Electronic Supplementary Information (ESI)

A near-infrared "on-off" fluorescent and colorimetric cyanide chemodosimeter based on phenothiazine with applications in living cell imaging

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Supplementary figures and tables

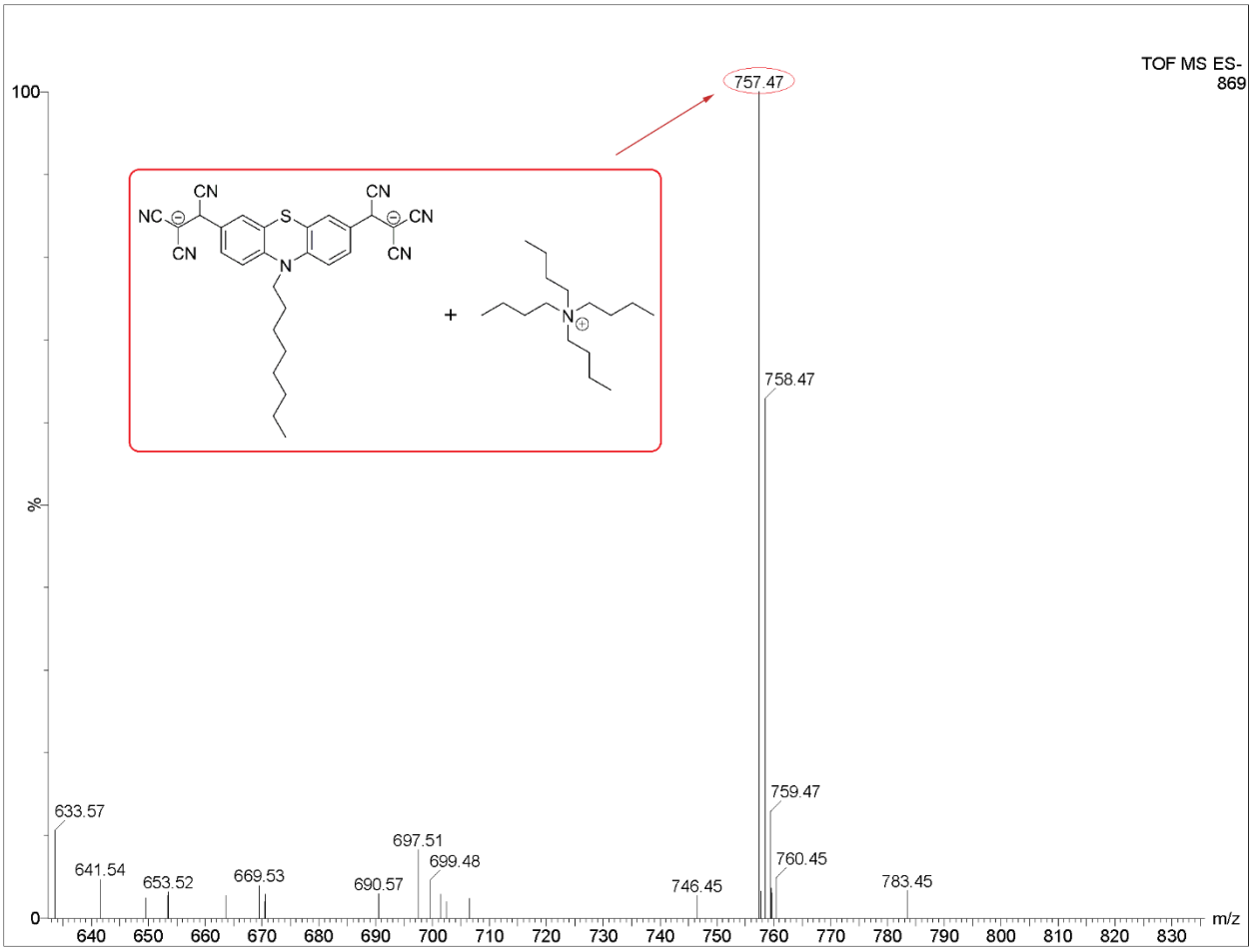


Fig. S1 MS (ESI-) spectrum of compound **PTZ** (10 μM) with CN^- (22 μM) in CH_3CN solution at 25 °C.

