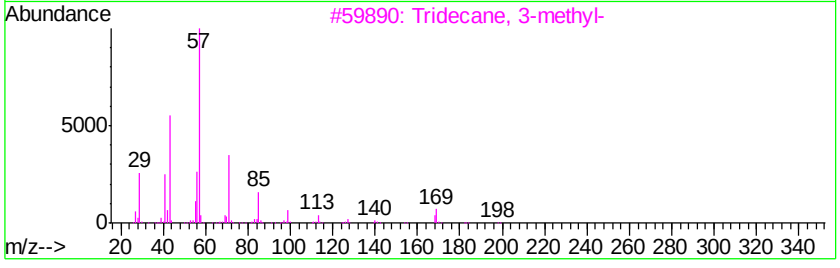



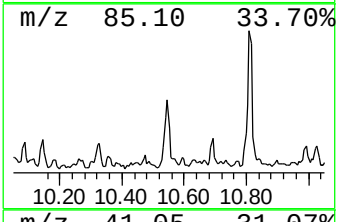



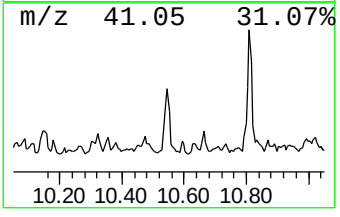



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

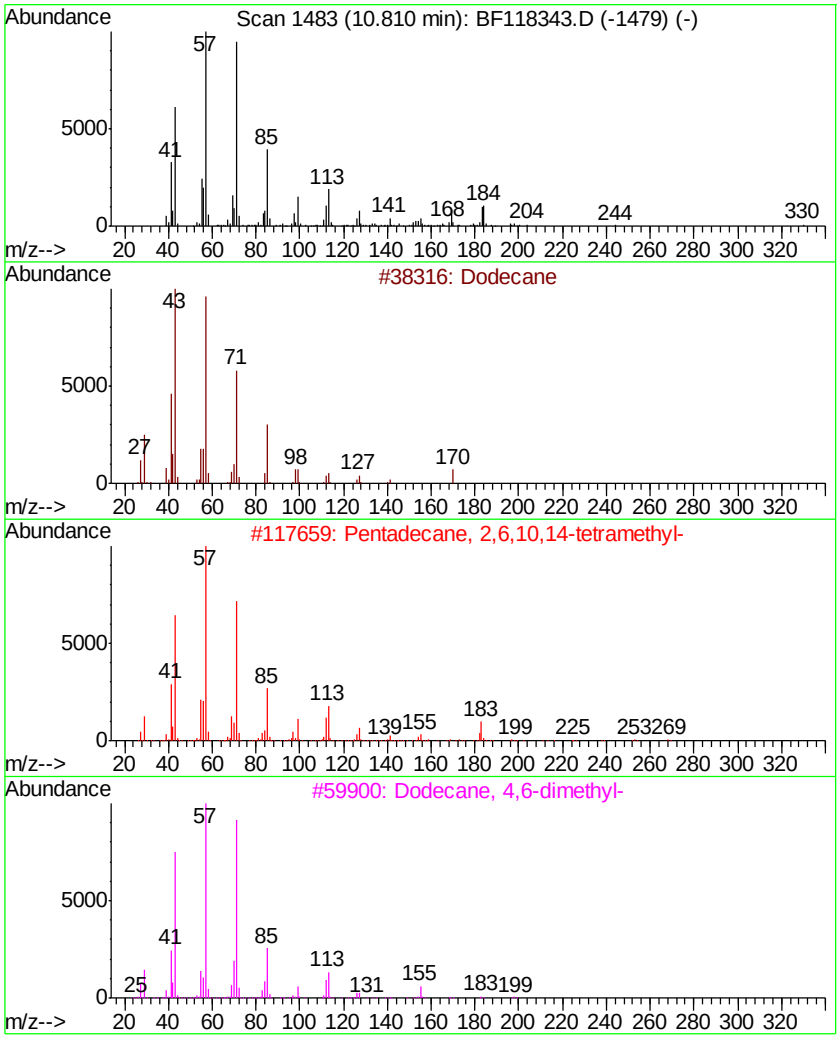
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

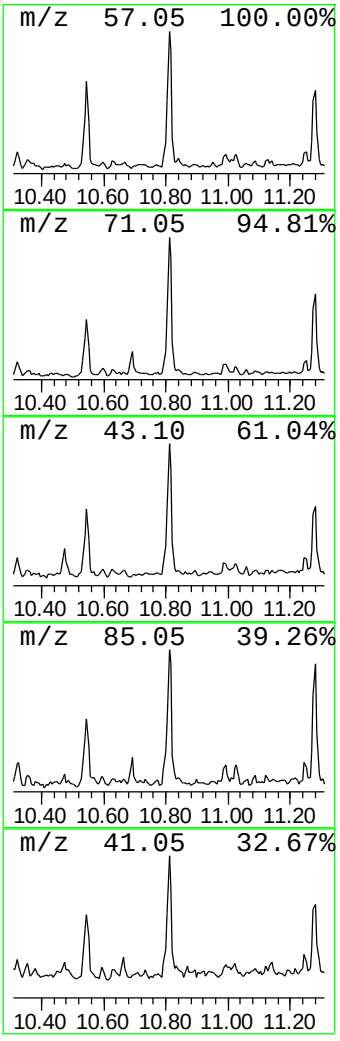
**********

Peak Number 6 Dodecane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.81 | 5.52 ng | 378090 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecane | 170 | C12H26 | 000112-40-3 | 83 |
| 2 | Pentadecane, 2,6,10,14-tetramethyl- | 268 | C19H40 | 001921-70-6 | 83 |
| 3 | Dodecane, 4,6-dimethyl- | 198 | C14H30 | 061141-72-8 | 76 |
| 4 | Hexadecane, 2,6,11,15-tetramethyl- | 282 | C20H42 | 000504-44-9 | 74 |
| 5 | Octane, 5-ethyl-2-methyl- | 156 | C11H24 | 062016-18-6 | 72 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

