LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** A010015

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-BF091521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125523.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.193 | 10 | 18 | 25 | rVB | 1093583 | 1369149 | 25.00% | 1.505% |
| 2 | 4.487 | 384 | 408 | 409 | rBV2 | 63168 | 282828 | 5.16% | 0.311% |
| 3 | 5.098 | 508 | 512 | 521 | rBV | 705649 | 993903 | 18.15% | 1.092% |
| 4 | 5.498 | 575 | 580 | 583 | rBV | 3904107 | 4183844 | 76.39% | 4.598% |
| 5 | 5.675 | 597 | 610 | 614 | rBV | 83220 | 255280 | 4.66% | 0.281% |
| 6 | 6.510 | 746 | 752 | 757 | rBV | 3649563 | 4513016 | 82.40% | 4.960% |
| 7 | 6.569 | 757 | 762 | 768 | rVV | 233265 | 488413 | 8.92% | 0.537% |
| 8 | 6.863 | 809 | 812 | 816 | rBV | 1147668 | 1043665 | 19.05% | 1.147% |
| 9 | 7.275 | 873 | 882 | 893 | rBV | 127581 | 185856 | 3.39% | 0.204% |
| 10 | 7.433 | 901 | 909 | 912 | rBV | 2769173 | 2938653 | 53.65% | 3.229% |
| 11 | 7.557 | 925 | 930 | 938 | rBV | 194731 | 303740 | 5.55% | 0.334% |
| 12 | 7.933 | 984 | 994 | 1001 | rBV2 | 445513 | 884253 | 16.14% | 0.972% |
| 13 | 8.063 | 1012 | 1016 | 1022 | rBV | 191980 | 355733 | 6.49% | 0.391% |
| 14 | 8.151 | 1027 | 1031 | 1033 | rVV | 1515973 | 1370705 | 25.03% | 1.506% |
| 15 | 8.169 | 1033 | 1034 | 1041 | rVB | 258624 | 188999 | 3.45% | 0.208% |
| 16 | 8.527 | 1088 | 1095 | 1103 | rBV | 650816 | 1001972 | 18.29% | 1.101% |
| 17 | 9.086 | 1186 | 1190 | 1197 | rVV | 509444 | 663578 | 12.12% | 0.729% |
| 18 | 9.227 | 1208 | 1214 | 1217 | rBV | 4886499 | 4620321 | 84.36% | 5.078% |
| 19 | 9.327 | 1227 | 1231 | 1234 | rVB | 1334266 | 1106186 | 20.20% | 1.216% |
| 20 | 9.486 | 1252 | 1258 | 1267 | rBV2 | 182859 | 534348 | 9.76% | 0.587% |
| 21 | 9.563 | 1268 | 1271 | 1274 | rVV2 | 139476 | 191601 | 3.50% | 0.211% |
| 22 | 9.610 | 1277 | 1279 | 1288 | rVV2 | 174981 | 265718 | 4.85% | 0.292% |
| 23 | 9.769 | 1302 | 1306 | 1313 | rVV | 389499 | 376895 | 6.88% | 0.414% |
| 24 | 9.904 | 1321 | 1329 | 1333 | rBV2 | 1455880 | 1591928 | 29.07% | 1.749% |
| 25 | 9.939 | 1333 | 1335 | 1338 | rVB2 | 195935 | 158996 | 2.90% | 0.175% |
| 26 | 10.110 | 1361 | 1364 | 1368 | rBV | 216070 | 196447 | 3.59% | 0.216% |
| 27 | 10.451 | 1419 | 1422 | 1427 | rVB3 | 118432 | 142425 | 2.60% | 0.157% |
| 28 | 10.616 | 1446 | 1450 | 1456 | rBV3 | 213175 | 299542 | 5.47% | 0.329% |
| 29 | 10.698 | 1460 | 1464 | 1470 | rVB | 2173695 | 1991702 | 36.36% | 2.189% |
| 30 | 11.004 | 1509 | 1516 | 1519 | rBV4 | 119770 | 179240 | 3.27% | 0.197% |
| 31 | 11.151 | 1539 | 1541 | 1546 | rVV2 | 107978 | 132190 | 2.41% | 0.145% |
| 32 | 11.204 | 1546 | 1550 | 1554 | rVV | 365469 | 336499 | 6.14% | 0.370% |
| 33 | 11.251 | 1554 | 1558 | 1560 | rVV2 | 126907 | 175459 | 3.20% | 0.193% |
| 34 | 11.292 | 1562 | 1565 | 1570 | rVB | 280605 | 266615 | 4.87% | 0.293% |
| 35 | 11.398 | 1579 | 1583 | 1585 | rBV | 1298068 | 1289424 | 23.54% | 1.417% |
| 36 | 11.427 | 1585 | 1588 | 1590 | rVV | 3712743 | 3216626 | 58.73% | 3.535% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** A010015

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-BF091521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 11.474 | 1590 | 1596 | 1598 | rVB | 883407 | 770449 | 14.07% | 0.847% |
| 38 | 11.510 | 1598 | 1602 | 1607 | rBV4 | 105778 | 229049 | 4.18% | 0.252% |
| 39 | 11.627 | 1616 | 1622 | 1628 | rBV2 | 326466 | 370683 | 6.77% | 0.407% |
| 40 | 11.692 | 1628 | 1633 | 1636 | rVB2 | 216602 | 230035 | 4.20% | 0.253% |
| 41 | 11.763 | 1642 | 1645 | 1651 | rVB | 846367 | 786596 | 14.36% | 0.864% |
| 42 | 11.851 | 1655 | 1660 | 1663 | rBV2 | 97177 | 149979 | 2.74% | 0.165% |
| 43 | 11.898 | 1665 | 1668 | 1670 | rVV | 643763 | 550684 | 10.05% | 0.605% |
| 44 | 11.927 | 1670 | 1673 | 1676 | rVB | 974545 | 897664 | 16.39% | 0.986% |
| 45 | 11.974 | 1676 | 1681 | 1684 | rVB | 299773 | 242997 | 4.44% | 0.267% |
| 46 | 12.010 | 1684 | 1687 | 1689 | rBV | 565017 | 615949 | 11.25% | 0.677% |
| 47 | 12.033 | 1689 | 1691 | 1695 | rVB | 464265 | 367942 | 6.72% | 0.404% |
| 48 | 12.080 | 1696 | 1699 | 1702 | rBV2 | 118894 | 152351 | 2.78% | 0.167% |
| 49 | 12.192 | 1715 | 1718 | 1721 | rVV | 592043 | 487752 | 8.91% | 0.536% |
| 50 | 12.451 | 1758 | 1762 | 1765 | rBV | 290747 | 362967 | 6.63% | 0.399% |
| 51 | 12.492 | 1765 | 1769 | 1771 | rVV2 | 190987 | 285838 | 5.22% | 0.314% |
| 52 | 12.545 | 1774 | 1778 | 1782 | rVB2 | 395343 | 435553 | 7.95% | 0.479% |
| 53 | 12.621 | 1786 | 1791 | 1795 | rBV | 4492222 | 5115700 | 93.40% | 5.622% |
| 54 | 12.710 | 1803 | 1806 | 1809 | rBV | 256082 | 225848 | 4.12% | 0.248% |
| 55 | 12.768 | 1809 | 1816 | 1819 | rBV2 | 214615 | 302096 | 5.52% | 0.332% |
| 56 | 12.851 | 1822 | 1830 | 1833 | rVV2 | 4202743 | 5477127 | 100.00% | 6.019% |
| 57 | 12.892 | 1834 | 1837 | 1841 | rVB2 | 376354 | 381504 | 6.97% | 0.419% |
| 58 | 12.963 | 1845 | 1849 | 1850 | rBV | 468692 | 459774 | 8.39% | 0.505% |
| 59 | 12.986 | 1850 | 1853 | 1855 | rVV | 3665128 | 3229928 | 58.97% | 3.550% |
| 60 | 13.004 | 1855 | 1856 | 1860 | rVB | 690905 | 500942 | 9.15% | 0.551% |
| 61 | 13.063 | 1861 | 1866 | 1870 | rBV3 | 405795 | 749958 | 13.69% | 0.824% |
| 62 | 13.145 | 1877 | 1880 | 1882 | rBV3 | 388666 | 489979 | 8.95% | 0.538% |
| 63 | 13.168 | 1882 | 1884 | 1887 | rVB2 | 450501 | 423150 | 7.73% | 0.465% |
| 64 | 13.204 | 1887 | 1890 | 1893 | rBV2 | 112390 | 138825 | 2.53% | 0.153% |
| 65 | 13.274 | 1898 | 1902 | 1906 | rBV2 | 690242 | 786824 | 14.37% | 0.865% |
| 66 | 13.368 | 1915 | 1918 | 1920 | rBV | 363489 | 296078 | 5.41% | 0.325% |
| 67 | 13.398 | 1920 | 1923 | 1926 | rBV2 | 333095 | 316585 | 5.78% | 0.348% |
| 68 | 13.480 | 1931 | 1937 | 1942 | rVB6 | 123105 | 202570 | 3.70% | 0.223% |
| 69 | 13.551 | 1945 | 1949 | 1954 | rBV6 | 150985 | 292470 | 5.34% | 0.321% |
| 70 | 13.680 | 1968 | 1971 | 1975 | rBV | 822332 | 705463 | 12.88% | 0.775% |
| 71 | 13.792 | 1986 | 1990 | 1992 | rBV2 | 523027 | 551909 | 10.08% | 0.607% |
| 72 | 13.815 | 1992 | 1994 | 1997 | rVV | 529128 | 549022 | 10.02% | 0.603% |
| 73 | 13.845 | 1997 | 1999 | 2005 | rVV3 | 428923 | 736643 | 13.45% | 0.810% |
| 74 | 13.892 | 2005 | 2007 | 2011 | rVB | 654033 | 555181 | 10.14% | 0.610% |
| 75 | 14.039 | 2025 | 2032 | 2036 | rBV2 | 2940021 | 4536785 | 82.83% | 4.986% |
| 76 | 14.074 | 2036 | 2038 | 2046 | rVV | 2516994 | 2588497 | 47.26% | 2.845% |

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Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** A010015

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-BF091521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 77 | 14.192 | 2055 | 2058 | 2061 | rVV2 | 285320 | 336431 | 6.14% | 0.370% |
| 78 | 14.233 | 2064 | 2065 | 2067 | rVV | 206496 | 165466 | 3.02% | 0.182% |
| 79 | 14.274 | 2067 | 2072 | 2075 | rVV2 | 341026 | 558305 | 10.19% | 0.614% |
| 80 | 14.392 | 2089 | 2092 | 2094 | rBV3 | 240234 | 263833 | 4.82% | 0.290% |
| 81 | 14.427 | 2095 | 2098 | 2101 | rVB | 563230 | 580940 | 10.61% | 0.638% |
| 82 | 14.462 | 2101 | 2104 | 2106 | rBV | 273888 | 228342 | 4.17% | 0.251% |
| 83 | 14.509 | 2108 | 2112 | 2116 | rVB3 | 156996 | 278018 | 5.08% | 0.306% |
| 84 | 14.557 | 2116 | 2120 | 2122 | rBV3 | 212076 | 217741 | 3.98% | 0.239% |
| 85 | 14.627 | 2129 | 2132 | 2138 | rVB3 | 281260 | 452802 | 8.27% | 0.498% |
| 86 | 14.751 | 2150 | 2153 | 2155 | rBV | 133615 | 148680 | 2.71% | 0.163% |
| 87 | 14.927 | 2179 | 2183 | 2188 | rBV2 | 230799 | 380475 | 6.95% | 0.418% |
| 88 | 15.104 | 2207 | 2213 | 2216 | rBV | 1952577 | 3361922 | 61.38% | 3.695% |
| 89 | 15.209 | 2227 | 2231 | 2234 | rBV | 436816 | 499750 | 9.12% | 0.549% |
| 90 | 15.298 | 2242 | 2246 | 2247 | rBV3 | 126869 | 154079 | 2.81% | 0.169% |
| 91 | 15.409 | 2260 | 2265 | 2271 | rVB | 1159353 | 1647871 | 30.09% | 1.811% |
| 92 | 15.480 | 2271 | 2277 | 2281 | rVB | 1641147 | 2187336 | 39.94% | 2.404% |
| 93 | 15.533 | 2281 | 2286 | 2289 | rBV | 684959 | 891044 | 16.27% | 0.979% |
| 94 | 15.568 | 2289 | 2292 | 2298 | rVB2 | 538282 | 738558 | 13.48% | 0.812% |
| 95 | 15.745 | 2319 | 2322 | 2328 | rVB5 | 109779 | 185964 | 3.40% | 0.204% |
| 96 | 17.033 | 2534 | 2541 | 2550 | rBV2 | 690555 | 1312853 | 23.97% | 1.443% |
| 97 | 17.209 | 2565 | 2571 | 2575 | rBV | 151840 | 298887 | 5.46% | 0.328% |
| 98 | 17.262 | 2575 | 2580 | 2585 | rVV2 | 129423 | 248597 | 4.54% | 0.273% |
| 99 | 17.486 | 2611 | 2618 | 2626 | rVB | 476029 | 953028 | 17.40% | 1.047% |
| 100 | 17.721 | 2653 | 2658 | 2664 | rBV | 123727 | 258867 | 4.73% | 0.284% |

