LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134597.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.157 | 7 | 12 | 19 | rVB3 | 50340 | 73840 | 2.18% | 0.259% |
| 2 | 5.416 | 561 | 566 | 570 | rBV | 3213913 | 3275811 | 96.75% | 11.487% |
| 3 | 6.422 | 732 | 737 | 740 | rBV | 3130800 | 3318028 | 98.00% | 11.635% |
| 4 | 6.622 | 768 | 771 | 776 | rBV | 110239 | 89855 | 2.65% | 0.315% |
| 5 | 6.792 | 797 | 800 | 804 | rBV | 1255059 | 1043595 | 30.82% | 3.659% |
| 6 | 7.351 | 890 | 895 | 898 | rBV | 2205238 | 2065641 | 61.01% | 7.243% |
| 7 | 8.069 | 1013 | 1017 | 1020 | rBV | 1470911 | 1321940 | 39.04% | 4.635% |
| 8 | 9.151 | 1196 | 1201 | 1204 | rBV | 4098287 | 3385723 | 100.00% | 11.872% |
| 9 | 9.269 | 1218 | 1221 | 1225 | rVB | 51533 | 41110 | 1.21% | 0.144% |
| 10 | 9.686 | 1288 | 1292 | 1295 | rBV | 64575 | 54396 | 1.61% | 0.191% |
| 11 | 9.827 | 1312 | 1316 | 1319 | rBV | 1355658 | 1164645 | 34.40% | 4.084% |
| 12 | 10.610 | 1445 | 1449 | 1453 | rBV | 1902757 | 1720746 | 50.82% | 6.034% |
| 13 | 11.310 | 1565 | 1568 | 1571 | rBV | 1185071 | 1087066 | 32.11% | 3.812% |
| 14 | 11.333 | 1571 | 1572 | 1576 | rVV | 362061 | 251870 | 7.44% | 0.883% |
| 15 | 11.386 | 1576 | 1581 | 1584 | rVB | 80220 | 72874 | 2.15% | 0.256% |
| 16 | 11.539 | 1602 | 1607 | 1610 | rBV2 | 47264 | 54417 | 1.61% | 0.191% |
| 17 | 11.816 | 1651 | 1654 | 1656 | rBV | 51278 | 39554 | 1.17% | 0.139% |
| 18 | 11.851 | 1656 | 1660 | 1664 | rBV2 | 254068 | 262533 | 7.75% | 0.921% |
| 19 | 11.927 | 1670 | 1673 | 1675 | rBV2 | 73400 | 76843 | 2.27% | 0.269% |
| 20 | 12.133 | 1706 | 1708 | 1711 | rVB | 77538 | 63148 | 1.87% | 0.221% |
| 21 | 12.363 | 1744 | 1747 | 1751 | rBV2 | 45607 | 49440 | 1.46% | 0.173% |
| 22 | 12.445 | 1759 | 1761 | 1767 | rVB2 | 41664 | 49088 | 1.45% | 0.172% |
| 23 | 12.527 | 1771 | 1775 | 1779 | rVB | 672289 | 590304 | 17.44% | 2.070% |
| 24 | 12.757 | 1808 | 1814 | 1817 | rBV | 656318 | 652205 | 19.26% | 2.287% |
| 25 | 12.804 | 1819 | 1822 | 1827 | rVB3 | 30912 | 48779 | 1.44% | 0.171% |
| 26 | 12.910 | 1836 | 1840 | 1843 | rBV | 3054398 | 2764969 | 81.67% | 9.696% |
| 27 | 12.974 | 1846 | 1851 | 1854 | rBV2 | 48603 | 67906 | 2.01% | 0.238% |
| 28 | 13.086 | 1867 | 1870 | 1873 | rVB | 86838 | 88244 | 2.61% | 0.309% |
| 29 | 13.151 | 1879 | 1881 | 1884 | rVB | 70615 | 54367 | 1.61% | 0.191% |
| 30 | 13.186 | 1884 | 1887 | 1890 | rBV | 75412 | 75340 | 2.23% | 0.264% |
| 31 | 13.310 | 1906 | 1908 | 1912 | rBV2 | 45958 | 48096 | 1.42% | 0.169% |
| 32 | 13.492 | 1937 | 1939 | 1945 | rVB4 | 37905 | 50823 | 1.50% | 0.178% |
| 33 | 13.592 | 1953 | 1956 | 1962 | rVB | 57121 | 63905 | 1.89% | 0.224% |
| 34 | 13.704 | 1970 | 1975 | 1978 | rBV2 | 66447 | 90394 | 2.67% | 0.317% |
| 35 | 13.733 | 1978 | 1980 | 1982 | rBV | 49390 | 39536 | 1.17% | 0.139% |
| 36 | 13.815 | 1989 | 1994 | 2002 | rVB2 | 267575 | 323773 | 9.56% | 1.135% |