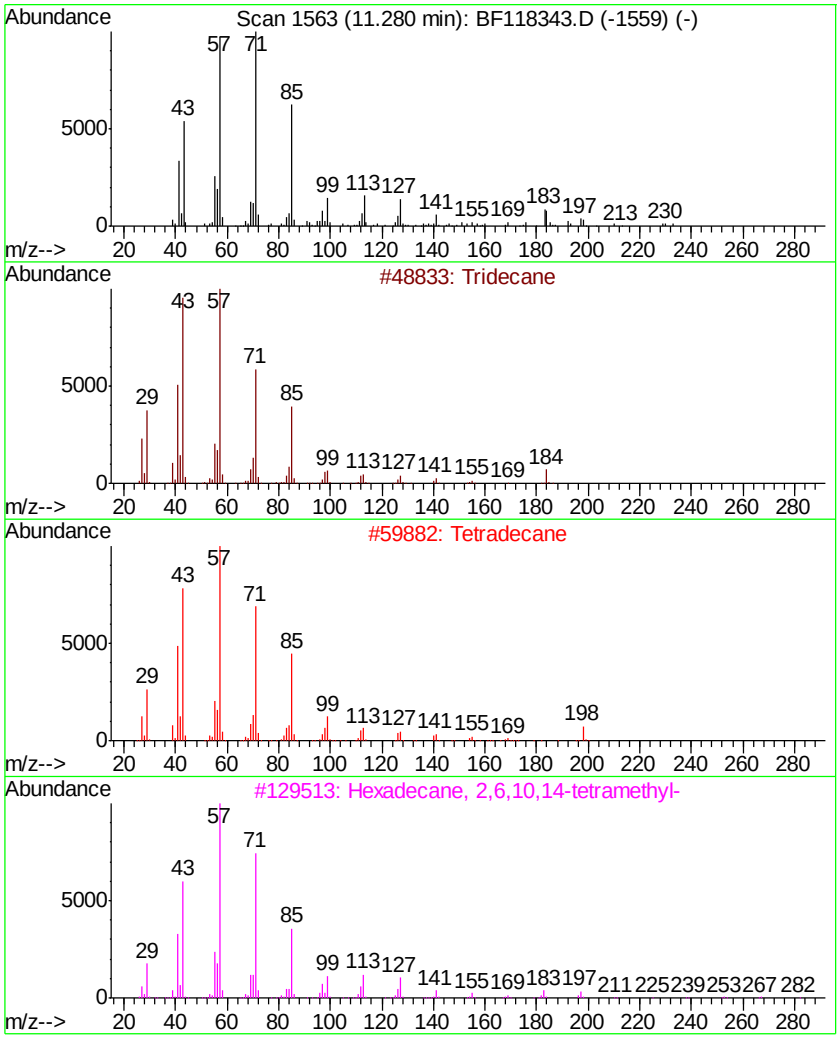
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

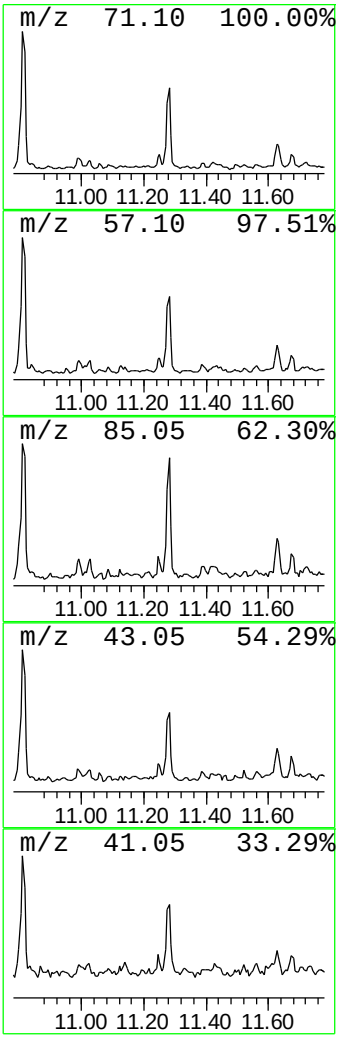
**********

Peak Number 7 Tridecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.28 | 3.72 ng | 255144 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecane | 184 | C13H28 | 000629-50-5 | 91 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 87 |
| 3 | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42 | 000638-36-8 | 74 |
| 4 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 72 |
| 5 | Nonane, 5-(2-methylpropyl)- | 184 | C13H28 | 062185-53-9 | 72 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

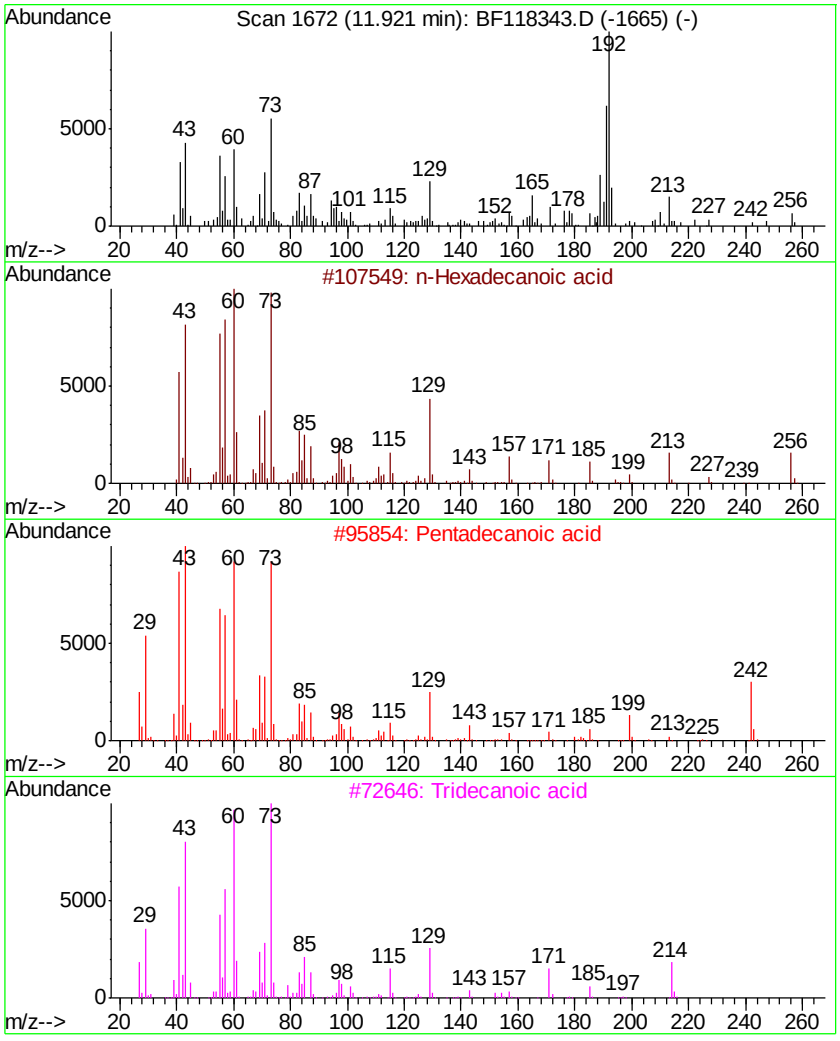
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

