

Supplementary information

Mitochondria-Targeted Aggregation Induced Emission Theranostics:

Crucial Importance of In Situ Activation

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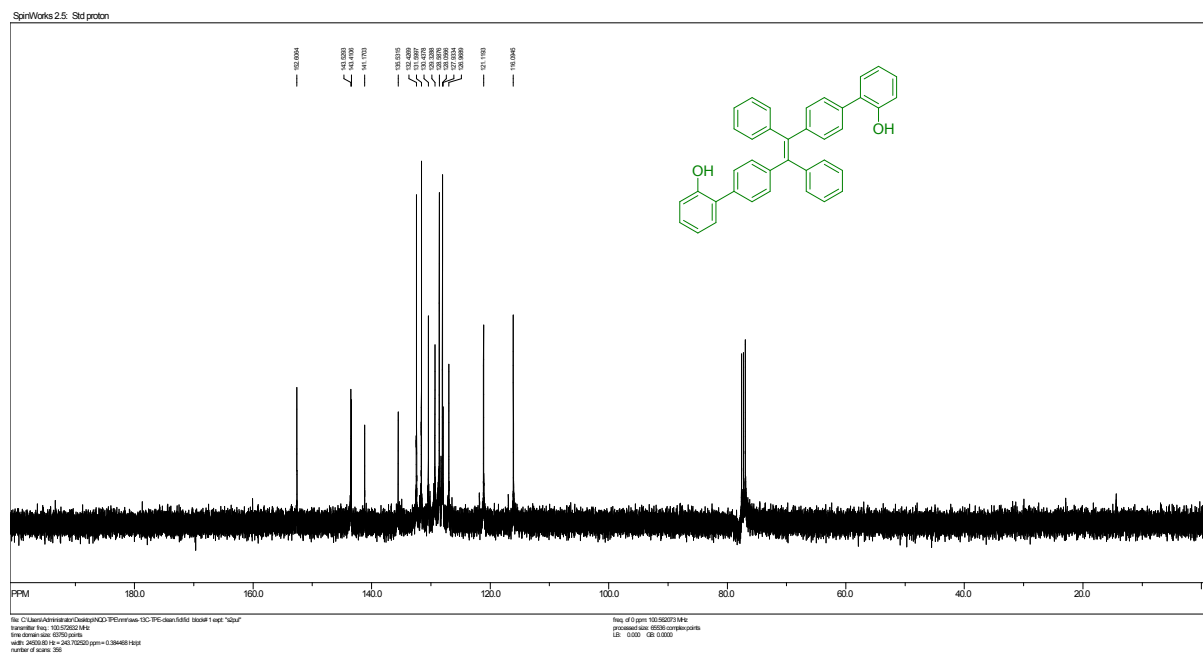


Figure S1: ^1H and ^{13}C NMR of **3**.

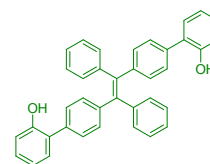
<Spectrum>

Line#:1 R.Time:0.500(Scan#:61)

MassPeaks:801

RawMode:Averaged 0.383-0.700(47-85) BasePeak:539.2500(192992)

