LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070822\
Data File : BF129177.D
Acq On : 08 Jul 2022 16:09
Operator : CG\JU
Sample : N3622-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220498A-SIM-C4A-COMPOSITE

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-BF062922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129177.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.569 | 550 | 558 | 561 | rBV | 5740790 | 5340646 | 94.85% | 9.496% |
| 2 | 6.569 | 722 | 728 | 731 | rBV | 5231883 | 5358905 | 95.18% | 9.529% |
| 3 | 6.945 | 788 | 792 | 795 | rBV | 1935932 | 1528735 | 27.15% | 2.718% |
| 4 | 7.057 | 808 | 811 | 814 | rBV2 | 100283 | 93070 | 1.65% | 0.165% |
| 5 | 7.339 | 855 | 859 | 862 | rBV2 | 52687 | 71254 | 1.27% | 0.127% |
| 6 | 7.504 | 883 | 887 | 891 | rBV | 3235182 | 3289340 | 58.42% | 5.849% |
| 7 | 8.228 | 1006 | 1010 | 1013 | rBV | 2480951 | 2055191 | 36.50% | 3.654% |
| 8 | 8.251 | 1013 | 1014 | 1016 | rVB | 145420 | 66664 | 1.18% | 0.119% |
| 9 | 9.304 | 1188 | 1193 | 1196 | rBV | 6735103 | 5630456 | 100.00% | 10.012% |
| 10 | 9.557 | 1233 | 1236 | 1243 | rVB2 | 79685 | 96353 | 1.71% | 0.171% |
| 11 | 9.692 | 1257 | 1259 | 1263 | rVB3 | 89205 | 73556 | 1.31% | 0.131% |
| 12 | 9.851 | 1283 | 1286 | 1288 | rBV | 64203 | 64650 | 1.15% | 0.115% |
| 13 | 9.986 | 1304 | 1309 | 1312 | rBV | 2626434 | 2240448 | 39.79% | 3.984% |
| 14 | 10.022 | 1312 | 1315 | 1318 | rVB | 256118 | 226072 | 4.02% | 0.402% |
| 15 | 10.192 | 1341 | 1344 | 1347 | rVB2 | 151594 | 133678 | 2.37% | 0.238% |
| 16 | 10.304 | 1359 | 1363 | 1365 | rBV2 | 63831 | 73753 | 1.31% | 0.131% |
| 17 | 10.392 | 1374 | 1378 | 1383 | rBV6 | 76086 | 104437 | 1.85% | 0.186% |
| 18 | 10.533 | 1399 | 1402 | 1408 | rBV | 240550 | 230408 | 4.09% | 0.410% |
| 19 | 10.621 | 1415 | 1417 | 1420 | rVB | 75948 | 68979 | 1.23% | 0.123% |
| 20 | 10.780 | 1440 | 1444 | 1447 | rBV | 4894672 | 4190561 | 74.43% | 7.451% |
| 21 | 10.892 | 1459 | 1463 | 1471 | rVB4 | 118951 | 194584 | 3.46% | 0.346% |
| 22 | 11.357 | 1539 | 1542 | 1544 | rBV2 | 82367 | 91388 | 1.62% | 0.162% |
| 23 | 11.374 | 1544 | 1545 | 1549 | rVB | 119881 | 95899 | 1.70% | 0.171% |
| 24 | 11.480 | 1559 | 1563 | 1565 | rBV | 2623875 | 2249628 | 39.95% | 4.000% |
| 25 | 11.504 | 1565 | 1567 | 1571 | rVV | 2094715 | 1665370 | 29.58% | 2.961% |
| 26 | 11.557 | 1571 | 1576 | 1579 | rVV | 533723 | 479890 | 8.52% | 0.853% |
| 27 | 11.710 | 1599 | 1602 | 1605 | rBV | 194239 | 156884 | 2.79% | 0.279% |
| 28 | 11.992 | 1645 | 1650 | 1652 | rBV2 | 275933 | 455794 | 8.10% | 0.810% |
| 29 | 12.010 | 1652 | 1653 | 1658 | rVB | 297319 | 184082 | 3.27% | 0.327% |
| 30 | 12.057 | 1659 | 1661 | 1664 | rVB | 122719 | 96895 | 1.72% | 0.172% |
| 31 | 12.098 | 1664 | 1668 | 1670 | rBV2 | 369098 | 382610 | 6.80% | 0.680% |
| 32 | 12.280 | 1696 | 1699 | 1701 | rVB | 146318 | 106740 | 1.90% | 0.190% |
| 33 | 12.427 | 1722 | 1724 | 1726 | rVB | 114988 | 80926 | 1.44% | 0.144% |
| 34 | 12.533 | 1739 | 1742 | 1745 | rBV | 131104 | 130479 | 2.32% | 0.232% |
| 35 | 12.698 | 1767 | 1770 | 1774 | rBV | 2187600 | 1873319 | 33.27% | 3.331% |
| 36 | 12.739 | 1774 | 1777 | 1779 | rVB2 | 141471 | 135278 | 2.40% | 0.241% |

