Electronic Supplementary Information

A mitochondria-targeted near-infrared probe for colorimetric and ratiometric fluorescence detection of hypochlorite in living cells

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Contents

1. ^{1}H NMR, ^{13}C NMR and HR-MS spectra of CMBI

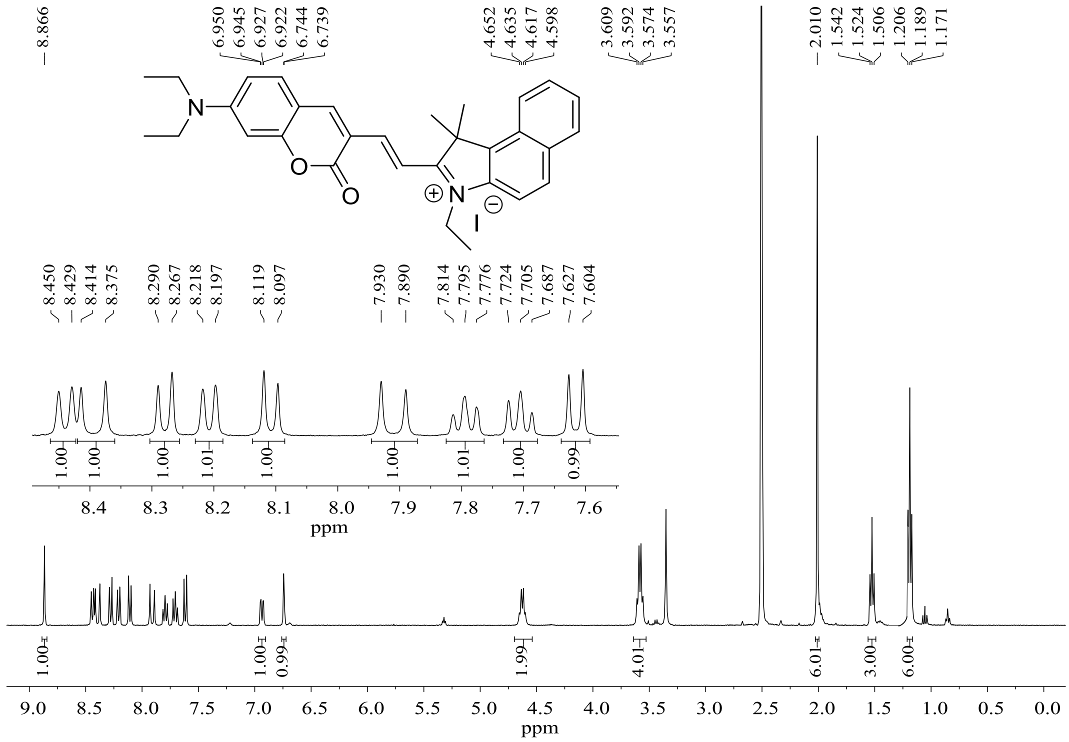

Fig. S1 ^{1}H NMR spectrum of **CMBI** in DMSO-d_6 (400 MHz).