BG Mode:None Segment 1 - Event 1



Exact Mass: 516.21

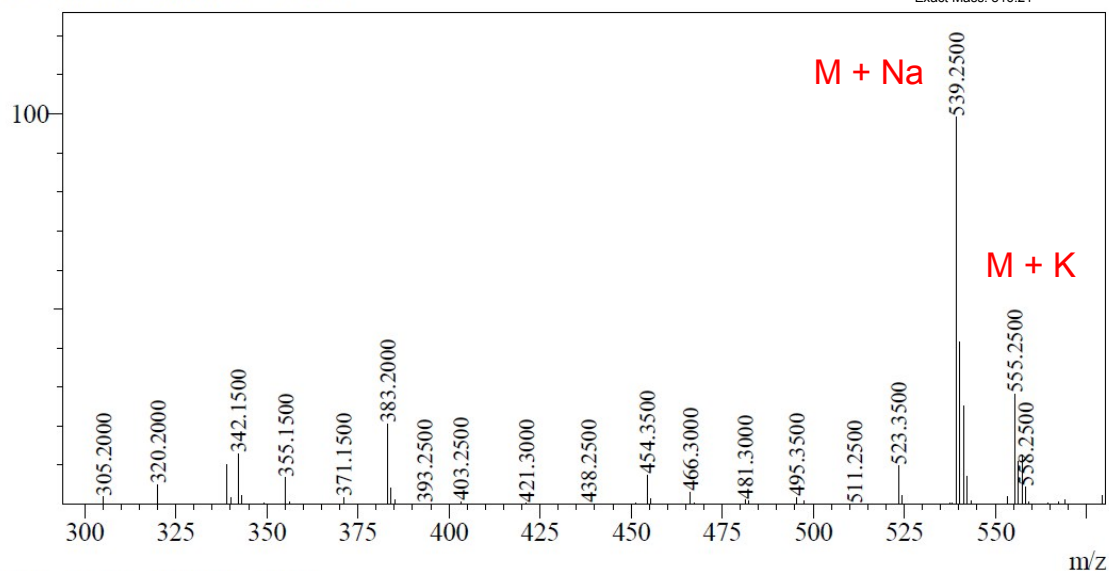


Figure S6: MS data of 3.

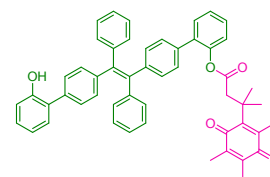
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Line#:1 R.Time:0.883(Scan#:107)

MassPeaks:400

RawMode:Averaged 0.717-1.117(87-135) BasePeak:771.3000(40154)

BG Mode:None Segment 1 - Event 1



Exact Mass: 748.32

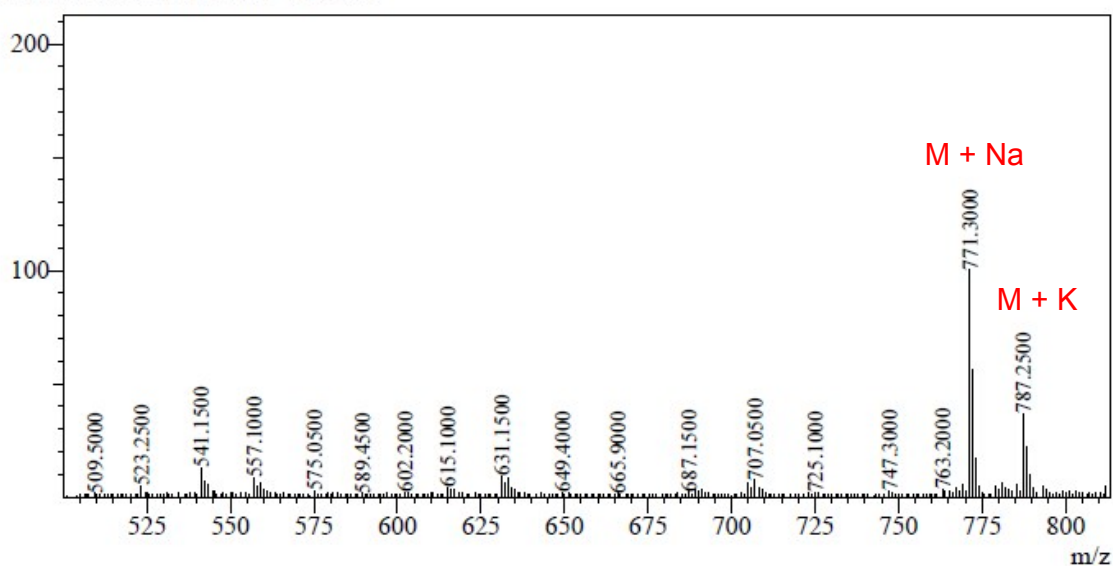


Figure S7: MS data of 2.