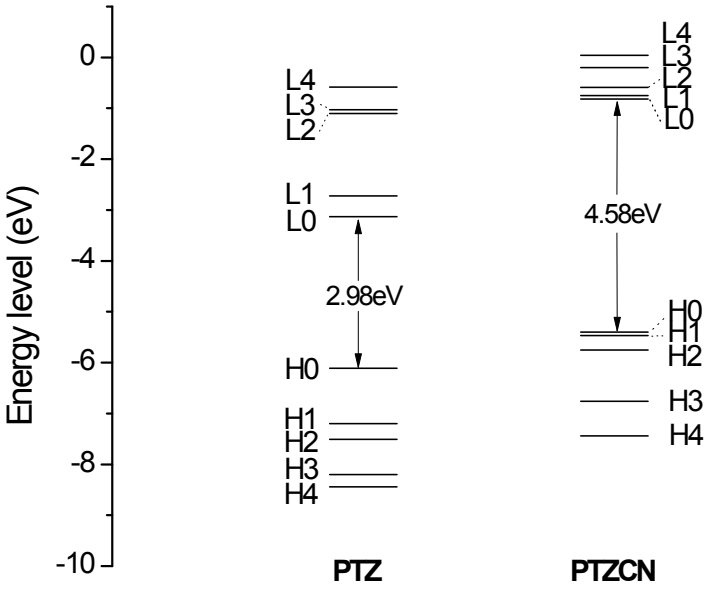


Fig. S2 Energy levels of the frontier molecular orbitals of compound **PTZ** and its adduct with CN^-. H0 = HOMO, L0 = LUMO, H1 = HOMO−1, L1 = LUMO+1, etc.

Table S1 Excitation energies, oscillator strengths and molecular orbital compositions of low-lying excited states of compound **PTZ**, computed at the TD-PBE0/6-311+G(2d,p) level of theory.

Compound	State	λ_{abs}	f	MO composition	Charge transfer
PTZ (S_0)	S_1	2.31 eV, 537 nm	0.6112	H-0 → L+0 (98%)	0.217 *e*
	S_2	2.86 eV, 433 nm	0.0572	H-0 → L+1 (96%)	0.242 *e*

	S_3	3.36 eV, 369 nm	0.7768	H-1 → L+0 (95%)	0.204 *e*
	S_6	4.04 eV, 307 nm	0.8348	H-0 → L+3 (80%)	−−
PTZ (S_1)	S_1	1.78 eV, 695 nm	0.4576	H-0 → L+0 (98%)	0.227 *e*

Table S2 Excitation energies, oscillator strengths and molecular orbital compositions of low-lying excited states of compound **PTZ**, computed at the TD-CAM-B3LYP/6-311+G(2d,p) level of theory.

Compound	State	λ_{abs}	*f*	MO composition	Charge transfer
PTZ	S_1	2.75 eV, 451 nm	0.9098	H-0 → L+0 (92%)	0.238 *e*
	S_2	3.45 eV, 359 nm	0.1248	H-0 → L+1 (90%)	0.291 *e*
	S_3	3.83 eV, 323 nm	0.7763	H-1 → L+0 (80%)	0.159 *e*
	S_5	4.32 eV, 287 nm	0.7747	H-0 → L+3 (67%)	−−

Table S3 Excitation energies, oscillator strengths and molecular orbital compositions of low-lying excited states of compound **PTZCN**, computed at the TD-PBE0/6-311+G(2d,p) level of theory.