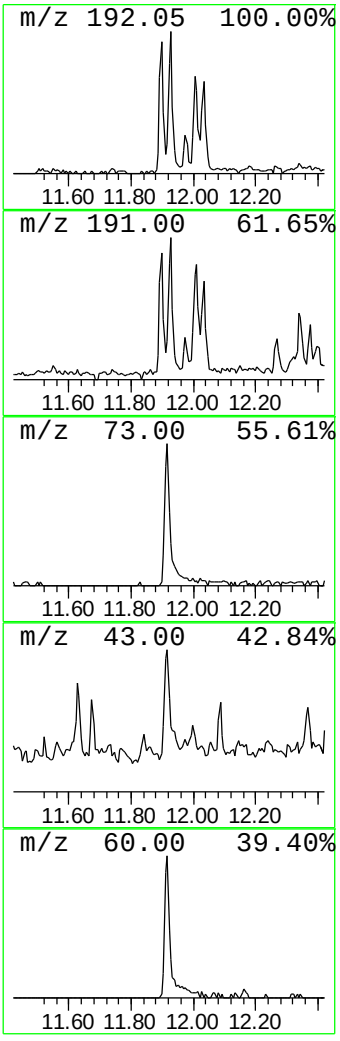
**********

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.92 | 4.59 ng | 314927 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 86 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 68 |
| 5 | Tetradecane | 198 | C14H30 | 000629-59-4 | 15 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

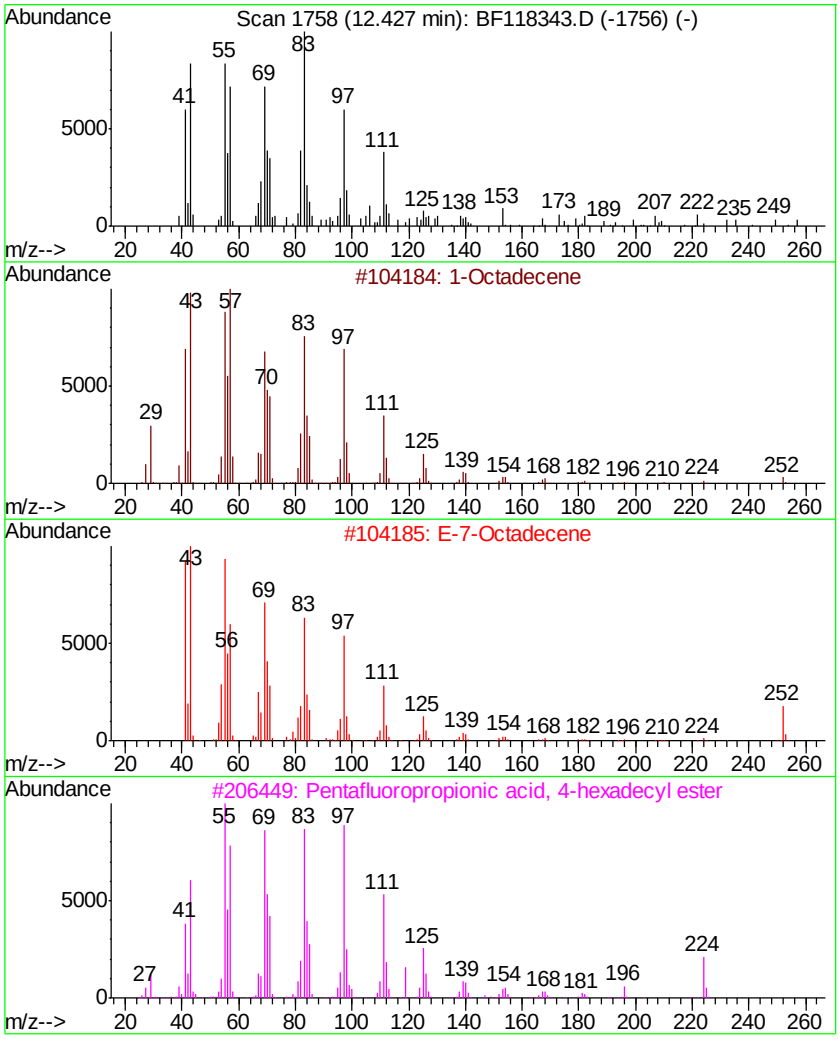
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