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Sample : N3622-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220498A-SIM-C4A-COMPOSITE

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-BF062922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 12.927 | 1803 | 1809 | 1815 | rBV | 1682191 | 2000926 | 35.54% | 3.558% |
| 38 | 12.980 | 1815 | 1818 | 1822 | rVB2 | 91584 | 103024 | 1.83% | 0.183% |
| 39 | 13.068 | 1829 | 1833 | 1836 | rBV | 5249181 | 4406636 | 78.26% | 7.836% |
| 40 | 13.145 | 1842 | 1846 | 1850 | rBV2 | 103263 | 172088 | 3.06% | 0.306% |
| 41 | 13.210 | 1853 | 1857 | 1859 | rVV | 447949 | 434219 | 7.71% | 0.772% |
| 42 | 13.257 | 1862 | 1865 | 1868 | rVB | 289176 | 266628 | 4.74% | 0.474% |
| 43 | 13.327 | 1874 | 1877 | 1879 | rBV | 181588 | 162175 | 2.88% | 0.288% |
| 44 | 13.362 | 1879 | 1883 | 1885 | rBV2 | 163413 | 160393 | 2.85% | 0.285% |
| 45 | 13.457 | 1897 | 1899 | 1901 | rVB | 95852 | 66699 | 1.18% | 0.119% |
| 46 | 13.486 | 1902 | 1904 | 1907 | rBV | 92468 | 79691 | 1.42% | 0.142% |
| 47 | 13.880 | 1969 | 1971 | 1973 | rVB | 97734 | 73439 | 1.30% | 0.131% |
| 48 | 13.909 | 1973 | 1976 | 1978 | rVB | 87304 | 68418 | 1.22% | 0.122% |
| 49 | 13.933 | 1978 | 1980 | 1983 | rBV2 | 71674 | 91472 | 1.62% | 0.163% |
| 50 | 14.098 | 2005 | 2008 | 2009 | rBV | 132409 | 98968 | 1.76% | 0.176% |
| 51 | 14.133 | 2009 | 2014 | 2016 | rVV2 | 1847027 | 2379476 | 42.26% | 4.231% |
| 52 | 14.157 | 2016 | 2018 | 2024 | rVB | 800261 | 654673 | 11.63% | 1.164% |
| 53 | 14.221 | 2024 | 2029 | 2036 | rBV2 | 856284 | 1037909 | 18.43% | 1.846% |
| 54 | 14.274 | 2036 | 2038 | 2042 | rBV3 | 80708 | 74539 | 1.32% | 0.133% |
| 55 | 14.515 | 2077 | 2079 | 2082 | rVB | 135265 | 112866 | 2.00% | 0.201% |
| 56 | 14.668 | 2103 | 2105 | 2109 | rVB2 | 100454 | 89028 | 1.58% | 0.158% |
| 57 | 14.986 | 2156 | 2159 | 2162 | rVB | 130158 | 122328 | 2.17% | 0.218% |
| 58 | 15.198 | 2191 | 2195 | 2199 | rBV | 536877 | 877842 | 15.59% | 1.561% |
| 59 | 15.309 | 2212 | 2214 | 2218 | rVB | 92870 | 96725 | 1.72% | 0.172% |
| 60 | 15.521 | 2246 | 2250 | 2256 | rVB | 328808 | 433498 | 7.70% | 0.771% |
| 61 | 15.586 | 2256 | 2261 | 2267 | rBV | 469773 | 607962 | 10.80% | 1.081% |
| 62 | 15.651 | 2267 | 2272 | 2276 | rBV | 1105444 | 1487892 | 26.43% | 2.646% |
| 63 | 17.198 | 2530 | 2535 | 2546 | rVB2 | 195278 | 394804 | 7.01% | 0.702% |
| 64 | 17.668 | 2610 | 2615 | 2627 | rVB | 168172 | 367569 | 6.53% | 0.654% |

