

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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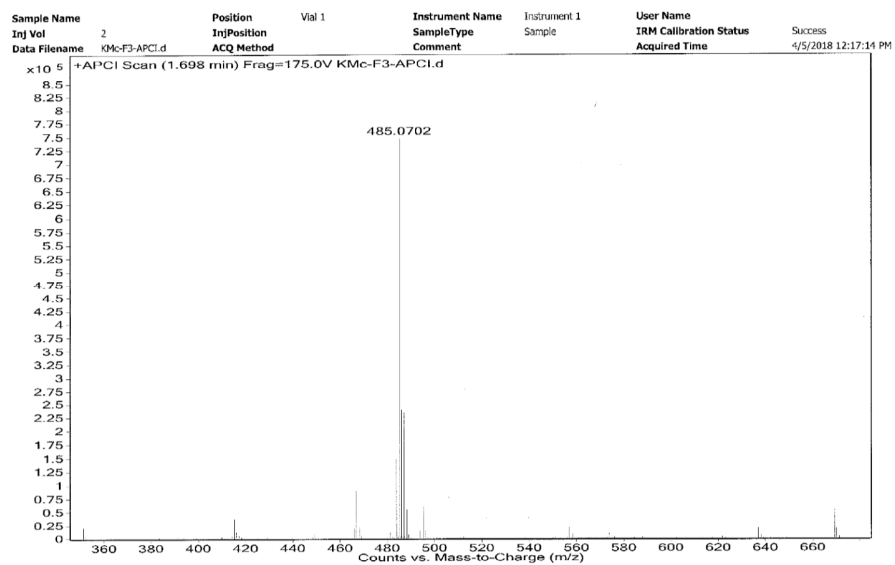


Figure S1. – HR APCI-MS F₃SPc(C₃).

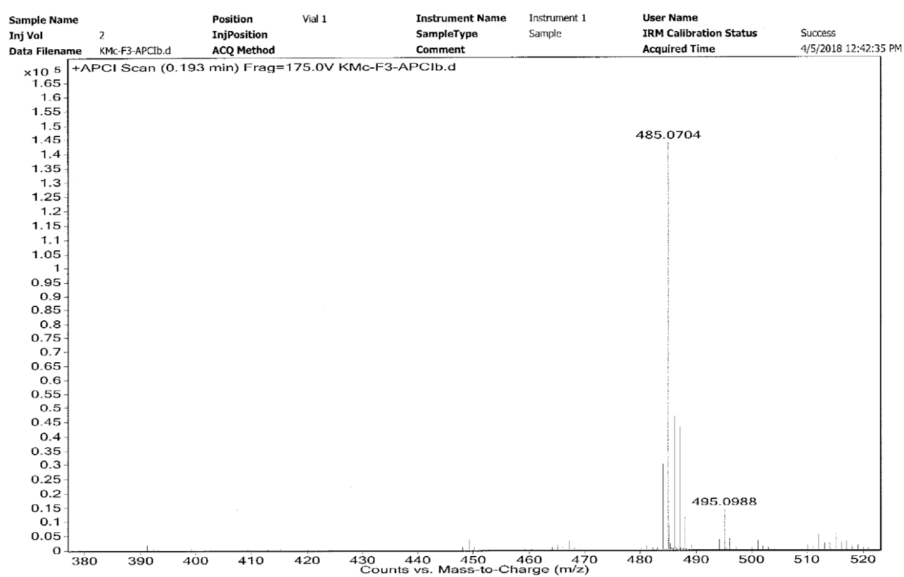


Figure S2. – HR APCI-MS F₃SPc(C₁).