Compound	State	λ_{abs}	f	MO composition
PTZCN	S_1	3.68 eV, 336 nm	0.0698	H-0 → L+0 (64%)
				H-2 → L+0 (21%)
	S_4	3.86 eV, 321 nm	0.0322	H-0 → L+1 (73%)
				H-1 → L+2 (13%)
	S_8	4.12 eV, 300 nm	0.0733	H-0 → L+0 (23%)
				H-2 → L+0 (20%)
				H-0 → L+5 (17%)
				H-1 → L+4 (12%)
	S_9	4.14 eV, 299 nm	0.2515	H-2 → L+2 (51%)
				H-1 → L+1 (24%)
				H-0 → L+2 (18%)

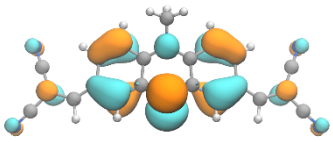
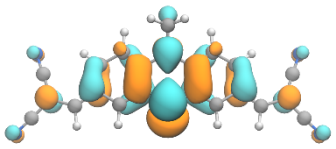
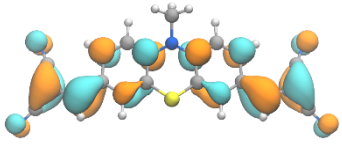
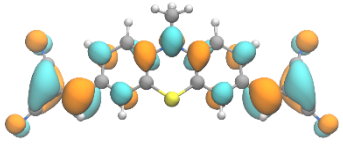
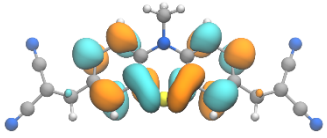
HOMO−1	HOMO	
		
LUMO	**LUMO+1**	**LUMO+3**
		

Fig. S3 Contour plots of frontier molecular orbitals of compound **PTZ**.

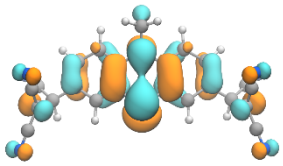
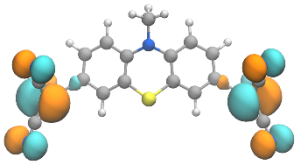
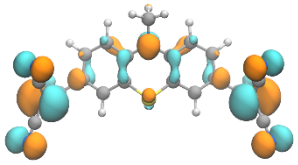
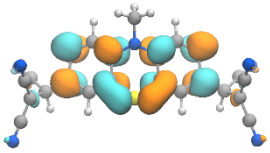
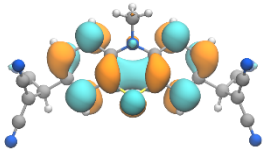
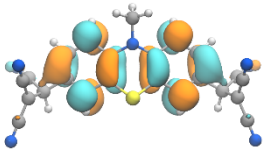
HOMO−2	HOMO−1	HOMO
		
LUMO	**LUMO+1**	**LUMO+2**
		

Fig. S4 Contour plots of frontier molecular orbitals of compound **PTZCN**.

