

Tailored BODIPY-based Fluorogenic Probes for Phosgene Detection: A Comparative Evaluation of Recognition Sites

Supporting Information

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1. Determination of Detection Limits

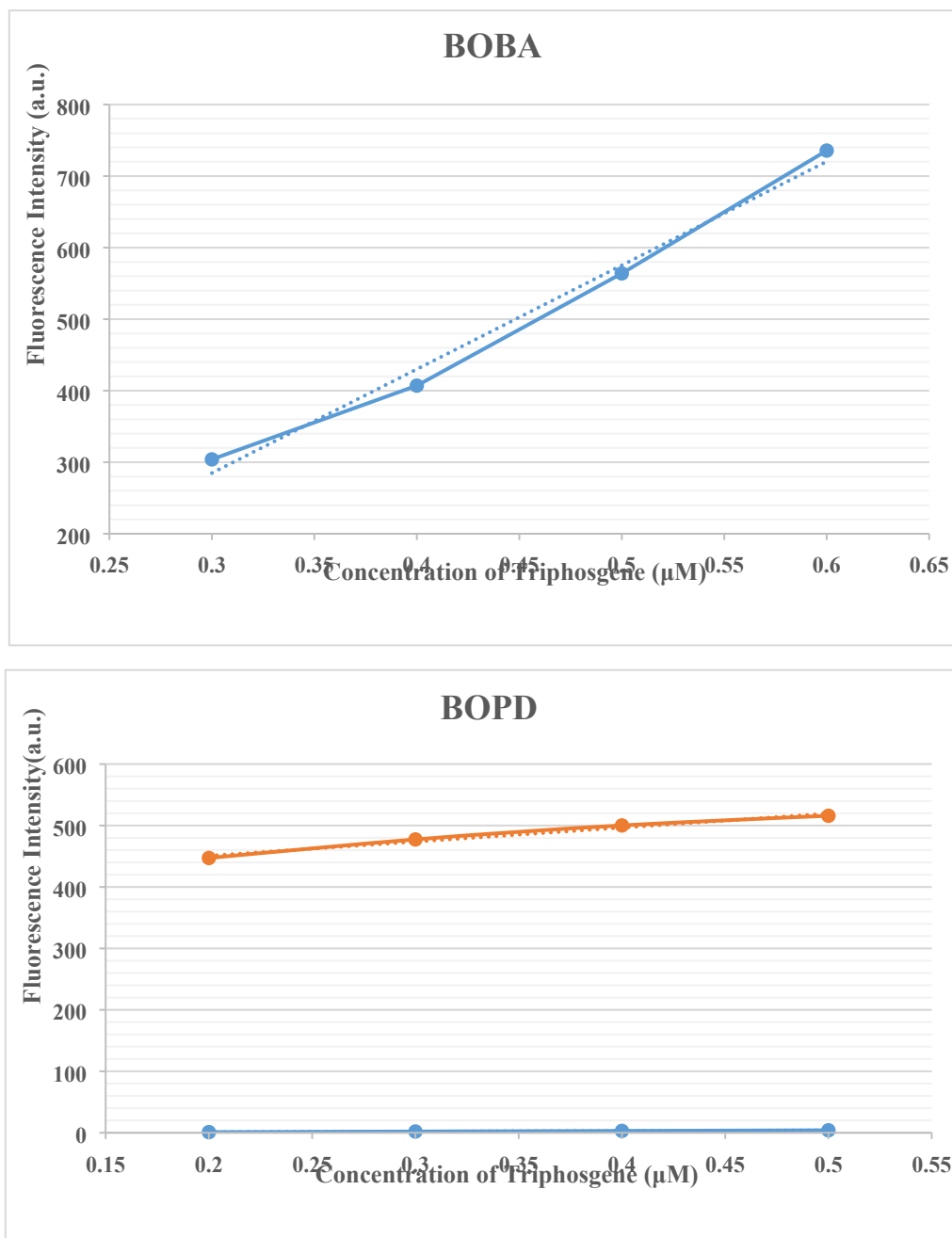


Figure S1. Fluorescence changes of **BOBA** (5 μM , λ_{ex} :500 nm) and **BOPD** (5 μM , λ_{ex} :500 nm) upon addition of triphosgene (0.1 to 0.9 μM) in CH_3CN .

