Electronic Supplementary Information

Distinct Optical and Kinetic Responses from E/Z Isomers of Caspase Probes with Aggregation-Induced Emission Characteristics

Jing Liang,†a Haibin Shi,†a Ryan T. K. Kwok, b Meng Gao, c Youyong Yuan, a Wenhua Zhang, c Ben Zhong Tang *bd and Bin Liu *ac

*a Department of Chemical and Biomolecular Engineering, 4 Engineering Drive 4, National University of Singapore, Singapore 117585

b Department of Chemistry, Division of Biomedical Engineering and Institute of Molecular Functional Materials, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China

c Institute of Materials Research and Engineering, 3 Research Link, Singapore 117602

d SCUT–HKUST Joint Research Laboratory, Guangdong Innovative Research Team, State Key Laboratory of Luminescent Materials and Devices, South China University of Technology, Guangzhou 510640, China

Corresponding author: cheliub@nus.edu.sg; tangbenz@ust.hk

†‡ These authors contributed equally to this work.
Fig. S1 (A) $^1$H and (B) $^{13}$C NMR spectra of TPE-2N$_3$ in CDCl$_3$. 

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A

18H, ph

4H, CH$_2$

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B

Chemical Shift (ppm)
**Fig. S2** $^1$H NMR (A) and $^{13}$C NMR (B) spectra of E-TPE-2DEVD (top) and Z-TPE-2DEVD (bottom), respectively.
Fig. S3 ¹H NMR and ¹³C NMR spectra of E-TPE-2N₃ (A & B) and Z-TPE-2N₃ (C & D), respectively.
**Fig. S4** Single crystal structure of E-TPE-2N$_3$ determined by XRD.

**Fig. S5** $^1$H NMR spectra of E-TPE-2DEVD synthesized from E-TPE-2N$_3$. 
Fig. S6 UV-vis absorption spectra of E/Z-TPE-2DEVD in DMSO/water (v/v = 1:199). [E-TPE-2DEVD] = [Z-TPE-2DEVD] = 10 µM.

Fig. S7 Plot of PL intensity of Z-TPE-2DEVD (10 µM) after incubation with caspase-3 at different concentrations (0–200 nM). $\lambda_{ex} = 320$ nm, $\lambda_{em} = 460$ nm.
Fig. S8 Another eight molecular docking models of E-TPE-2DEVD with caspase-3. Caspase-3 is shown in sky blue. E-TPE-2DEVD is shown in multiple colors.