Supplementary Data

for

Sensitive and selective detection of phosgene with a bis-(1H-benzimidazol-2–yl)-based turn-on fluorescent probe in solution and gas phase

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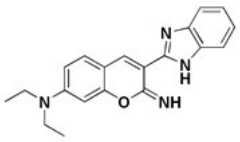
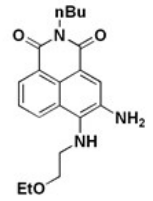
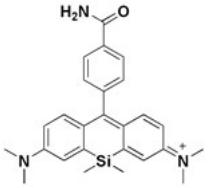
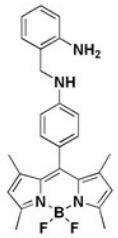
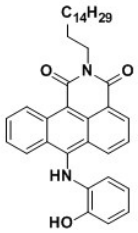
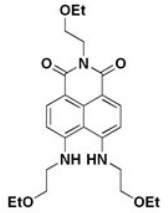
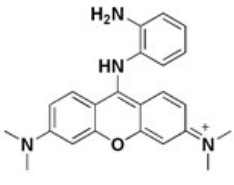
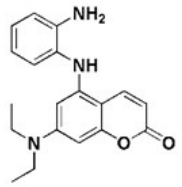
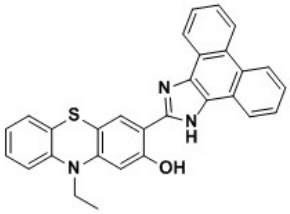
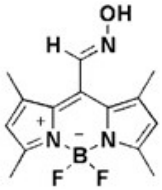
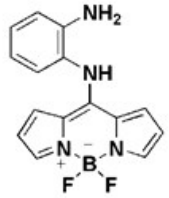
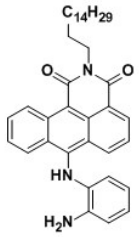
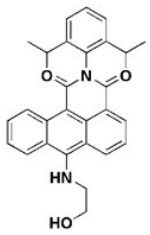
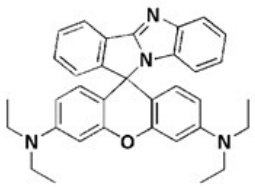
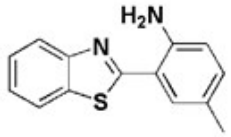
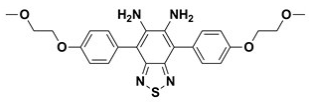
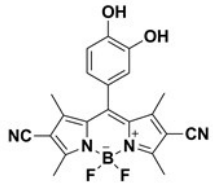
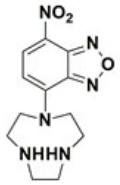
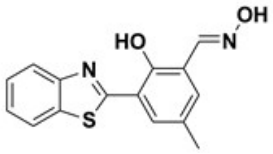
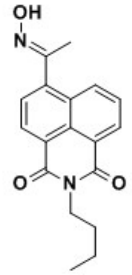
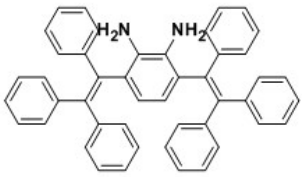
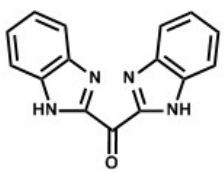
1. A mini review about recent reported phosgene fluorescent probes.

Table S1. Comparisons of recently reported strategies for phosgene detection.

Structures	Fluorescence Mode	Fluorophore	Detection limit	Response time	References
	Ratiometric	Coumarin	27 nM (Phosgene)	2 min	1
	Turn-on	Naphthalimide	0.2 nM (Triphosgene)	30 s	2
	Turn-on	Rhodamine	8.9 nM (Triphosgene)	4 min	3
	Turn-on	BODIPY	179 nM (Triphosgene)	10 s	4
	Turn-on	Anthracene carboximide	4.6 nM (Phosgene)	15 s	5
	Ratiometric	Naphthalimide	1.3 nM (Triphosgene)	20 min	6
	Turn-on	Pyronin	20 nM (Triphosgene)	2 min	7