Sum of corrected areas: 90994884

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
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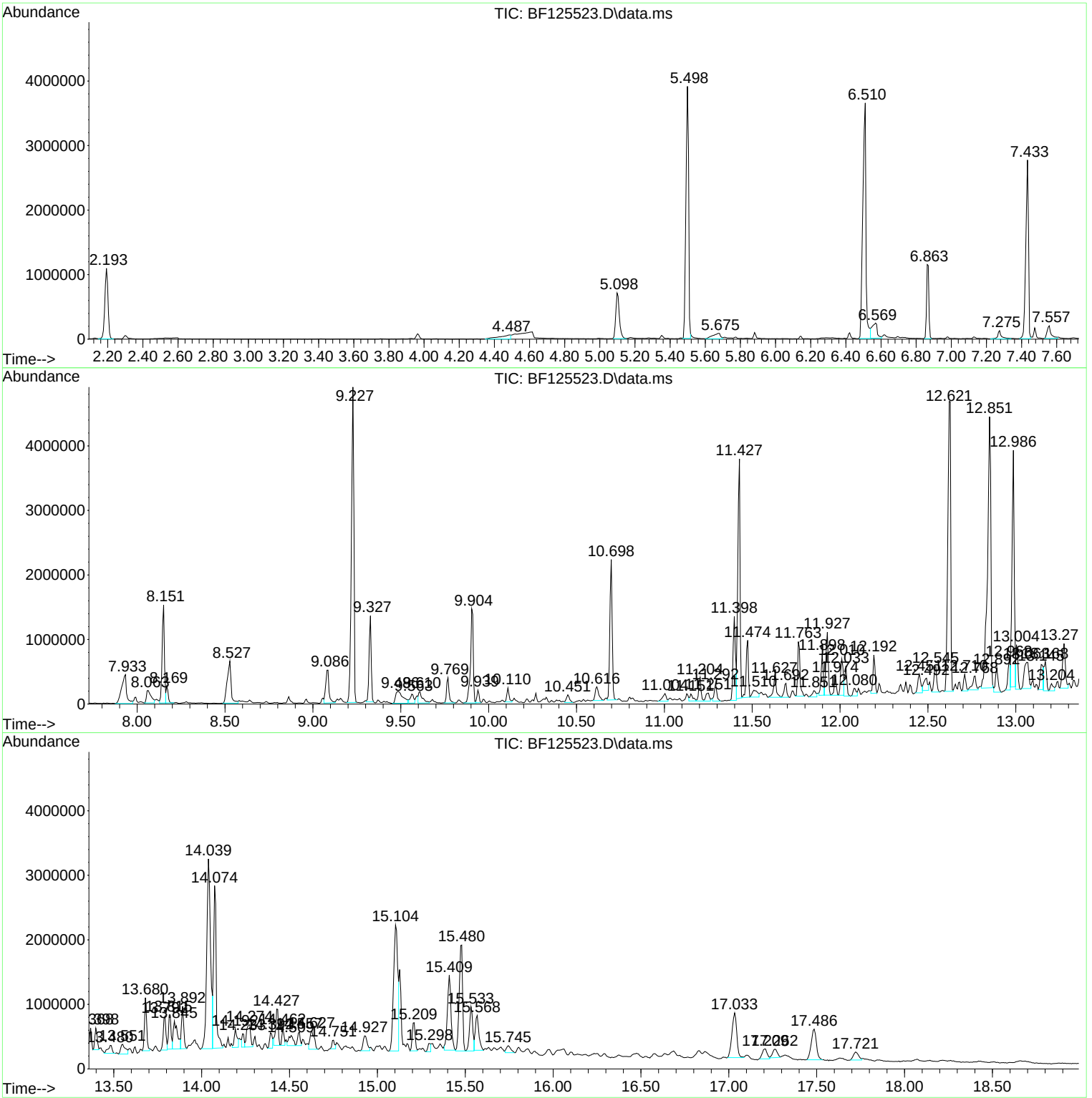
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

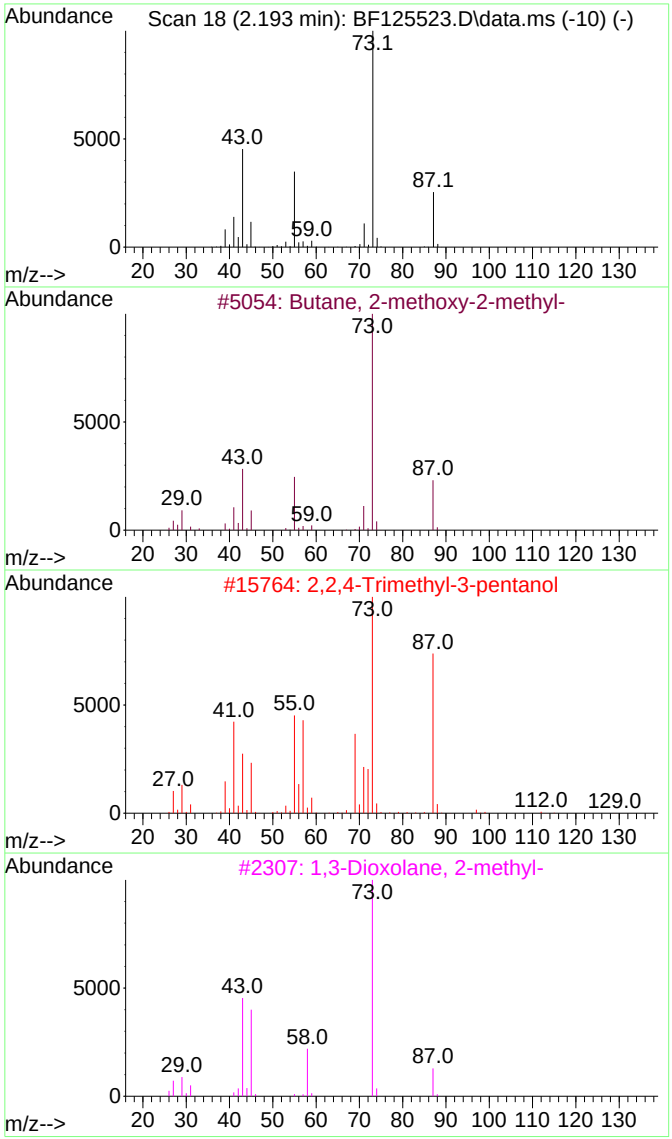
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

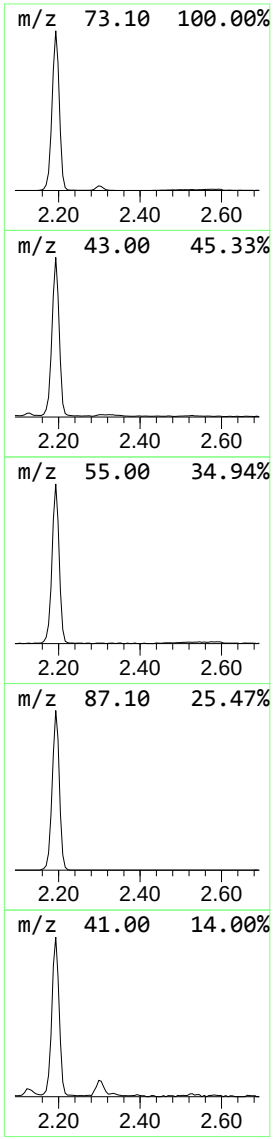
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.193 | 26.24 ng | 1369150 | 1,4-Dichlorobenzene-d4 | 6.869 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 37 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 25 |
| 5 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

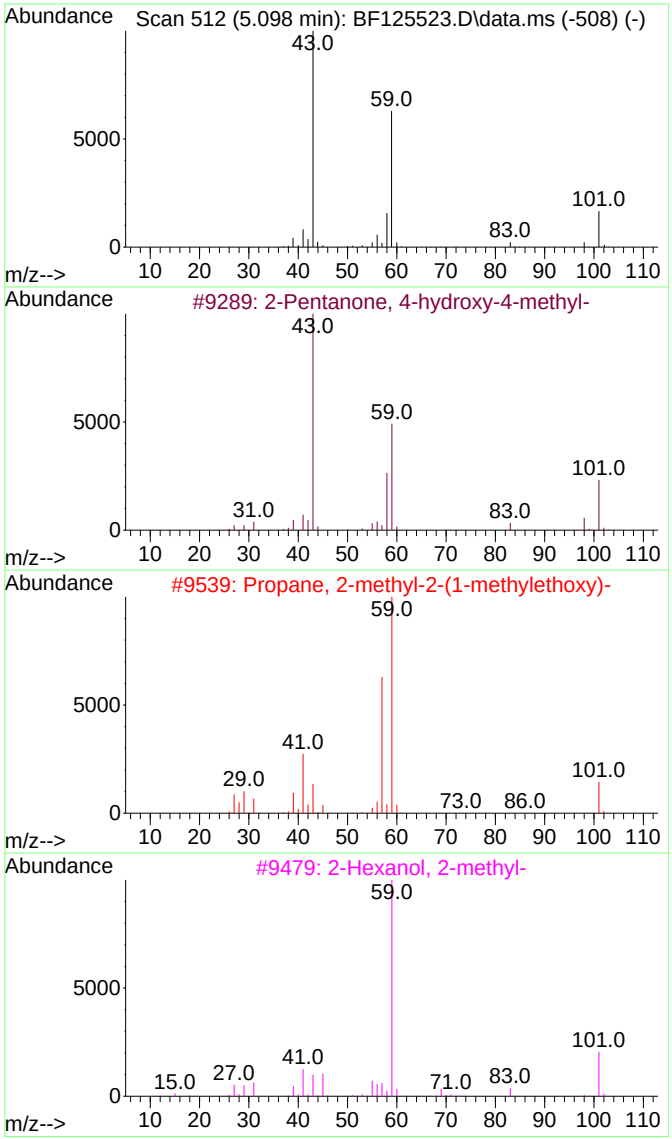
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

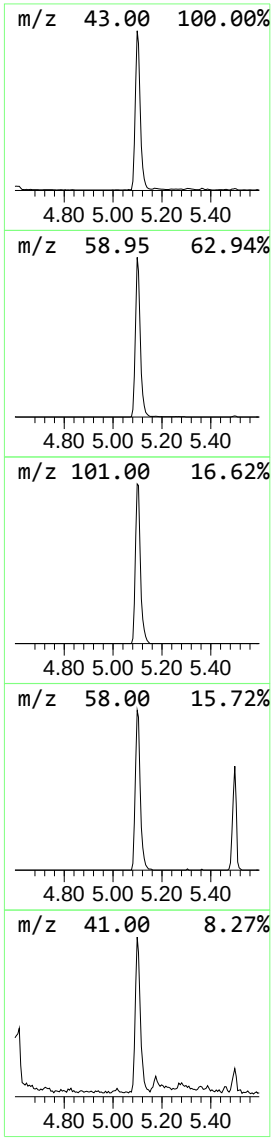
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.098 | 19.05 ng | 993903 | 1,4-Dichlorobenzene-d4 | 6.869 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 42 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 4 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