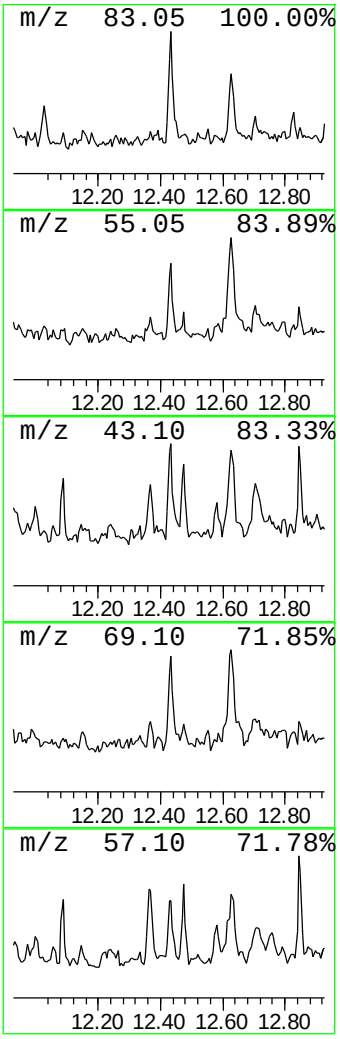
**********

Peak Number 9 1-Octadecene Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.43 | 2.92 ng | 200340 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 64 |
| 2 | E-7-Octadecene | 252 | C18H36 | 1000130-92-0 | 64 |
| 3 | Pentafluoropropionic acid, 4-hex... | 388 | C19H33F5O2 | 1000283-04-1 | 58 |
| 4 | Cyclopropane, 1-(1,2-dimethylpro... | 252 | C18H36 | 041977-42-8 | 53 |
| 5 | Cyclopentane, 1-pentyl-2-propyl- | 182 | C13H26 | 062199-51-3 | 49 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

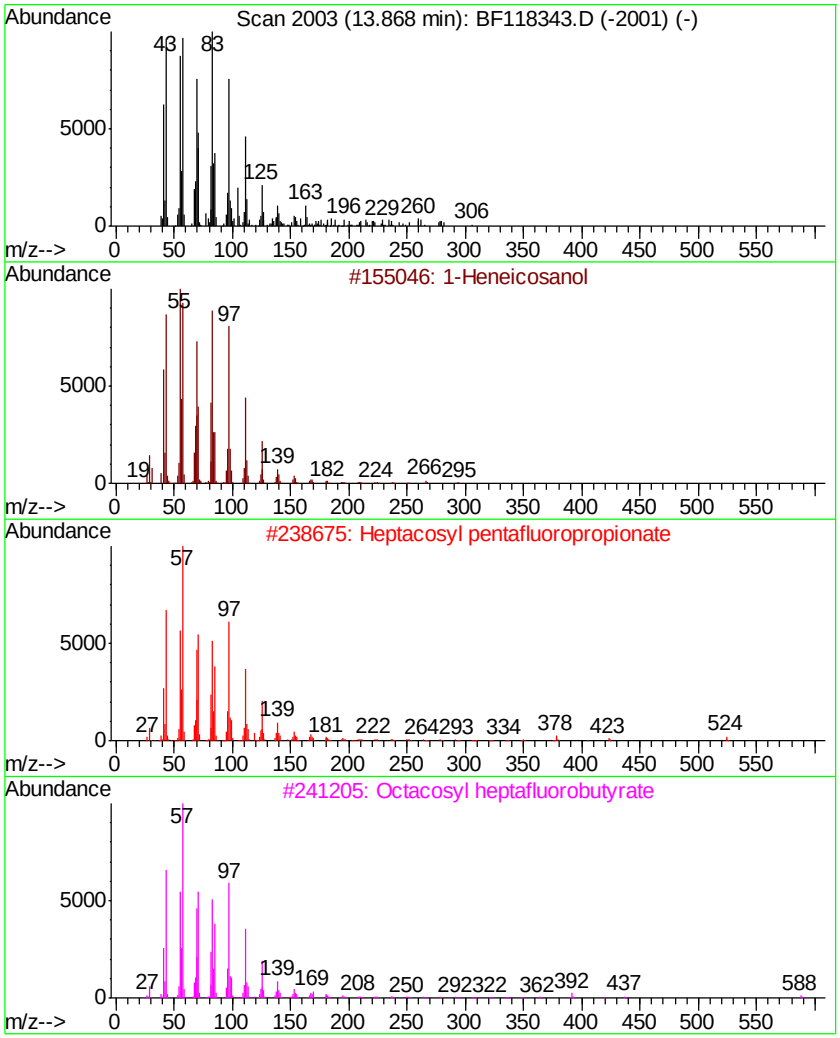
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

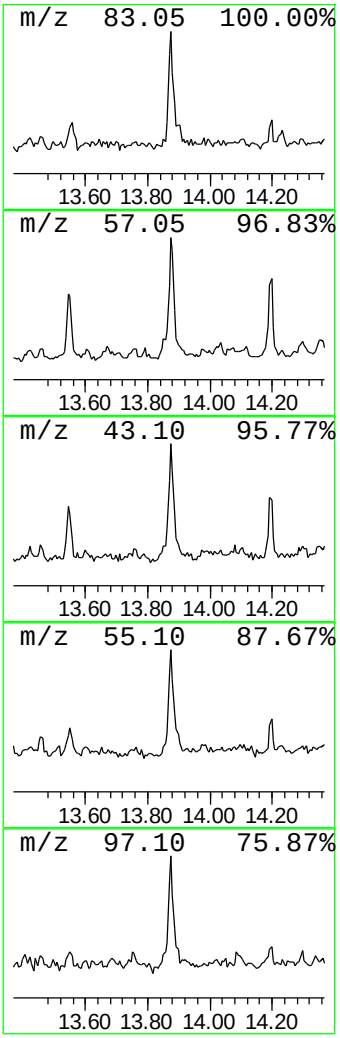
**********

Peak Number 10 1-Heneicosanol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.87 | 6.38 ng | 336287 | Chrysene-d12 | 14.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 2 | Heptacosyl pentafluoropropionate | 542 | C30H55F5O2 | 1000351-81-6 | 91 |
| 3 | Octacosyl heptafluorobutyrate | 606 | C32H57F7O2 | 1000351-83-6 | 91 |
| 4 | Octacosyl trifluoroacetate | 506 | C30H57F3O2 | 1000351-74-9 | 91 |
| 5 | Triacontyl pentafluoropropionate | 584 | C33H61F5O2 | 1000351-80-0 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