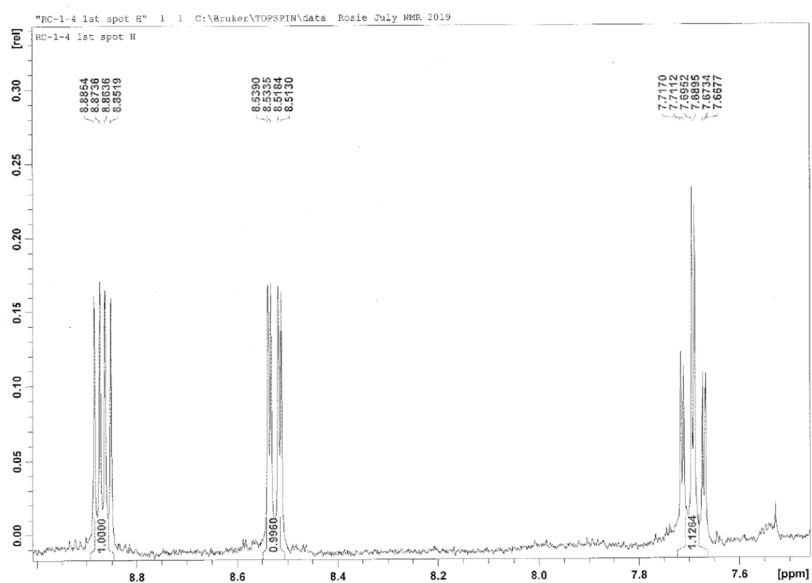


Figure S3. – Aromatic ^1H NMR $\text{F}_3\text{SPc}(\text{C}_3)$.

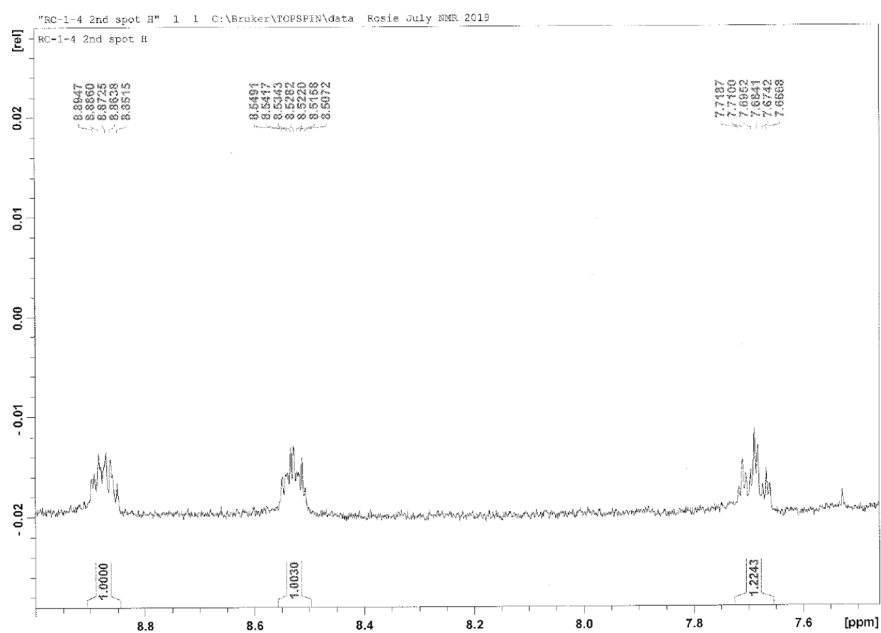


Figure S4. – Aromatic ^1H NMR $\text{F}_3\text{SPc}(\text{C}_1)$.

