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Electronic Supplementary Information

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

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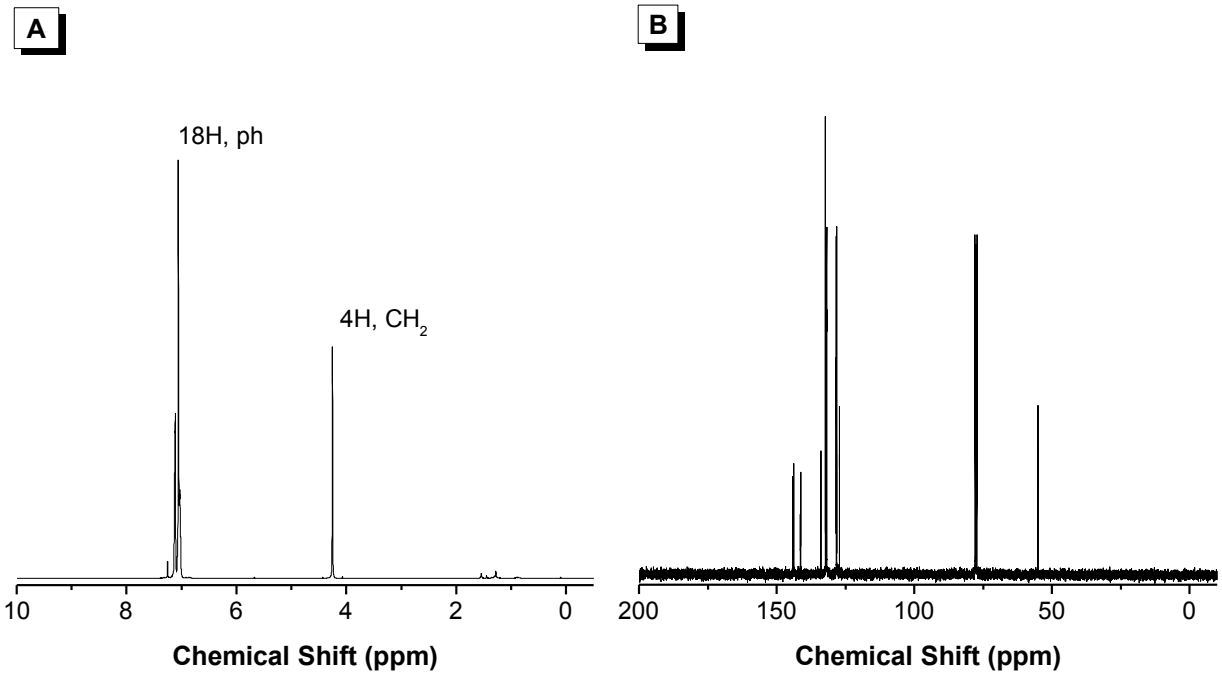
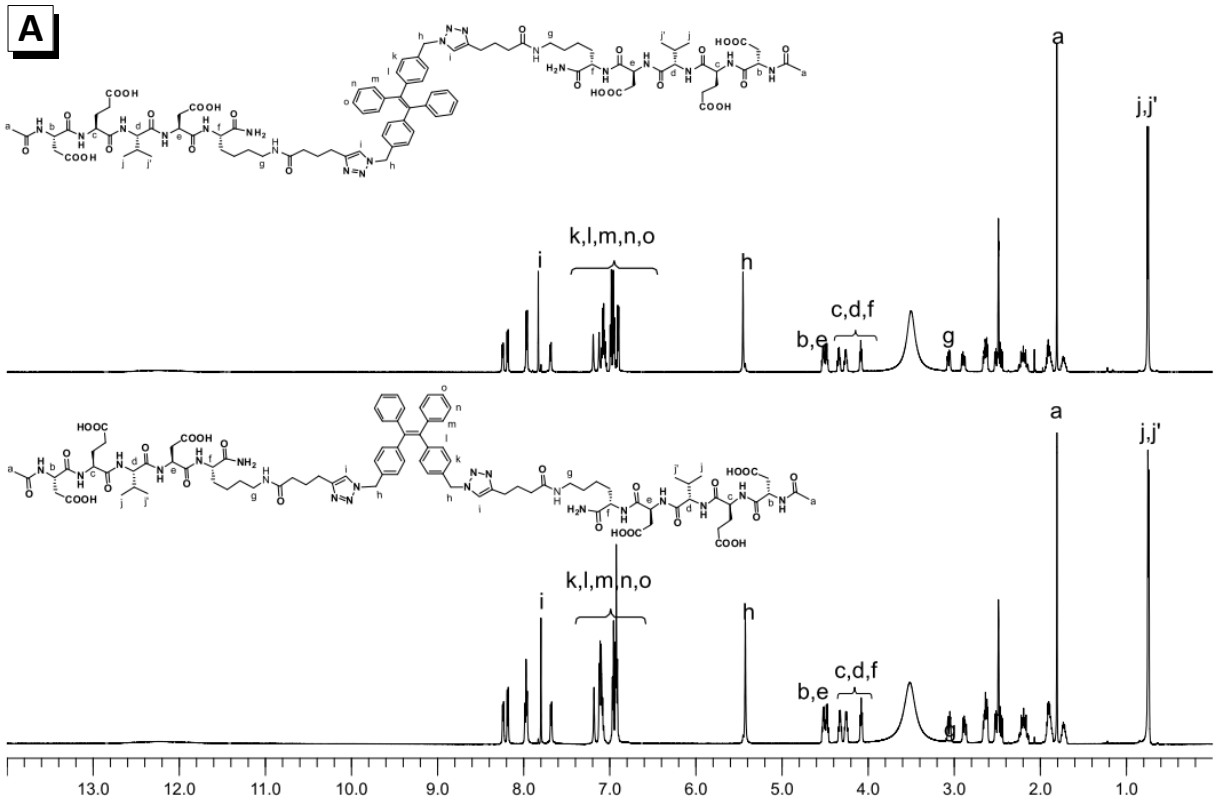


