

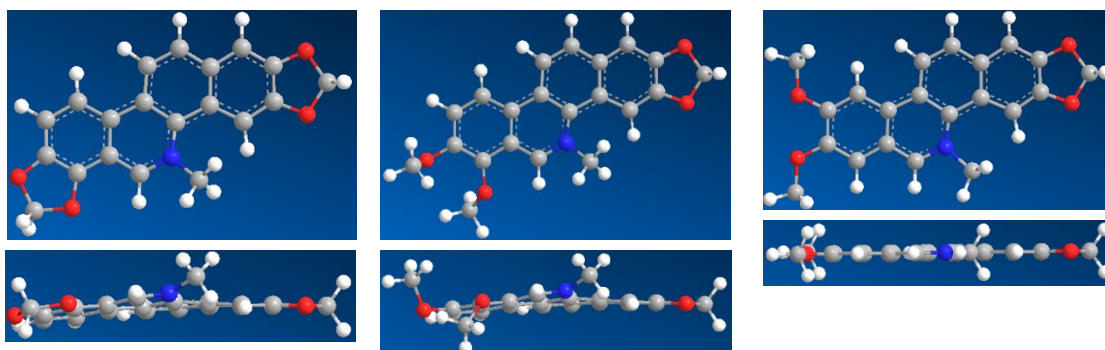
# Structuring polarity-inverted TBA to G- quadruplex for selective recognition of planarity of natural isoquinoline alkaloids

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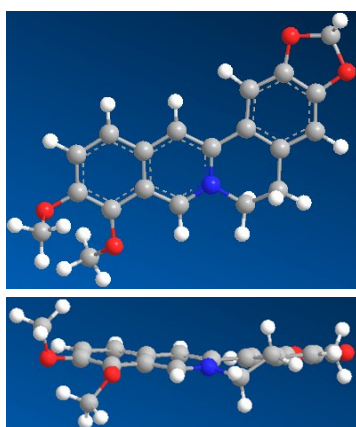
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SAN

