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

Yufeng Zhou,† Yali Yu,† Longlong Gao,† Yifan Fei,† Ting Ye,† Qiusha Li,† Xiaoshun Zhou,† Ning Gan,§ and Yong Shao*†

†Institute of Physical Chemistry, College of Chemistry and Life Sciences, Zhejiang Normal University, Jinhua 321004, Zhejiang, China
†Faculty of Material Science and Chemical Engineering, Ningbo University, Ningbo 315211, Zhejiang, China
*E-mail: yshao@zjnu.cn (S. Y.). Fax: 86 579 82282595
Scheme S1. Top-viewed (up) ans 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 μM 3iTBA and 5iTBA in 0.05 M Tris-HCl buffer (pH 7.0) containing 0.1 M K⁺.
**Figure S2.** Melting curves of 3 μM 3iTBA in 0.05 M Tris-HCl buffer (pH 7.0) containing 0.1 M Li⁺, Na⁺, Rb⁺, and Cs⁺, respectively. That of mTBA in K⁺ is also shown as a control.
Figure S3. (A) Absorption spectra of 3iTBA (2 µM), NIT (10 µM), 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 μM) in the absence and presence of NIT (10 μM) in 0.1 M PBS buffer (pH 7.0, K+). The absorbance at the starting temperature of 3 °C was normalized for comparison.
**Figure S5.** Absorption spectra of AuNPs in PBS buffer (pH 7.0, 35 mM K\(^+\)) containing 3iTBA and TBA, respectively.