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 13.957 | 2013 | 2018 | 2021 | rBV2 | 1087965 | 1226453 | 36.22% | 4.301% |
| 38 | 13.980 | 2021 | 2022 | 2025 | rVB | 296654 | 205794 | 6.08% | 0.722% |
| 39 | 14.062 | 2034 | 2036 | 2040 | rBV2 | 34108 | 42577 | 1.26% | 0.149% |
| 40 | 14.145 | 2047 | 2050 | 2053 | rBV3 | 52479 | 45738 | 1.35% | 0.160% |
| 41 | 14.345 | 2080 | 2084 | 2087 | rVB | 60820 | 60410 | 1.78% | 0.212% |
| 42 | 14.380 | 2087 | 2090 | 2094 | rVB2 | 52129 | 44315 | 1.31% | 0.155% |
| 43 | 14.457 | 2097 | 2103 | 2107 | rBV4 | 84103 | 153393 | 4.53% | 0.538% |
| 44 | 14.904 | 2176 | 2179 | 2183 | rBV2 | 109143 | 113317 | 3.35% | 0.397% |
| 45 | 14.992 | 2190 | 2194 | 2197 | rBV | 239192 | 344771 | 10.18% | 1.209% |
| 46 | 15.104 | 2209 | 2213 | 2215 | rBV2 | 91192 | 113387 | 3.35% | 0.398% |
| 47 | 15.127 | 2215 | 2217 | 2224 | rVB | 123326 | 155664 | 4.60% | 0.546% |
| 48 | 15.292 | 2242 | 2245 | 2251 | rVB | 144978 | 171805 | 5.07% | 0.602% |
| 49 | 15.356 | 2251 | 2256 | 2261 | rVB | 193794 | 232131 | 6.86% | 0.814% |
| 50 | 15.421 | 2262 | 2267 | 2271 | rBV | 531981 | 680112 | 20.09% | 2.385% |
| 51 | 15.698 | 2310 | 2314 | 2318 | rBV5 | 32809 | 45908 | 1.36% | 0.161% |
| 52 | 15.939 | 2352 | 2355 | 2359 | rBV2 | 36069 | 45861 | 1.35% | 0.161% |
| 53 | 16.886 | 2511 | 2516 | 2525 | rVB2 | 77862 | 164060 | 4.85% | 0.575% |
| 54 | 17.080 | 2545 | 2549 | 2554 | rBV5 | 20910 | 44118 | 1.30% | 0.155% |
| 55 | 17.327 | 2587 | 2591 | 2600 | rVB | 56259 | 107131 | 3.16% | 0.376% |