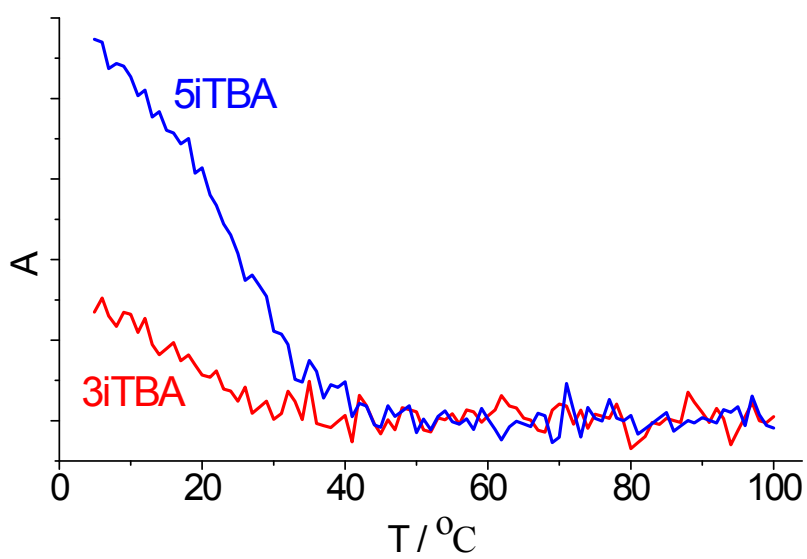
CHE

NIT

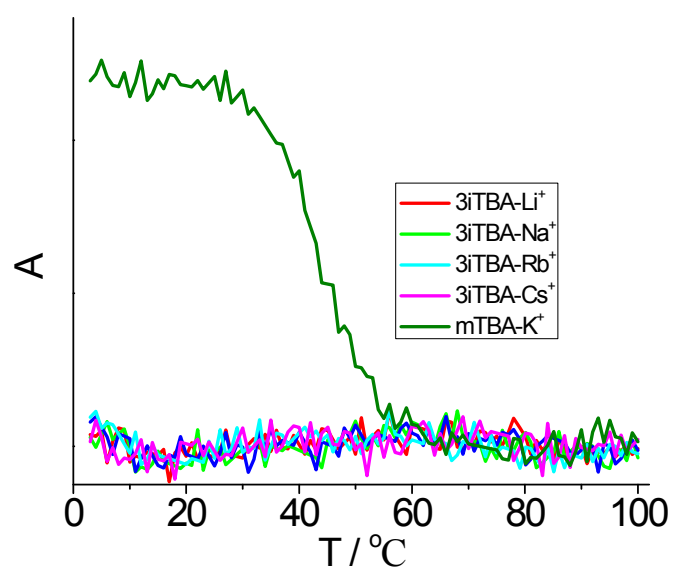


BER

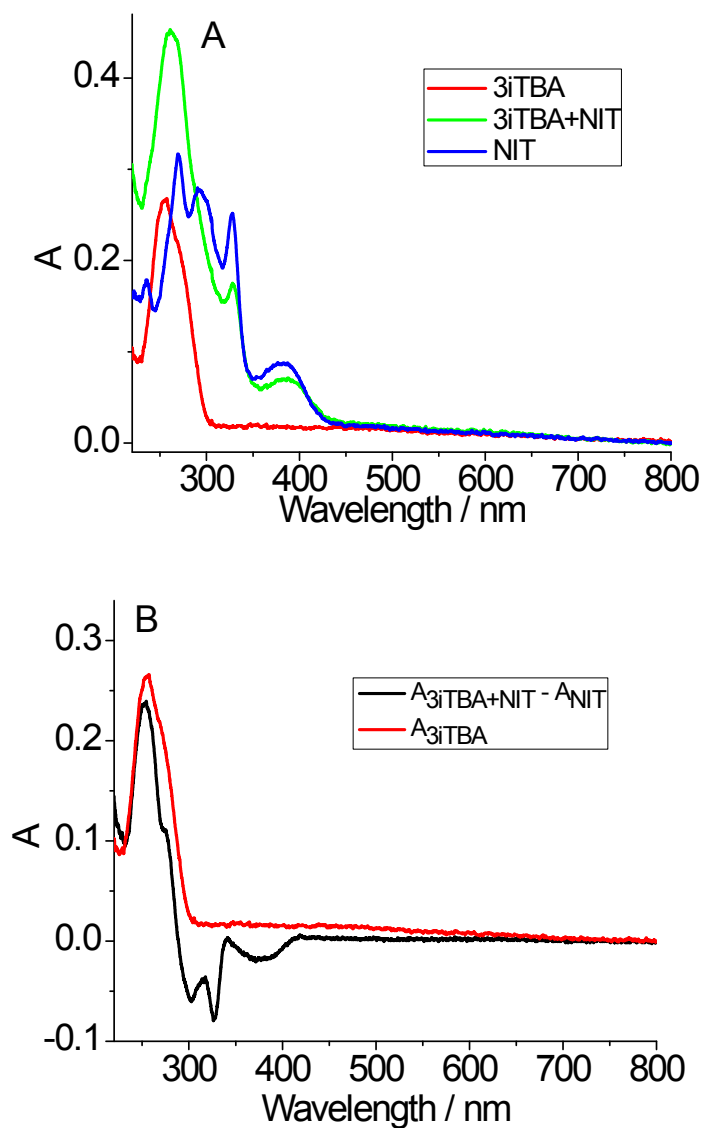
**Scheme S1.** Top-viewed (up) and side-viewed (down) structures of IAs. For PAs, only BER is presented because of the structure similarity to show the saturated ring B induced non-planarity.