	Turn-on	Coumarin	3 nM (Triphosgene)	0.5 min	8
	Turn-on	1H-phenanthro[9,10-d]imidazolyl	84.2 nM (Phosgene)	2 min	9
	Turn-on	BODIPY	0.09 ppb (Triphosgene)	10 s	10
	Turn-on	BODIPY	2.7 nM (Triphosgene)	15 s	11
	Turn-on	Anthracene carboxyimide	72 nM (Phosgene)	2 min	12
	Ratiometric	Anthracene carboxyimide	2.3 nM (Phosgene)	5 min	13
	Turn-on	Rhodamine	3.2 ppb (Triphosgene)	2 min	14

	Ratiometric	Benzothiazole	0.14 ppm (Phosgene)	5 min	15
	Turn-on	Benzothiadiazole	20 nM (Phosgene)	20 min	16
	Turn-on	BODIPY	24 pM (Phosgene)	within 3 s	17
	Turn-on	NBD	1.2 nM (Triphosgene)	within 20 s	18
	Turn-on	Benzothiazole	0.48 nM (Phosgene)	20 min	19
	Turn-on	Naphthalimide	6.3 nM (Phosgene)	15 min	20
	Turn-on	TPE	21 nM (Triphosgene)	2 min	21
	Turn-on	Bis-(1H-benzimidazol-2–yl)	3.3 nM (Phosgene)	Within 30 s	This Work

46 **“—” Not mentioned.**

2. NMR, ESI-MS and chromatogram spectra of Probe 1 and Compound 2.

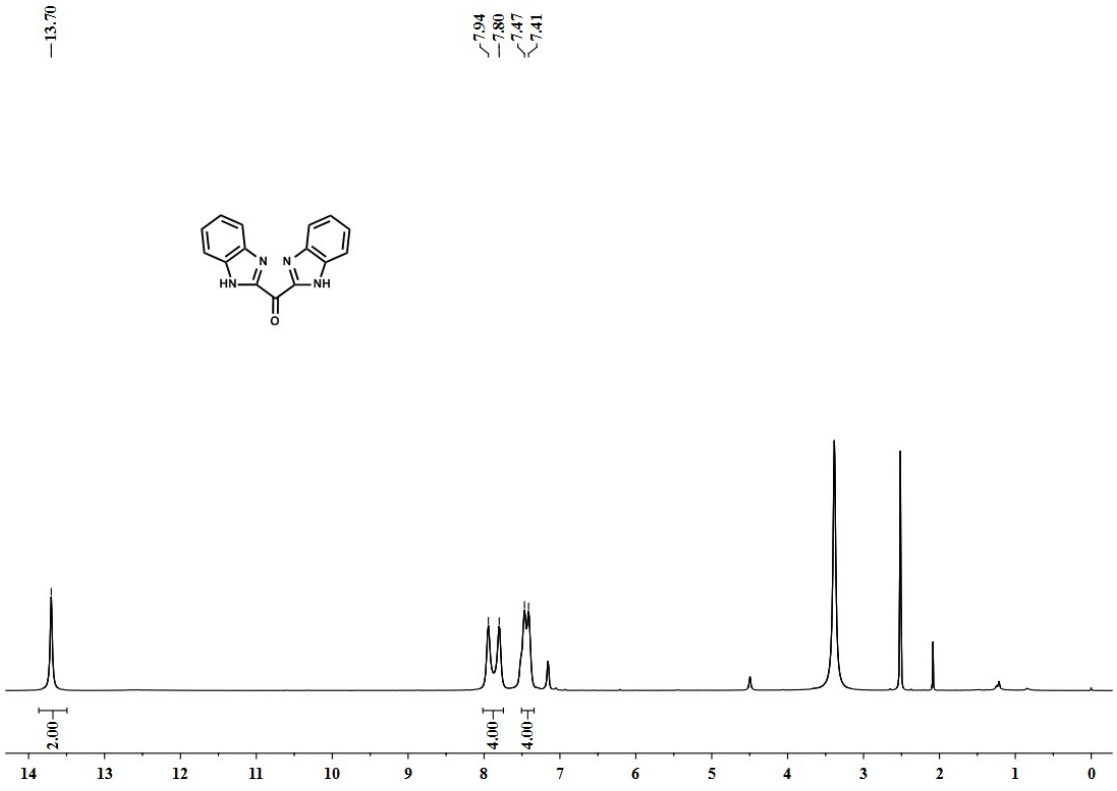


Figure S1. ^{1}H NMR spectrum of Probe 1 in DMSO-d_6 (500 MHz).