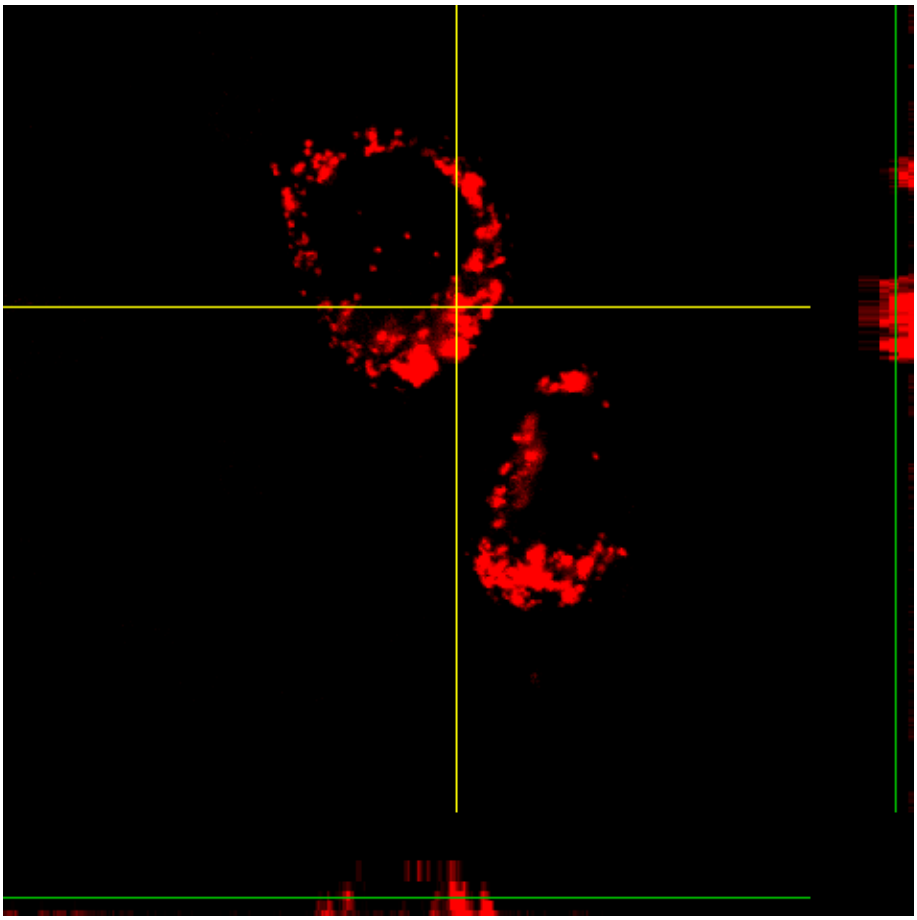


Fig. S5 Z-scan images of HeLa cells supplemented with 20 μM CN^- in the growth media for 20 min at 37 °C and then incubated with compound **PTZ** (10 μM) for 30 min at 37 °C. λ_{ex} = 488 nm. Collecting region: 650–750 nm.