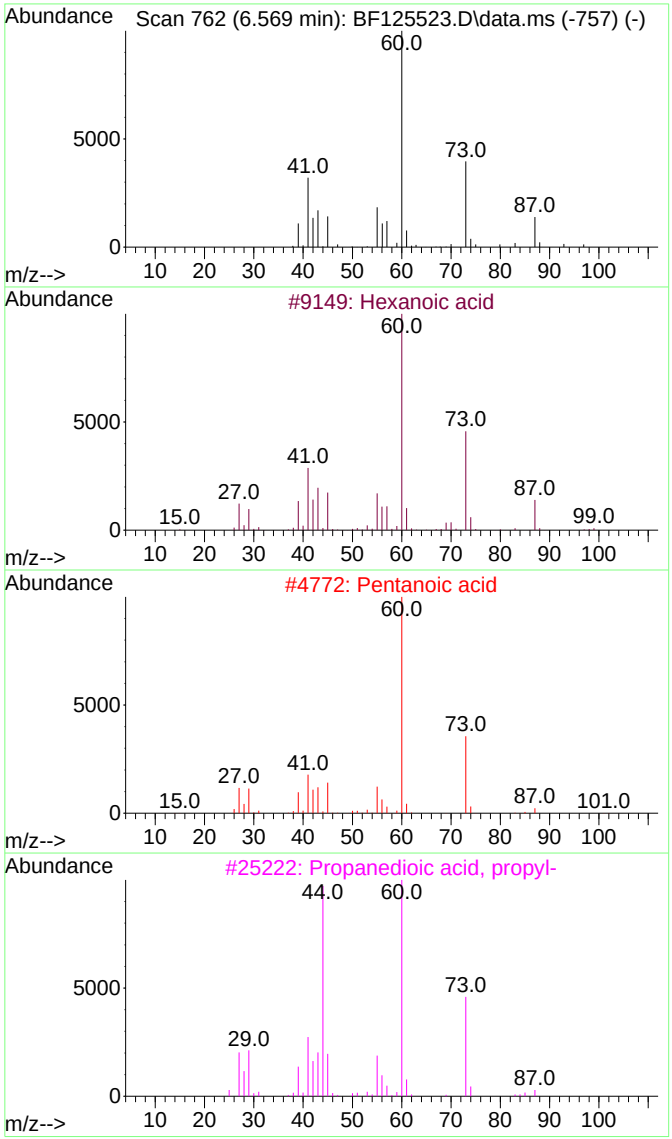
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

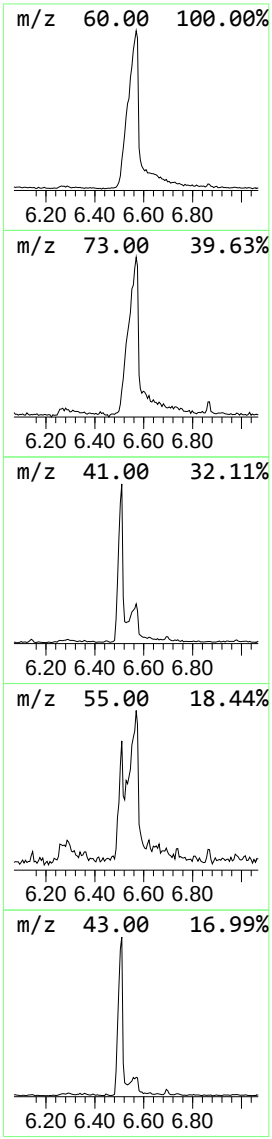
**********

Peak Number 3 Hexanoic acid Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.569 | 9.36 ng | 488413 | 1,4-Dichlorobenzene-d4 | 6.869 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanoic acid | 116 | C6H12O2 | 000142-62-1 | 78 |
| 2 | Pentanoic acid | 102 | C5H10O2 | 000109-52-4 | 72 |
| 3 | Propanedioic acid, propyl- | 146 | C6H10O4 | 000616-62-6 | 72 |
| 4 | Butanoic acid | 88 | C4H8O2 | 000107-92-6 | 64 |
| 5 | Butanoic acid, 3-methyl- | 102 | C5H10O2 | 000503-74-2 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

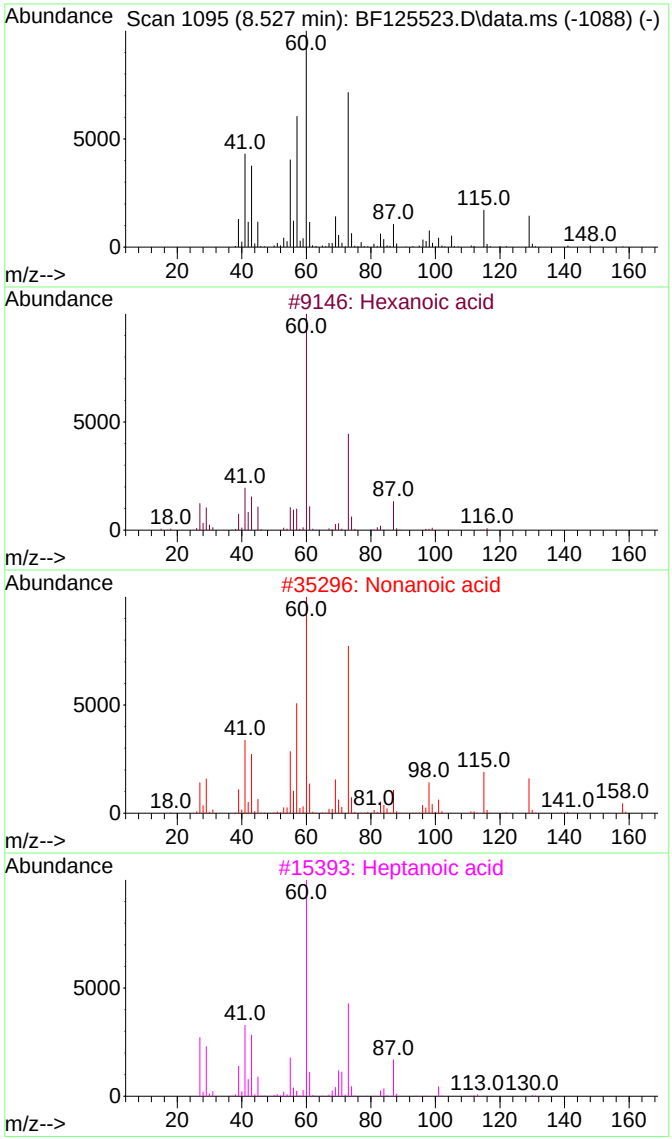
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

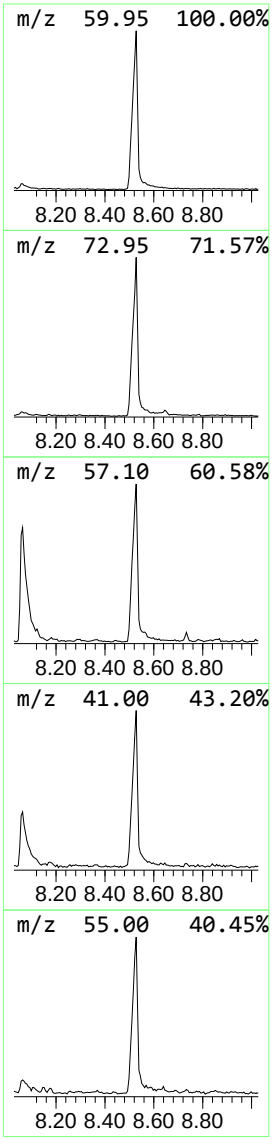
**********

Peak Number 4 Nonanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.527 | 14.62 ng | 1001970 | Naphthalene-d8 | 8.151 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanoic acid | 116 | C6H12O2 | 000142-62-1 | 72 |
| 2 | Nonanoic acid | 158 | C9H18O2 | 000112-05-0 | 64 |
| 3 | Heptanoic acid | 130 | C7H14O2 | 000111-14-8 | 59 |
| 4 | Butanoic acid | 88 | C4H8O2 | 000107-92-6 | 53 |
| 5 | Octanoic acid, silver(1+) salt | 250 | C8H15AgO2 | 024927-67-1 | 53 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

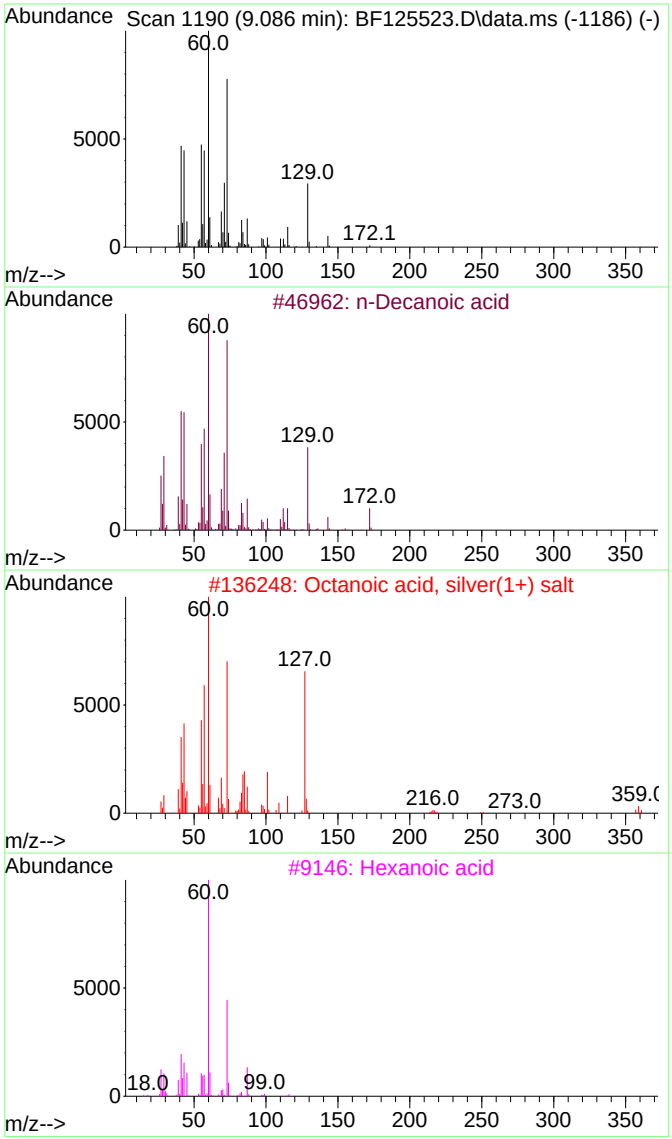
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

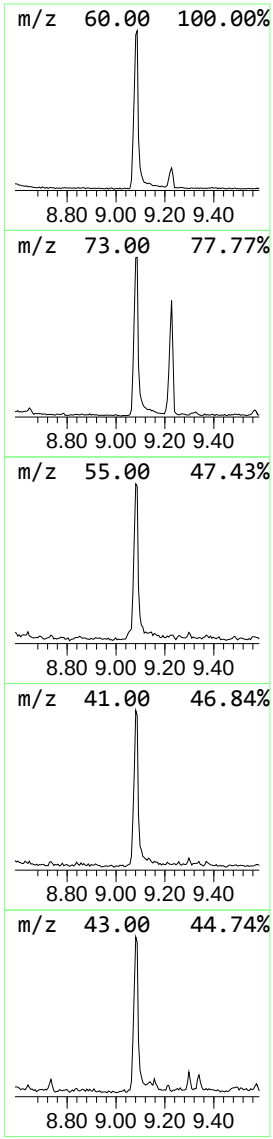
**********

Peak Number 5 n-Decanoic acid Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.086 | 8.34 ng | 663578 | Acenaphthene-d10 | 9.904 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 90 |
| 2 | Octanoic acid, silver(1+) salt | 250 | C8H15AgO2 | 024927-67-1 | 52 |
| 3 | Hexanoic acid | 116 | C6H12O2 | 000142-62-1 | 52 |
| 4 | Heptanoic acid | 130 | C7H14O2 | 000111-14-8 | 52 |
| 5 | Xylose | 150 | C5H10O5 | 000058-86-6 | 47 |



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Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

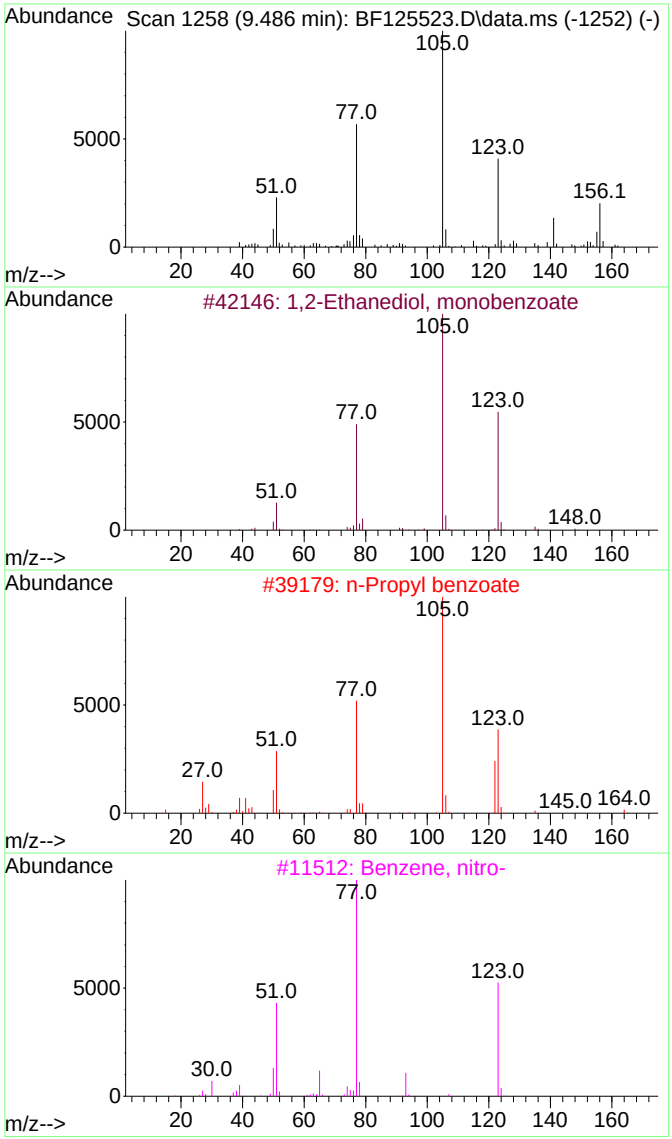
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