Fig. S1 (A) ^{1}H and (B) ^{13}C NMR spectra of TPE-2N$_3$ in CDCl$_3$.



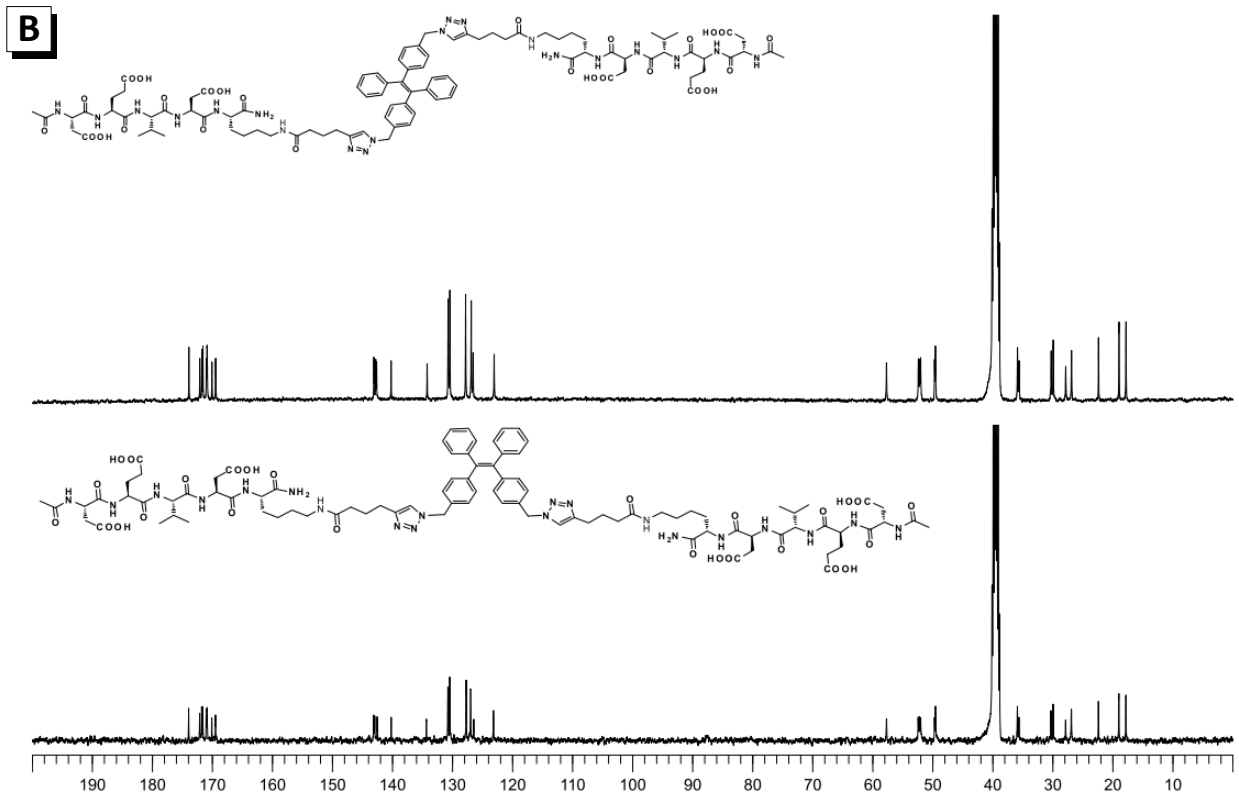