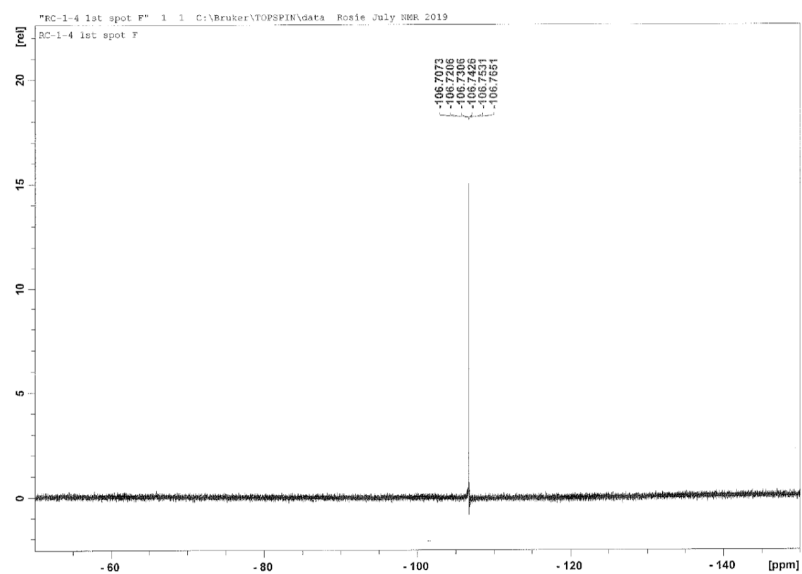


Figure S5. – ^{19}F NMR $\text{F}_3\text{SPc}(\text{C}_3)$.

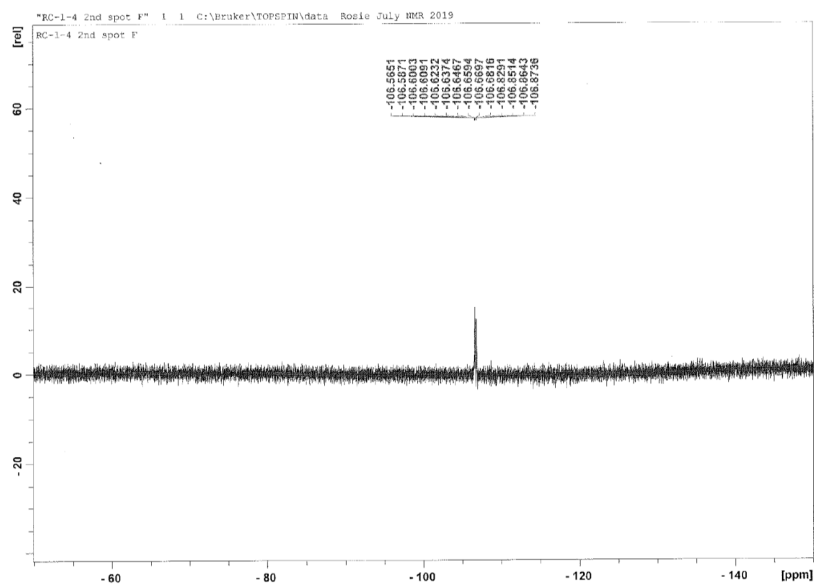
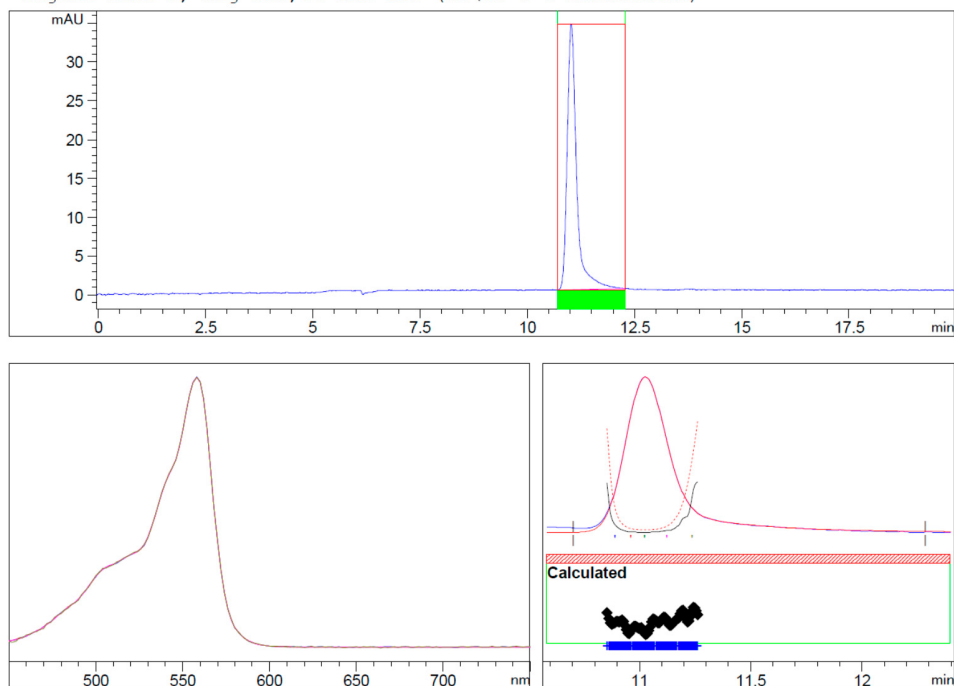