Sum of corrected areas: 56238809

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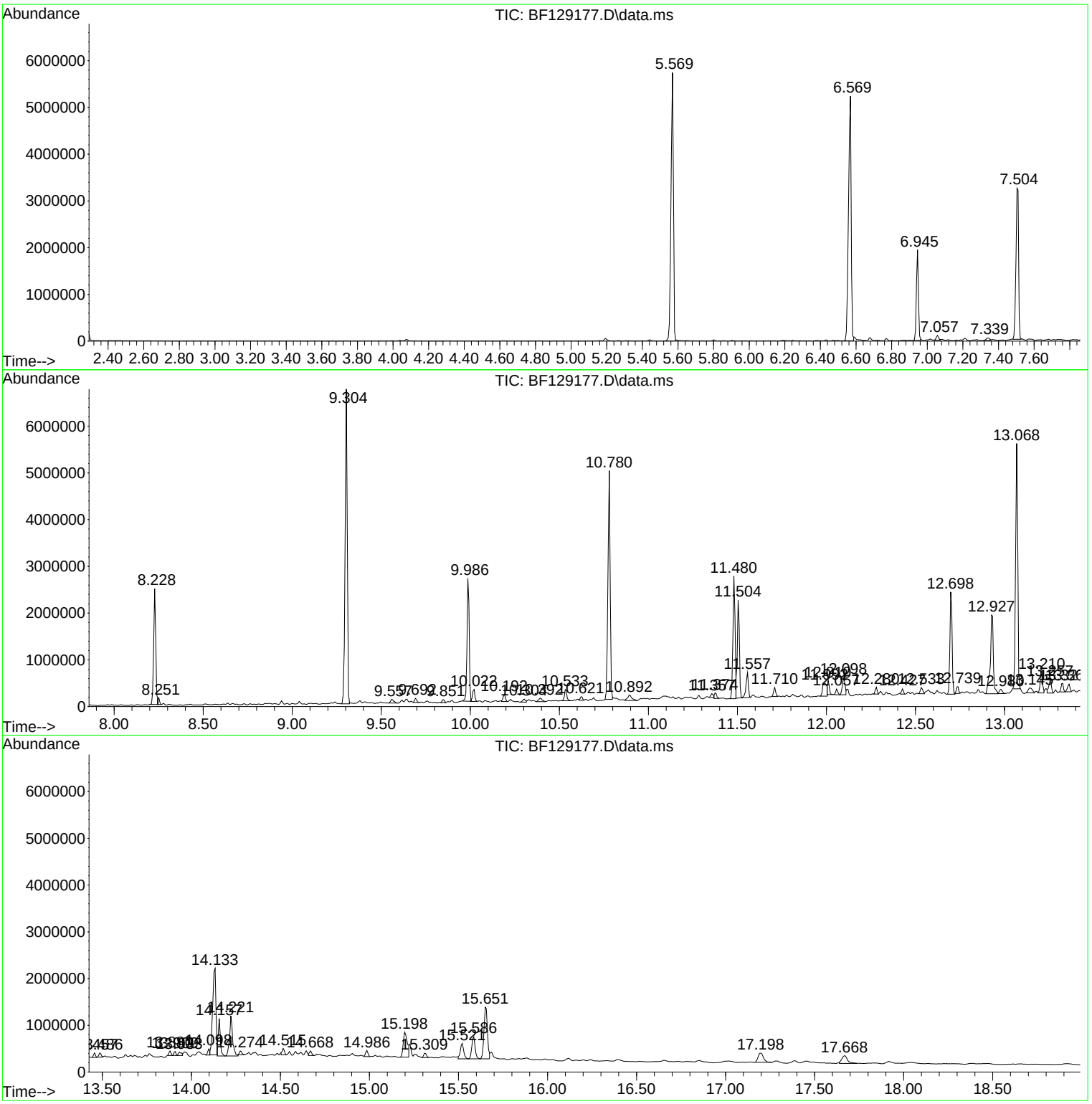
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220498A-SIM-C4A-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.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\BF070822\
Data File : BF129177.D
Acq On : 08 Jul 2022 16:09
Operator : CG\JU
Sample : N3622-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220498A-SIM-C4A-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

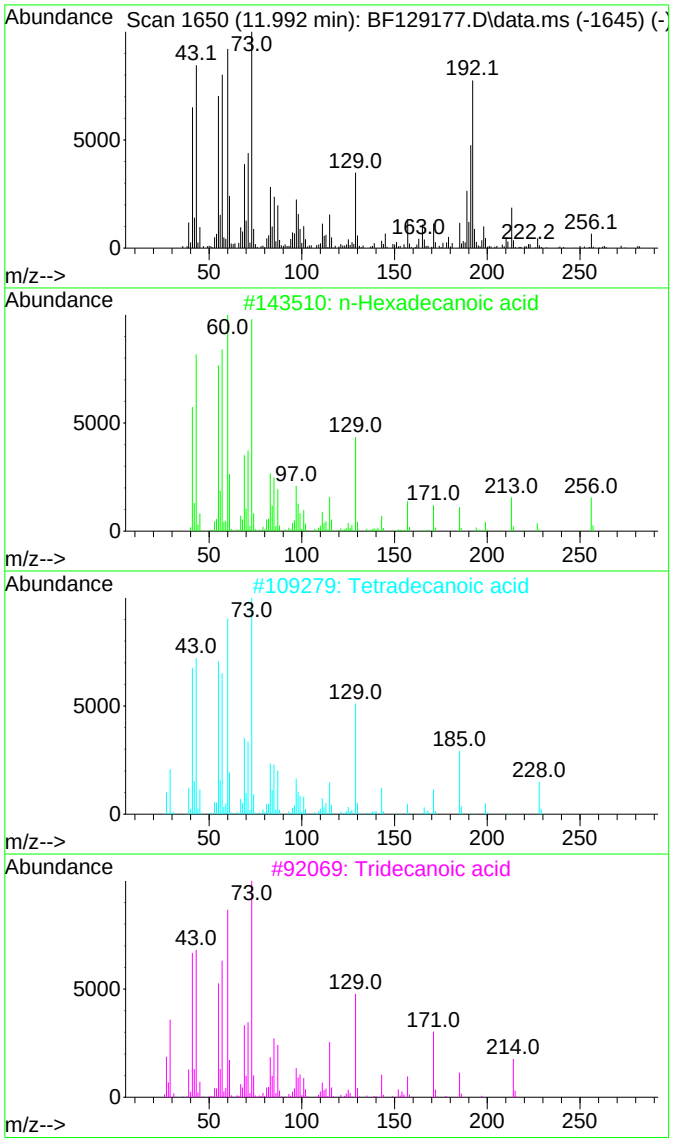
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