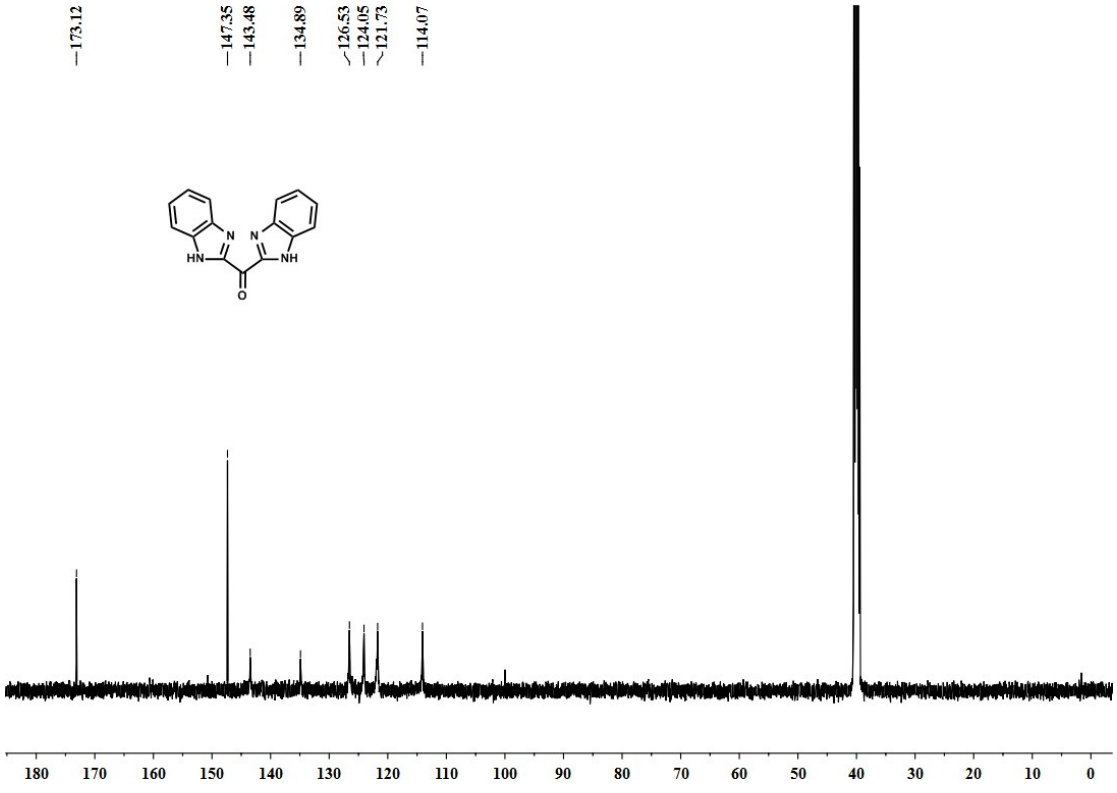


Figure S2. ^{13}C NMR spectrum of Probe 1 in DMSO-d_6 (125 MHz).

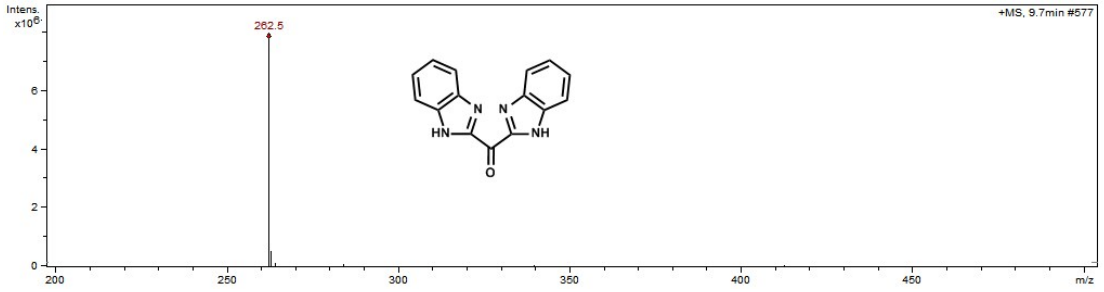


Figure S3. ESI-MS spectrum of Probe 1.