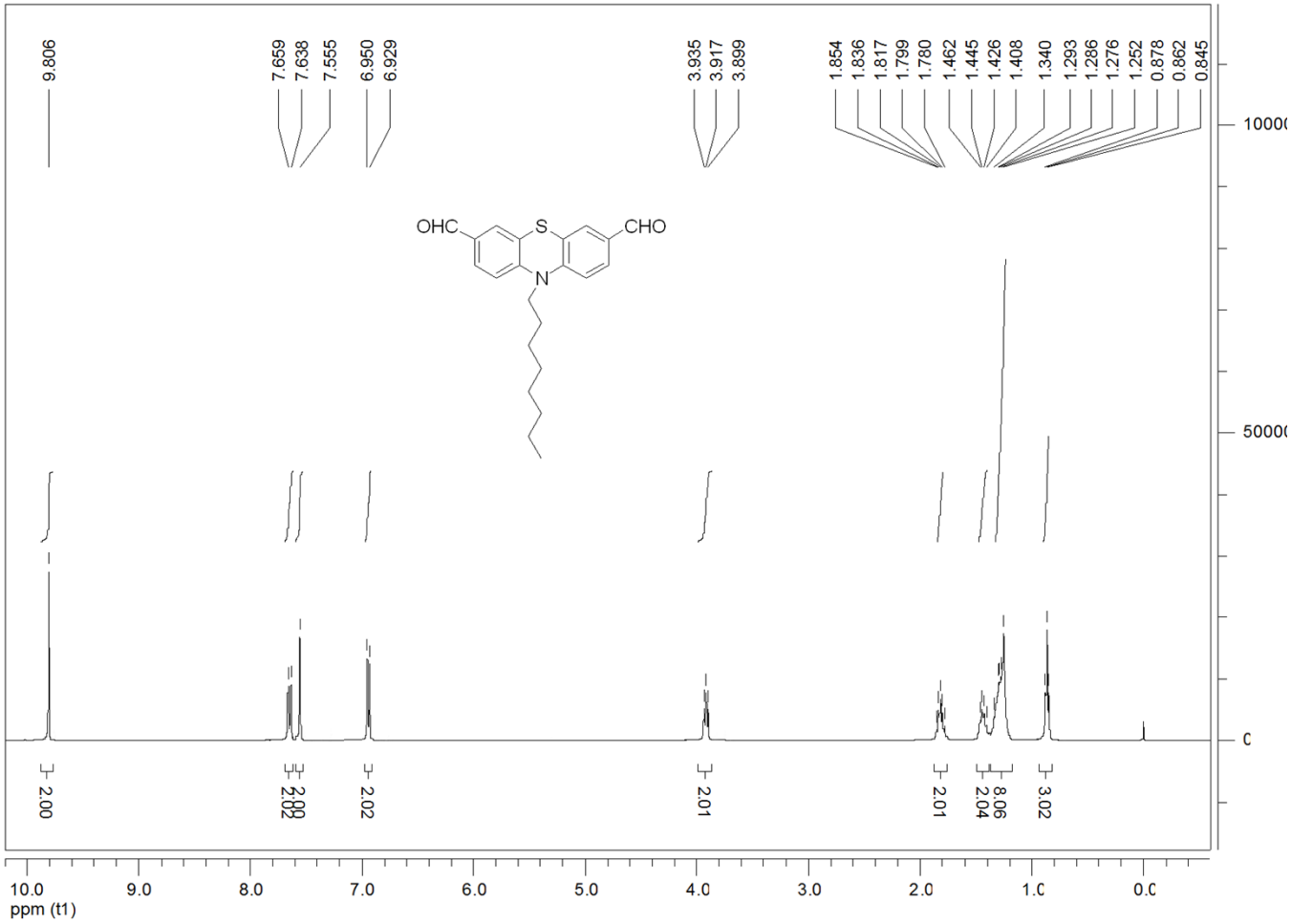


Fig. S6 ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **2**.