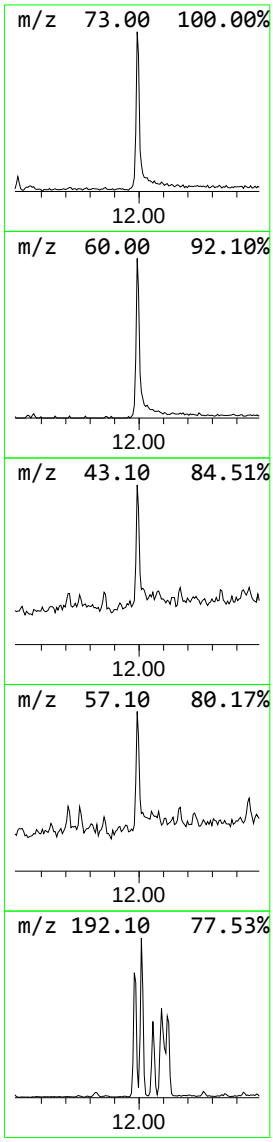
**********

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.992 | 4.05 ng | 455794 | Phenanthrene-d10 | 11.480 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 96 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 87 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 64 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 55 |
| 5 | Anthracene, 9-methyl- | 192 | C15H12 | 000779-02-2 | 47 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070822\
Data File : BF129177.D
Acq On : 08 Jul 2022 16:09
Operator : CG\JU
Sample : N3622-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220498A-SIM-C4A-COMPOSITE

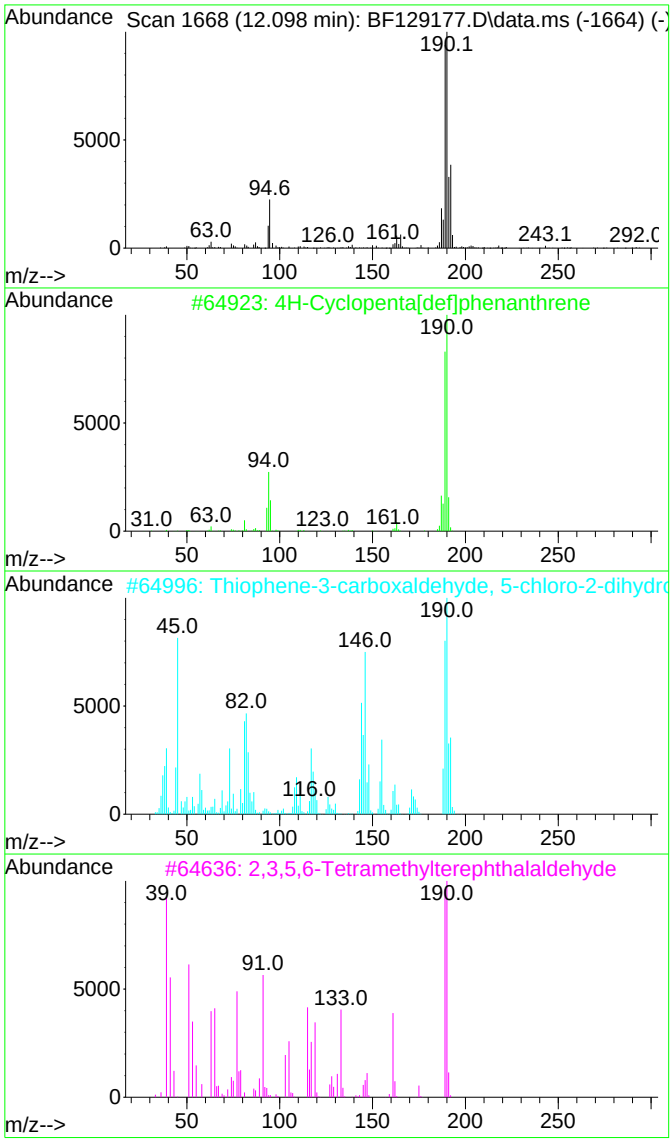
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