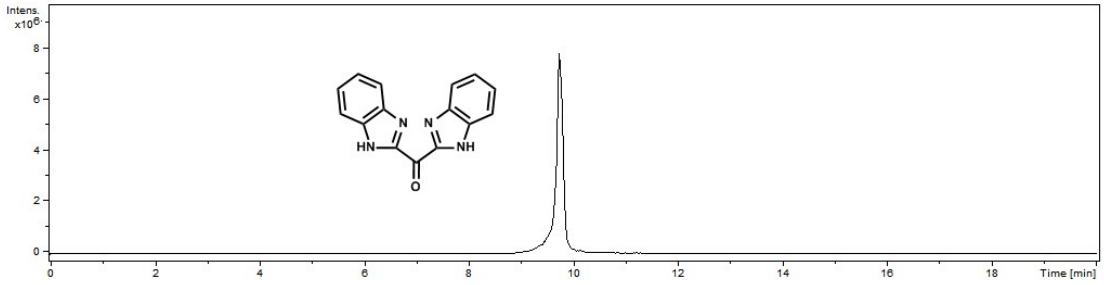


Figure S4. Chromatogram of Probe 1.

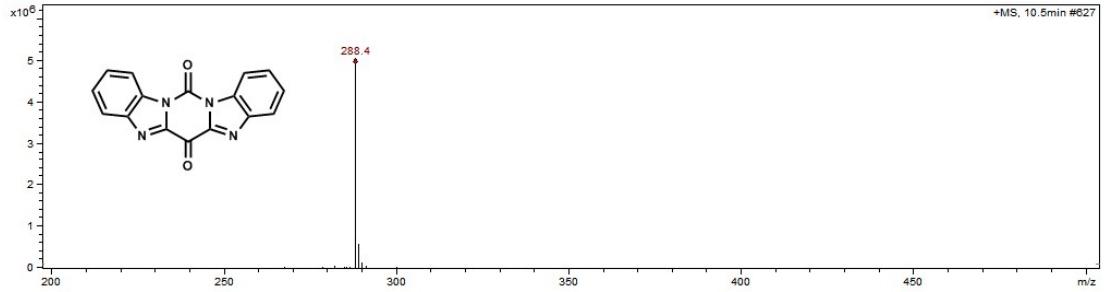


Figure S5. ESI-MS spectrum of Compound 2.

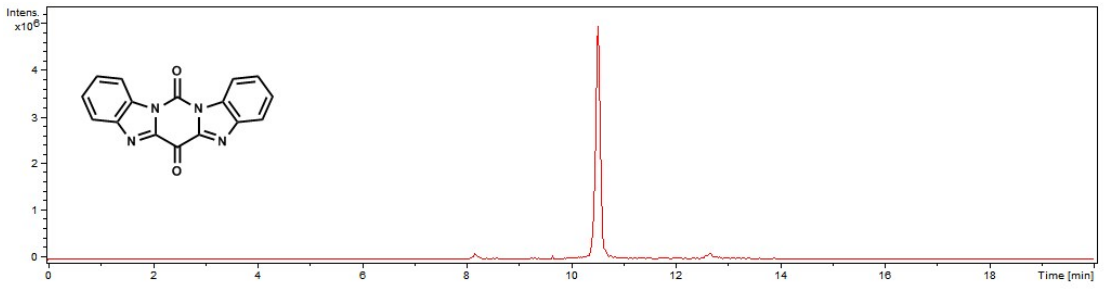


Figure S6. Chromatogram of Compound 2.

3. Determination of the fluorescence quantum yields of Probe 1 and Compound 2.

The relative quantum yield of probes was calculated according to the following equation:

$$\varphi_S = \varphi_A \times \frac{F_S}{F_A} \times \frac{A_A}{A_S} \times \frac{\eta_S^2}{\eta_A^2}$$

Where φ_S and φ_A are quantum yields of sample solutions and reference standard (Quinine sulphate in 0.1 M H_2SO_4 was used in this work, φ_A = 0.54); F_S and F_A are the corresponding integrated fluorescence intensities of quinine sulphate and sample solutions (λ_{ex}=360 nm); A_A and A_S are the absorbance of quinine sulphate and sample solutions at the same excitation; η_S and η_A are the refractive index of the solvents used.

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