<Spectrum>

Line#:1 R.Time:0.500(Scan#:61)

MassPeaks:301

RawMode:Averaged 0.417-0.617(51-75) BasePeak:875.35(47008)

BG Mode:None Segment 1 - Event 1

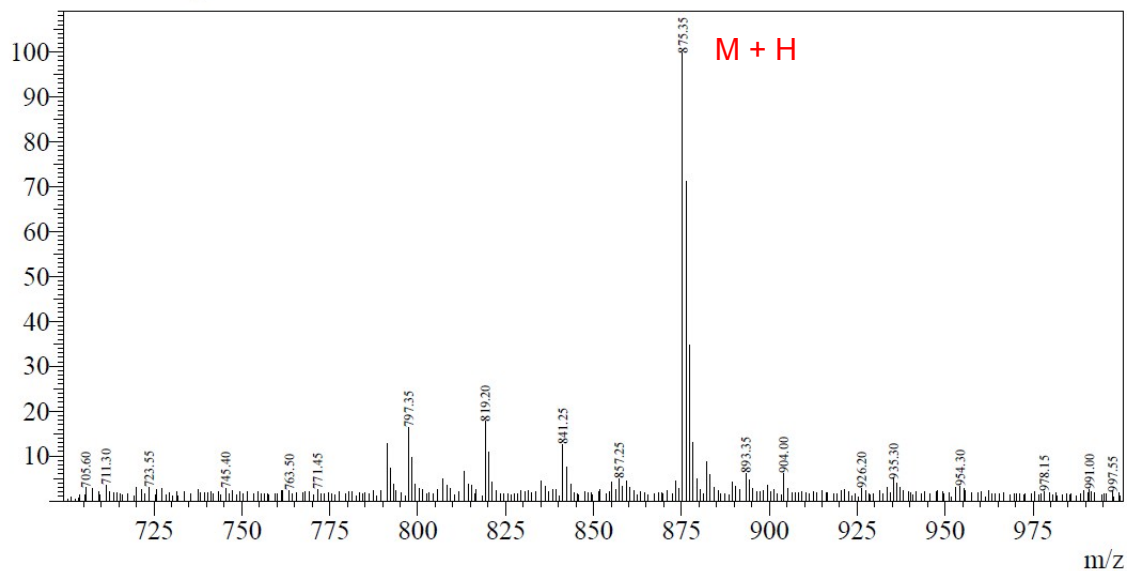
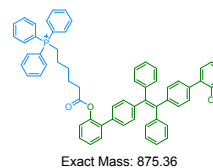


Figure S8: MS data of **8**.

<Spectrum>

Line#:1 R.Time:0.467(Scan#:57)

MassPeaks:523

RawMode:Single 0.467(57) BasePeak:777.20(255159)

BG Mode:None Segment 1 - Event 1

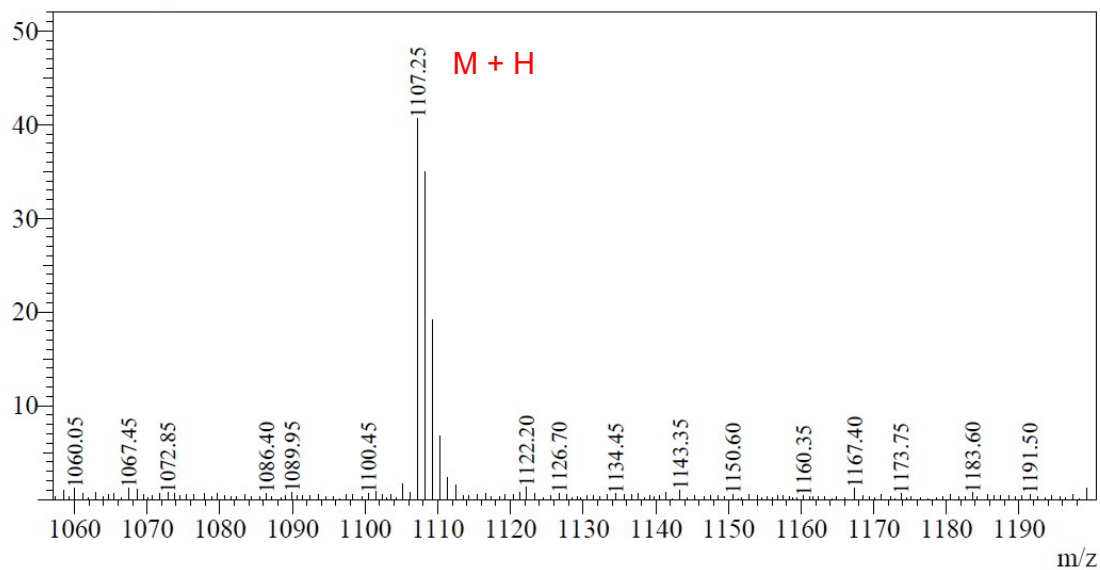
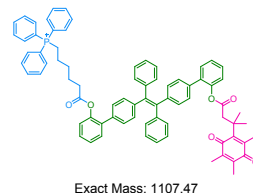


Figure S9: MS data of **1**.