2. Time Profiles of BOPD and BOBA towards Triphosgene

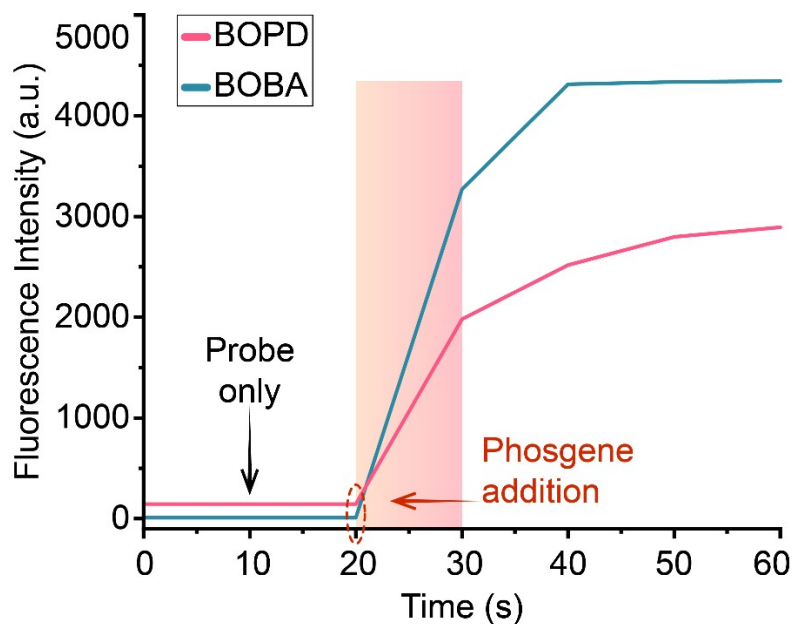


Figure S2. Time-dependent fluorescence change **BOBA** ($5 \mu\text{M}$, λ_{ex} :500 nm) and **BOPD** ($5 \mu\text{M}$, λ_{ex} :500 nm) in the presence of triphosgene (5 equiv.) in CH_3CN .

3. Images of BOPD-loaded TLC Plates

For the solid-state performance of **BOPD**, silica TLC plates were treated with 200 μL **BOPD** solution. After air drying process, TLC plates were exposed to different concentrations of phosgene gas (from 0.1 ppm to 30 ppm). The production of phosgene gas was mentioned in the paper.



Figure S3. Images of fluorescence responses of TLC plates impregnated with **BOPD** (200 μM) upon exposure to various concentrations of phosgene gas (left to right: 0 ppm, 0.1 ppm, 5 ppm, 10 ppm, 30 ppm).

4. SEM micrographs of BOPD-loaded melt-blown nonwovens

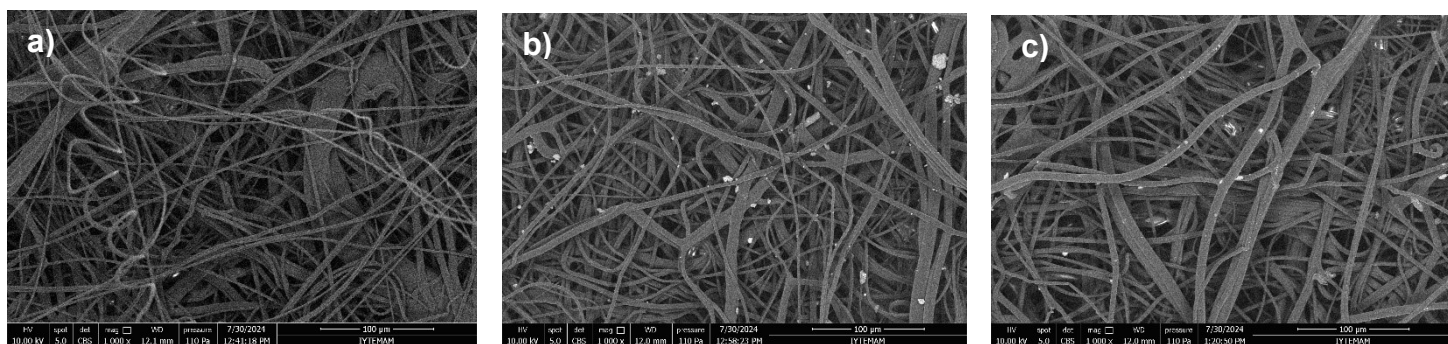


Figure S4. SEM images of a) only melt-blown nonwovens b) loaded with **BOPD** (200µM) c) after exposure to phosgene gas (30 ppm).