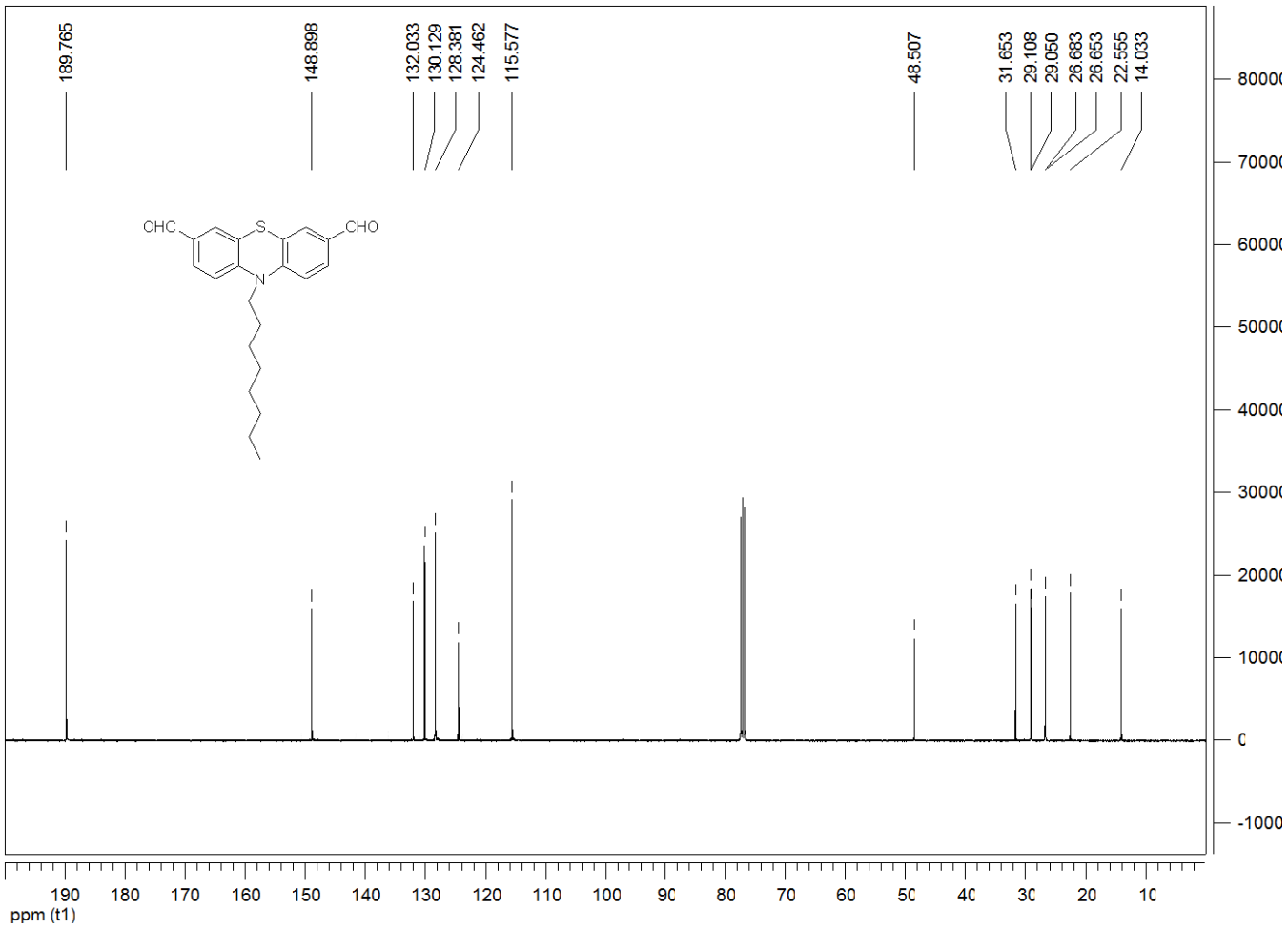


Fig. S7 ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **2**.