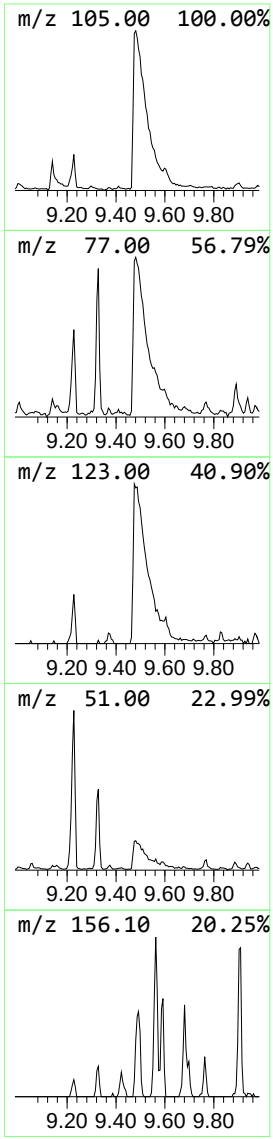
**********

Peak Number 6 1,2-Ethanediol, monobenzoate Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.486 | 6.71 ng | 534348 | Acenaphthene-d10 | 9.904 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2-Ethanediol, monobenzoate | 166 | C9H10O3 | 000094-33-7 | 64 |
| 2 | n-Propyl benzoate | 164 | C10H12O2 | 002315-68-6 | 59 |
| 3 | Benzene, nitro- | 123 | C6H5NO2 | 000098-95-3 | 53 |
| 4 | Sulfone, methyl phenyl | 156 | C7H8O2S | 003112-85-4 | 43 |
| 5 | Acetophenone, 2-chloro- | 154 | C8H7ClO | 000532-27-4 | 43 |



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Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

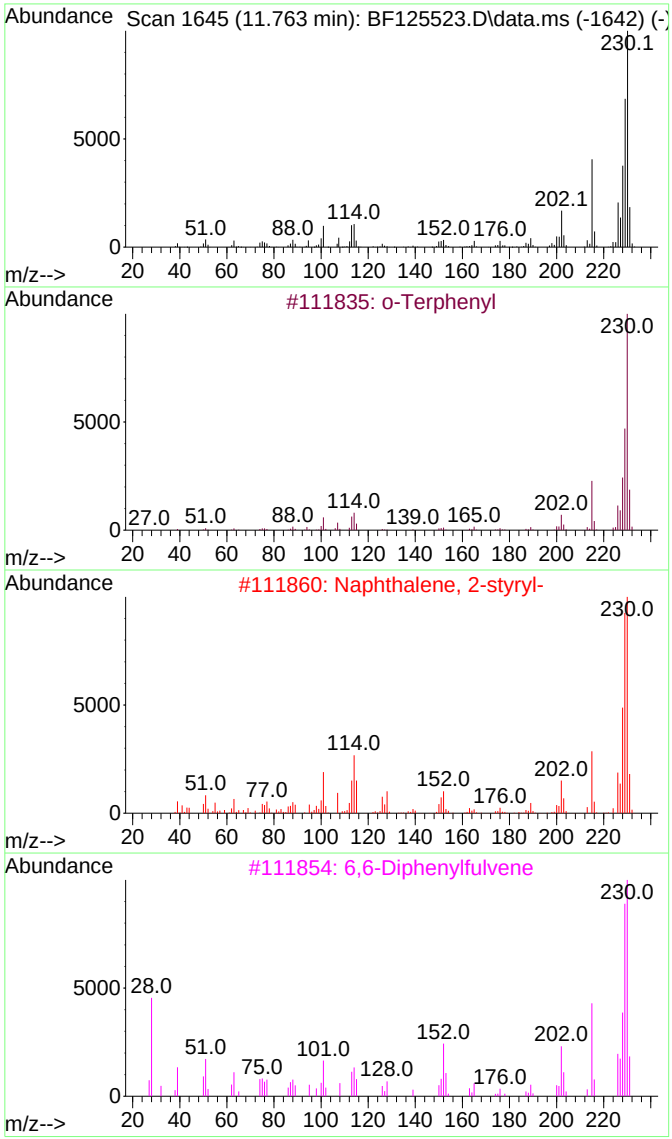
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

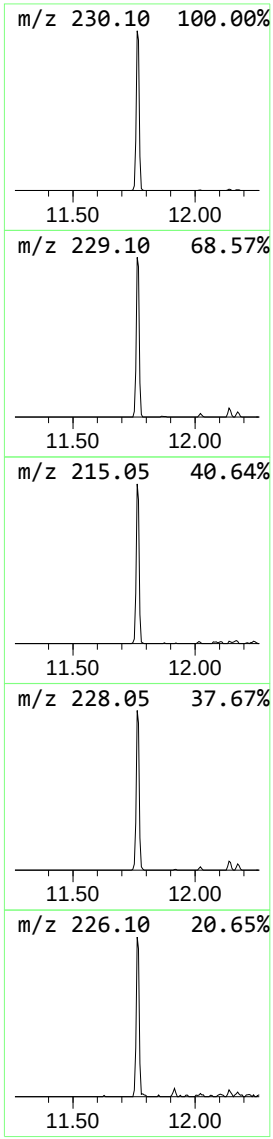
**********

Peak Number 7 o-Terphenyl Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.763 | 12.20 ng | 786596 | Phenanthrene-d10 | 11.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | o-Terphenyl | 230 | C18H14 | 000084-15-1 | 97 |
| 2 | Naphthalene, 2-styryl- | 230 | C18H14 | 002039-70-5 | 93 |
| 3 | 6,6-Diphenylfulvene | 230 | C18H14 | 002175-90-8 | 90 |
| 4 | Pyrene, 1,3-dimethyl- | 230 | C18H14 | 064401-21-4 | 83 |
| 5 | Naphthacene, 5,12-dihydro- | 230 | C18H14 | 000959-02-4 | 60 |



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Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

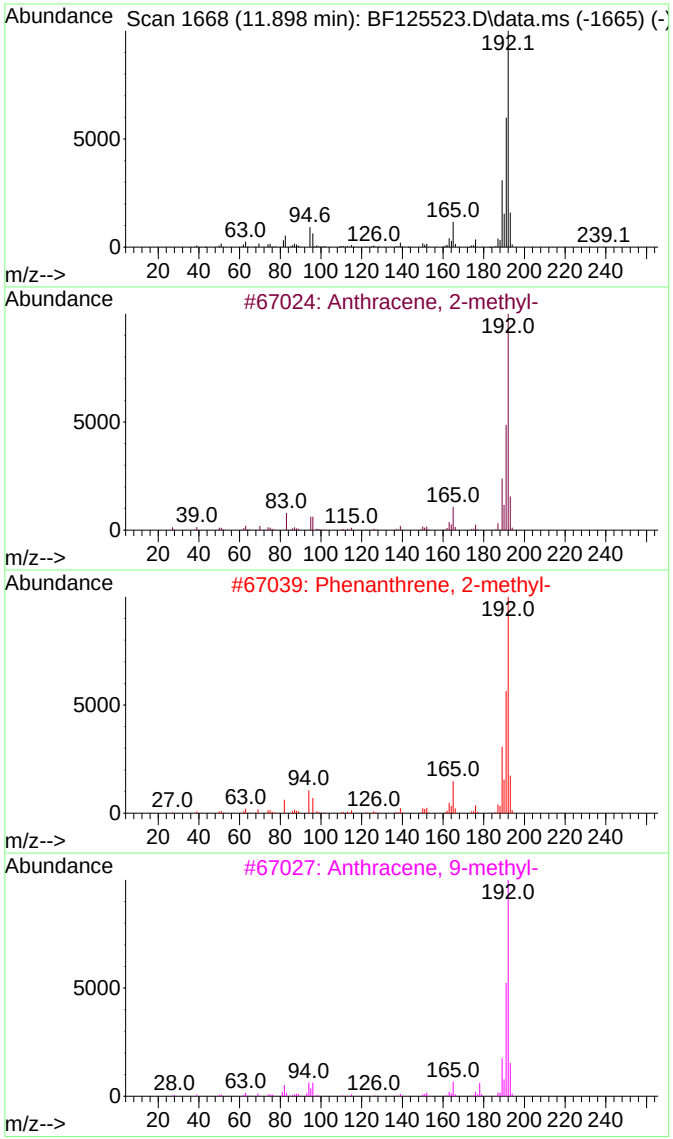
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

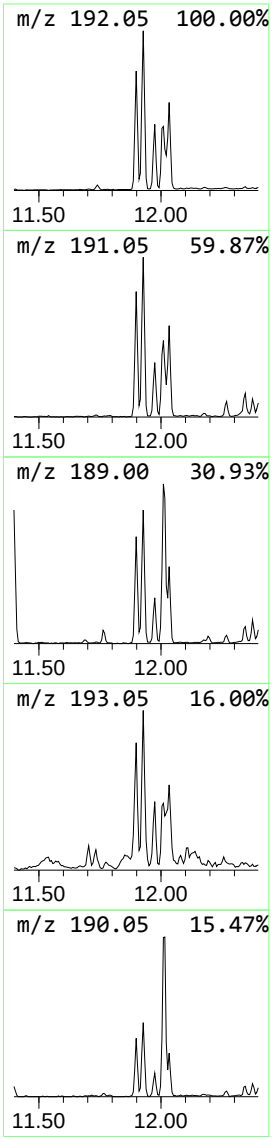
**********

Peak Number 8 Anthracene, 2-methyl- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.898 | 8.54 ng | 550684 | Phenanthrene-d10 | 11.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Anthracene, 2-methyl- | 192 | C15H12 | 000613-12-7 | 96 |
| 2 | Phenanthrene, 2-methyl- | 192 | C15H12 | 002531-84-2 | 95 |
| 3 | Anthracene, 9-methyl- | 192 | C15H12 | 000779-02-2 | 95 |
| 4 | 1H-Cyclopropa[l]phenanthrene,1a,... | 192 | C15H12 | 000949-41-7 | 95 |
| 5 | Anthracene, 1-methyl- | 192 | C15H12 | 000610-48-0 | 94 |



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Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

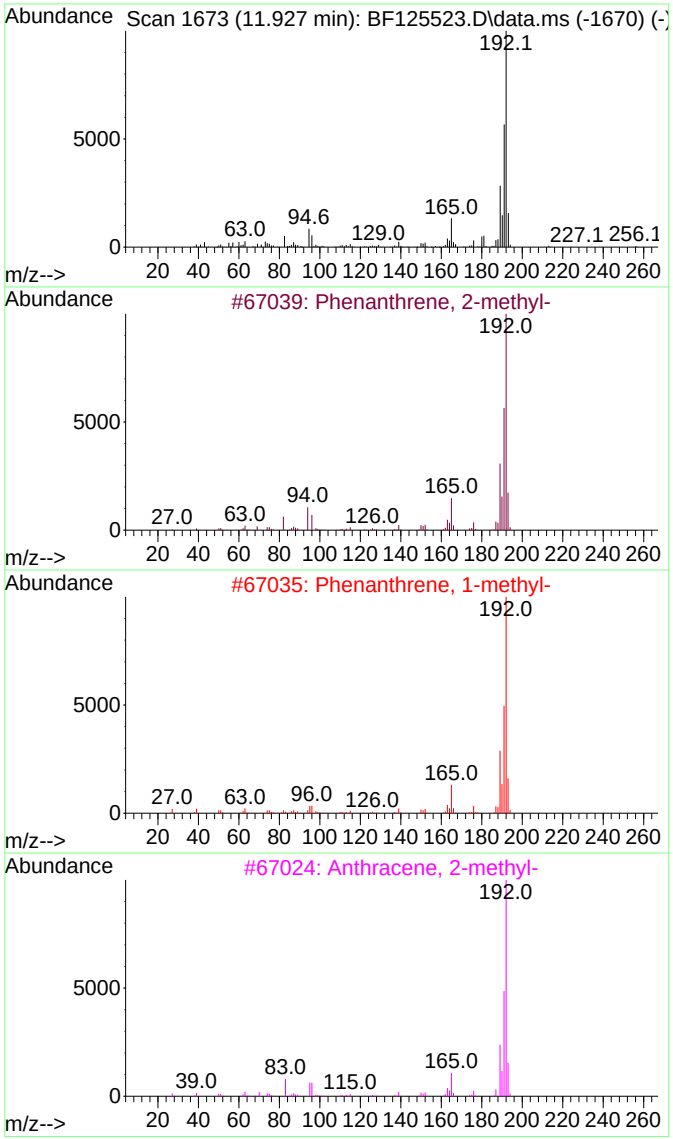
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