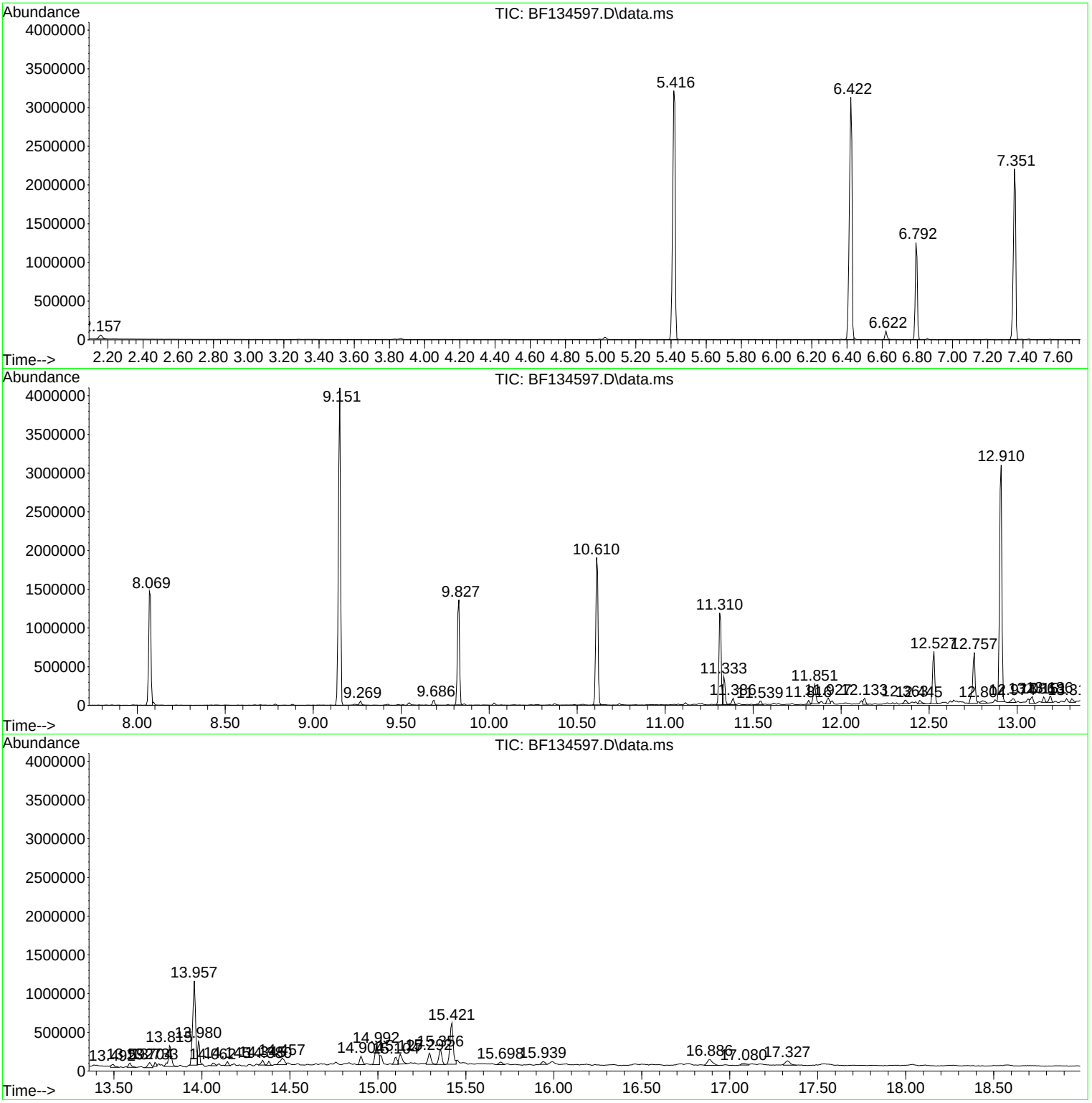
Sum of corrected areas: 28517749

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

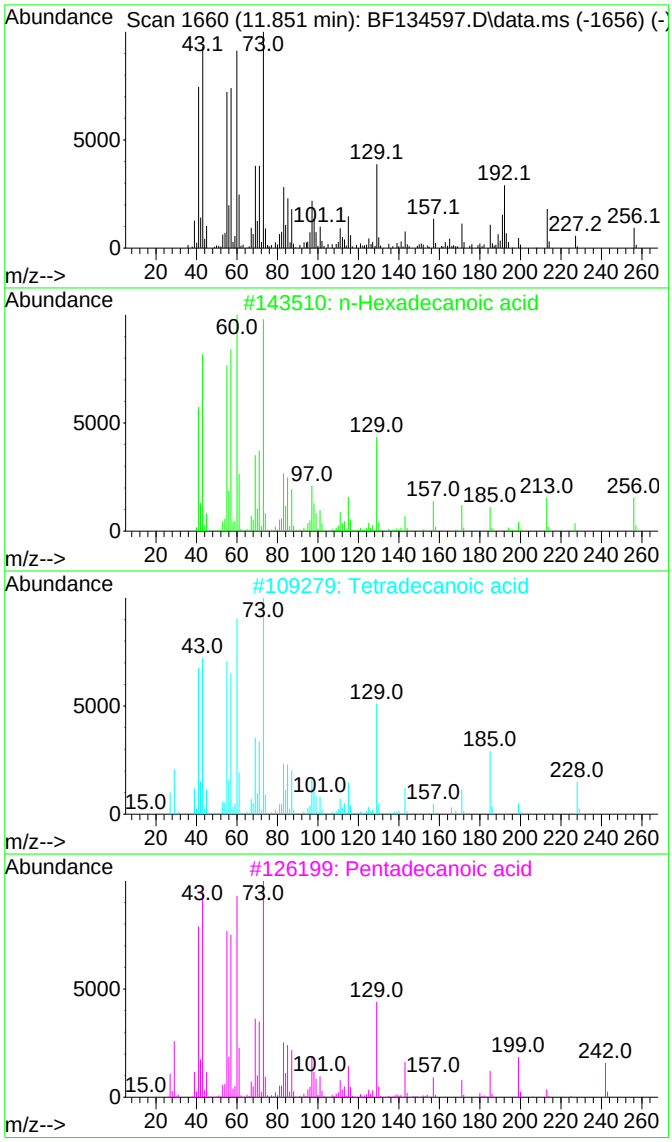
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

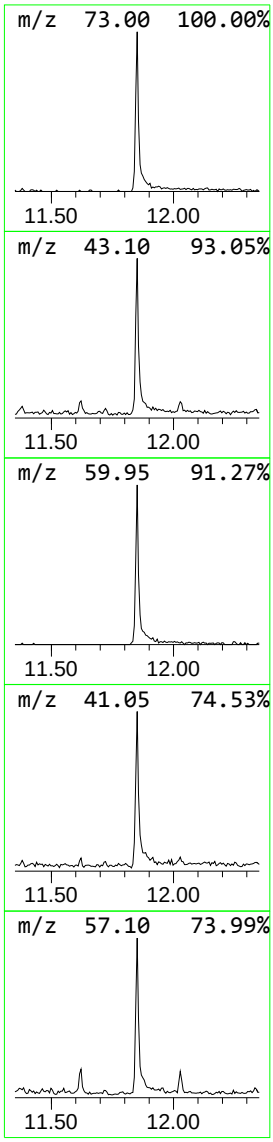
**********

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.851 | 4.83 ng | 262533 | Phenanthrene-d10 | 11.310 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 97 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 81 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 62 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