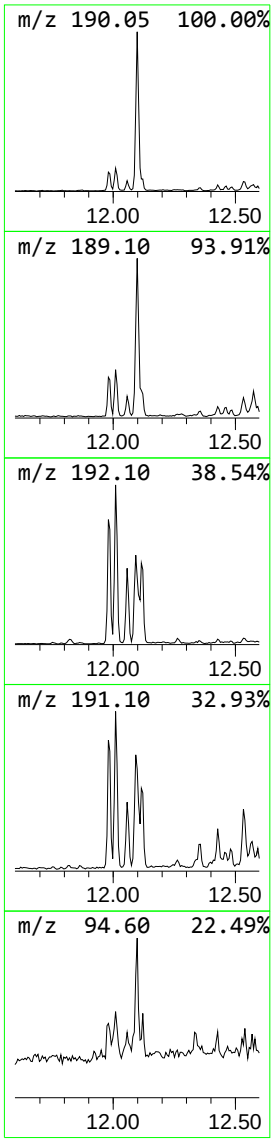
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.098 | 3.40 ng | 382610 | Phenanthrene-d10 | 11.480 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4H-Cyclopenta[def]phenanthrene | 190 | C15H10 | 000203-64-5 | 93 |
| 2 | Thiophene-3-carboxaldehyde, 5-ch... | 190 | C5H4BClO3S | 036155-87-0 | 53 |
| 3 | 2,3,5,6-Tetramethylterephthalald... | 190 | C12H14O2 | 007072-01-7 | 47 |
| 4 | 2,2'-Bis(4,5-dimethylimidazole) | 190 | C10H14N4 | 069286-06-2 | 42 |
| 5 | 2,4(1H,3H)-Pyrimidinedione, 5-br... | 190 | C4H3BrN2O2 | 000051-20-7 | 32 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070822\
Data File : BF129177.D
Acq On : 08 Jul 2022 16:09
Operator : CG\JU
Sample : N3622-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220498A-SIM-C4A-COMPOSITE

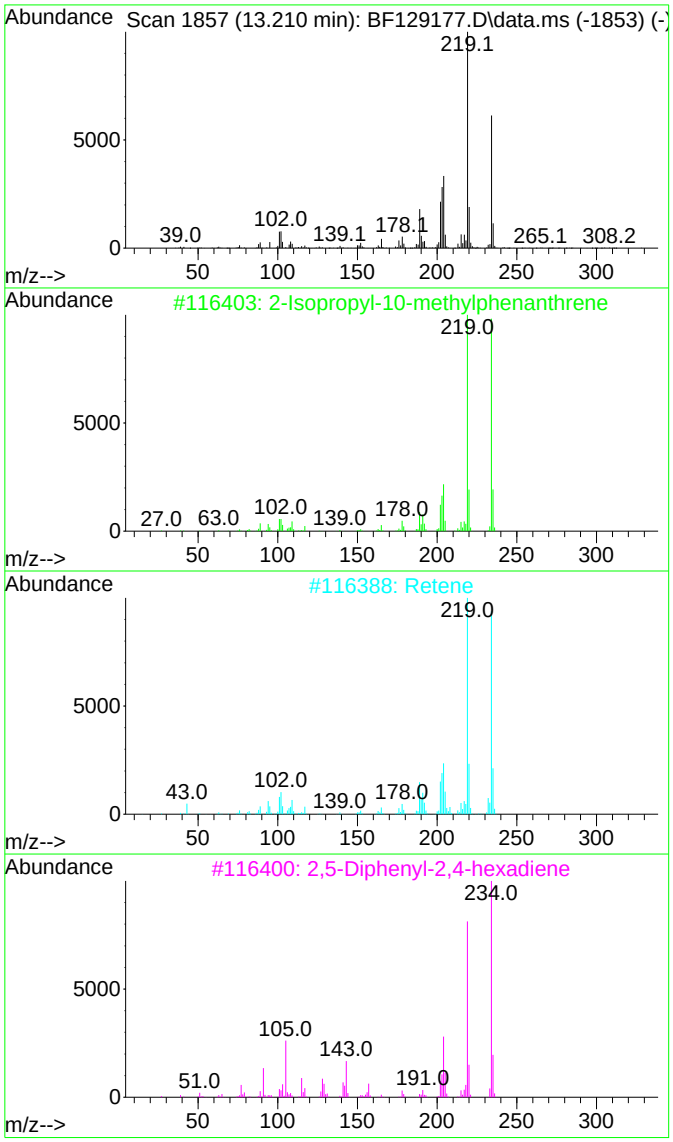
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