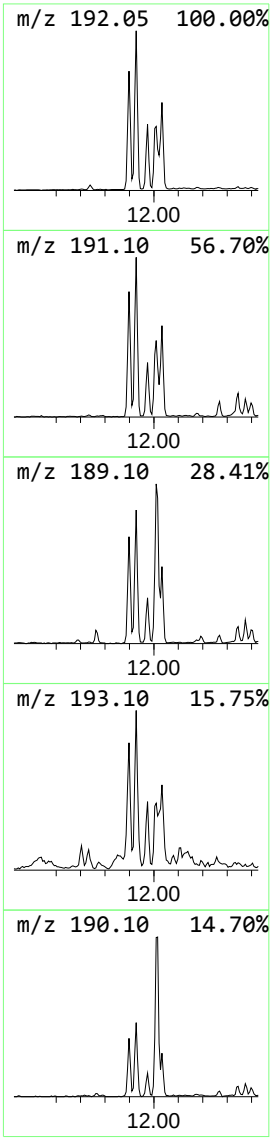
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 9 Phenanthrene, 2-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.927 | 13.92 ng | 897664 | Phenanthrene-d10 | 11.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenanthrene, 2-methyl- | 192 | C15H12 | 002531-84-2 | 98 |
| 2 | Phenanthrene, 1-methyl- | 192 | C15H12 | 000832-69-9 | 97 |
| 3 | Anthracene, 2-methyl- | 192 | C15H12 | 000613-12-7 | 96 |
| 4 | Phenanthrene, 4-methyl- | 192 | C15H12 | 000832-64-4 | 95 |
| 5 | 1H-Cyclopropa[l]phenanthrene,1a,... | 192 | C15H12 | 000949-41-7 | 95 |



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Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

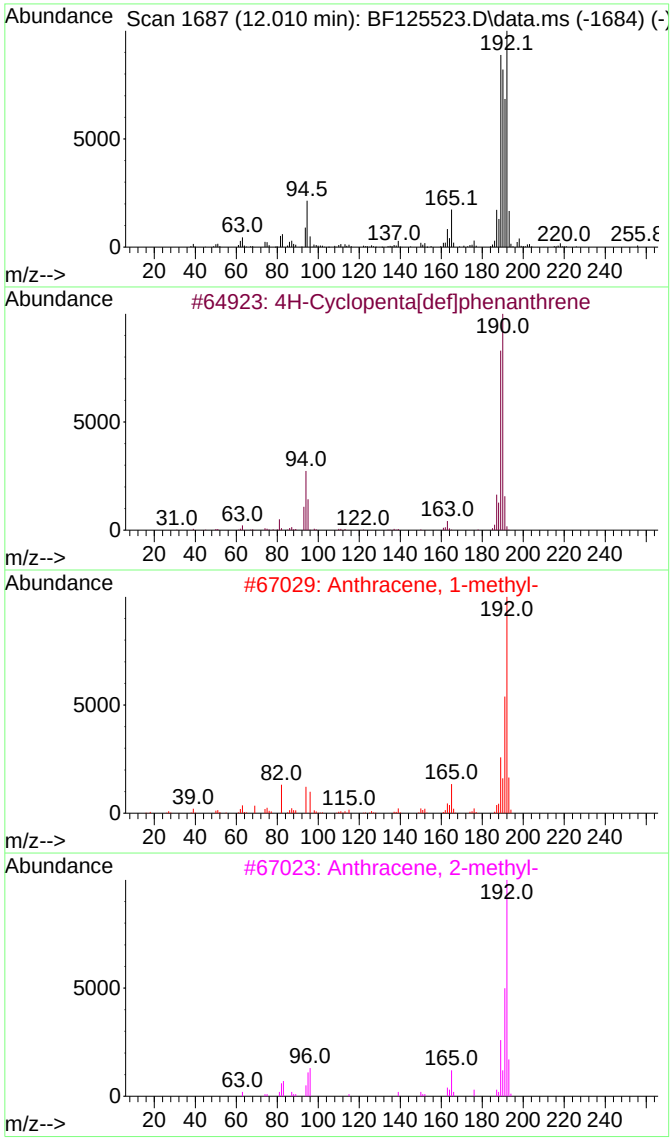
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

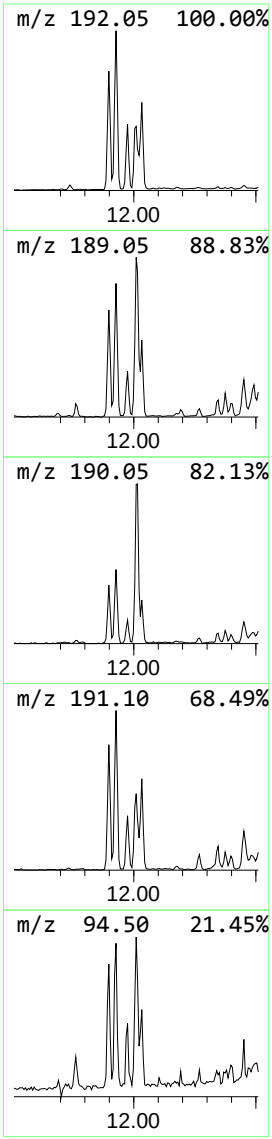
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.010 | 9.55 ng | 615949 | Phenanthrene-d10 | 11.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4H-Cyclopenta[def]phenanthrene | 190 | C15H10 | 000203-64-5 | 60 |
| 2 | Anthracene, 1-methyl- | 192 | C15H12 | 000610-48-0 | 46 |
| 3 | Anthracene, 2-methyl- | 192 | C15H12 | 000613-12-7 | 46 |
| 4 | Phenanthrene, 1-methyl- | 192 | C15H12 | 000832-69-9 | 46 |
| 5 | 1H-Indene, 2-phenyl- | 192 | C15H12 | 004505-48-0 | 42 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
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Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

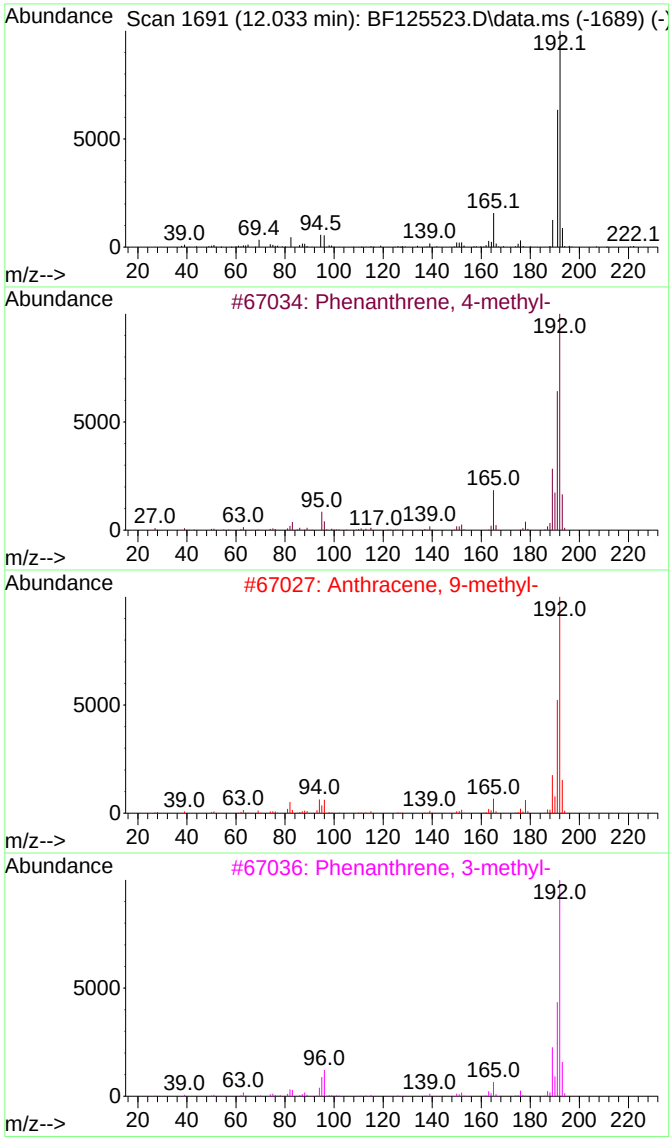
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

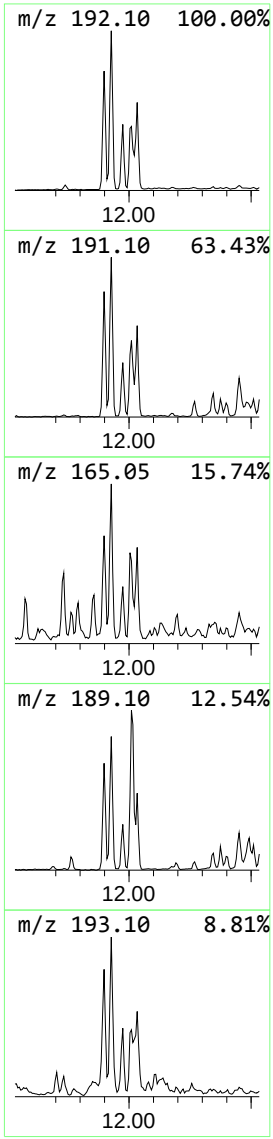
**********

Peak Number 11 Phenanthrene, 4-methyl- Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.033 | 5.71 ng | 367942 | Phenanthrene-d10 | 11.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenanthrene, 4-methyl- | 192 | C15H12 | 000832-64-4 | 74 |
| 2 | Anthracene, 9-methyl- | 192 | C15H12 | 000779-02-2 | 74 |
| 3 | Phenanthrene, 3-methyl- | 192 | C15H12 | 000832-71-3 | 72 |
| 4 | Anthracene, 2-methyl- | 192 | C15H12 | 000613-12-7 | 72 |
| 5 | 1H-Indene, 1-phenyl- | 192 | C15H12 | 001961-96-2 | 72 |



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Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

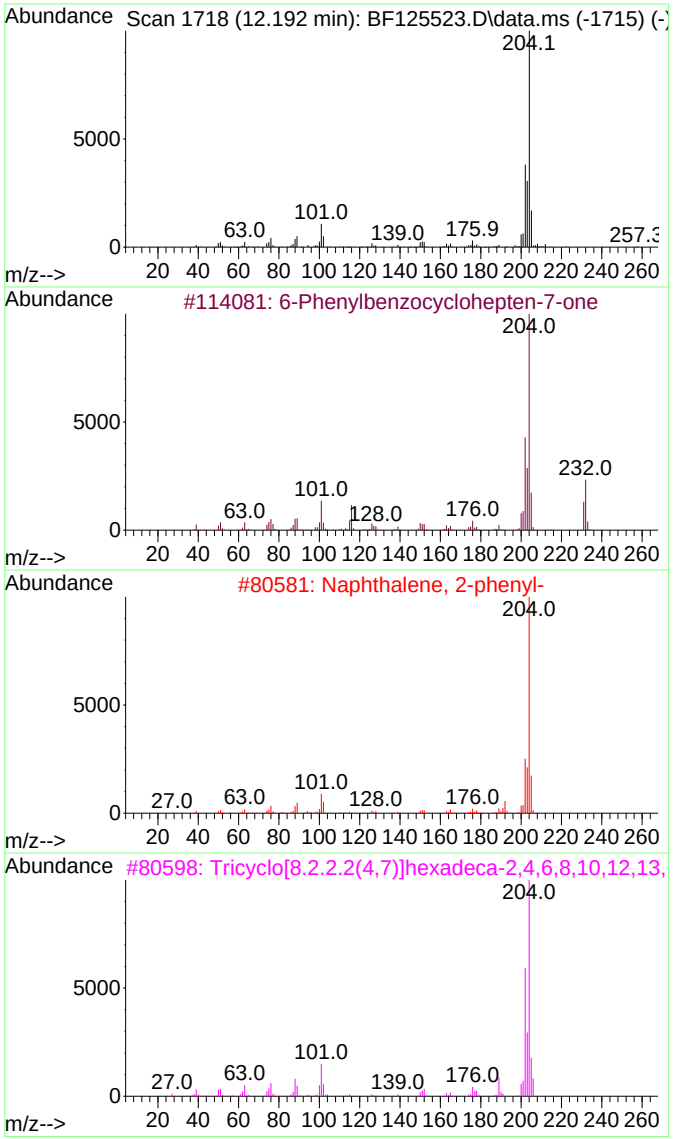
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