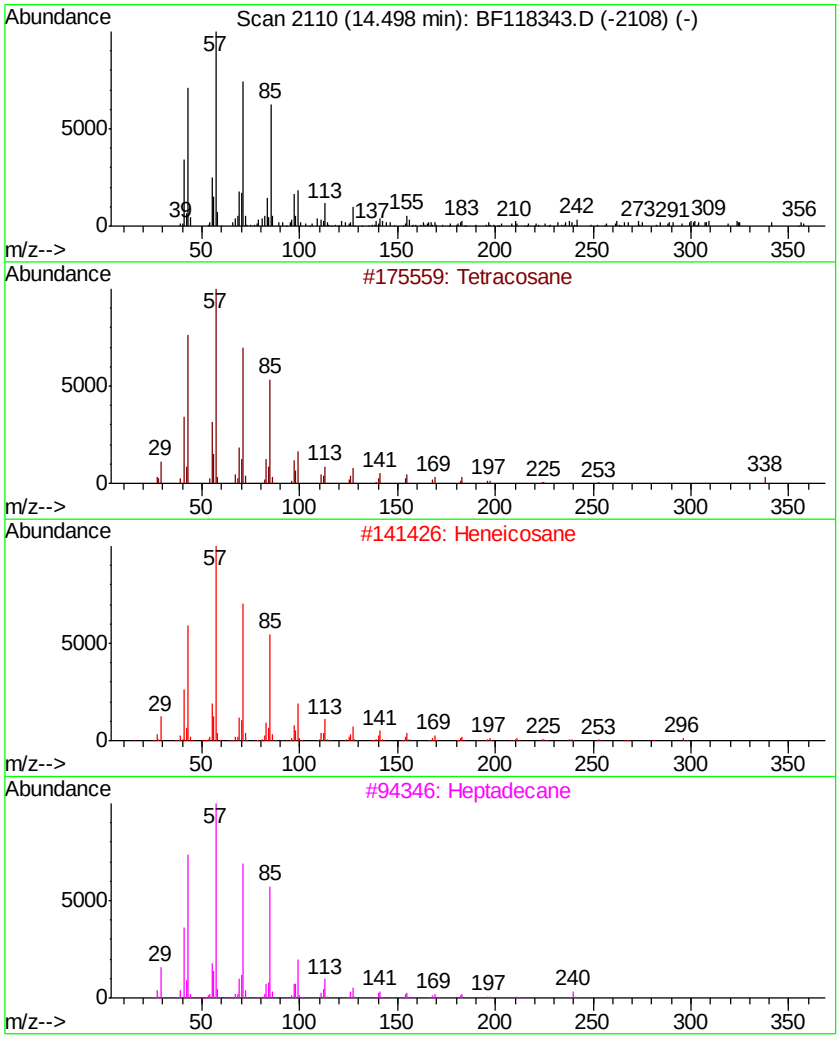
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

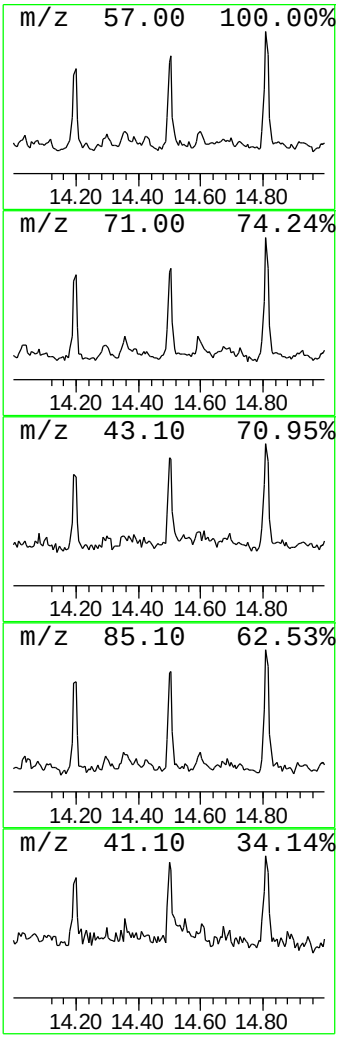
**********

Peak Number 11 Tetracosane Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.50 | 2.62 ng | 137932 | Chrysene-d12 | 14.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |
| 4 | Dodecane, 2-methyl- | 184 | C13H28 | 001560-97-0 | 86 |
| 5 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 83 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

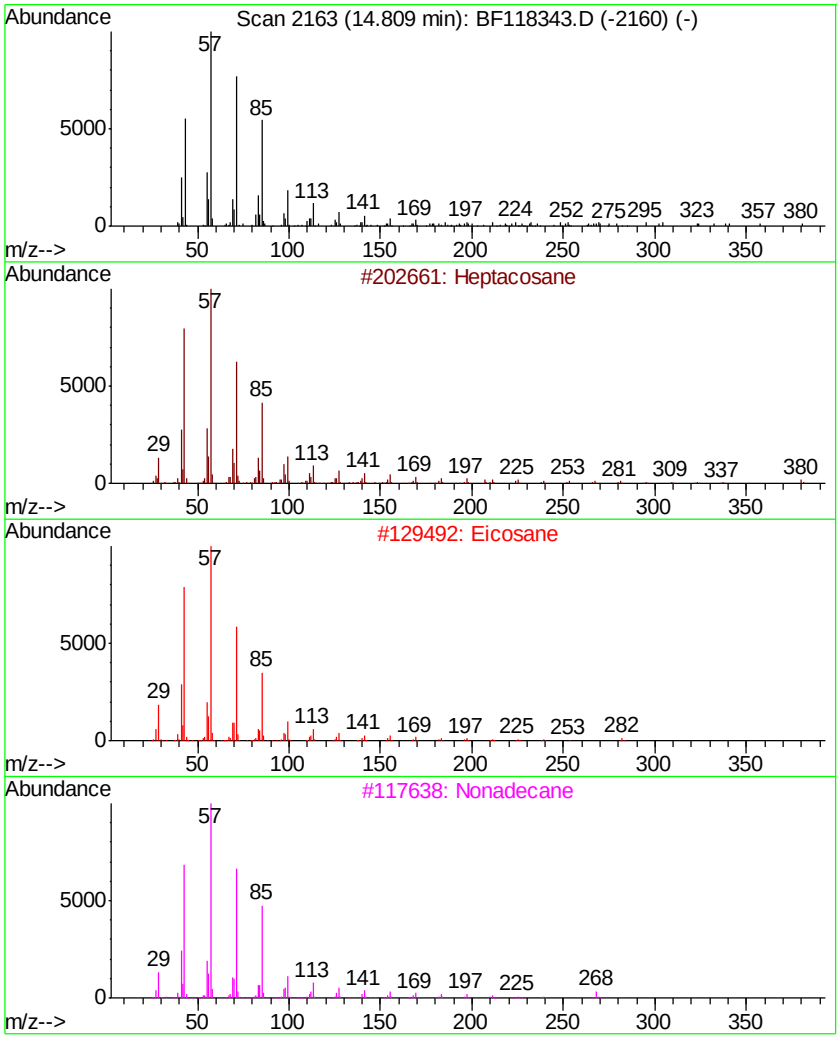
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