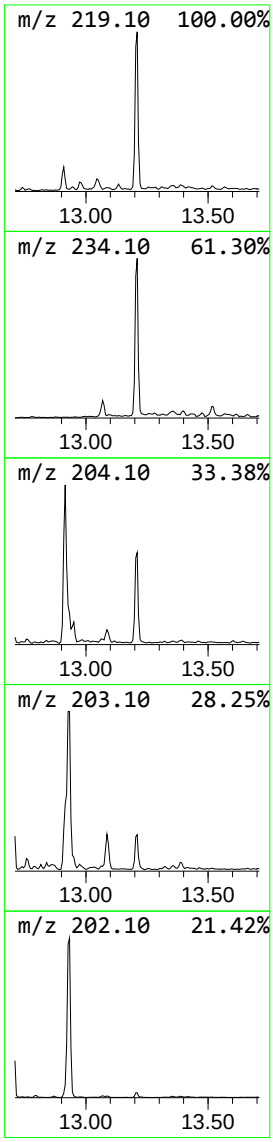
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 2-Isopropyl-10-methylphenan... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.210 | 3.65 ng | 434219 | Chrysene-d12 | 14.133 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Isopropyl-10-methylphenanthrene | 234 | C18H18 | 066552-97-4 | 94 |
| 2 | Retene | 234 | C18H18 | 000483-65-8 | 94 |
| 3 | 2,5-Diphenyl-2,4-hexadiene | 234 | C18H18 | 016819-47-9 | 80 |
| 4 | Benzene, 1,3-bis(1,1-dimethyleth... | 234 | C16H26O | 001518-53-2 | 52 |
| 5 | 3-Isopropylamino-6-methyl-6,7-di... | 234 | C13H18N2O2 | 145220-69-5 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070822\
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Sample : N3622-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220498A-SIM-C4A-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

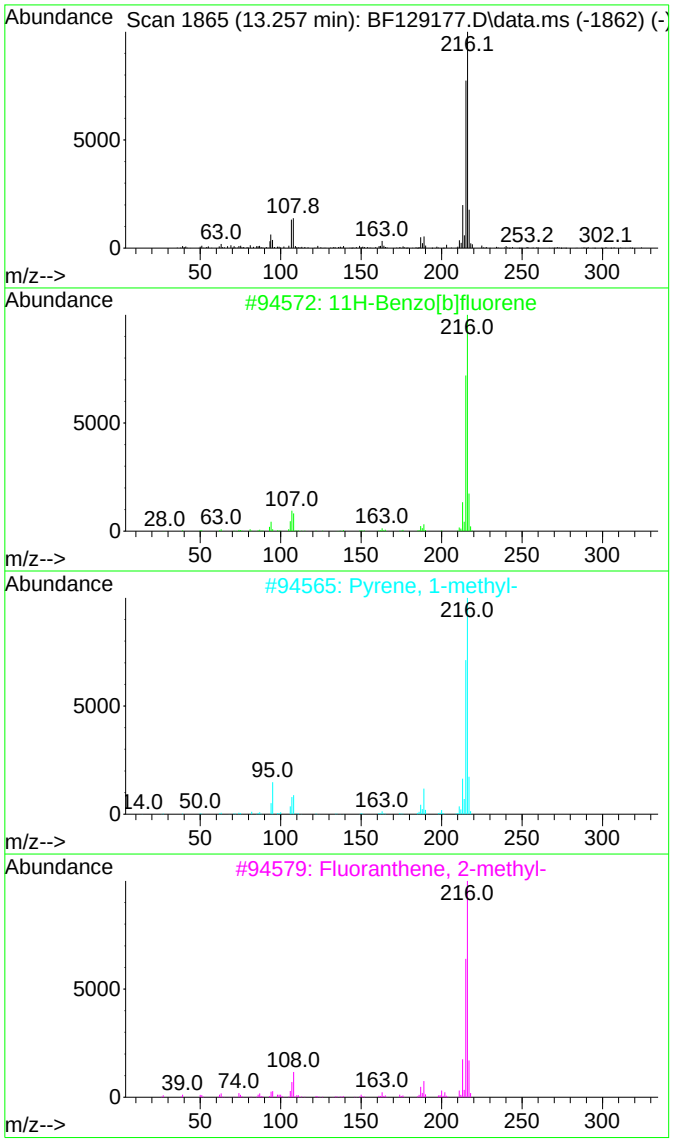
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

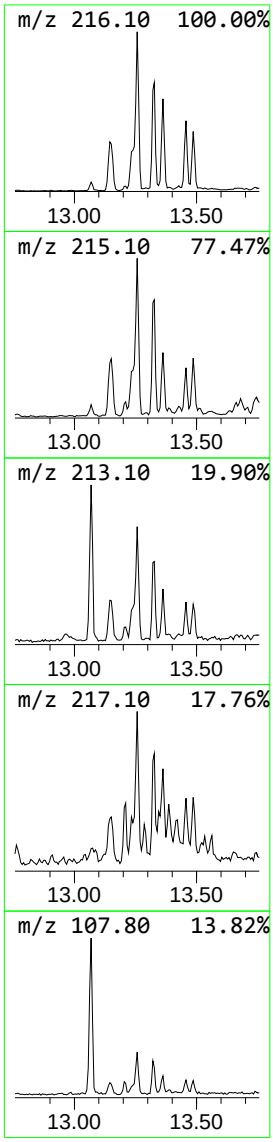
**********

Peak Number 4 11H-Benzo[b]fluorene Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.257 | 2.24 ng | 266628 | Chrysene-d12 | 14.133 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 11H-Benzo[b]fluorene | 216 | C17H12 | 000243-17-4 | 94 |
| 2 | Pyrene, 1-methyl- | 216 | C17H12 | 002381-21-7 | 94 |
| 3 | Fluoranthene, 2-methyl- | 216 | C17H12 | 033543-31-6 | 93 |
| 4 | 11H-Benzo[a]fluorene | 216 | C17H12 | 000238-84-6 | 91 |
| 5 | Pyrene, 2-methyl- | 216 | C17H12 | 003442-78-2 | 91 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070822\
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Acq On : 08 Jul 2022 16:09
Operator : CG\JU
Sample : N3622-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220498A-SIM-C4A-COMPOSITE