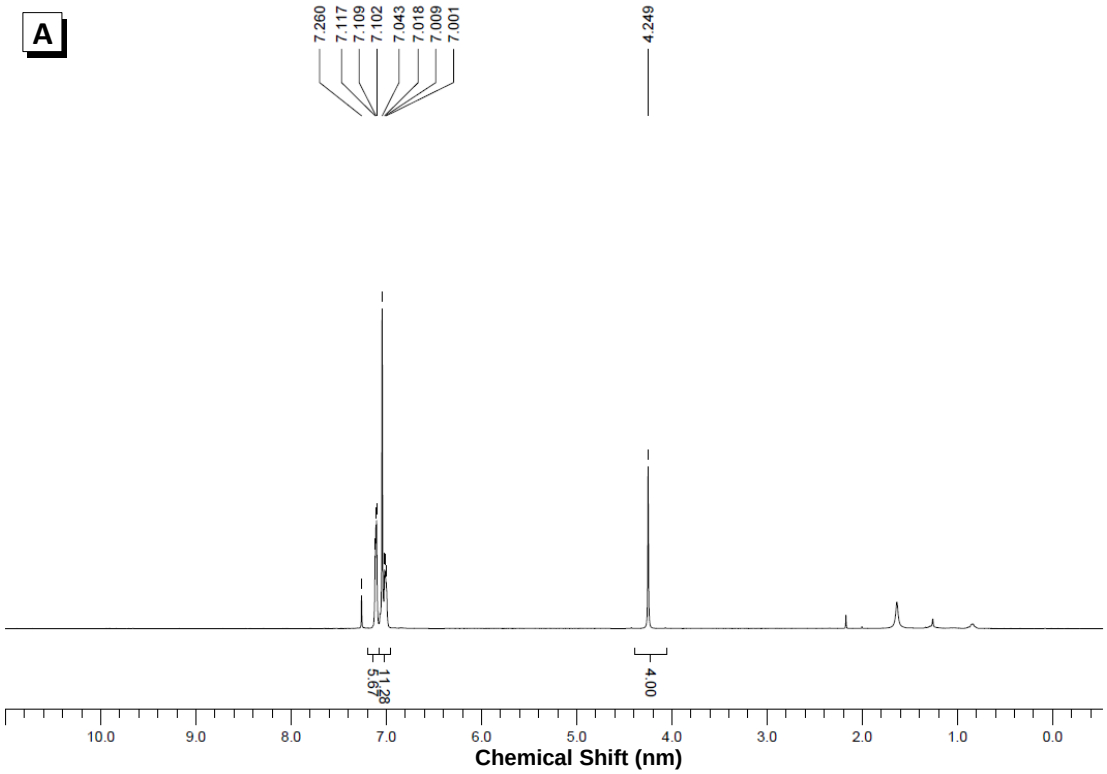
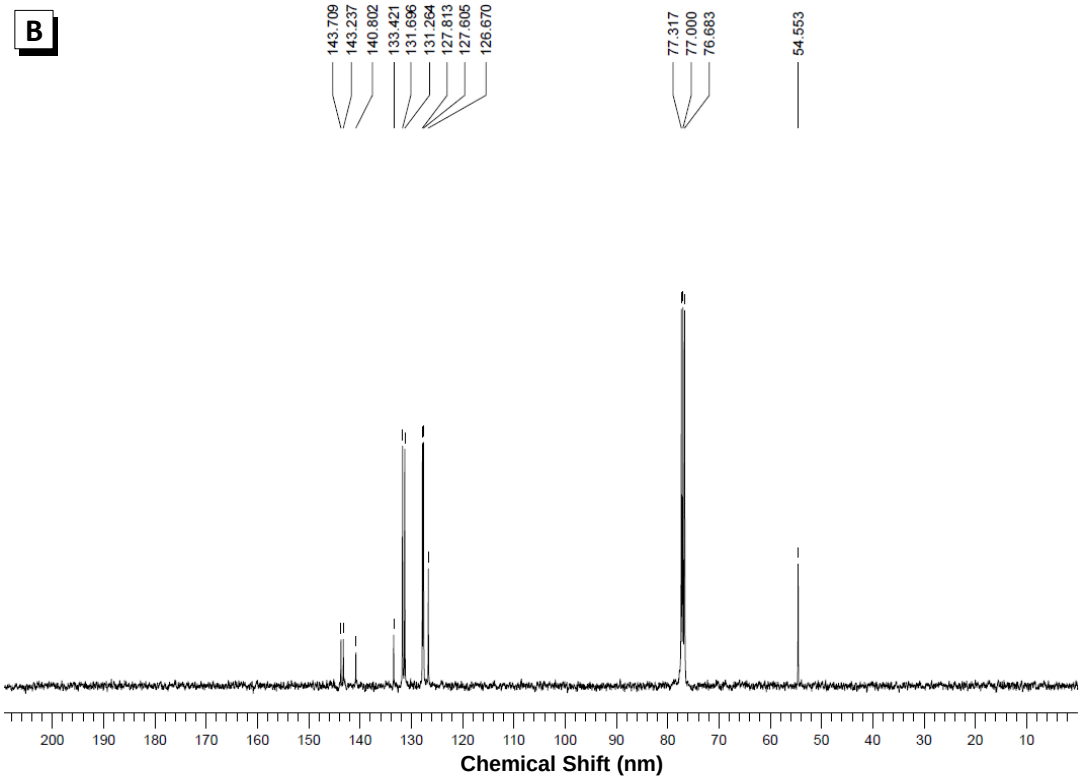


