Supporting Information for:

**Synthesis of the C₃ and C₁ Constitutional Isomers of Trifluorosubphthalocyanine and their Fluorescence within MDA-MB-231 Breast Tumor Cells**

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Figure S1. – HR APCI-MS F3SPc(C3).

| Sample Name | Instrument Name | Instrument Type | Instrument Method | Instrument Setting | Instrument Condition | Instrument Time | Instrument Date |
|-------------|-----------------|-----------------|-------------------|--------------------|----------------------|----------------|----------------|
|             |                  |                 |                   |                    | x10.5                |                |                |
|             |                  |                 |                   |                    | 8.5                  |                |                |
|             |                  |                 |                   |                    | 8.25                 |                |                |
|             |                  |                 |                   |                    | 8                    |                |                |
|             |                  |                 |                   |                    | 7.75                 |                |                |
|             |                  |                 |                   |                    | 8                    |                |                |
|             |                  |                 |                   |                    | 7.25                 |                |                |
|             |                  |                 |                   |                    | 7                    |                |                |
|             |                  |                 |                   |                    | 6.75                 |                |                |
|             |                  |                 |                   |                    | 6.3                  |                |                |
|             |                  |                 |                   |                    | 5.9                  |                |                |
|             |                  |                 |                   |                    | 5.5                  |                |                |
|             |                  |                 |                   |                    | 5.1                  |                |                |
|             |                  |                 |                   |                    | 4.8                  |                |                |
|             |                  |                 |                   |                    | 4.5                  |                |                |
|             |                  |                 |                   |                    | 4.25                 |                |                |
|             |                  |                 |                   |                    | 3.75                 |                |                |
|             |                  |                 |                   |                    | 3.5                  |                |                |
|             |                  |                 |                   |                    | 3.25                 |                |                |
|             |                  |                 |                   |                    | 3                    |                |                |
|             |                  |                 |                   |                    | 2.75                 |                |                |
|             |                  |                 |                   |                    | 2.5                  |                |                |
|             |                  |                 |                   |                    | 2                    |                |                |
|             |                  |                 |                   |                    | 1.75                 |                |                |
|             |                  |                 |                   |                    | 1.5                  |                |                |
|             |                  |                 |                   |                    | 1.25                 |                |                |
|             |                  |                 |                   |                    | 1                    |                |                |
|             |                  |                 |                   |                    | 0.75                 |                |                |
|             |                  |                 |                   |                    | 0.5                  |                |                |
|             |                  |                 |                   |                    | 0.25                 |                |                |

Counts vs. Mass-to-Charge (m/z)

Figure S2. – HR APCI-MS F3SPc(C1).

| Sample Name | Instrument Name | Instrument Type | Instrument Method | Instrument Setting | Instrument Condition | Instrument Time | Instrument Date |
|-------------|-----------------|-----------------|-------------------|--------------------|----------------------|----------------|----------------|
|             |                  |                 |                   |                    | x10.5                |                |                |
|             |                  |                 |                   |                    | 10.5                 |                |                |
|             |                  |                 |                   |                    | 10.0                 |                |                |
|             |                  |                 |                   |                    | 10.5                 |                |                |
|             |                  |                 |                   |                    | 10.0                 |                |                |
|             |                  |                 |                   |                    | 9.5                  |                |                |
|             |                  |                 |                   |                    | 9.5                  |                |                |
|             |                  |                 |                   |                    | 9.0                  |                |                |
|             |                  |                 |                   |                    | 9.0                  |                |                |
|             |                  |                 |                   |                    | 8.5                  |                |                |
|             |                  |                 |                   |                    | 8.5                  |                |                |
|             |                  |                 |                   |                    | 8.0                  |                |                |
|             |                  |                 |                   |                    | 8.0                  |                |                |
|             |                  |                 |                   |                    | 7.5                  |                |                |
|             |                  |                 |                   |                    | 7.5                  |                |                |
|             |                  |                 |                   |                    | 7.0                  |                |                |
|             |                  |                 |                   |                    | 7.0                  |                |                |
|             |                  |                 |                   |                    | 6.5                  |                |                |
|             |                  |                 |                   |                    | 6.5                  |                |                |
|             |                  |                 |                   |                    | 6.0                  |                |                |
|             |                  |                 |                   |                    | 6.0                  |                |                |
|             |                  |                 |                   |                    | 5.5                  |                |                |
|             |                  |                 |                   |                    | 5.5                  |                |                |
|             |                  |                 |                   |                    | 5.0                  |                |                |
|             |                  |                 |                   |                    | 5.0                  |                |                |
|             |                  |                 |                   |                    | 4.5                  |                |                |
|             |                  |                 |                   |                    | 4.5                  |                |                |
|             |                  |                 |                   |                    | 4.0                  |                |                |
|             |                  |                 |                   |                    | 4.0                  |                |                |
|             |                  |                 |                   |                    | 3.5                  |                |                |
|             |                  |                 |                   |                    | 3.5                  |                |                |
|             |                  |                 |                   |                    | 3.0                  |                |                |
|             |                  |                 |                   |                    | 3.0                  |                |                |
|             |                  |                 |                   |                    | 2.5                  |                |                |
|             |                  |                 |                   |                    | 2.5                  |                |                |
|             |                  |                 |                   |                    | 2.0                  |                |                |
|             |                  |                 |                   |                    | 2.0                  |                |                |
|             |                  |                 |                   |                    | 1.5                  |                |                |
|             |                  |                 |                   |                    | 1.5                  |                |                |
|             |                  |                 |                   |                    | 1.0                  |                |                |
|             |                  |                 |                   |                    | 1.0                  |                |                |
|             |                  |                 |                   |                    | 0.5                  |                |                |
|             |                  |                 |                   |                    | 0.5                  |                |                |

Counts vs. Mass-to-Charge (m/z)
Figure S3. – Aromatic $^1$H NMR FeSPc(C₃).

Figure S4. – Aromatic $^1$H NMR FeSPc(C₄).
Figure S5. $^{19}$F NMR F$_3$SPc(C$_3$).

Figure S6. $^{19}$F NMR F$_3$SPc(C$_1$).
Purity results peak 1 at 11.025 min.

Signal DAD1 B, Sig=550,16 Ref-off (RC\RC-1-4-2MDCDL02.D)

-> The purity factor is within the calculated threshold limit. <=

Purity factor : 999.985 (62 of 62 spectra are within the calculated threshold limit.)
Threshold : 999.961 (Calculated with 62 of 62 spectra)
Reference : Peak start and end spectra (integrated) (10.703 / 12.283)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 0.018 (12 spectra, St.Dev 0.009 + 3 * 0.003)

*** End of Report ***

Figure S7. – HPLC purity report FsSPc(C).
Purity results peak 1 at 10.708 min.

Signal DAD1 B, Sig=550,16 Ref=off (RC\RC-1-4-2NDCOL03.D)

-> The purity factor is within the calculated threshold limit. <-

Purity factor : 999.984 (106 of 106 spectra are within the calculated threshold limit.)
Threshold : 999.936 (Calculated with 106 of 106 spectra)
Reference : Peak start and end spectra (integrated) (10.384 / 12.418)
Spectra : 5 (Selection automatic, 5)
Noise Threshold : 0.024 (12 spectra, St.Dev 0.0111 + 3 * 0.0043)

*** End of Report ***

Figure S8. – HPLC purity report for F3SPc(C).