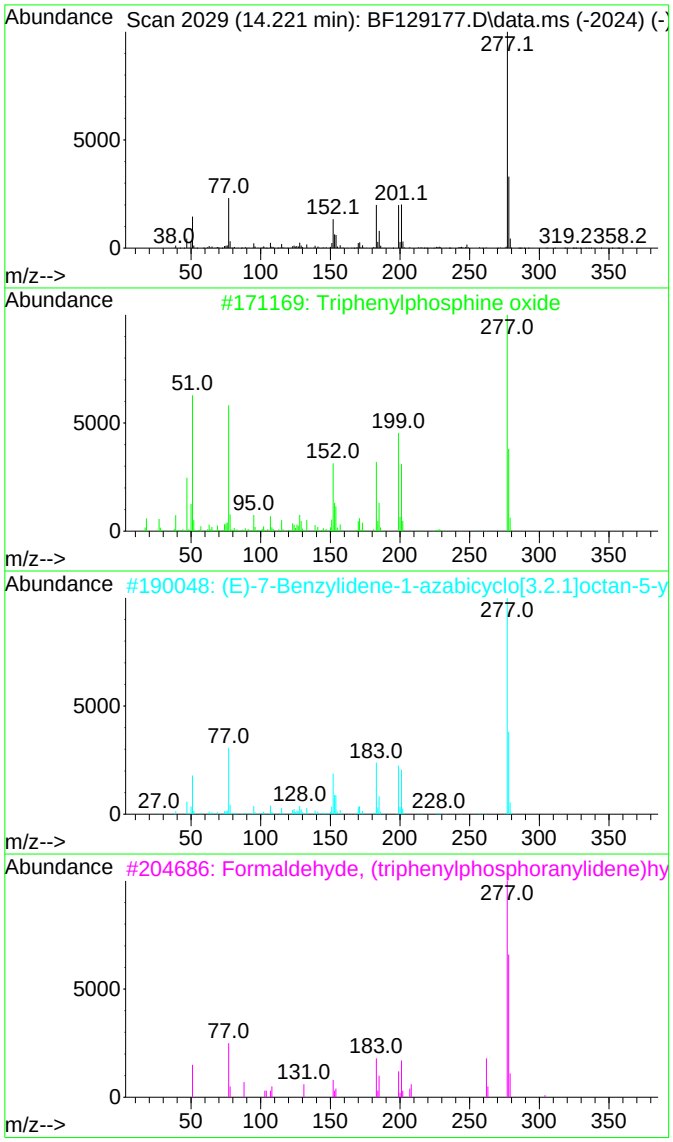
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

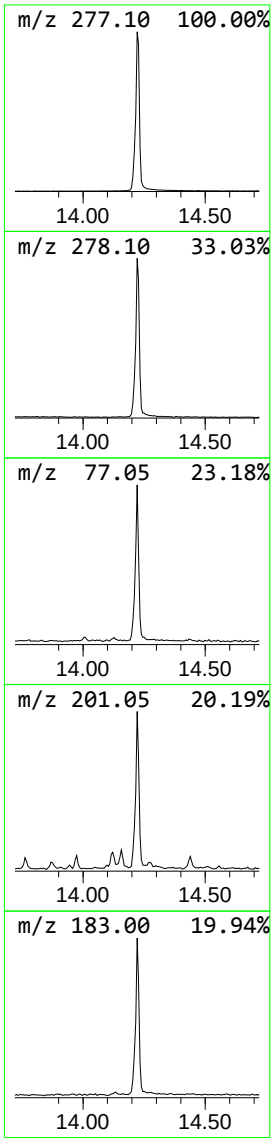
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.221 | 8.72 ng | 1037910 | Chrysene-d12 | 14.133 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triphenylphosphine oxide | 278 | C18H15OP | 000791-28-6 | 92 |
| 2 | (E)-7-Benzylidene-1-azabicyclo[3... | 293 | C15H19NO3S | 1000483-83-4 | 91 |
| 3 | Formaldehyde, (triphenylphosphor... | 304 | C19H17N2P | 015990-54-2 | 64 |
| 4 | Cobalt,(.eta.<5>-2,4-cyclopentad... | 277 | C16H15BCo | 036682-12-9 | 25 |
| 5 | Vanadium, cycloheptatrienyl-(pen... | 277 | C17H22V | 1000155-20-5 | 23 |



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Data File : BF129177.D
Acq On : 08 Jul 2022 16:09
Operator : CG\JU
Sample : N3622-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220498A-SIM-C4A-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