Fig. S2 ^{1}H NMR (A) and ^{13}C NMR (B) spectra of *E*-TPE-2DEVD (top) and *Z*-TPE-2DEVD (bottom), respectively.


A
7.260
7.117
7.109
7.102
7.043
7.018
7.009
7.001
4.249
5.67
11.28
4.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Chemical Shift (nm)


B
143.709
143.237
140.802
133.421
131.696
131.264
127.813
127.605
126.670
77.317
77.000
76.683
54.553
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
Chemical Shift (nm)

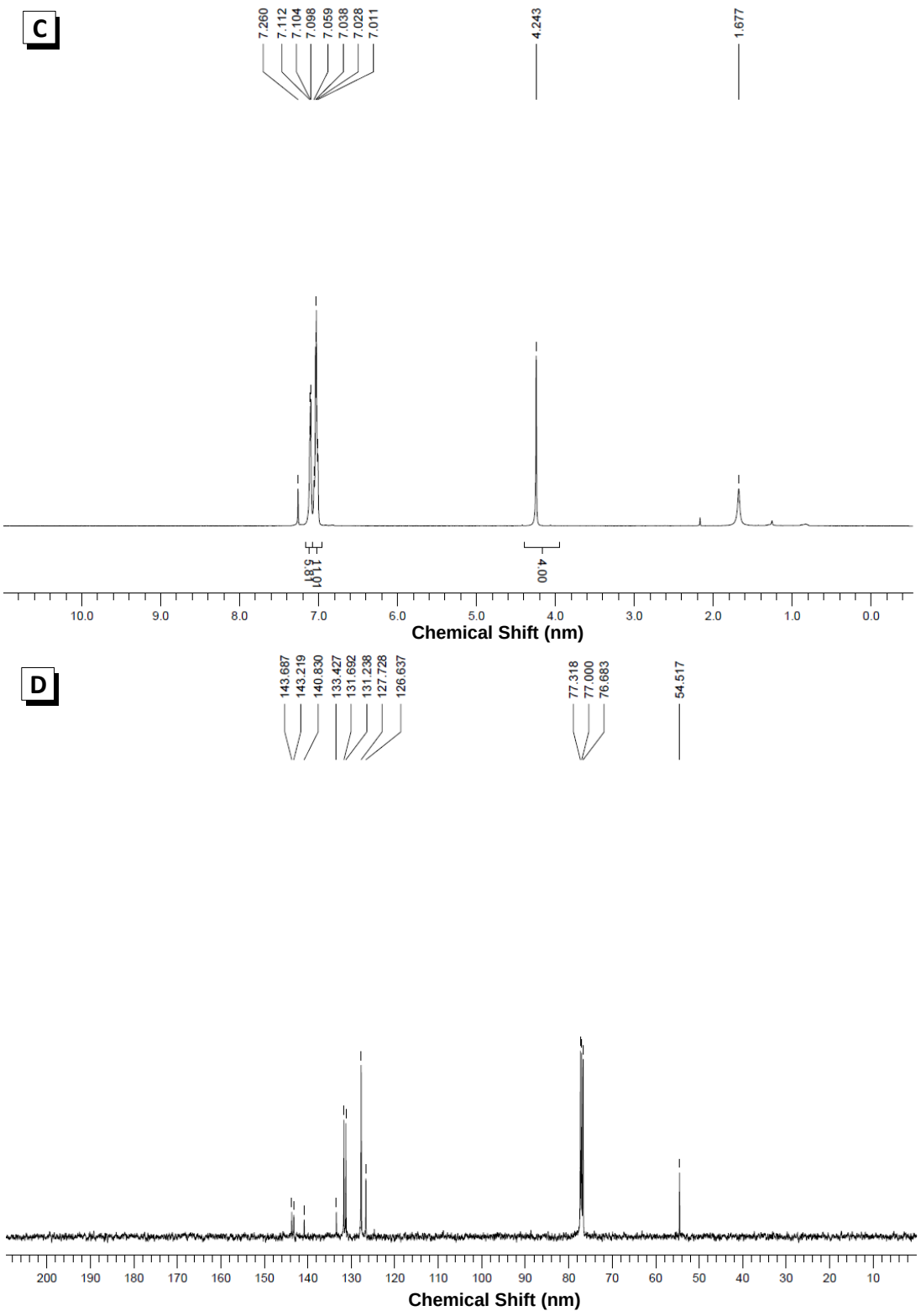


Fig. S3 ^{1}H NMR and ^{13}C NMR spectra of *E*-TPE-2N$_3$ (A & B) and *Z*-TPE-2N$_3$ (C & D), respectively.

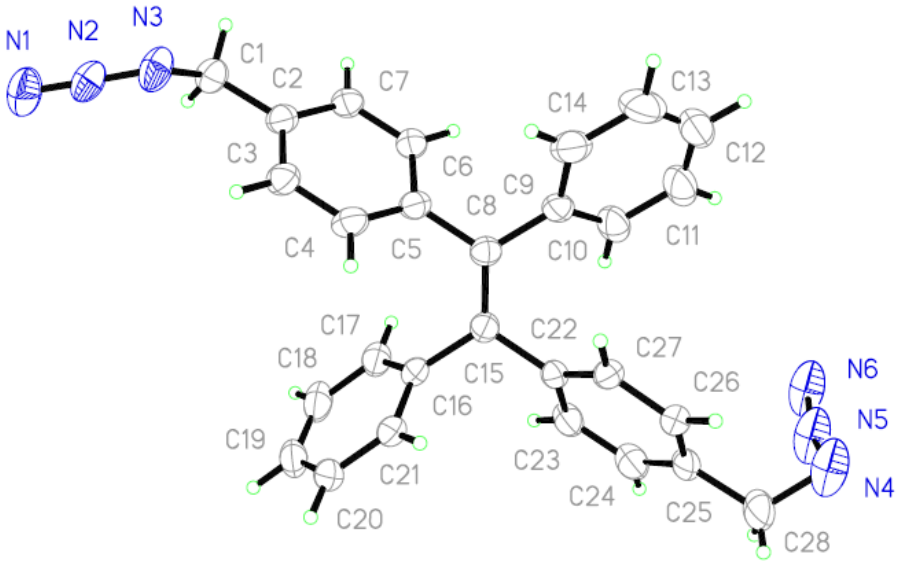


Fig. S4 Single crystal structure of *E*-TPE-2N_3 determined by XRD.