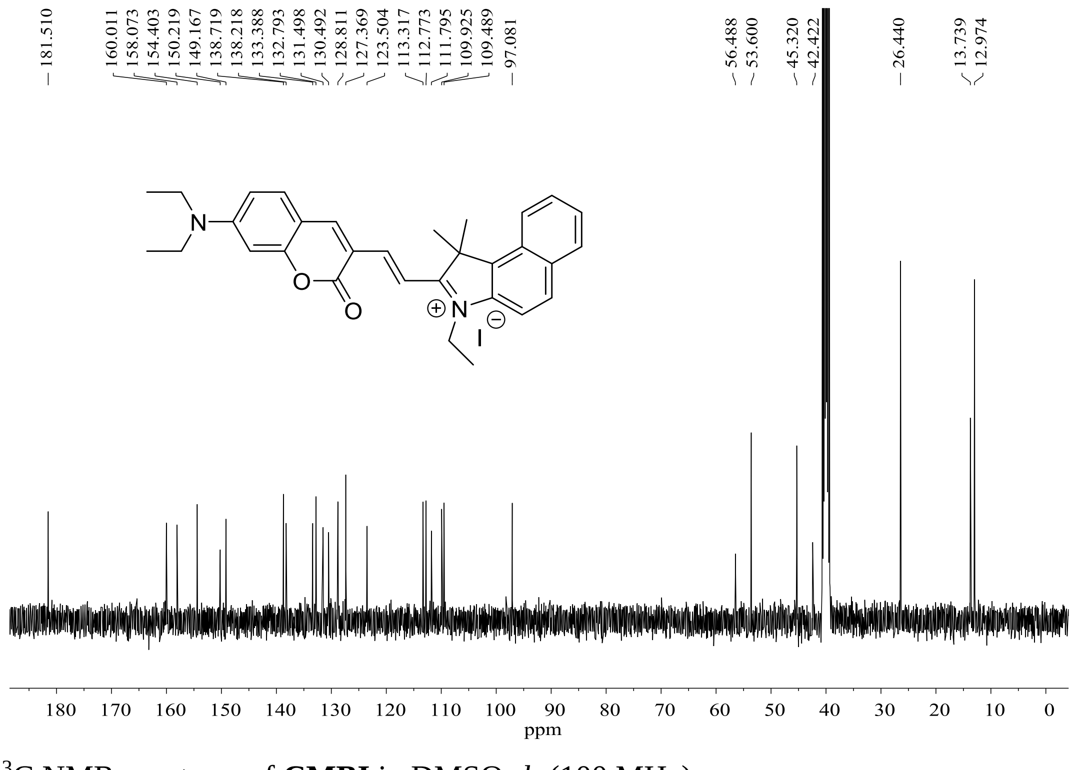

Fig. S2 ^{13}C NMR spectrum of **CMBI** in DMSO-d_6 (100 MHz).

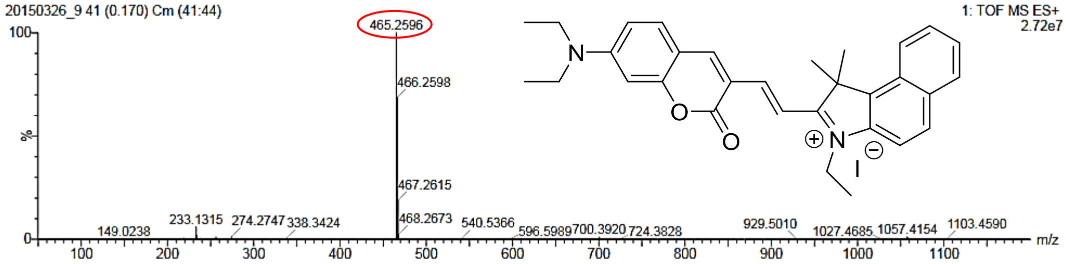

Fig. S3 HR-MS (ESI) spectrum of **CMBI**.

2. Summary of photophysical properties

Table S1 Spectroscopic properties of **CMBI** (10 μM) and **CMBI** (10 μM) with ClO^- (100 μM) in EtOH/PBS solution (v/v = 1/9, pH 7.4, 10 mM).

Compound	λ_{abs} (nm)	λ_{em} (nm)	Φ	Δν (cm^{-1})
CMBI	592	658	0.012	1694
CMBI + ClO^-	400	475	0.141	3947

3. Ratiometric response of CMBI toward ClO^- at low concentrations

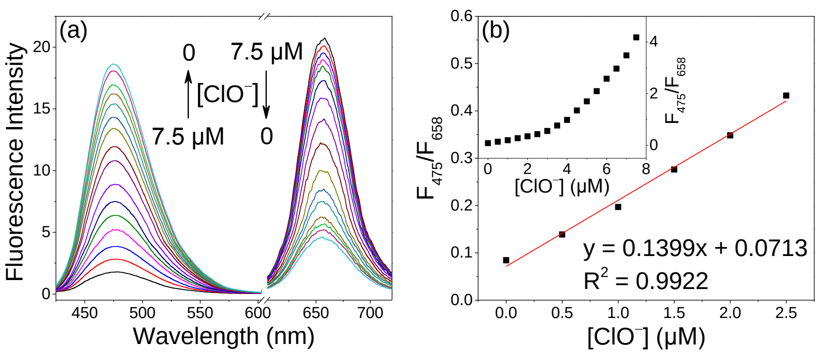

Fig. S4 (a) Fluorescence spectra changes of 1 μM **CMBI** in EtOH/PBS solution (v/v = 1/9, pH 7.4, 10 mM) upon addition of increasing amount of ClO^- (0 – 7.5 μM). (b) Linear relationship between fluorescence intensity of 1.0 μM **CMBI** *versus* concentrations of ClO^- in EtOH/PBS solution (v/v = 1/9, pH 7.4, 10 mM). Each spectrum was recorded after 3 min.