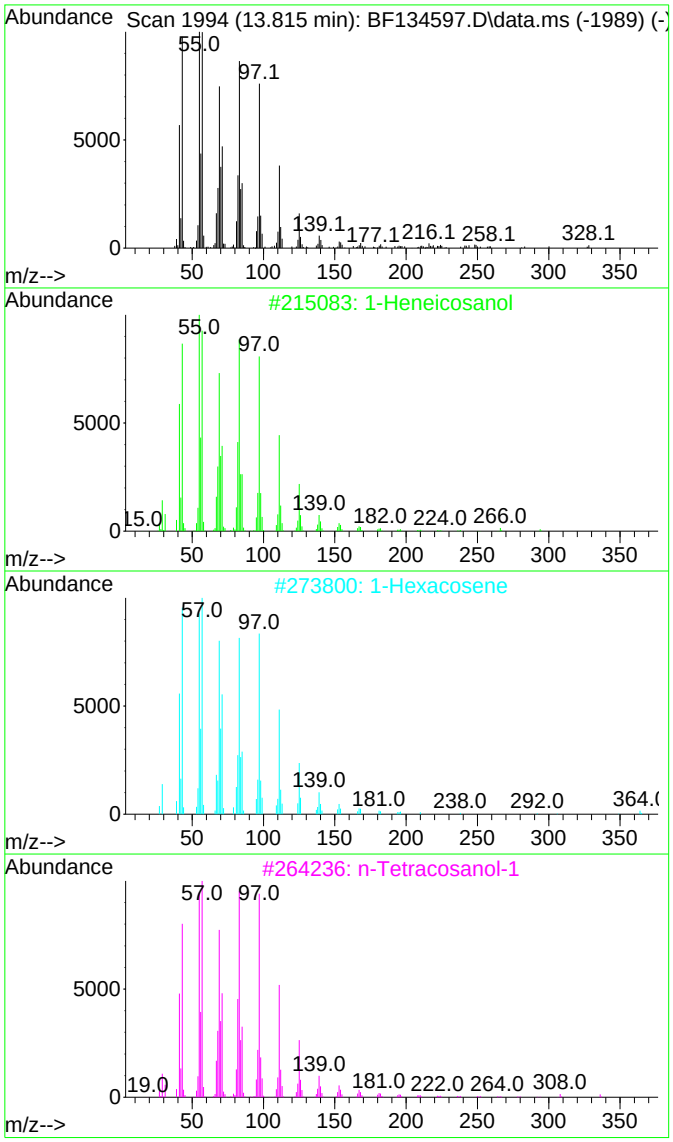
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

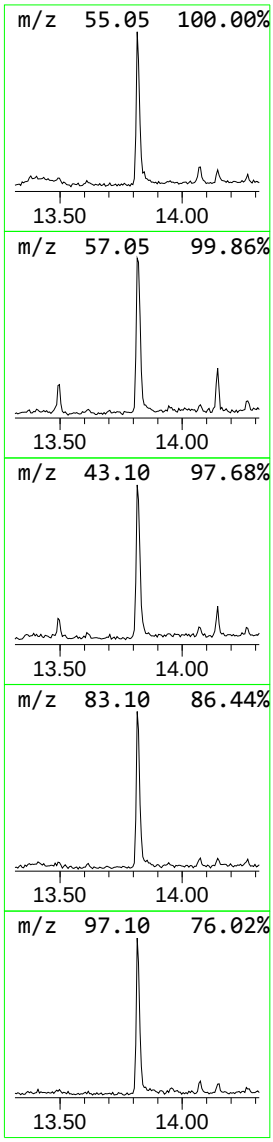
**********

Peak Number 2 1-Heneicosanol Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.815 | 5.28 ng | 323773 | Chrysene-d12 | 13.957 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 2 | 1-Hexacosene | 364 | C26H52 | 018835-33-1 | 94 |
| 3 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 4 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 93 |
| 5 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 91 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