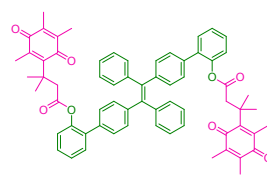
<Spectrum>

Line#:1 R.Time:0.933(Scan#:113)

MassPeaks:848

RawMode:Single 0.933(113) BasePeak:1019.3500(9902)

BG Mode:None Segment 1 - Event 1



Exact Mass: 980.43

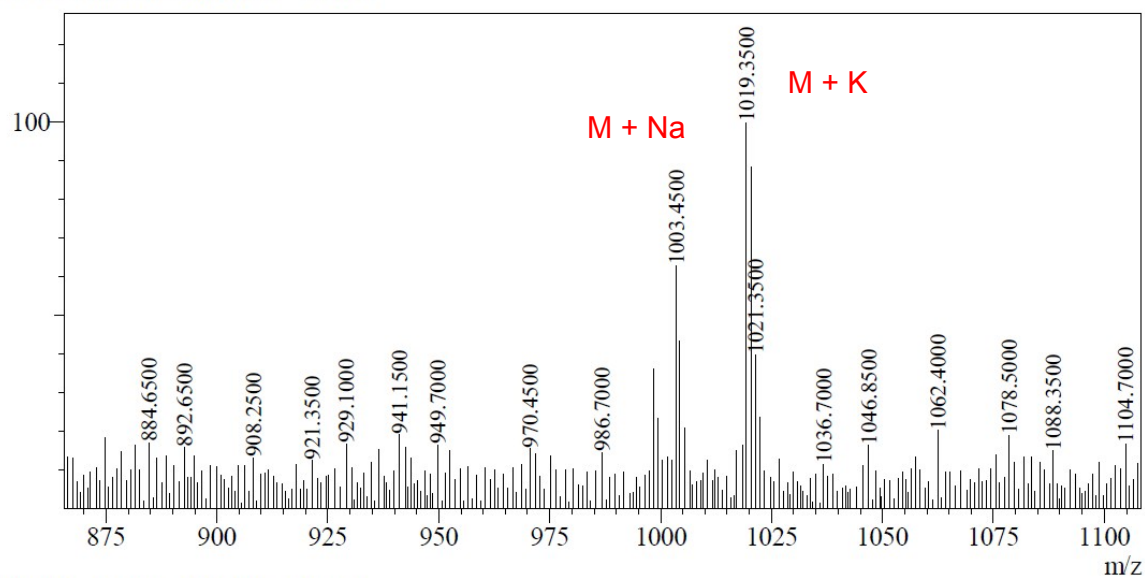


Figure S10: MS data of 9.