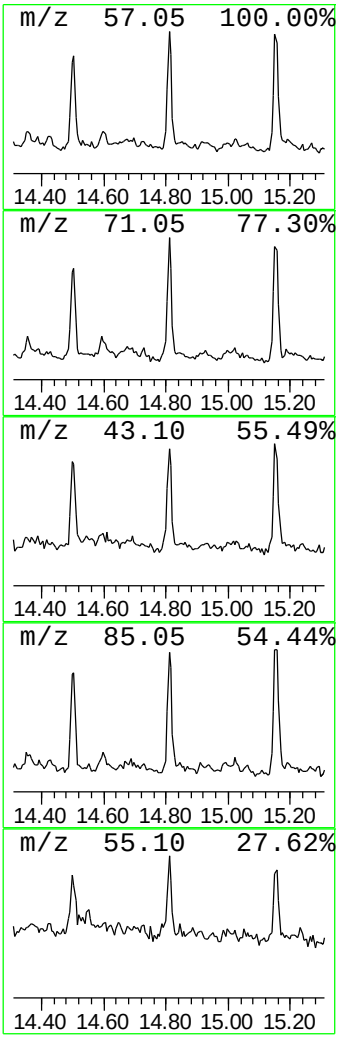
**********

Peak Number 12 Heptacosane Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.81 | 2.45 ng | 159855 | Perylene-d12 | 15.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptacosane | 380 | C27H56 | 000593-49-7 | 95 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 93 |
| 3 | Nonadecane | 268 | C19H40 | 000629-92-5 | 93 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

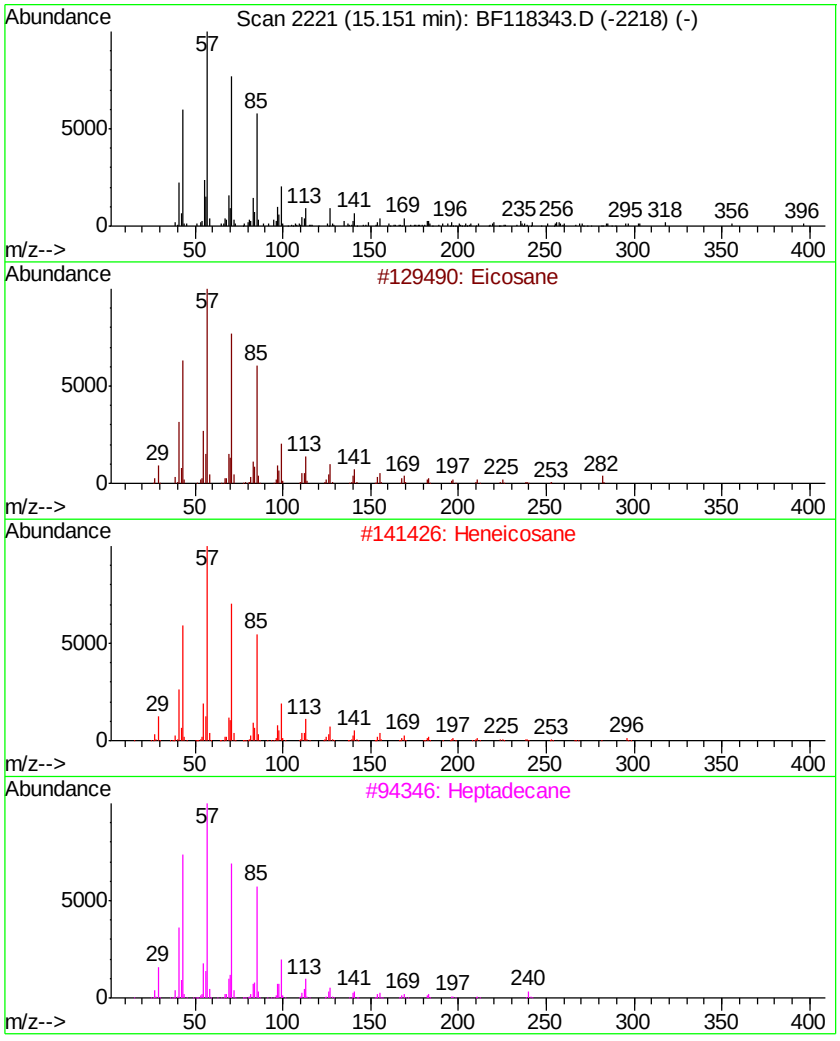
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