Figure S6. – ^{19}F NMR $\text{F}_3\text{SPc}(\text{C}_1)$.

Purity results peak 1 at 11.025 min.

Signal DAD1 B, Sig=550,16 Ref=off (RC\RC-1-4-2NDCOL02.D)



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

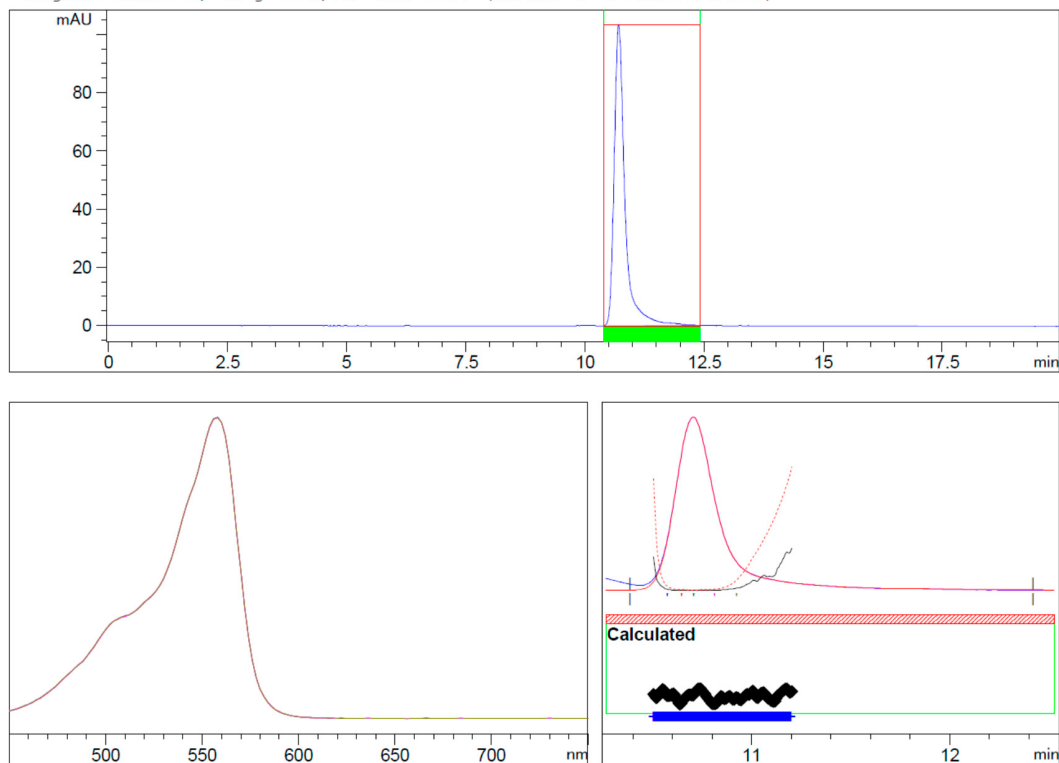
Purity factor : 999.985 (62 of 62 spectra are within the calculated threshold limit.)
Threshold : 999.961 (Calculated with 62 of 62 spectra)
Reference : Peak start and end spectra (integrated) (10.703 / 12.283)
Spectra : 5 (Selection automatic, 5)
Noise Threshold: 0.018 (12 spectra, St.Dev 0.009 + 3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

*** End of Report ***

Figure S7. – HPLC purity report F₃SPc(C₃).

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(C₁).