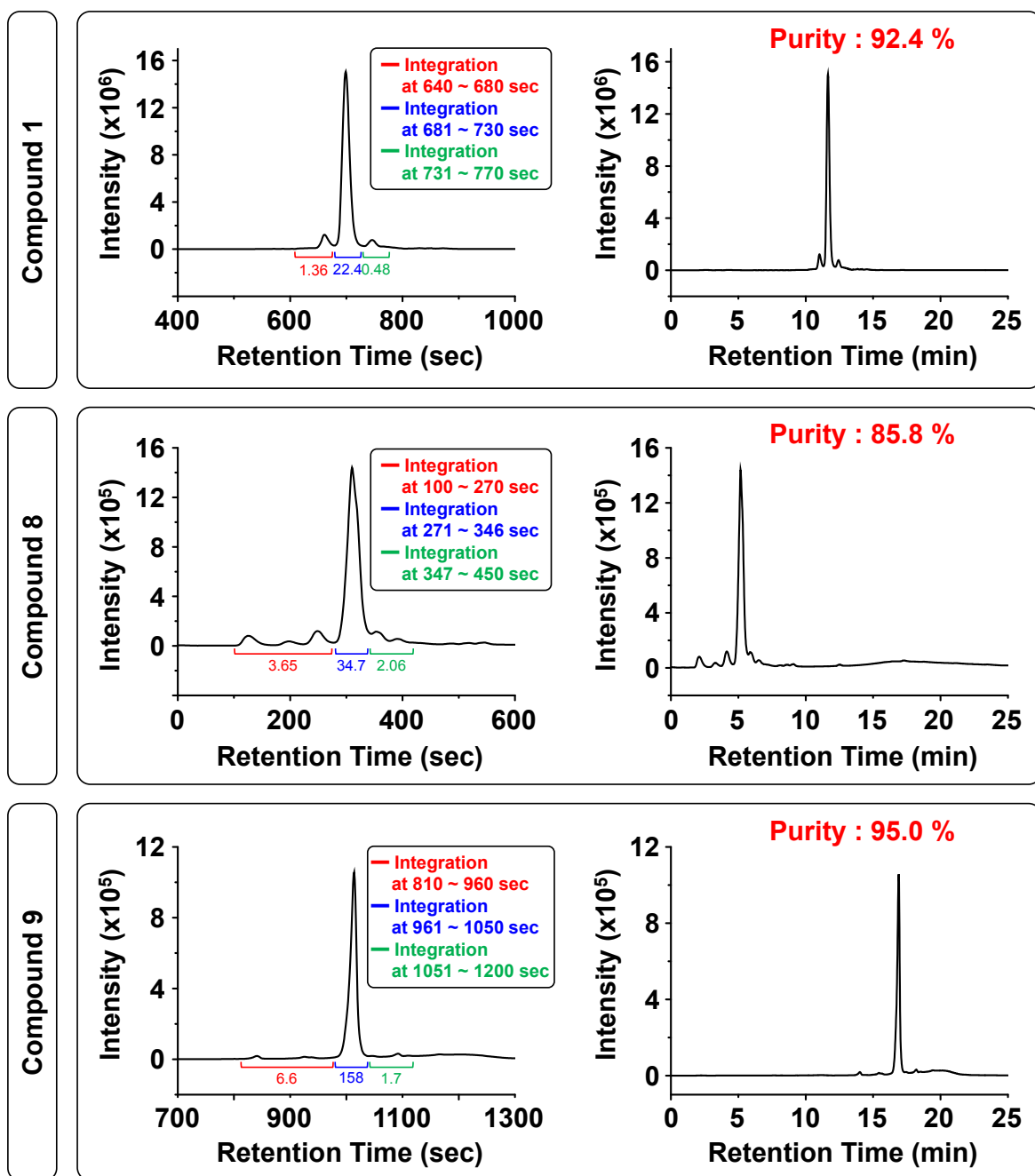


Figure S11: Purity determination of compounds **1**, **8** and **9** by HPLC (Wavelength: black 340 nm, gradient: 70 % B to 100 % B for 15 min, then 100% B during 10 min; A: Water, B: ACN).