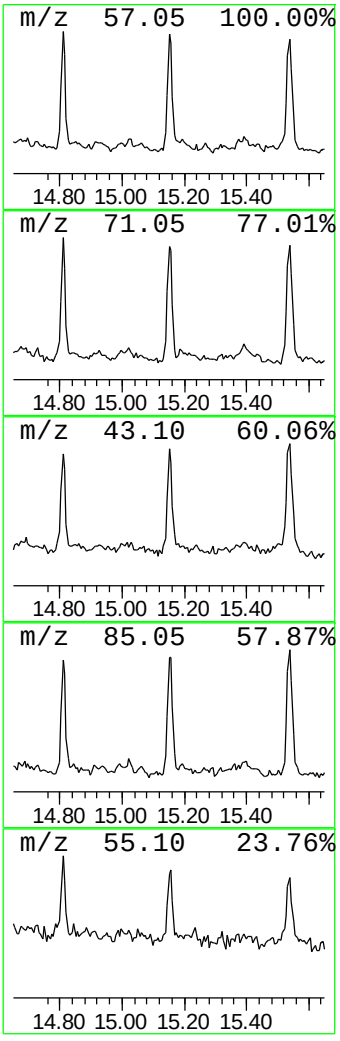
**********

Peak Number 13 Eicosane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.15 | 2.82 ng | 184112 | Perylene-d12 | 15.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 97 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 91 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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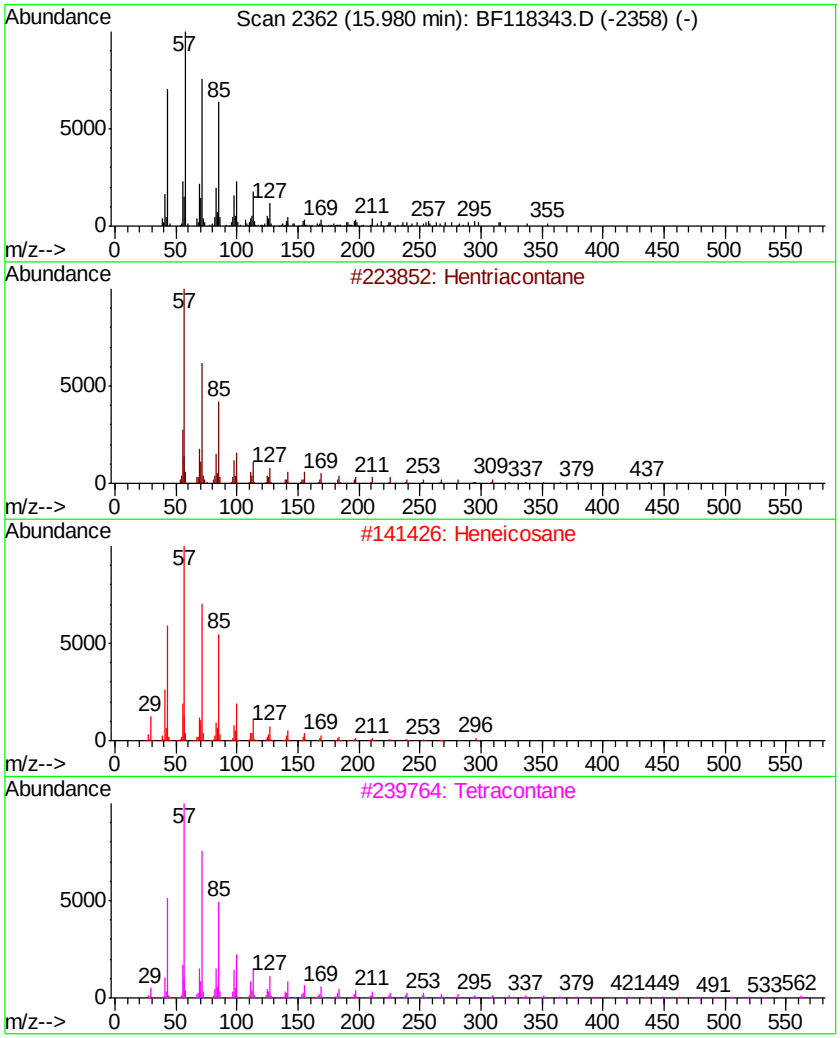
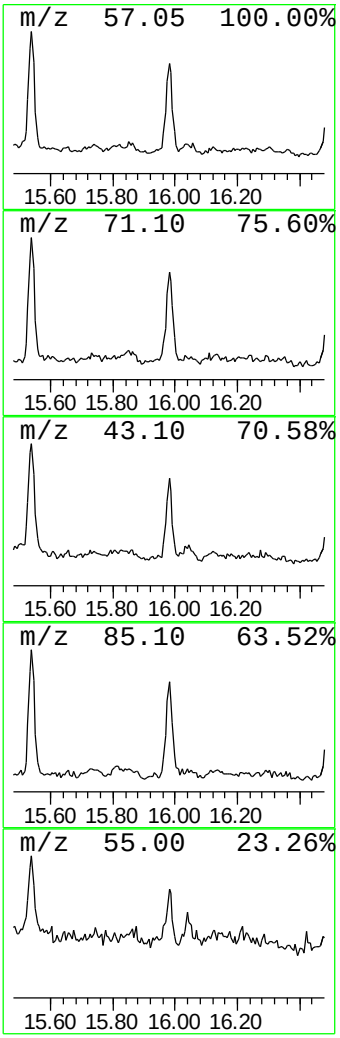
Peak Number 14 Hentriacontane Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.98 | 2.63 ng | 172077 | Perylene-d12 | 15.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 90 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 3 | Tetracontane | 563 | C40H82 | 004181-95-7 | 86 |
| 4 | Sulfurous acid, butyl undecyl ester | 292 | C15H32O3S | 1000309-17-8 | 86 |
| 5 | Triacontane | 422 | C30H62 | 000638-68-6 | 83 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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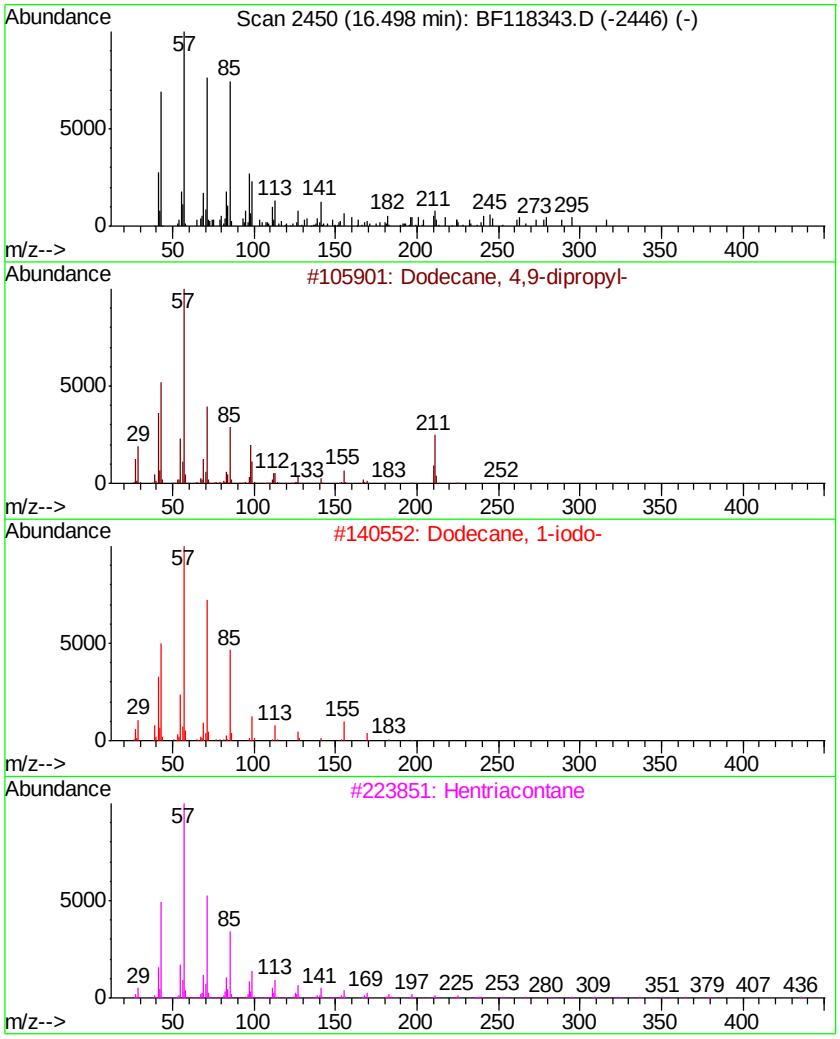
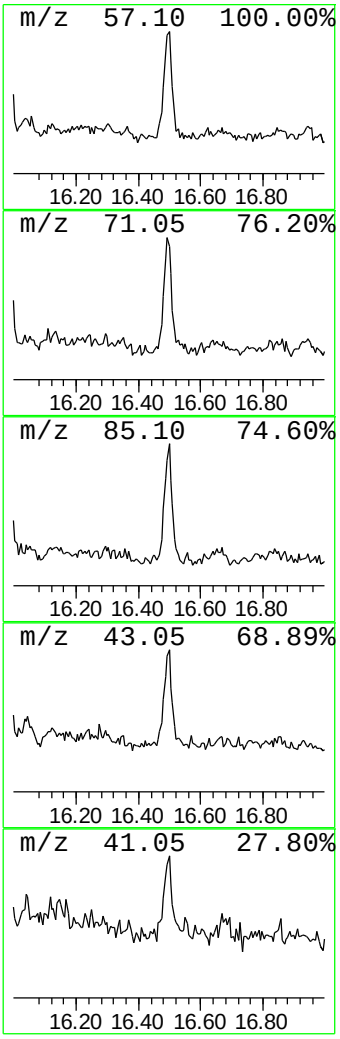
Peak Number 15 Dodecane, 4,9-dipropyl- Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.50 | 2.03 ng | 132570 | Perylene-d12 | 15.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecane, 4,9-dipropyl- | 254 | C18H38 | 003054-63-5 | 59 |
| 2 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 59 |
| 3 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 52 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 49 |