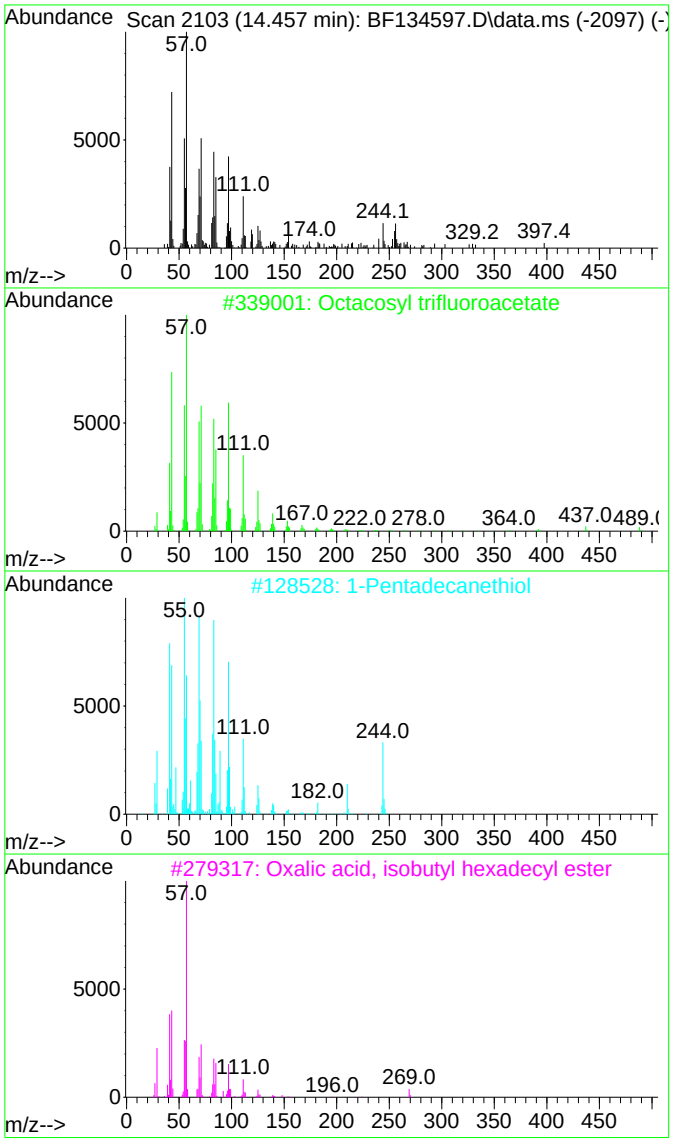
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

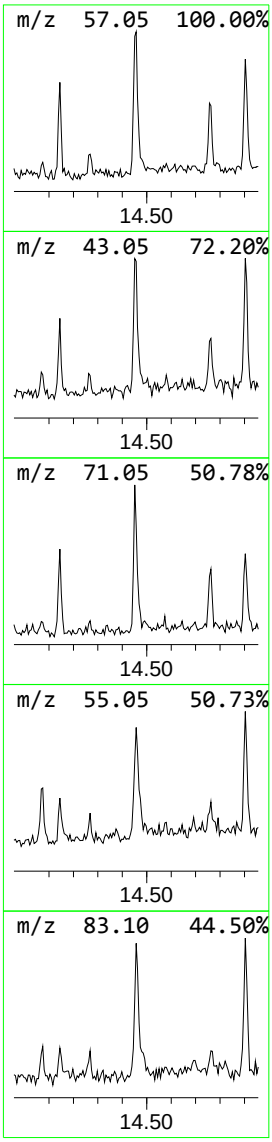
**********

Peak Number 3 Octacosyl trifluoroacetate Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.457 | 2.50 ng | 153393 | Chrysene-d12 | 13.957 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosyl trifluoroacetate | 506 | C30H57F3O2 | 1000351-74-9 | 87 |
| 2 | 1-Pentadecanethiol | 244 | C15H32S | 025276-70-4 | 83 |
| 3 | Oxalic acid, isobutyl hexadecyl ... | 370 | C22H42O4 | 1000309-38-1 | 83 |
| 4 | Tetratriacontyl pentafluoropropi... | 641 | C37H69F5O2 | 1000351-81-5 | 83 |
| 5 | Triacontyl pentafluoropropionate | 584 | C33H61F5O2 | 1000351-80-0 | 83 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

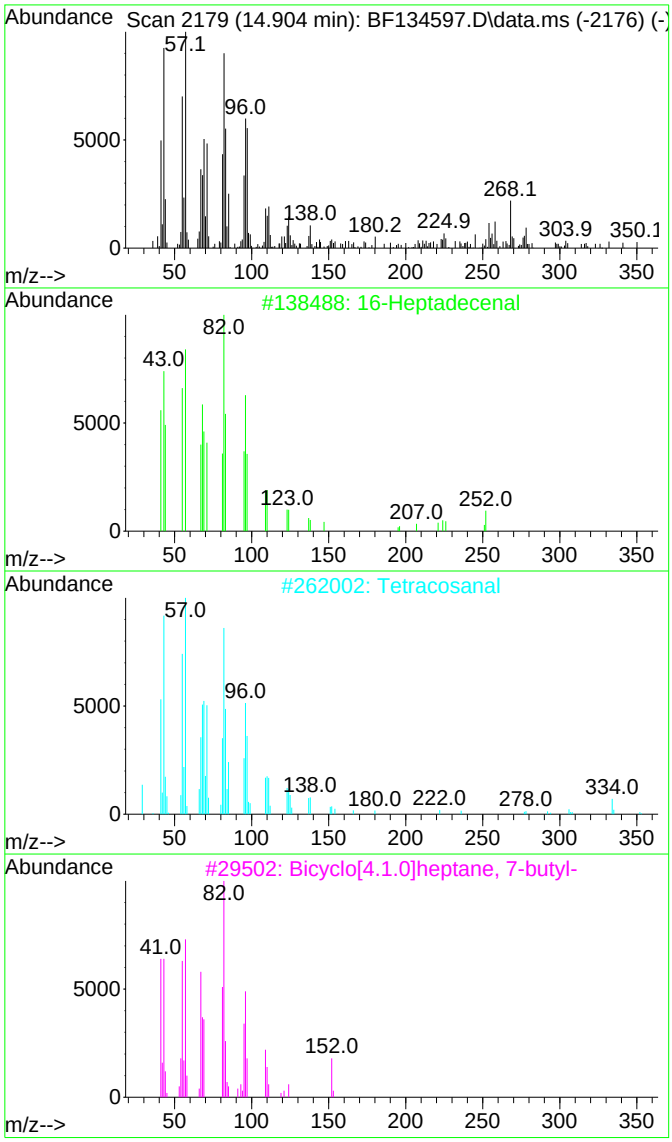
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