4. Selectivity of CMBI toward ClO⁻

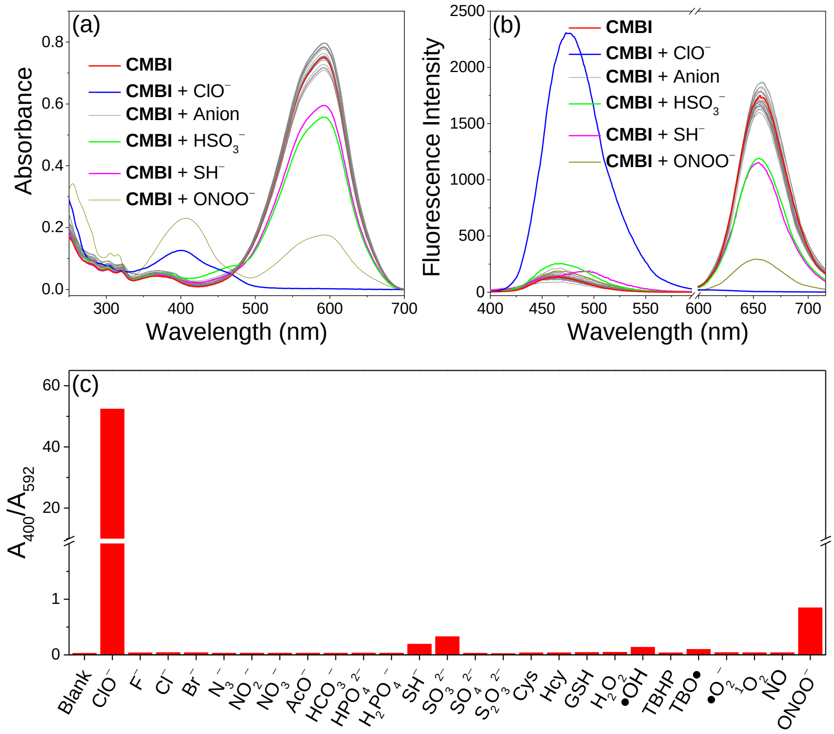

Fig. S5 (a) UV-vis absorption, (b) fluorescence spectra changes and (c) UV-vis absorption ratios (A_{400}/A_{592}) of 10 μM **CMBI** in EtOH/PBS solution (v/v = 1/9, pH 7.4, 10 mM) in the presence of various small molecular species (500 μM) and ROS/RNS (100 μM). Each spectrum was recorded after 3 min.

5. Kinetics research for CMBI towards ClO^-, HSO_3^- and HS^-

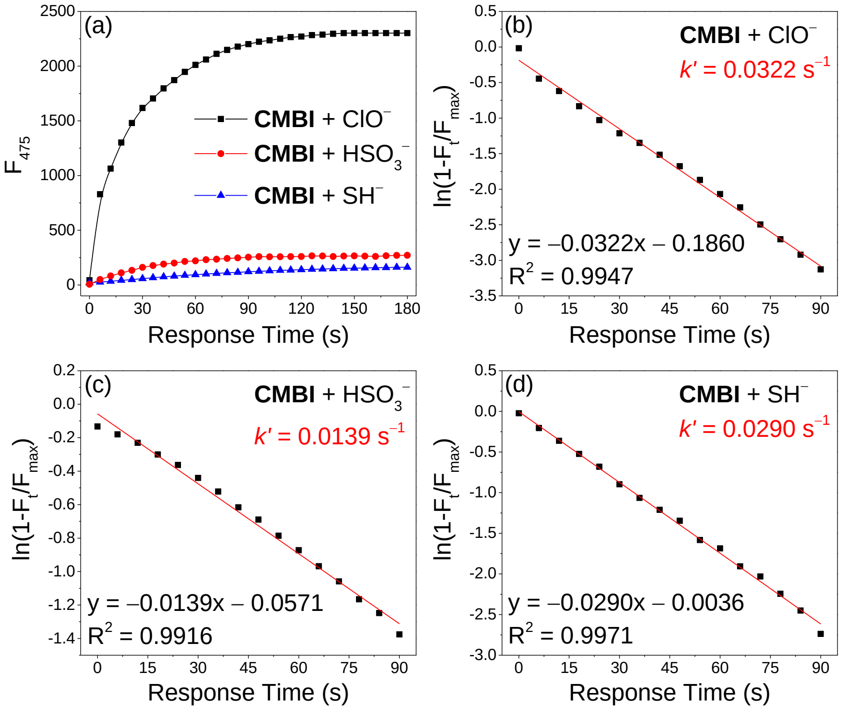

Fig. S6 Time-resolved fluorescence responses (a) and Pseudo-first-order kinetic plot of 10 μM **CMBI** towards 100 μM ClO^- (b), HSO_3^- (c) and HS^- (d) in EtOH/PBS solution (v/v = 1/9, pH 7.4, 10 mM).