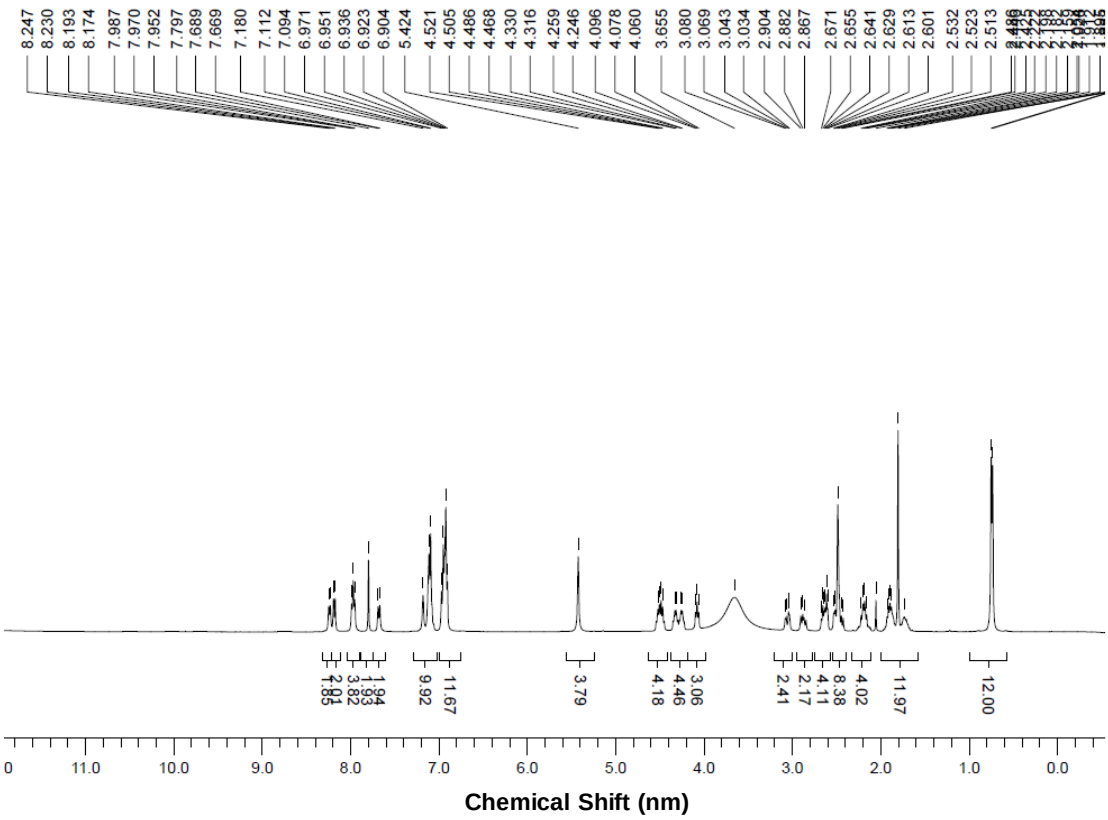


Fig. S5 ^{1}H NMR spectra of *E*-TPE-2DEVD synthesized from *E*-TPE-2N_3.

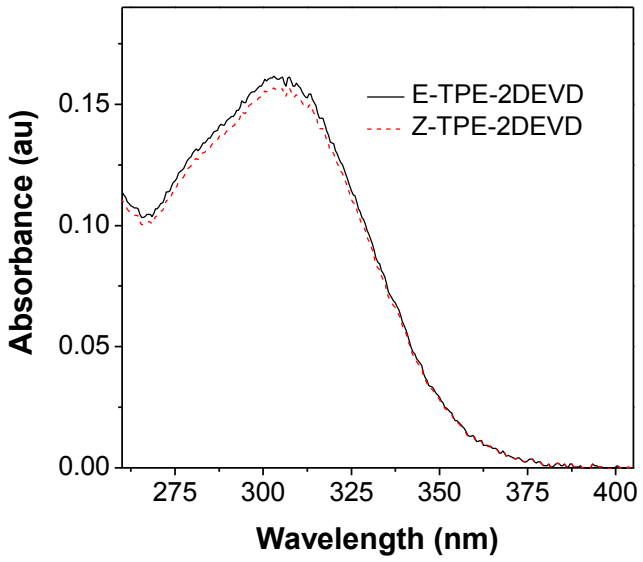


Fig. S6 UV-vis absorption spectra of *E*/*Z*-TPE-2DEVD in DMSO/water (v/v = 1:199). [*E*-TPE-2DEVD] = [*Z*-TPE-2DEVD] = 10 μM.