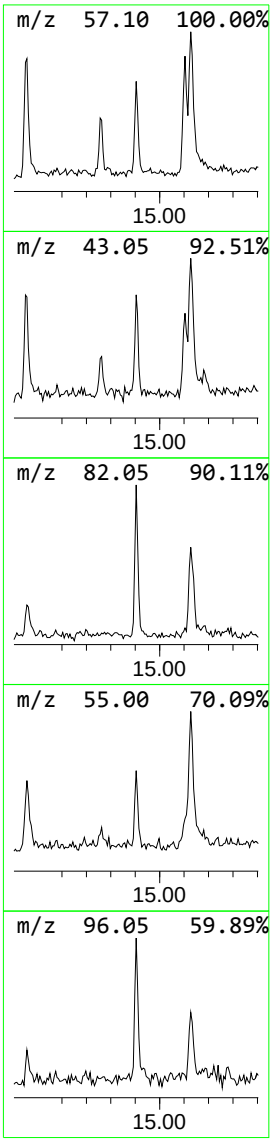
**********

Peak Number 4 16-Heptadecenal Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.904 | 3.33 ng | 113317 | Perylene-d12 | 15.421 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 16-Heptadecenal | 252 | C17H32O | 1010144-57-9 | 90 |
| 2 | Tetracosanal | 352 | C24H48O | 057866-08-7 | 68 |
| 3 | Bicyclo[4.1.0]heptane, 7-butyl- | 152 | C11H20 | 018645-10-8 | 60 |
| 4 | Oxirane, heptadecyl- | 282 | C19H38O | 067860-04-2 | 58 |
| 5 | 15-Octadecenal | 266 | C18H34O | 056554-93-9 | 58 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

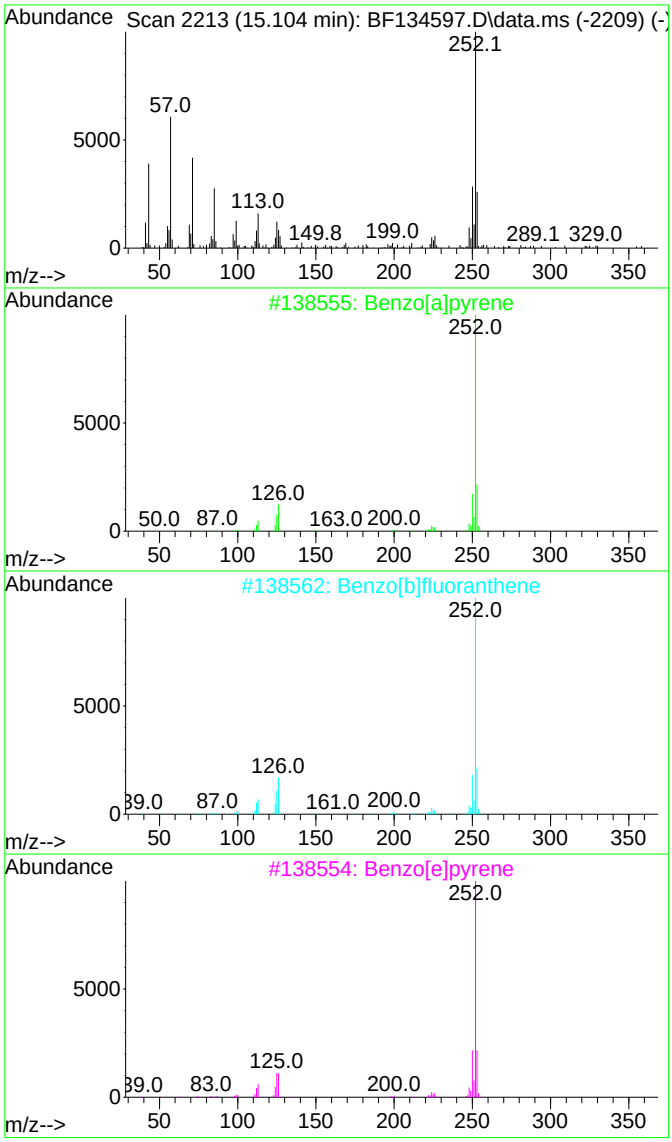
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