5. NMR Characterization of Molecules

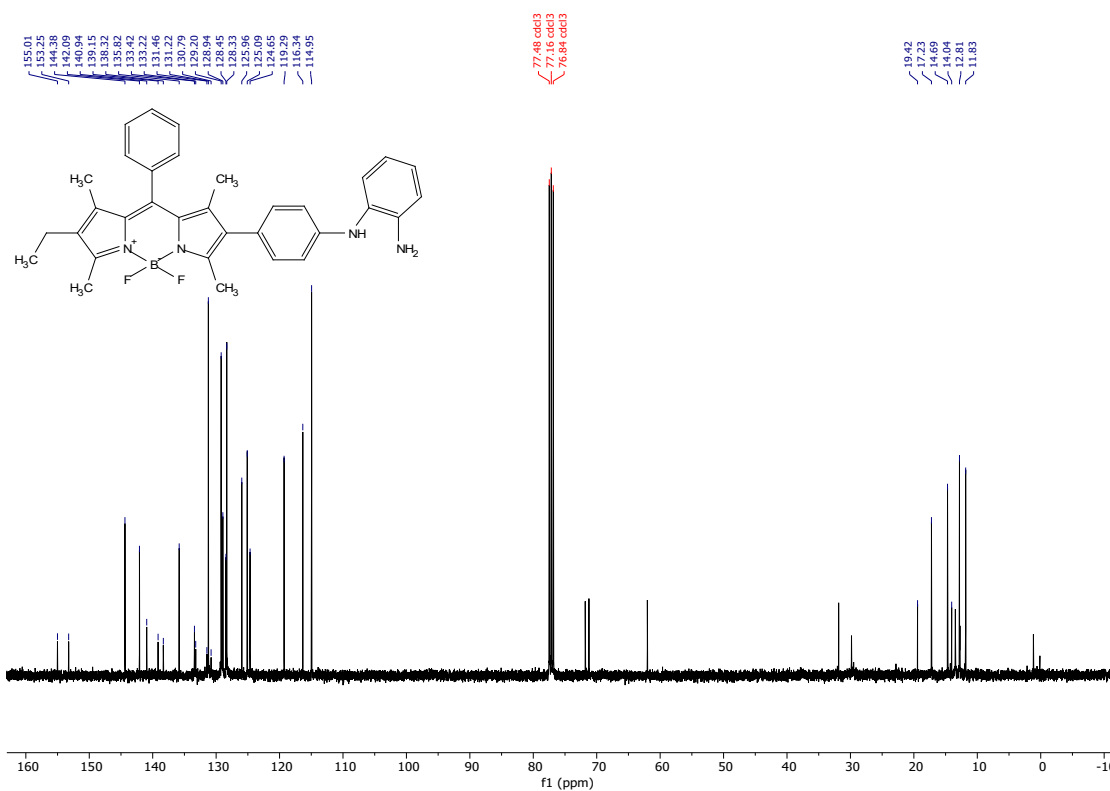
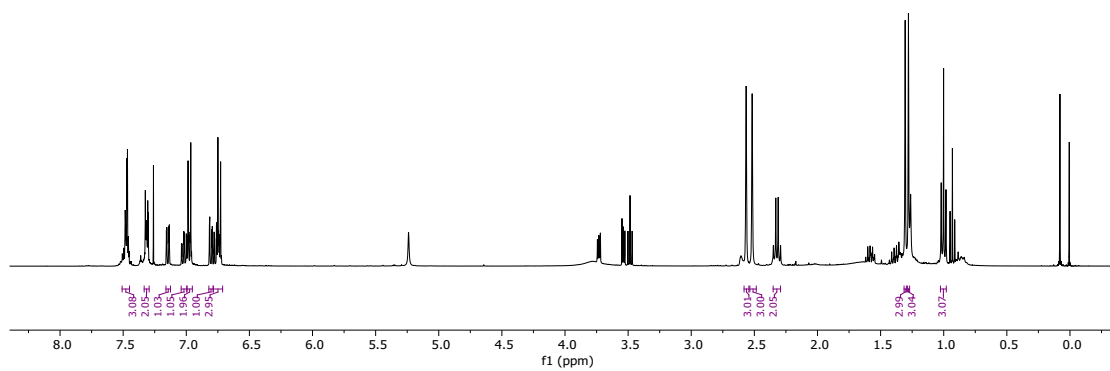
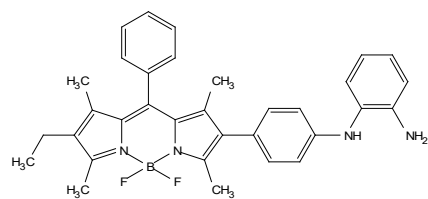