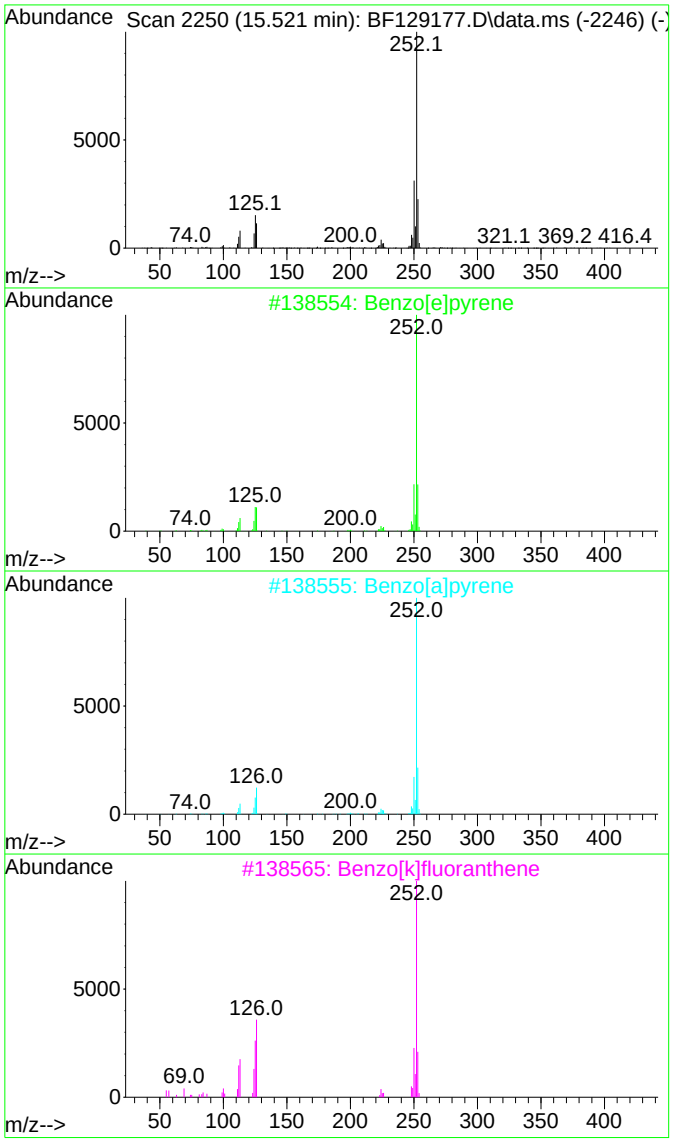
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

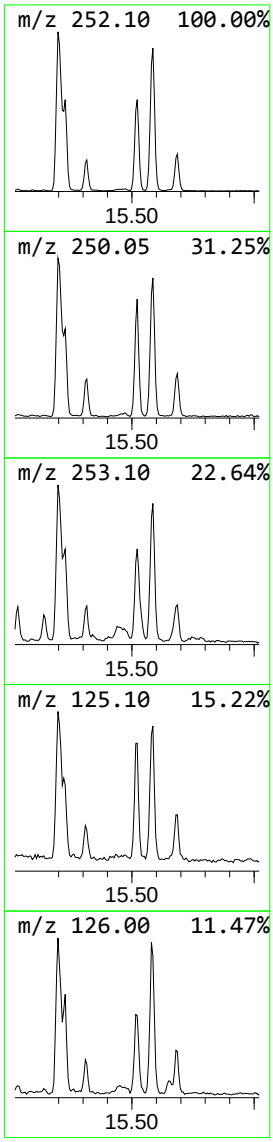
**********

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.521 | 5.83 ng | 433498 | Perylene-d12 | 15.651 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 98 |
| 2 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 97 |
| 3 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 96 |
| 4 | Perylene | 252 | C20H12 | 000198-55-0 | 96 |
| 5 | Benzo[b]fluoranthene | 252 | C20H12 | 000205-99-2 | 95 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070822\
Data File : BF129177.D
Acq On : 08 Jul 2022 16:09
Operator : CG\JU
Sample : N3622-09
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
20220498A-SIM-C4A-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.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 |
| n-Hexadecanoic ... | 11.992 | 4.0 | ng | 455794 | 4 | 11.480 | 2249630 | 20.0 |
| 4H-Cyclopenta[d... | 12.098 | 3.4 | ng | 382610 | 4 | 11.480 | 2249630 | 20.0 |
| 2-Isopropyl-10-... | 13.210 | 3.6 | ng | 434219 | 5 | 14.133 | 2379480 | 20.0 |
| 11H-Benzo[b]flu... | 13.257 | 2.2 | ng | 266628 | 5 | 14.133 | 2379480 | 20.0 |
| Triphenylphosph... | 14.221 | 8.7 | ng | 1037910 | 5 | 14.133 | 2379480 | 20.0 |
| Benzo[e]pyrene | 15.521 | 5.8 | ng | 433498 | 6 | 15.651 | 1487890 | 20.0 |