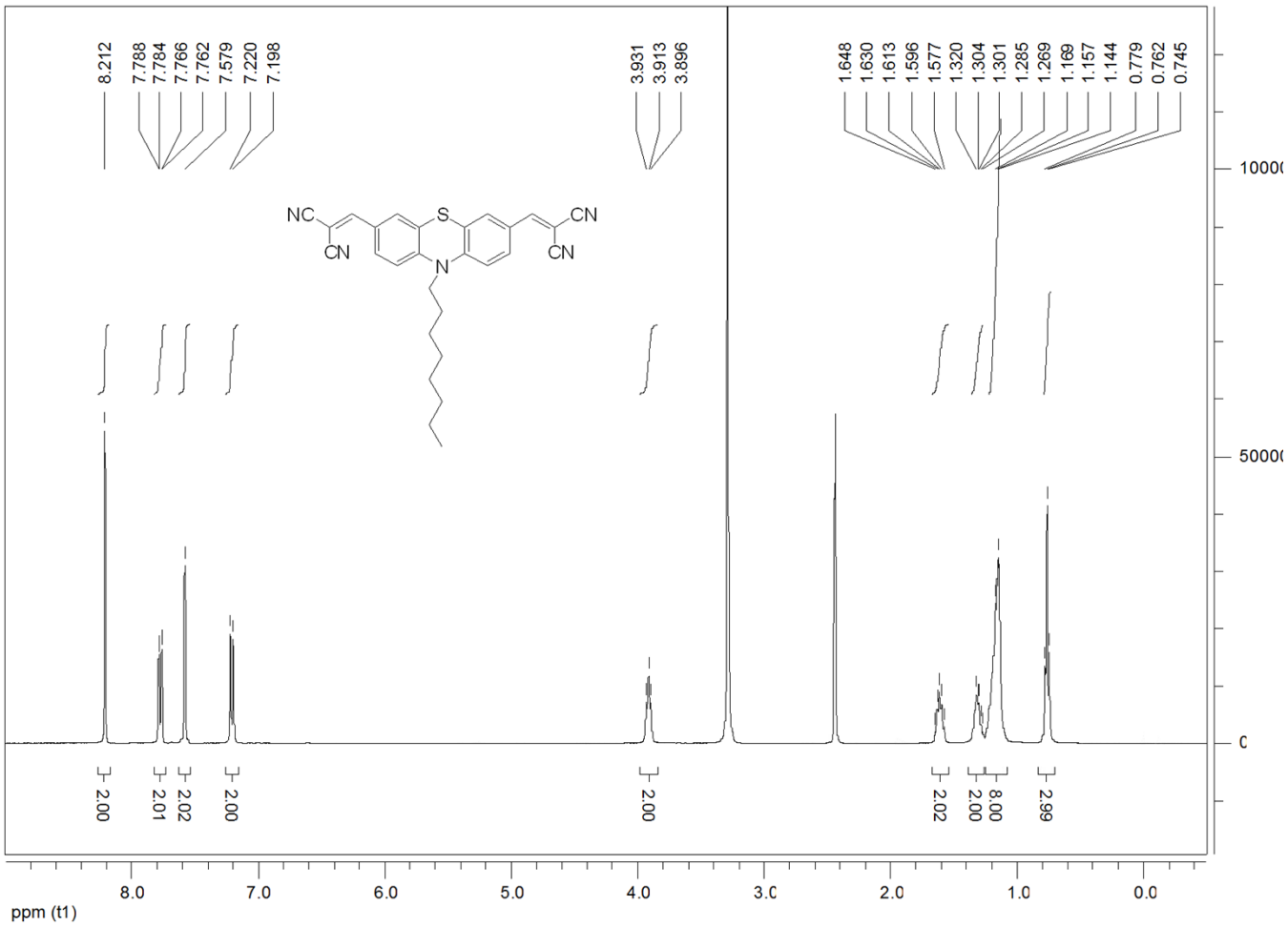


Fig. S8 ^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of compound **PTZ**.