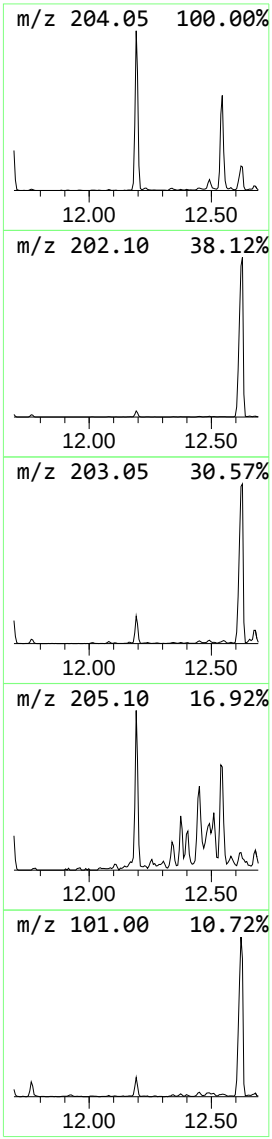
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 12 6-Phenylbenzocyclohepten-7-one Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.192 | 7.57 ng | 487752 | Phenanthrene-d10 | 11.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6-Phenylbenzocyclohepten-7-one | 232 | C17H12O | 093327-56-1 | 90 |
| 2 | Naphthalene, 2-phenyl- | 204 | C16H12 | 000612-94-2 | 89 |
| 3 | Tricyclo[8.2.2.2(4,7)]hexadeca-2... | 204 | C16H12 | 006572-60-7 | 68 |
| 4 | 9,10-Bis(bromomethyl)anthracene | 362 | C16H12Br2 | 034373-96-1 | 64 |
| 5 | Naphthalene, 1-phenyl- | 204 | C16H12 | 000605-02-7 | 55 |



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Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

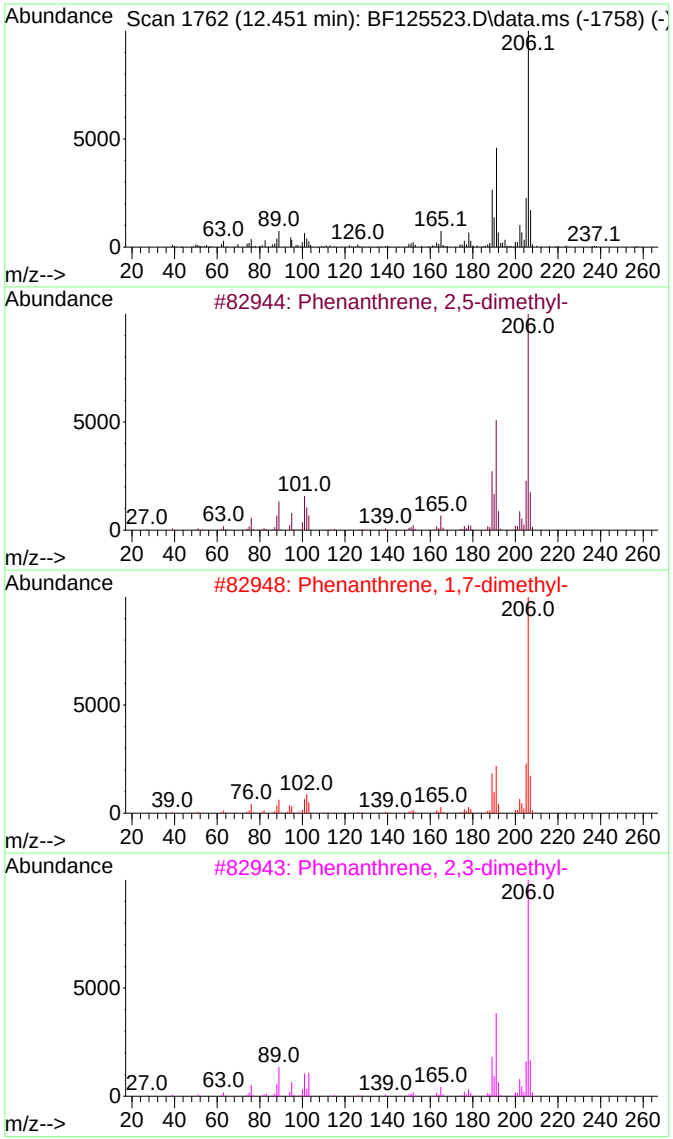
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

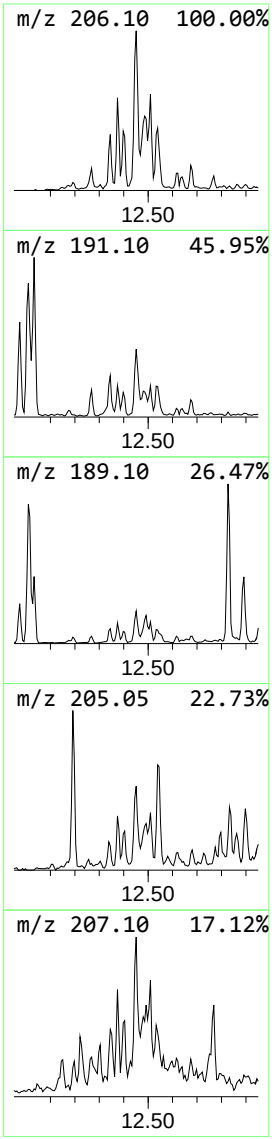
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 13 Phenanthrene, 2,5-dimethyl- Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.451 | 5.63 ng | 362967 | Phenanthrene-d10 | 11.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenanthrene, 2,5-dimethyl- | 206 | C16H14 | 003674-66-6 | 97 |
| 2 | Phenanthrene, 1,7-dimethyl- | 206 | C16H14 | 000483-87-4 | 93 |
| 3 | Phenanthrene, 2,3-dimethyl- | 206 | C16H14 | 003674-65-5 | 93 |
| 4 | Phenanthrene, 3,6-dimethyl- | 206 | C16H14 | 001576-67-6 | 91 |
| 5 | 9,10-Dimethylanthracene | 206 | C16H14 | 000781-43-1 | 91 |



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Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

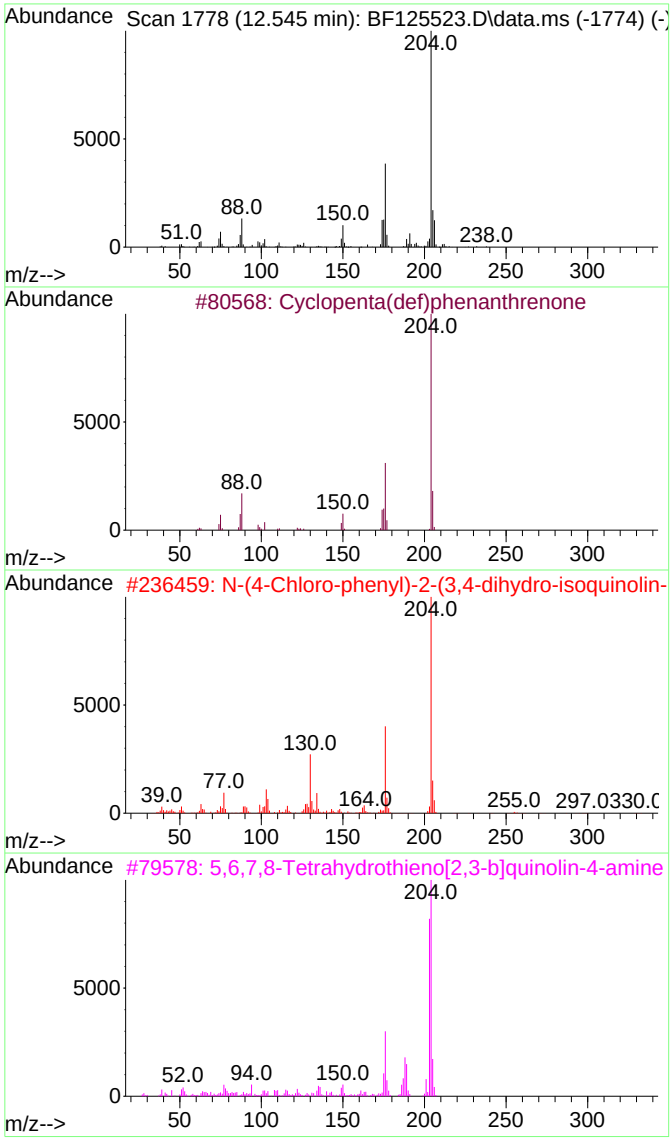
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

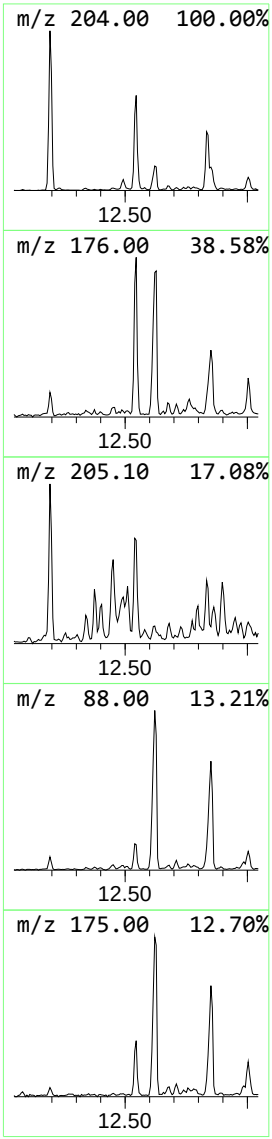
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 14 Cyclopenta(def)phenanthrenone Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.545 | 6.76 ng | 435553 | Phenanthrene-d10 | 11.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopenta(def)phenanthrenone | 204 | C15H8O | 005737-13-3 | 95 |
| 2 | N-(4-Chloro-phenyl)-2-(3,4-dihyd... | 330 | C17H15ClN2OS | 1010296-34-3 | 59 |
| 3 | 5,6,7,8-Tetrahydrothieno[2,3-b]q... | 204 | C11H12N2S | 122914-50-5 | 50 |
| 4 | [1,1'-Biphenyl]-2,2'-dicarbonitrile | 204 | C14H8N2 | 004341-02-0 | 43 |
| 5 | Ethyl .alpha.-D-glucopyranoside,... | 496 | C20H48O6Si4 | 1000365-90-0 | 43 |



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Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** A010015

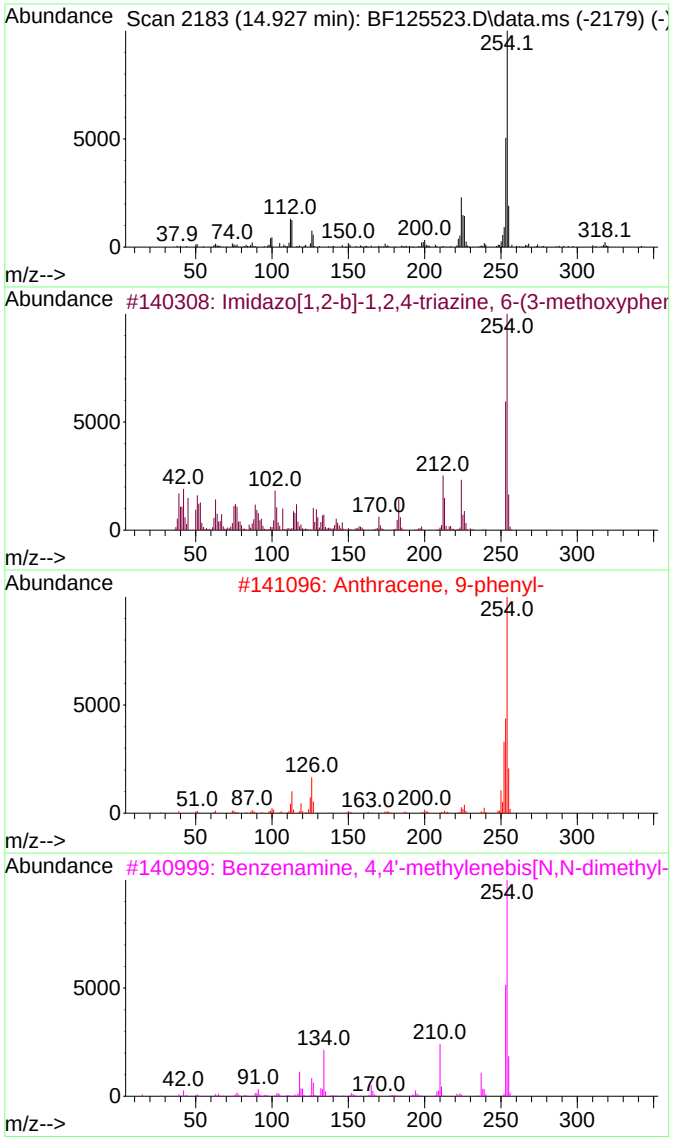
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

