

AIE Dye Mono-Functionalized i-Motif Forming Nucleic Acids for pH-Responsive Fluorescence Probe

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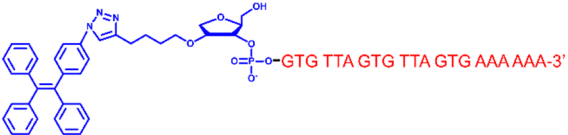
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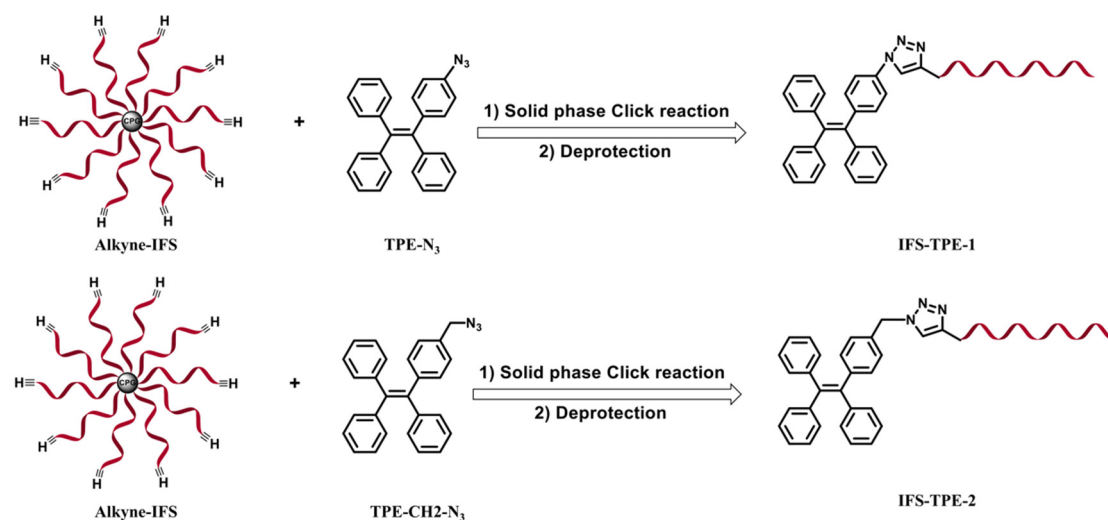
1. Synthesis of IFS-TPE-1 and IFS-TPE-2.

1.1 Synthesis of alkyne terminated DNA strands.

Table S1. DNA Sequences used in this work

Name	Sequence (from 5' to 3')
IFS	CCC TAA CCC TAA CCC TAA CCC
Functionalized IFS	alkyne-CCC TAA CCC TAA CCC TAA CCC
RS	GTG TTA GTG TTA GTG AAA AAA
Functionalized RS	alkyne-GTG TTA GTG TTA GTG AAA AAA
RS-TPE-1	

1.2 Synthesis of IFS-TPE-1 and IFS-TPE-2 through solid phase “click reaction”



Scheme S1. Solid-phase “click” chemistry approach for the synthesis of IFS-TPE-1 and IFS-TPE-2.