6. Proposed mensing mechanism

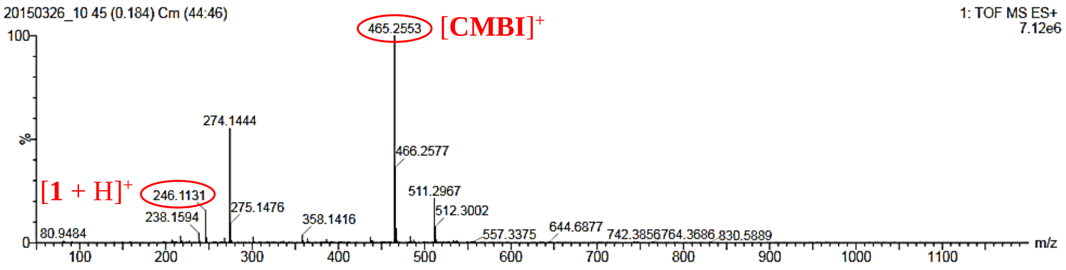

Fig. S7 HR-MS (ESI) spectrum of **CMBI** with ClO^{-}.

7. Cell toxicity test of CMBI

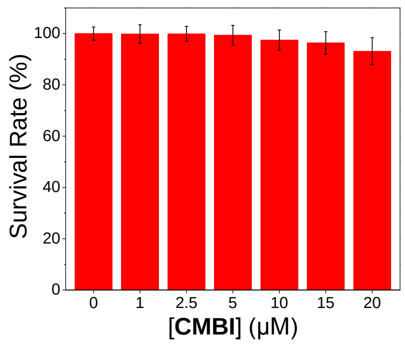

Fig. S8 Cell toxicity effect of **CMBI**. HeLa cells were incubated with **CMBI** (0–20 μM) for 24 h. Results are mean ± SD, $n = 3$.

8. Comparison of ratiometric fluorescent probes for ClO^-

Table S2 Comparison of ratiometric fluorescent probes for ClO^-

Probes	λ_{ex} /nm	λ_{em} /nm	Reagents	Detection limit/nM	Response time/s	Application
Phenanthroimidazole Probe **1**[1]	394	439 509	pH 9.0 PBS (80% DMF)	—	Within seconds	—
1b[2]	540 464	585 505	pH 7.4 PBS (20% DMF)	200	< 600	MCF-7 cells (Ex) Ex = exogenous
Cou-Rho-HOCl[3]	410	473 594	pH 7.4 PBS (50% DMF)	52	< 60	Bel 7702 cells (Ex) RAW 264.7 cells (En) En = endogenous
BODIPY-DCDHF Probe **1**[4]	465	629 520	pH 7.4 PBS (1% EtOH, 0.1 % Triton X-100)	500	~ 400	RAW 264.7 cells (Ex, En)
Cy7-NR1[5]	540	780 566	pH 7.4 PBS (0.5% DMF)	19.5	~ 360	HeLa cells (Ex)
Z2[6]	460	509 600	pH 7.4 PBS	63	< 120	Test paper
CDH[7]	316	376 456	pH 7.4 HEPES (40% CH_3CN)	1070	< 60	Water samples TLC plate strips
HRS1[8]	410 554	501 578	pH 8.5 PBS (40% DMF)	24	< 60	Water samples
DPNO[9]	305	354 430	pH 7.4 HEPES (60% CH_3CN)	56	< 60	Water samples TLC plate strips
DPH[10]	344	495 375	pH 7.4 HEPES (50% EtOH)	350	—	Water samples
CMCY[11]	460	631 480	pH 7.4 PBS	80	< 120	HeLa cells (Ex)
Coumarin-Pyridinium Probe **1**[12]	420	631 488	pH 7.4 PBS (75% THF)	93	~ 20	Water samples RAW 264.7 cells (En)
1,8-diaminonaphthalene[13]	325	440 518	pH 7.0 HEPES	20	< 20	Water samples HepG2 cells (Ex)
Coumarin-Rhodamine Probe **2**[14]	410	580 470	pH 5.0 PBS (40% DMF)	—	< 50	RAW 264.7 cells (En)