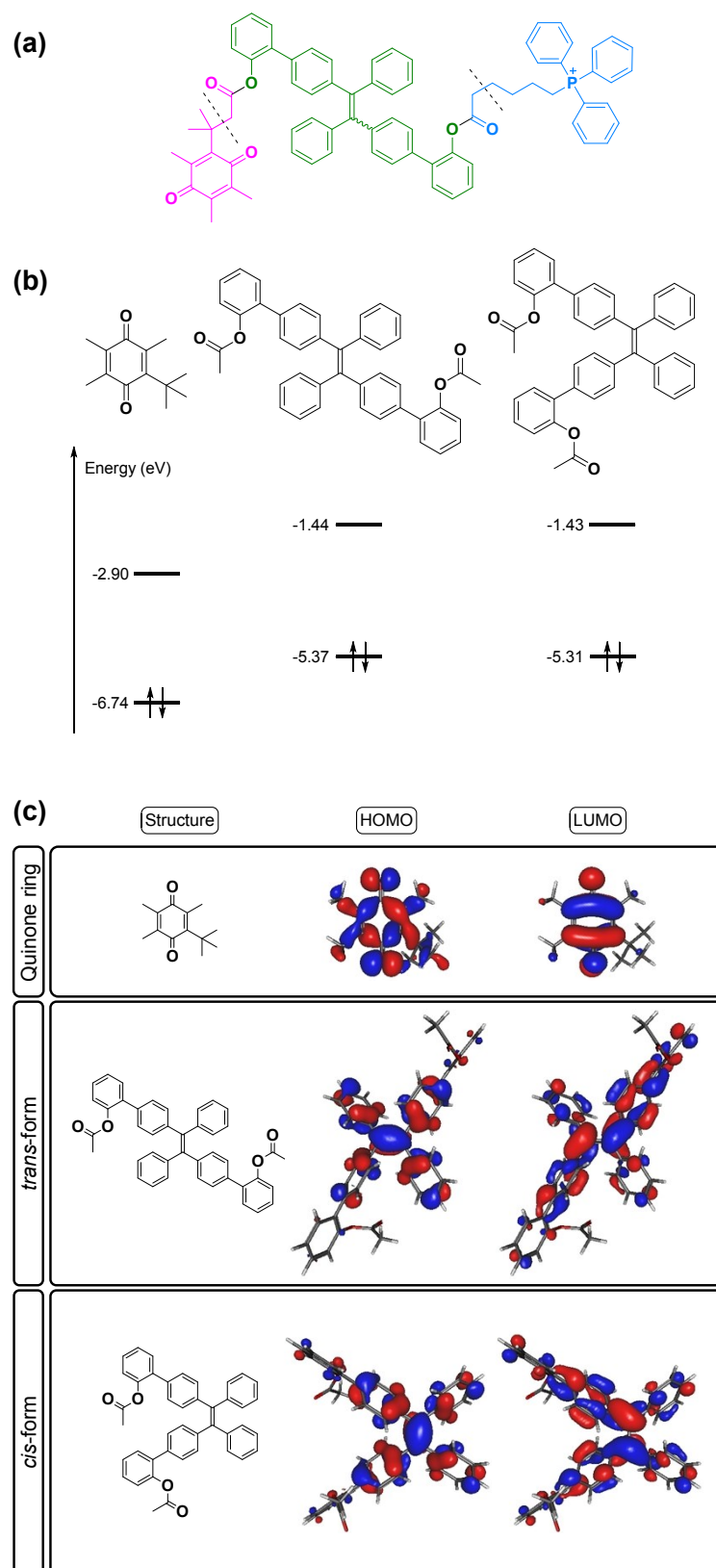


Figure S12. DFT theoretical calculations B3LYP at the 6-31G(d) level of theory. (a) The structure of **1** showing the truncation sites. (b) Energy diagram of the frontier orbitals of the trigger's quinone unit and the trans and cis substituted dyes. (c) The electron distributions of the frontier orbitals at the $0.03 \text{ e.}(\text{bohr})^{-3}$ isovalue.