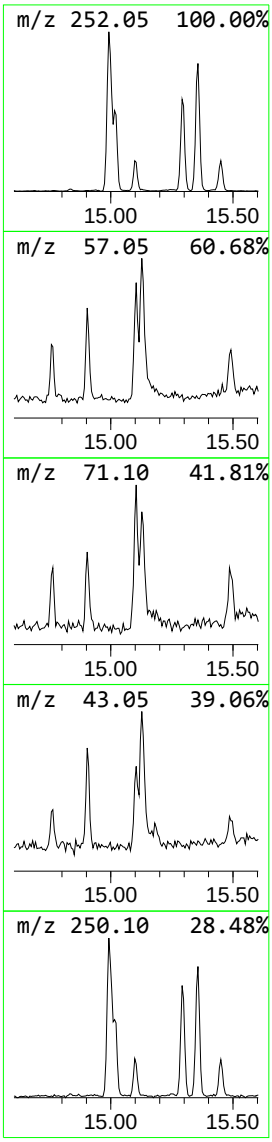
**********

Peak Number 5 Benzo[e]pyrene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.104 | 3.33 ng | 113387 | Perylene-d12 | 15.421 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 87 |
| 2 | Benzo[b]fluoranthene | 252 | C20H12 | 000205-99-2 | 76 |
| 3 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 76 |
| 4 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 58 |
| 5 | Perylene | 252 | C20H12 | 000198-55-0 | 55 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

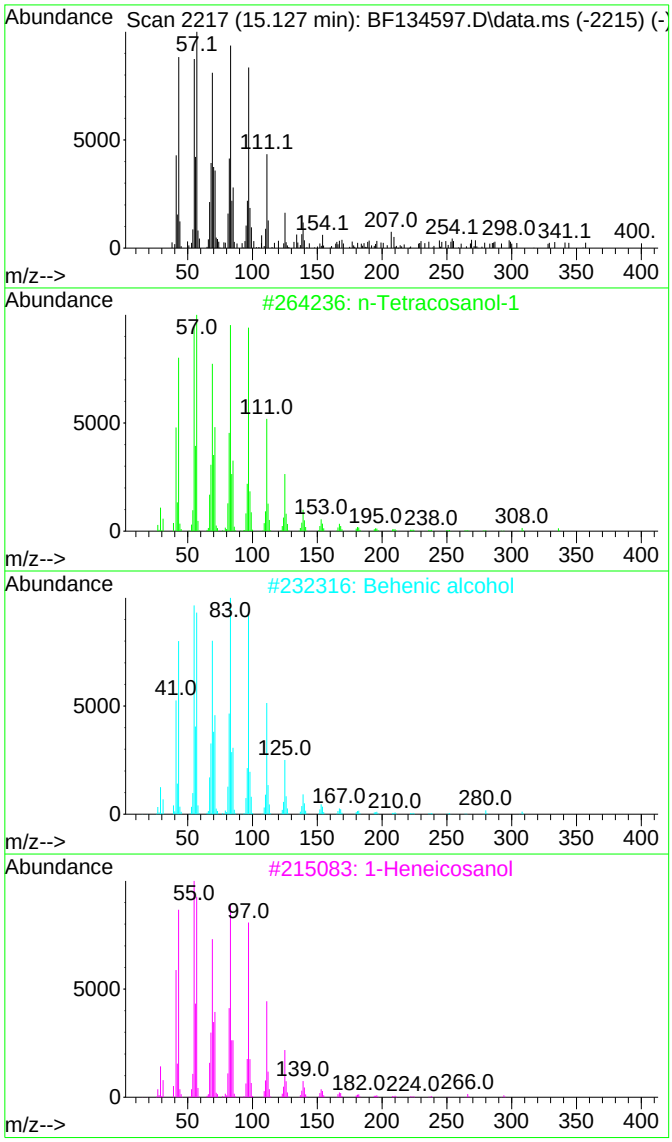
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

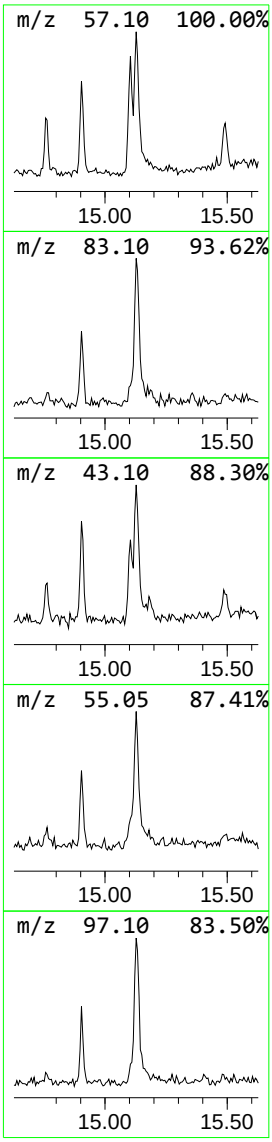
**********

Peak Number 6 n-Tetracosanol-1 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.127 | 4.58 ng | 155664 | Perylene-d12 | 15.421 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 94 |
| 2 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 94 |
| 3 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 4 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 91 |
| 5 | Eicosyl methyl ether | 312 | C21H44O | 1000406-29-4 | 91 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