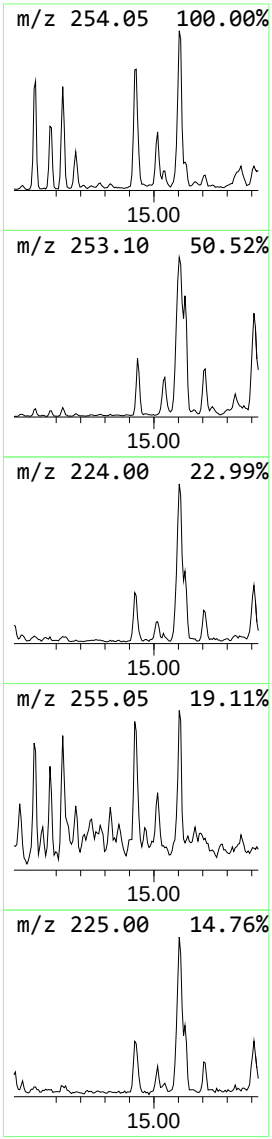
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 15 Imidazo[1,2-b]-1,2,4-triazi... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.927 | 8.54 ng | 380475 | Perylene-d12 | 15.533 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Imidazo[1,2-b]-1,2,4-triazine, 6... | 254 | C14H14N4O | 1000277-24-4 | 59 |
| 2 | Anthracene, 9-phenyl- | 254 | C20H14 | 000602-55-1 | 52 |
| 3 | Benzenamine, 4,4'-methylenebis[N... | 254 | C17H22N2 | 000101-61-1 | 50 |
| 4 | 3-Hydroxy-1-methoxyanthraquinone | 254 | C15H10O4 | 028504-24-7 | 50 |
| 5 | Raseglurant, N-methyl | 254 | C16H15FN2 | 1000498-91-9 | 47 |



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Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

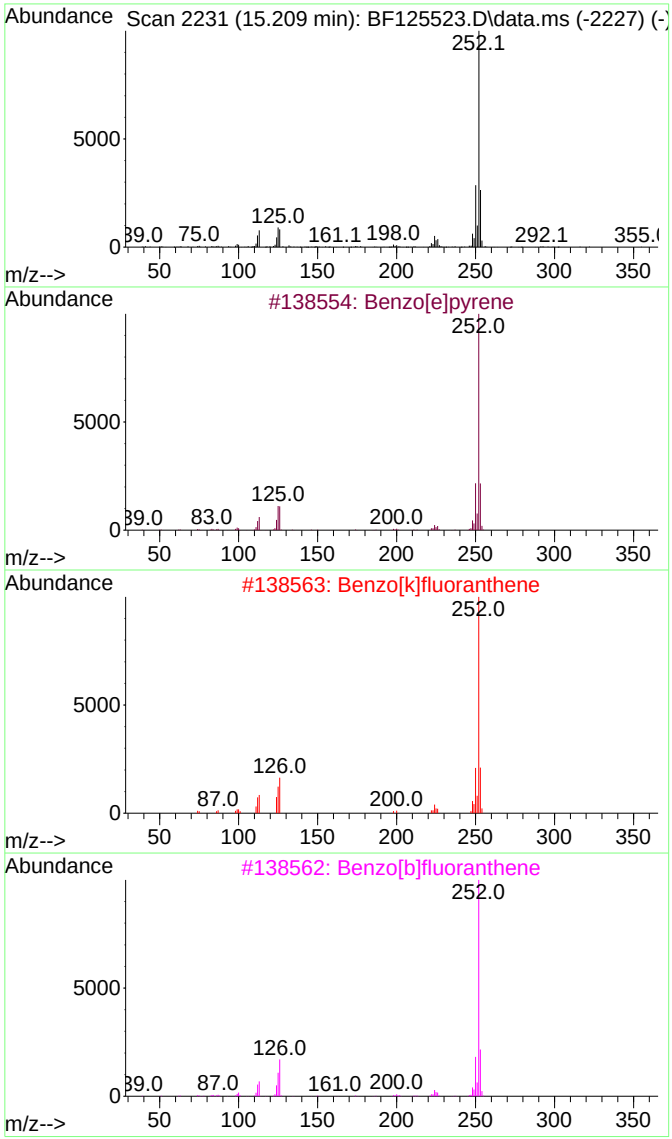
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

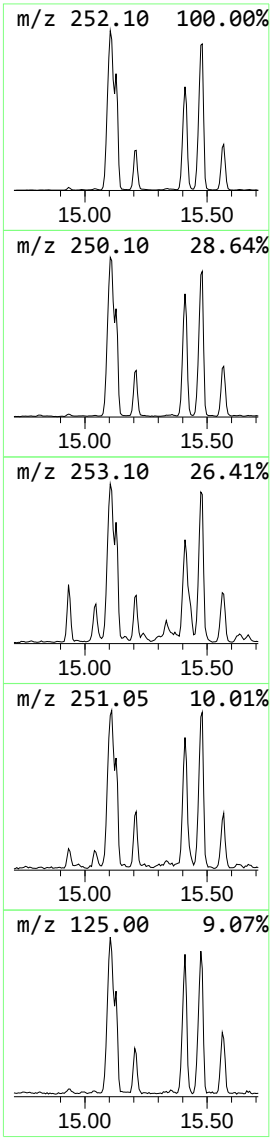
**********

Peak Number 16 Benzo[e]pyrene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.209 | 11.22 ng | 499750 | Perylene-d12 | 15.533 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 94 |
| 2 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 93 |
| 3 | Benzo[b]fluoranthene | 252 | C20H12 | 000205-99-2 | 93 |
| 4 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 91 |
| 5 | Perylene | 252 | C20H12 | 000198-55-0 | 76 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

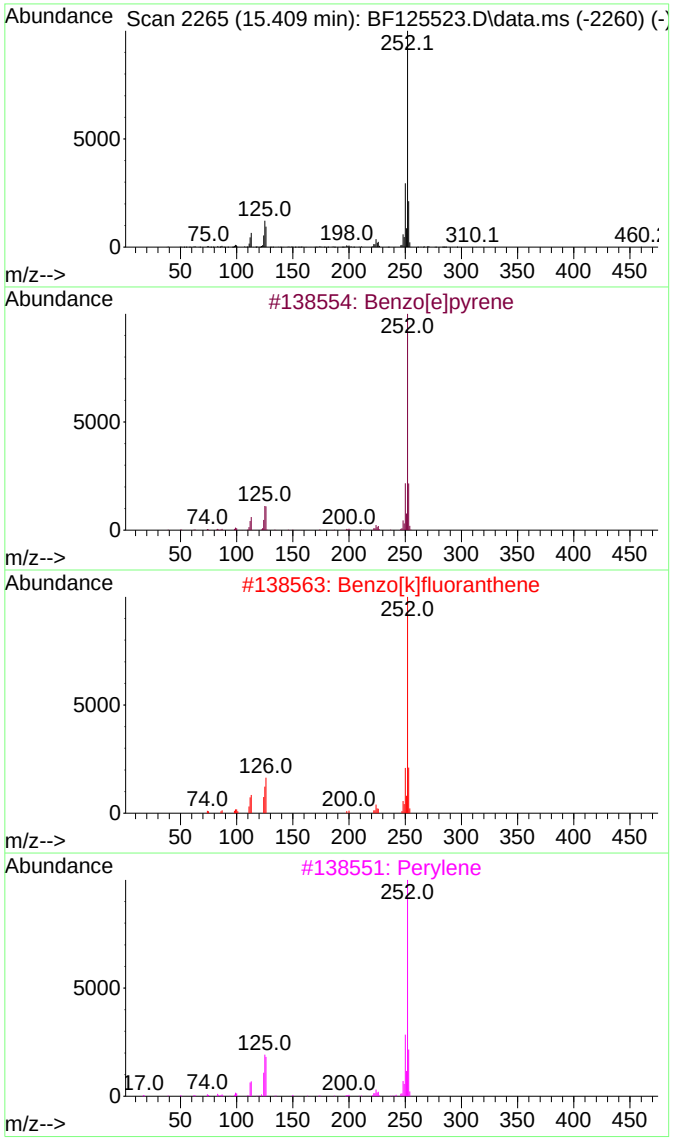
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