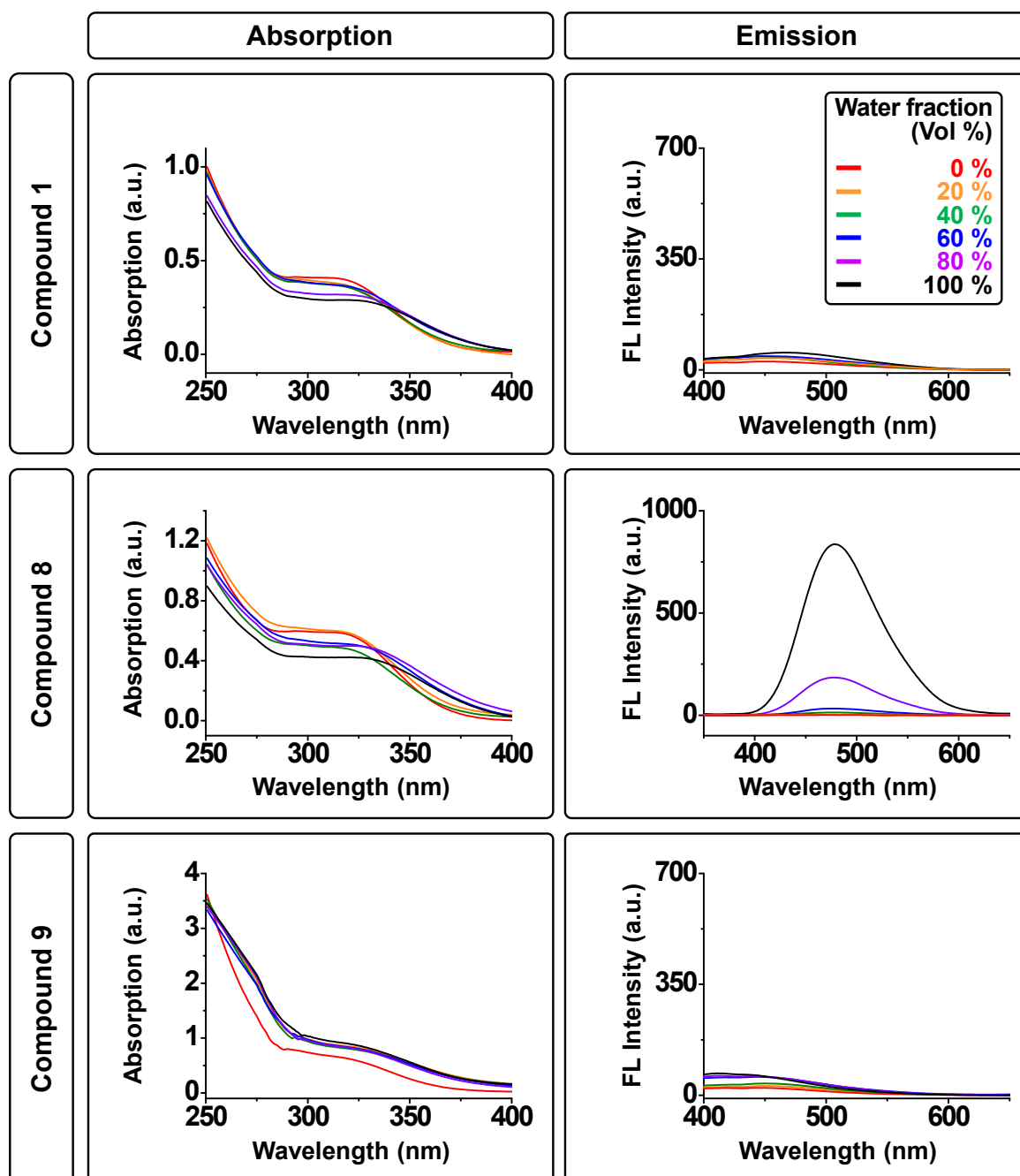
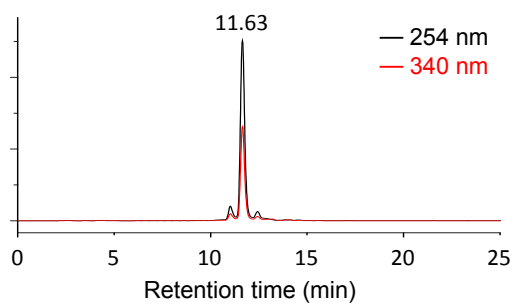
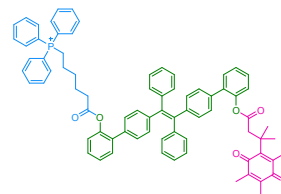


Figure S13: The dependence of water content (in methanol) on the AIE absorption of probe **1**, **8** and **9** (Concentration : 50 μ M, T = 24 $^{\circ}$ C). emission of probe **1**, **8** and **9** (concentration : 10 μ M, T = 24 $^{\circ}$ C, slit : 5/5 nm, sensitivity : high)

Before adding sodium dithionite



reduction



After adding sodium dithionite

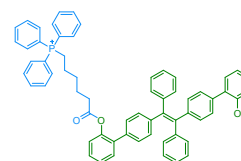
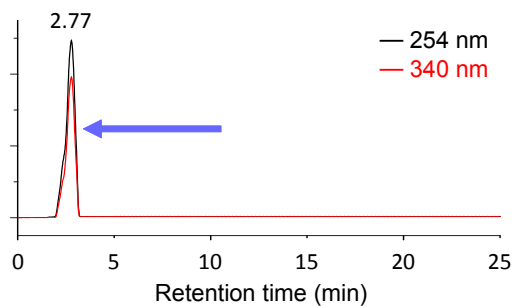


Figure S14: HPLC analysis of **1** upon the addition of sodium dithionite. (dual wavelength: black 254 nm, red 340 nm, gradient: 70 % B to 100 % B for 15 min, then 100% B during 10 min; A: Water, B: ACN).