BTHT[15]	365	562 476	pH 7.4 HEPES (50% CH_3CN)	140	< 480	Water samples TLC plate strips
NIR-1 thiospirolactone Probe **1**[16]	430 650	486 707	pH 7.4 PBS (30% CH_3CN)	40	Within seconds	Water samples HeLa cells (Ex) RAW 264.7 cells (En)
TAM[17]	430	630 485	pH 7.1 H_2O (40% THF)	70	~ 100	TLC plate strips PBMCs (Ex)
Dansyl-Rhodamine Probe **1**[18]	400	494 578	pH 8.0 PBS (10% CH_3CN)	1130	< 120	Water samples Test paper
PMN-TPP[19]	410	522 640	pH 7.3 PBS (0.5% DMSO, 1 mM Triton X-100)	430	Few seconds	RAW 264.7 cells (En) Nude mouse (En)
Naph-Rh[20]	350	440 585	pH 6.0 PBS (30% EtOH)	100	< 50	RAW 264.7 cells (En)
RMClO-2[21]	412 540	476 570	pH 7.4 PBS (0.1% DMSO)	0.84	Within seconds	Normal and cancer cells
HPQ-Cy$_2$[22]	365	575 435	pH 7.4 PBS (0.5% EtOH)	28	< 50	A375 cells (En)
CRSH[23]	350	470 580	pH 5.0 PBS (50% EtOH)	210	~ 60	RAW 264.7 cells (En)
STBR[24]	370	514 595	pH 7.5 PBS (20% CH_3CN)	220	—	TLC plate strips Baker’s yeast (Ex)
AETU-HOCl[25]	380	533 473	pH 7.4 PBS (50% EtOH)	3.9	~ 60	RAW 264.7 cells (En)
QC1[26]	400	482 381	pH 7.4 HEPES (1% DMSO)	410	—	—
Naphthalimide-Indolium Probe **1**[27]	430	620 515	pH 7.0 HEPES (50% MeOH)	53	~ 50	HepG2 cells (Ex)
HES-BODIPY[28]	480	562 532	pH 7.1 PBS (10% EtOH)	430	Within seconds	RAW 264.7 cells (En)
BRT[29]	525	540 580	pH 5.0 PBS (60% EtOH)	38	~ 15	RAW 264.7 cells (En)
CARSH[30]	350	490 580	pH 5.0 PBS (50% EtOH)	200	~ 60	RAW 264.7 cells (En)
Lyso-HA[31]	420	450 586	pH 5.0 PBS (30% DMSO)	110	Within seconds	HeLa cells (Ex) RAW 264.7 cells (En)

MTPE-M[32]	340	595 498	pH 7.4 PBS (1% DMSO, 1mM CTAB)	470	~ 180	RAW 264.7 cells (En) Zebrafish (En)
Py-Cy[33]	430	613 470	pH 7.4 PBS (5% DMSO)	350	4200	Water samples HeLa cells (Ex) RAW 264.7 cells (En)
CMBI (This work)	585 390	658 475	pH 7.4 PBS (10% EtOH)	33	~ 90	HeLa cells (Ex)

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9. ^{1}H NMR spectra of compounds 1 and 2