1.3 Purification of IFS-TPE-1 and IFS-TPE-2.

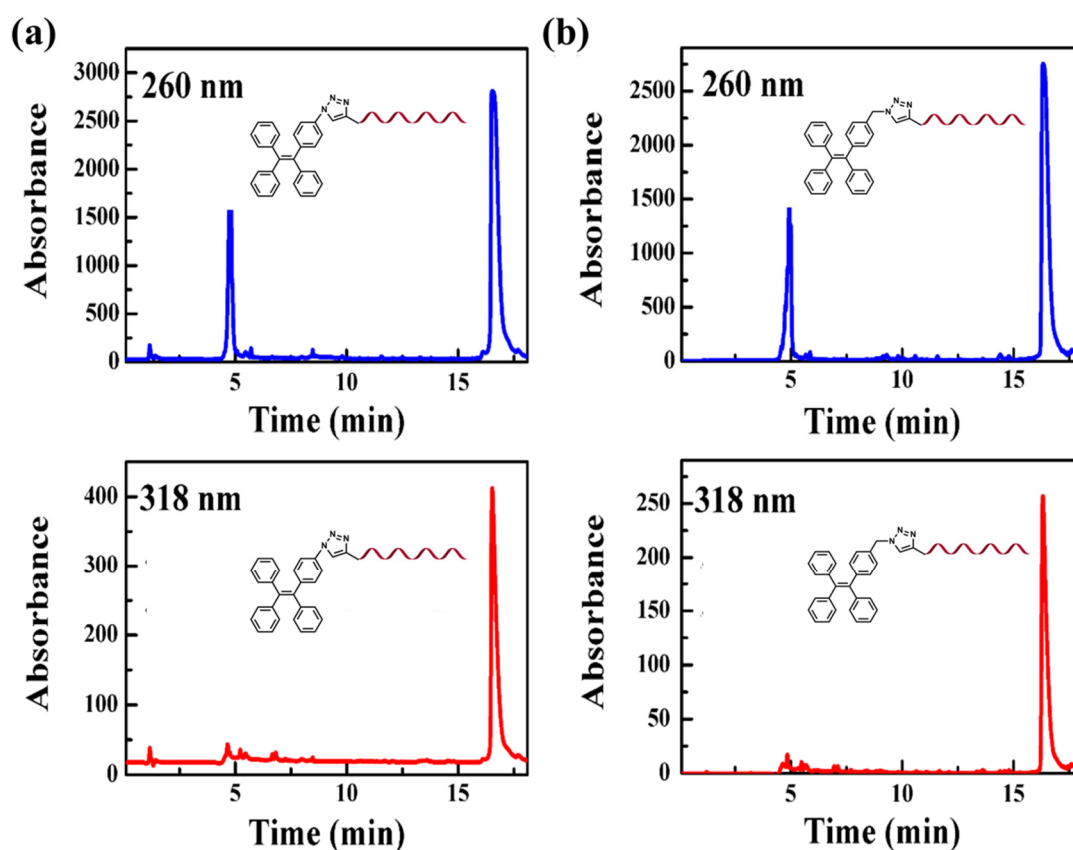


Figure S1. Reverse phase-HPLC analysis of IFS-TPE-1 (a) and IFS-TPE-2 (b) with absorbance at both 260 nm and 318 nm. Retention time of target molecule lies at 17.0 min.

1.4 MALDI-TOF characterization.

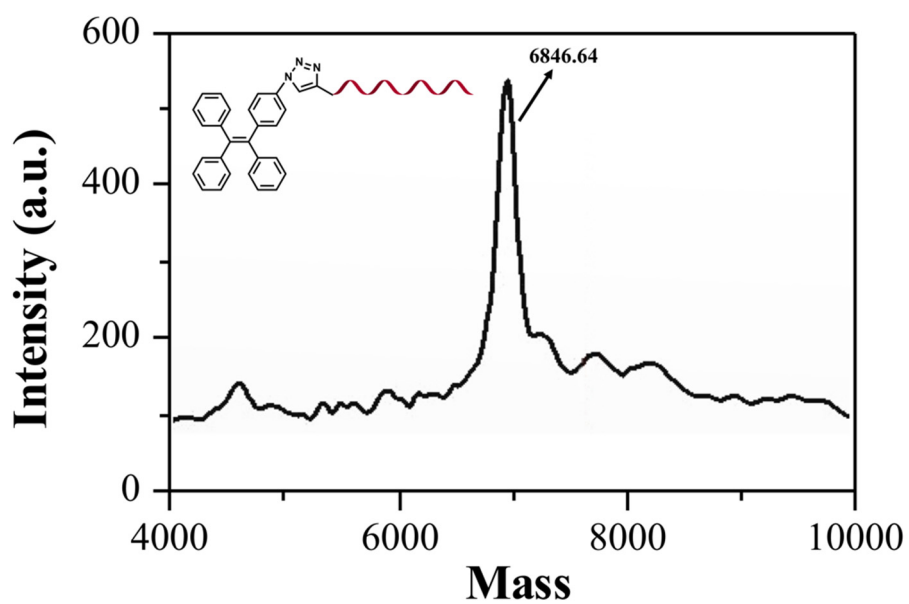


Figure S2. Chemical structure and MALDI-TOF spectrum of IFS-TPE-1 $m/z = 6846.64$ (6848.83 theoretically).