| 5 | Pentacosane | 352 | C25H52 | 000629-99-2 | 49 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122719\
Data File : BF118343.D
Acq On : 27 Dec 2019 17:43
Operator : JU
Sample : K6435-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-3E-(09.5-11.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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 |
| 2-Pentanone, 4-hy... | 5.06 | 11.9 | ng | 502473 | 1 | 6.85 | 841413 | 20.0 |
| unknown6.62 | 6.62 | 65.8 | ng | 2769840 | 1 | 6.85 | 841413 | 20.0 |
| 2,4,7,9-Tetrameth... | 9.33 | 2.4 | ng | 161201 | 3 | 9.90 | 1347720 | 20.0 |
| Bacchotricuneatin c | 10.55 | 3.0 | ng | 203728 | 3 | 9.90 | 1347720 | 20.0 |
| Dodecane | 10.81 | 5.5 | ng | 378090 | 4 | 11.39 | 1370800 | 20.0 |
| Tridecane | 11.28 | 3.7 | ng | 255144 | 4 | 11.39 | 1370800 | 20.0 |
| n-Hexadecanoic acid | 11.92 | 4.6 | ng | 314927 | 4 | 11.39 | 1370800 | 20.0 |
| 1-Octadecene | 12.43 | 2.9 | ng | 200340 | 4 | 11.39 | 1370800 | 20.0 |
| 1-Heneicosanol | 13.87 | 6.4 | ng | 336287 | 5 | 14.04 | 1053730 | 20.0 |
| Tetracosane | 14.50 | 2.6 | ng | 137932 | 5 | 14.04 | 1053730 | 20.0 |
| Heptacosane | 14.81 | 2.5 | ng | 159855 | 6 | 15.54 | 1306770 | 20.0 |
| Eicosane | 15.15 | 2.8 | ng | 184112 | 6 | 15.54 | 1306770 | 20.0 |
| Hentriacontane | 15.98 | 2.6 | ng | 172077 | 6 | 15.54 | 1306770 | 20.0 |
| Dodecane, 4,9-dip... | 16.50 | 2.0 | ng | 132570 | 6 | 15.54 | 1306770 | 20.0 |