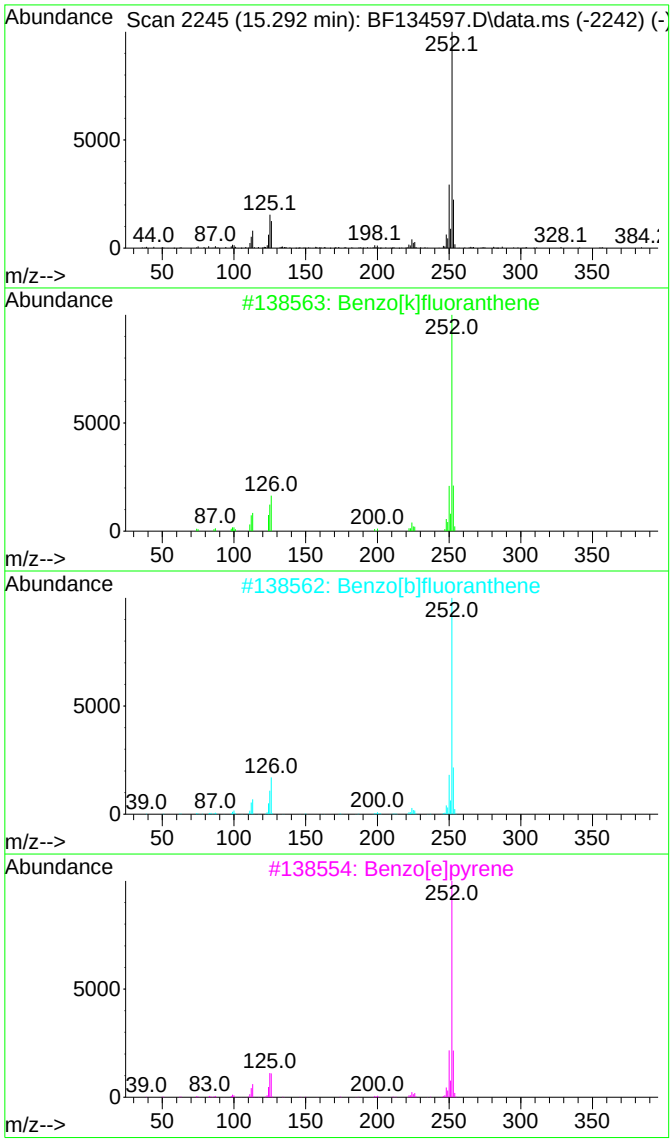
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

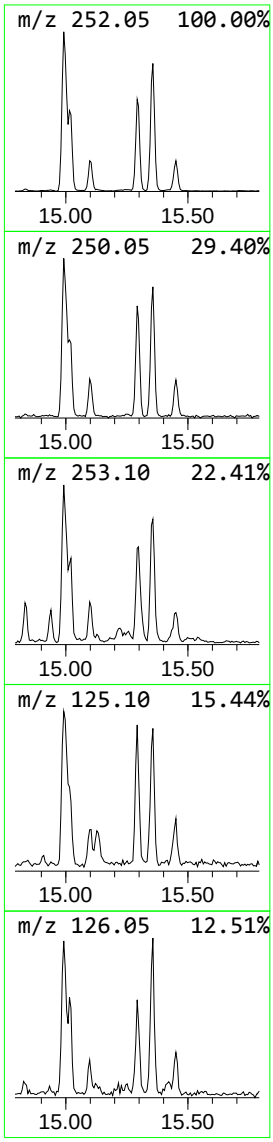
**********

Peak Number 7 Perylene Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.292 | 5.05 ng | 171805 | Perylene-d12 | 15.421 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 99 |
| 2 | Benzo[b]fluoranthene | 252 | C20H12 | 000205-99-2 | 98 |
| 3 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 98 |
| 4 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 93 |
| 5 | Perylene | 252 | C20H12 | 000198-55-0 | 93 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080223\
Data File : BF134597.D
Acq On : 03 Aug 2023 00:23
Operator : CG\JU
Sample : 03598-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
RB-55-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.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 ... | 11.851 | 4.8 | ng | 262533 | 4 | 11.310 | 1087070 | 20.0 |
| 1-Heneicosanol | 13.815 | 5.3 | ng | 323773 | 5 | 13.957 | 1226450 | 20.0 |
| Octacosyl trifl... | 14.457 | 2.5 | ng | 153393 | 5 | 13.957 | 1226450 | 20.0 |
| 16-Heptadecenal | 14.904 | 3.3 | ng | 113317 | 6 | 15.421 | 680112 | 20.0 |
| Benzo[e]pyrene | 15.104 | 3.3 | ng | 113387 | 6 | 15.421 | 680112 | 20.0 |
| n-Tetracosanol-1 | 15.127 | 4.6 | ng | 155664 | 6 | 15.421 | 680112 | 20.0 |
| Perylene | 15.292 | 5.0 | ng | 171805 | 6 | 15.421 | 680112 | 20.0 |