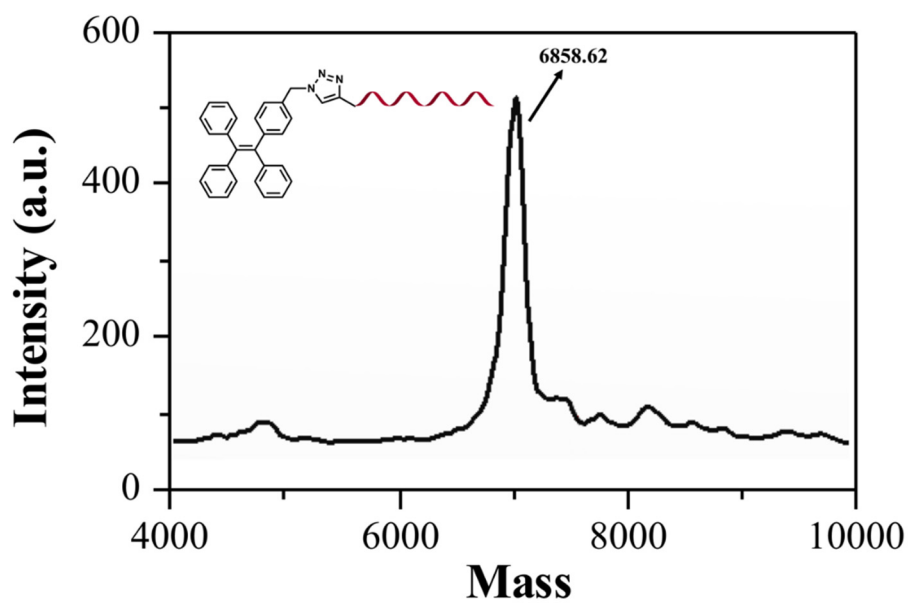


Figure S3. Chemical structure and MALDI-TOF spectrum of IFS-TPE-2 $m/z = 6858.62$ (6862.39 theoretically).

2. Absorption and CD characterizations.

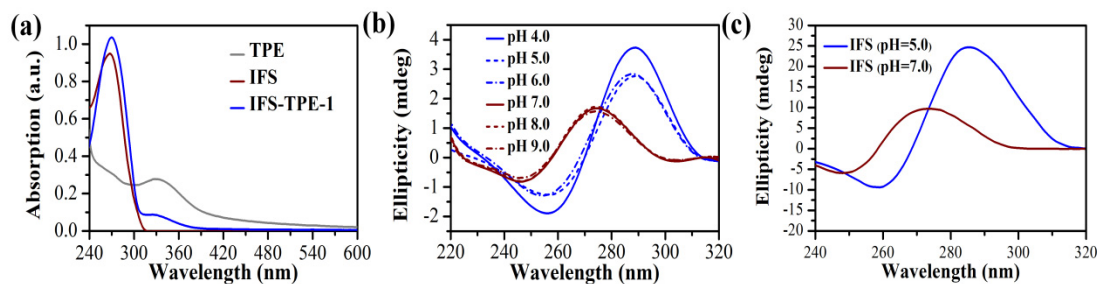


Figure S4. (a) The absorption spectra of TPE, IFS, and IFS-TPE-1. (b) The CD spectra of IFS-TPE-1 under different pH values. (c) The CD spectra of IFS strand at pH 7.0 and pH 5.0, respectively.

3. Gel electrophoresis analysis.

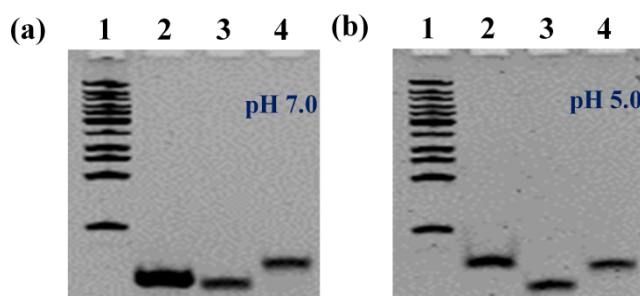


Figure S5. (a) and (b) The PAGE characterizations at pH 7.0 and pH 5.0, respectively; For both images: Lane 1: DNA marker; Lane 2: RS sequence; Lane 3: IFS sequence; Lane 4: IFS-TPE-1.

4. MTT assay.

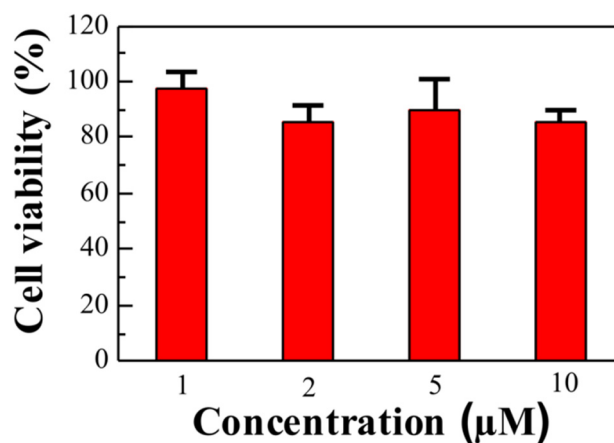


Figure S6. Cell viability (%) of HeLa cells treated with different concentrations of IFS-TPE-1 for 24 h by MTT assays. Data as mean values \pm SD ($n = 3$).