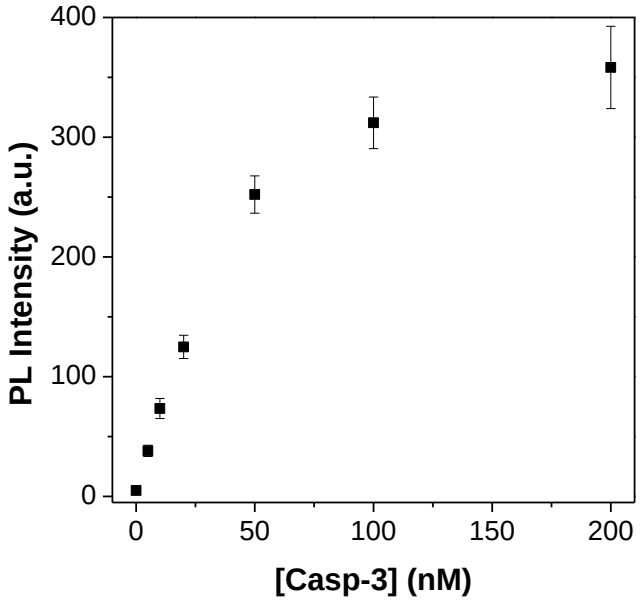


Fig. S7 Plot of PL intensity of *Z*-TPE-2DEVD (10 μM) after incubation with caspase-3 at different concentrations (0–200 nM). λ_{ex} = 320 nm, λ_{em} = 460 nm.

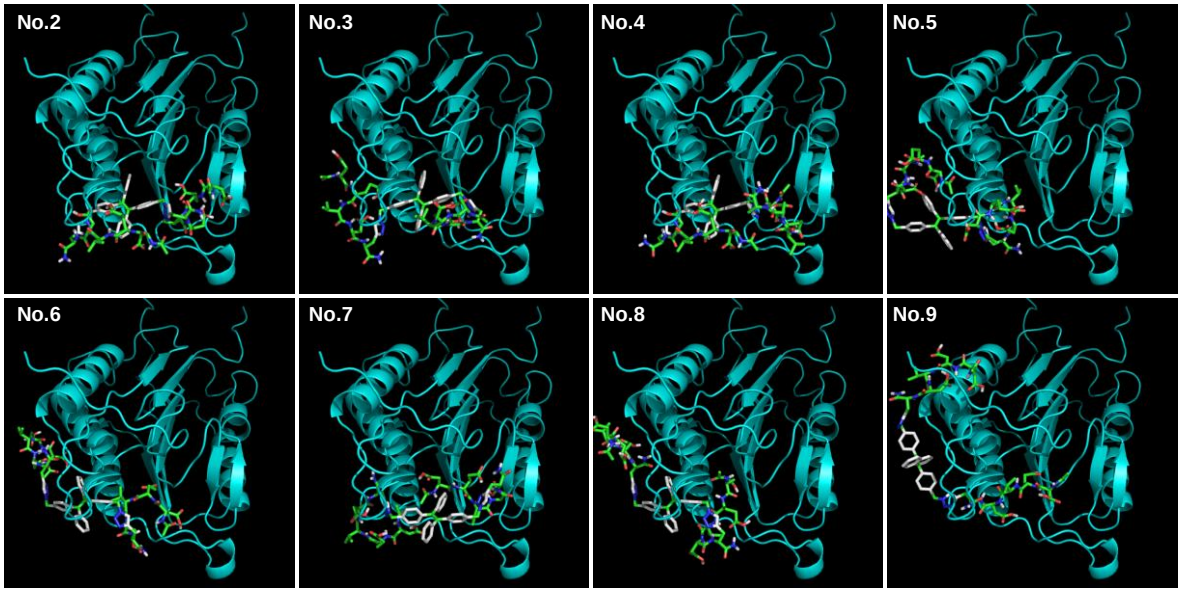


Fig. S8 Another eight molecular docking models of *E*-TPE-2DEVD with caspase-3. Caspase-3 is shown in sky blue. *E*-TPE-2DEVD is shown in multiple colors.