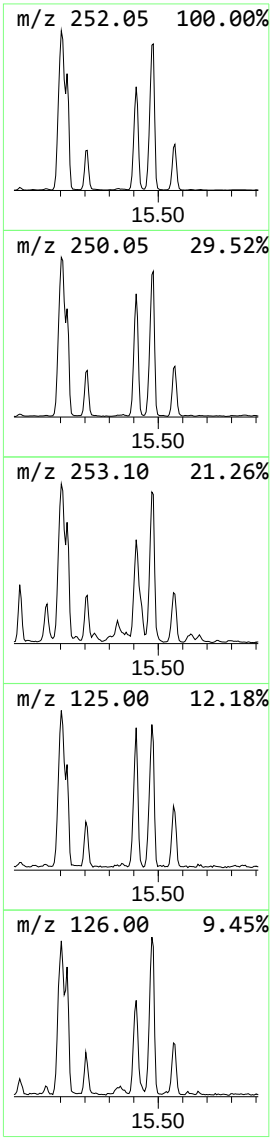
**********

Peak Number 17 Perylene Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.409 | 36.99 ng | 1647870 | Perylene-d12 | 15.533 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 99 |
| 2 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 97 |
| 3 | Perylene | 252 | C20H12 | 000198-55-0 | 95 |
| 4 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 94 |
| 5 | Benzo[b]fluoranthene | 252 | C20H12 | 000205-99-2 | 94 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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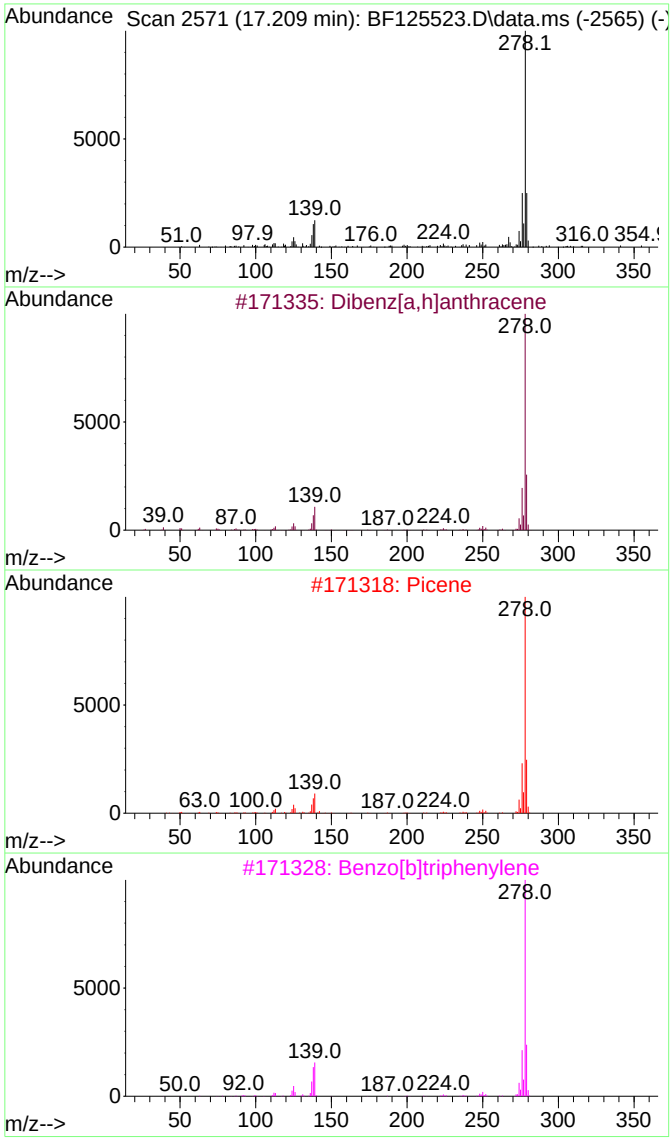
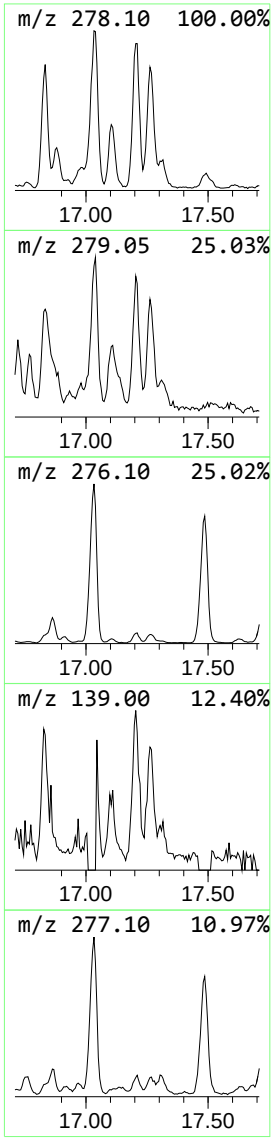
Peak Number 18 Picene Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.209 | 6.71 ng | 298887 | Perylene-d12 | 15.533 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dibenz[a,h]anthracene | 278 | C22H14 | 000053-70-3 | 99 |
| 2 | Picene | 278 | C22H14 | 000213-46-7 | 98 |
| 3 | Benzo[b]triphenylene | 278 | C22H14 | 000215-58-7 | 98 |
| 4 | Pentaphene | 278 | C22H14 | 000222-93-5 | 97 |
| 5 | Benzo[b]chrysene | 278 | C22H14 | 000214-17-5 | 95 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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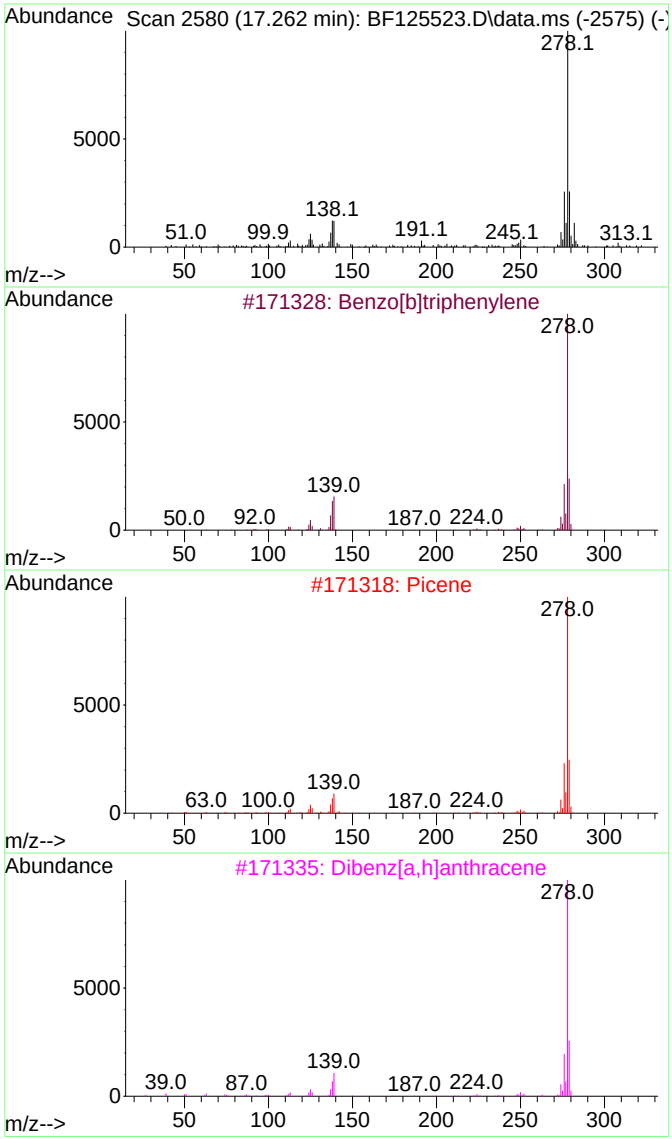
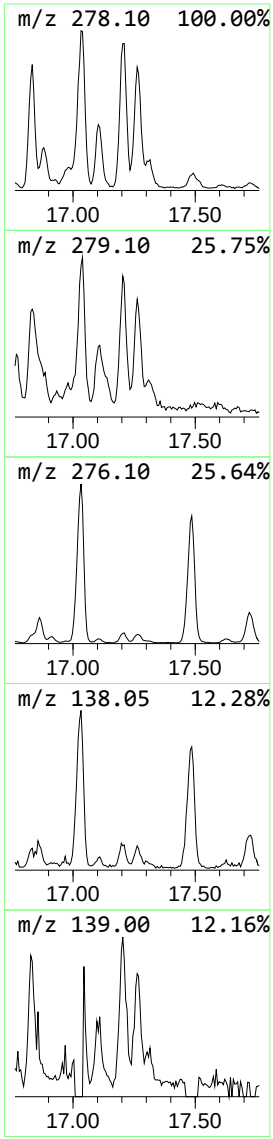
Peak Number 19 Benzo[b]triphenylene Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.262 | 5.58 ng | 248597 | Perylene-d12 | 15.533 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[b]triphenylene | 278 | C22H14 | 000215-58-7 | 95 |
| 2 | Picene | 278 | C22H14 | 000213-46-7 | 95 |
| 3 | Dibenz[a,h]anthracene | 278 | C22H14 | 000053-70-3 | 93 |
| 4 | Pentacene | 278 | C22H14 | 000135-48-8 | 93 |
| 5 | Benzo[b]chrysene | 278 | C22H14 | 000214-17-5 | 89 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
A010015

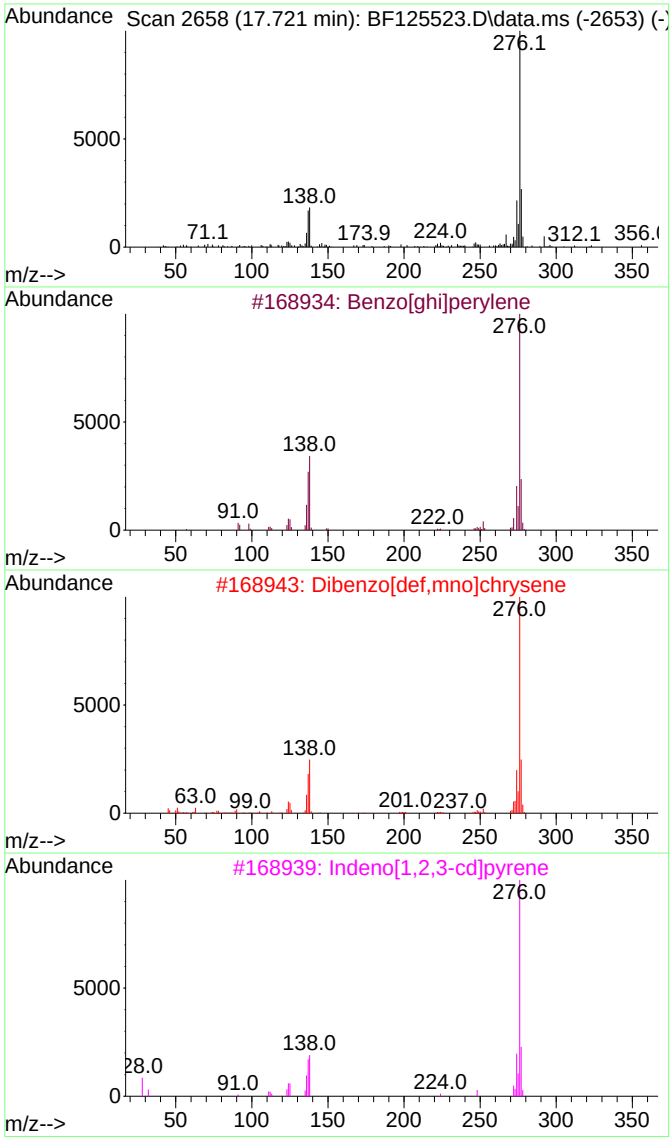
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

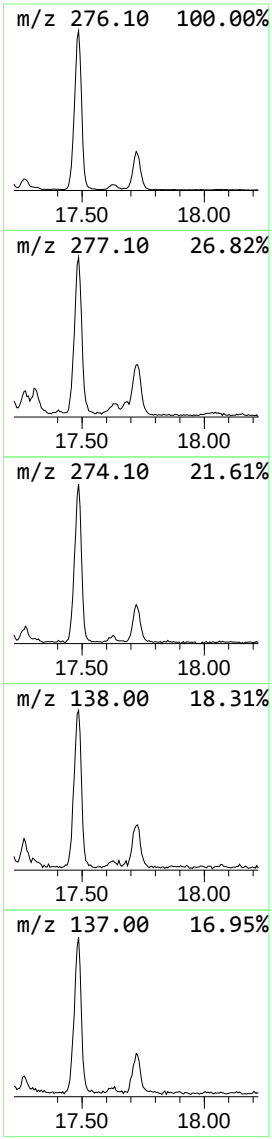
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 20 Dibenzo[def,mno]chrysene Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.721 | 5.81 ng | 258867 | Perylene-d12 | 15.533 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[ghi]perylene | 276 | C22H12 | 000191-24-2 | 93 |
| 2 | Dibenzo[def,mno]chrysene | 276 | C22H12 | 000191-26-4 | 90 |
| 3 | Indeno[1,2,3-cd]pyrene | 276 | C22H12 | 000193-39-5 | 81 |
| 4 | Indeno[1,2,3-cd]fluoranthene | 276 | C22H12 | 000193-43-1 | 62 |
| 5 | 6H-Pyrido[4,3-b]carbazole, 9-met... | 276 | C18H16N2O | 010371-86-5 | 53 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125523.D
Acq On : 16 Sep 2021 1:24
Operator : JU/CG
Sample : M3687-23
Misc :
ALS Vial : 18 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** A010015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-metho... | 2.193 | 26.2 | ng | 1369150 | 1 | 6.869 | 1043670 | 20.0 |
| 2-Pentanone, 4-... | 5.098 | 19.1 | ng | 993903 | 1 | 6.869 | 1043670 | 20.0 |
| Hexanoic acid | 6.569 | 9.4 | ng | 488413 | 1 | 6.869 | 1043670 | 20.0 |
| Nonanoic acid | 8.527 | 14.6 | ng | 1001970 | 2 | 8.151 | 1370710 | 20.0 |
| n-Decanoic acid | 9.086 | 8.3 | ng | 663578 | 3 | 9.904 | 1591930 | 20.0 |
| 1,2-Ethanediol,... | 9.486 | 6.7 | ng | 534348 | 3 | 9.904 | 1591930 | 20.0 |
| o-Terphenyl | 11.763 | 12.2 | ng | 786596 | 4 | 11.398 | 1289420 | 20.0 |
| Anthracene, 2-m... | 11.898 | 8.5 | ng | 550684 | 4 | 11.398 | 1289420 | 20.0 |
| Phenanthrene, 2... | 11.927 | 13.9 | ng | 897664 | 4 | 11.398 | 1289420 | 20.0 |
| 4H-Cyclopenta[d... | 12.010 | 9.6 | ng | 615949 | 4 | 11.398 | 1289420 | 20.0 |
| Phenanthrene, 4... | 12.033 | 5.7 | ng | 367942 | 4 | 11.398 | 1289420 | 20.0 |
| 6-Phenylbenzocy... | 12.192 | 7.6 | ng | 487752 | 4 | 11.398 | 1289420 | 20.0 |
| Phenanthrene, 2... | 12.451 | 5.6 | ng | 362967 | 4 | 11.398 | 1289420 | 20.0 |
| Cyclopenta(def)... | 12.545 | 6.8 | ng | 435553 | 4 | 11.398 | 1289420 | 20.0 |
| Imidazo[1,2-b]-... | 14.927 | 8.5 | ng | 380475 | 6 | 15.533 | 891044 | 20.0 |
| Benzo[e]pyrene | 15.209 | 11.2 | ng | 499750 | 6 | 15.533 | 891044 | 20.0 |
| Perylene | 15.409 | 37.0 | ng | 1647870 | 6 | 15.533 | 891044 | 20.0 |
| Picene | 17.209 | 6.7 | ng | 298887 | 6 | 15.533 | 891044 | 20.0 |
| Benzo[b]triphen... | 17.262 | 5.6 | ng | 248597 | 6 | 15.533 | 891044 | 20.0 |
| Dibenzo[def,mno... | 17.721 | 5.8 | ng | 258867 | 6 | 15.533 | 891044 | 20.0 |