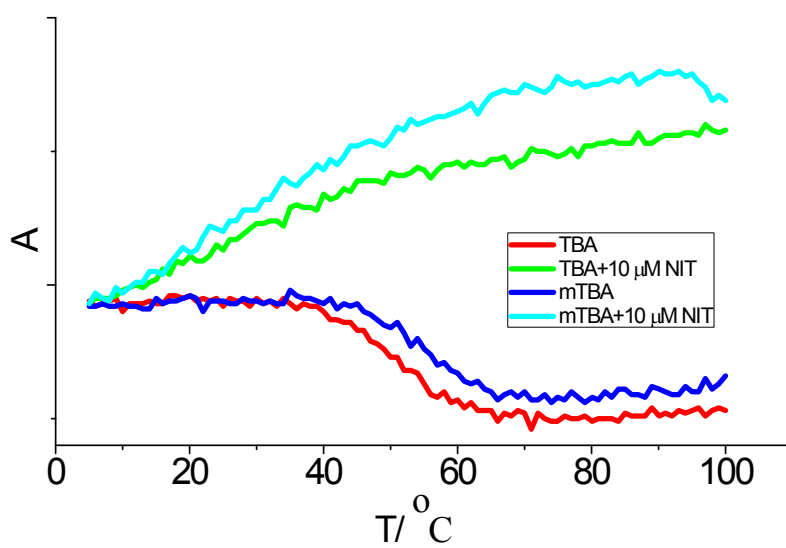
**Figure S1.** Melting curves of 3  $\mu$ M 3iTBA and 5iTBA in 0.05 M Tris-HCl buffer (pH 7.0) containing 0.1 M  $K^+$ .



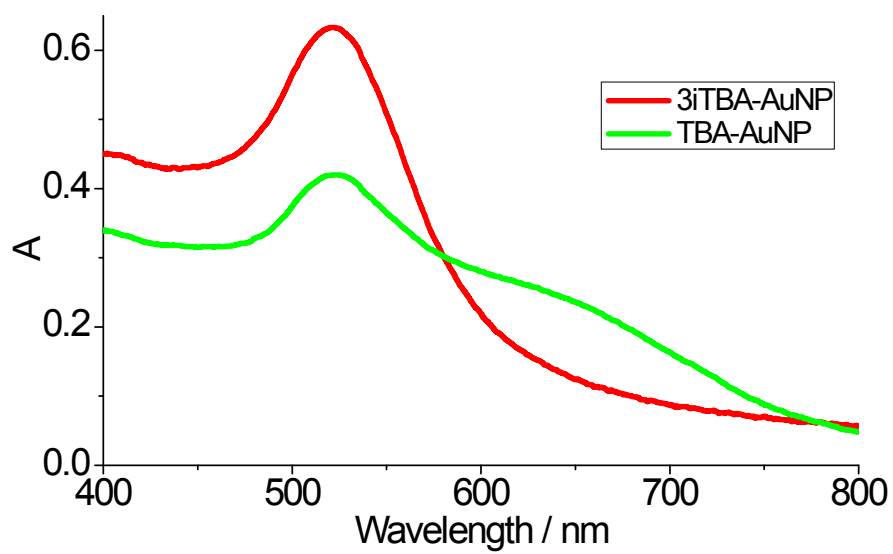
**Figure S2.** Melting curves of 3  $\mu\text{M}$  3iTBA in 0.05 M Tris-HCl buffer (pH 7.0) containing 0.1 M  $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{Rb}^+$ , and  $\text{Cs}^+$ , respectively. That of mTBA in  $\text{K}^+$  is also shown as a control.



**Figure S3.** (A) Absorption spectra of 3iTBA (2  $\mu$ M), NIT (10  $\mu$ M), and their mixture in 0.1 M PBS buffer (pH 7.0). (B) Absorption difference spectra of 3iTBA in the presence of NIT after subtracting that of NIT alone. Also shown is that of 3iTBA alone for a comparison to show the 3iTBA folding upon the NIT addition.



**Figure S4.** Melting curves of TBA and mTBA (3  $\mu\text{M}$ ) in the absence and presence of NIT (10  $\mu\text{M}$ ) in 0.1 M PBS buffer (pH 7.0,  $\text{K}^+$ ). The absorbance at the starting temperature of 3  $^{\circ}\text{C}$  was normalized for comparison.



**Figure S5.** Absorption spectra of AuNPs in PBS buffer (pH 7.0, 35 mM K<sup>+</sup>) containing 3iTBA and TBA, respectively.