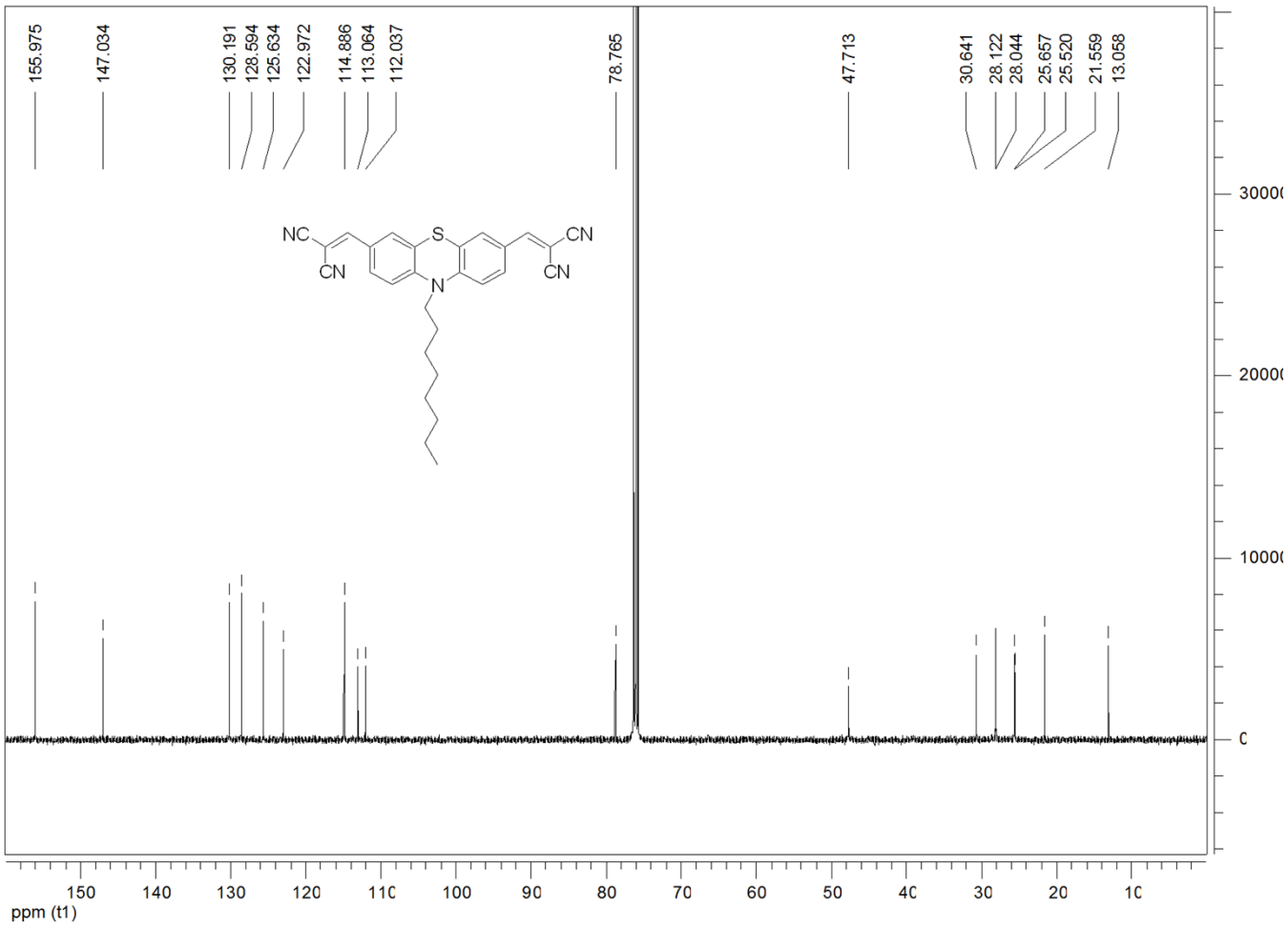
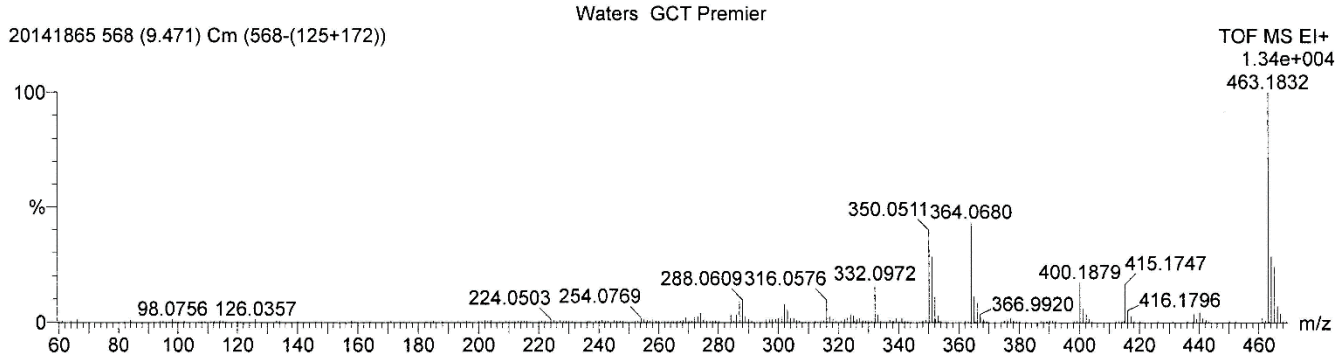


Fig. S9 ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **PTZ**.

Multiple Mass Analysis: 29 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
558 formula(e) evaluated with 32 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-28 H: 0-25 N: 0-5 S: 0-1



Minimum:	3.00			-1.5
Maximum:	100.00	5.0	10.0	50.0

Fig. S10 HRMS (EI+) spectrum of compound **PTZ**.