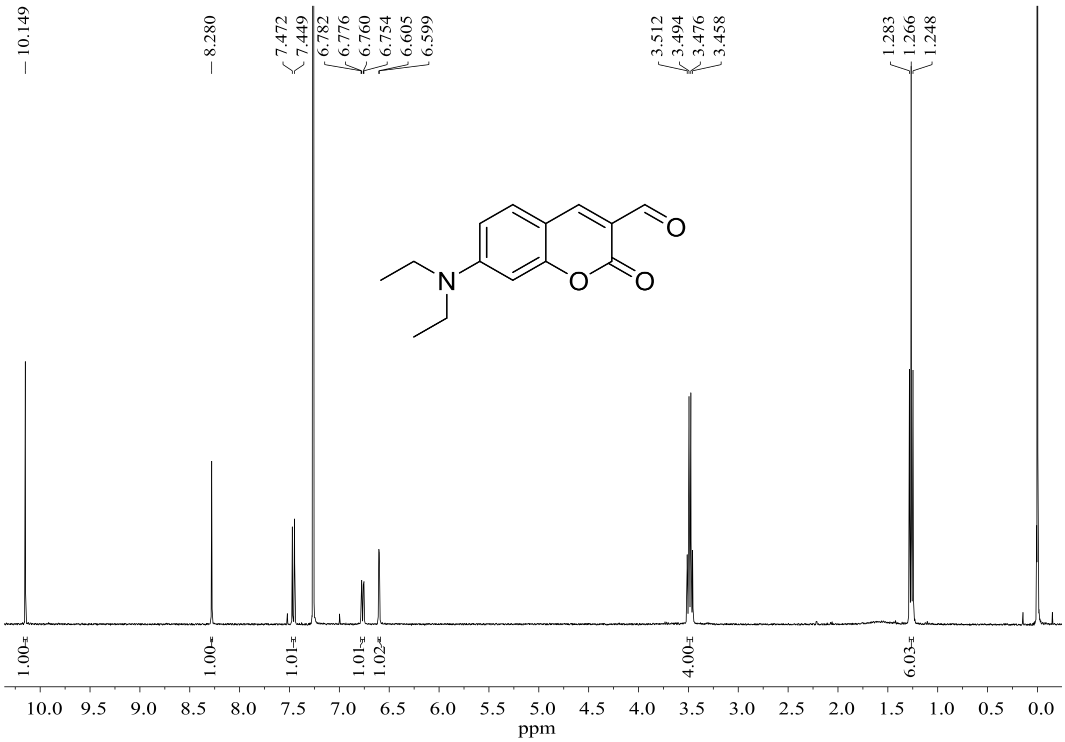

Fig. S9 ^{1}H NMR spectrum of compound **1** in $CDCl_3$ (400 MHz).

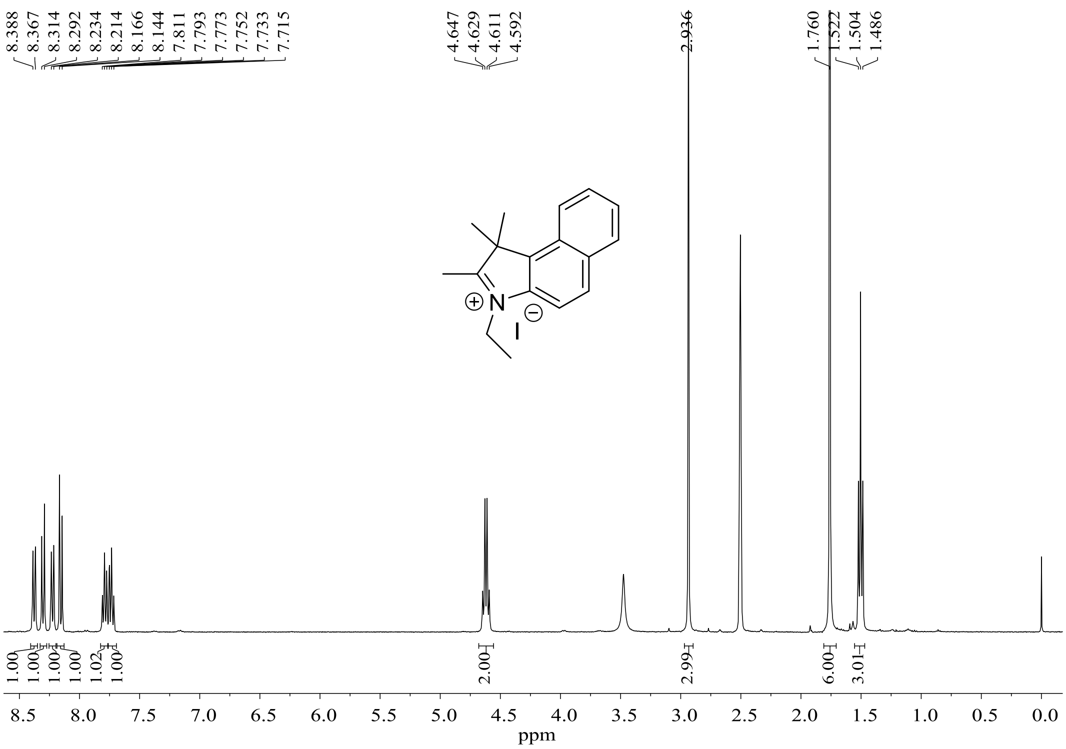

Fig. S10 ^{1}H NMR spectrum of compound **2** in DMSO-d_6 (400 MHz).