Figure S5. ^1H NMR and ^{13}C NMR Spectra of BOPD

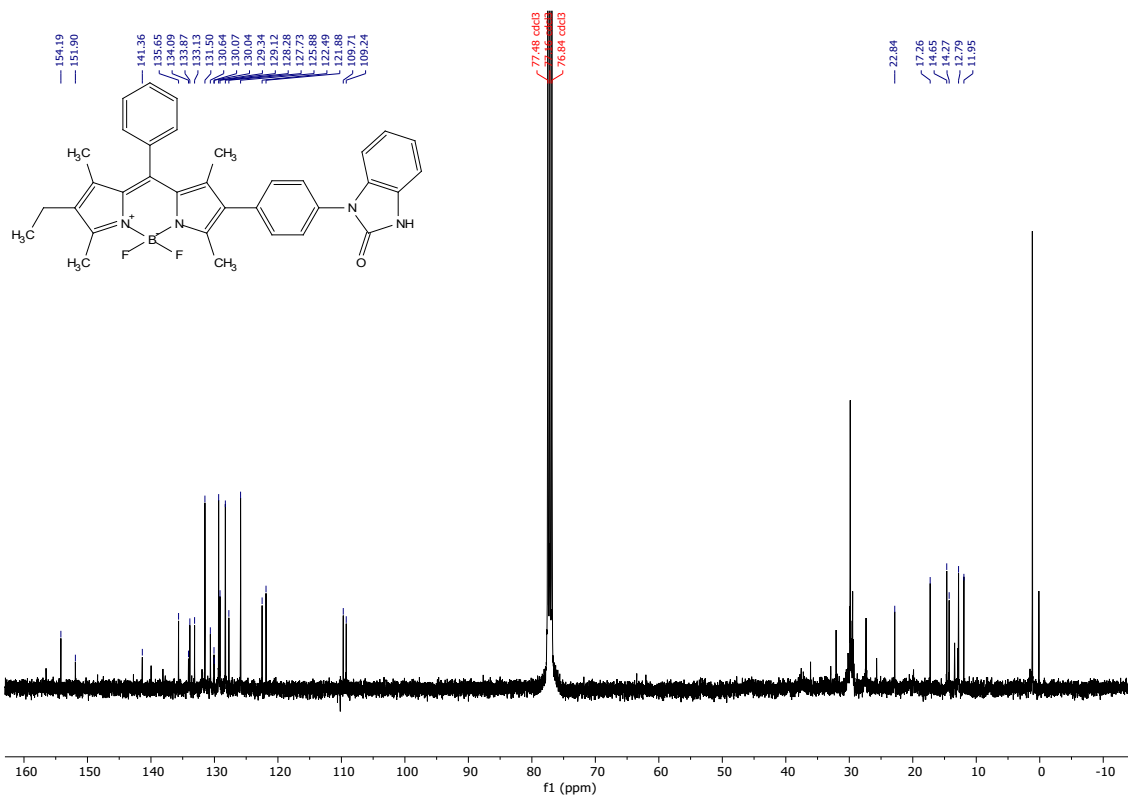
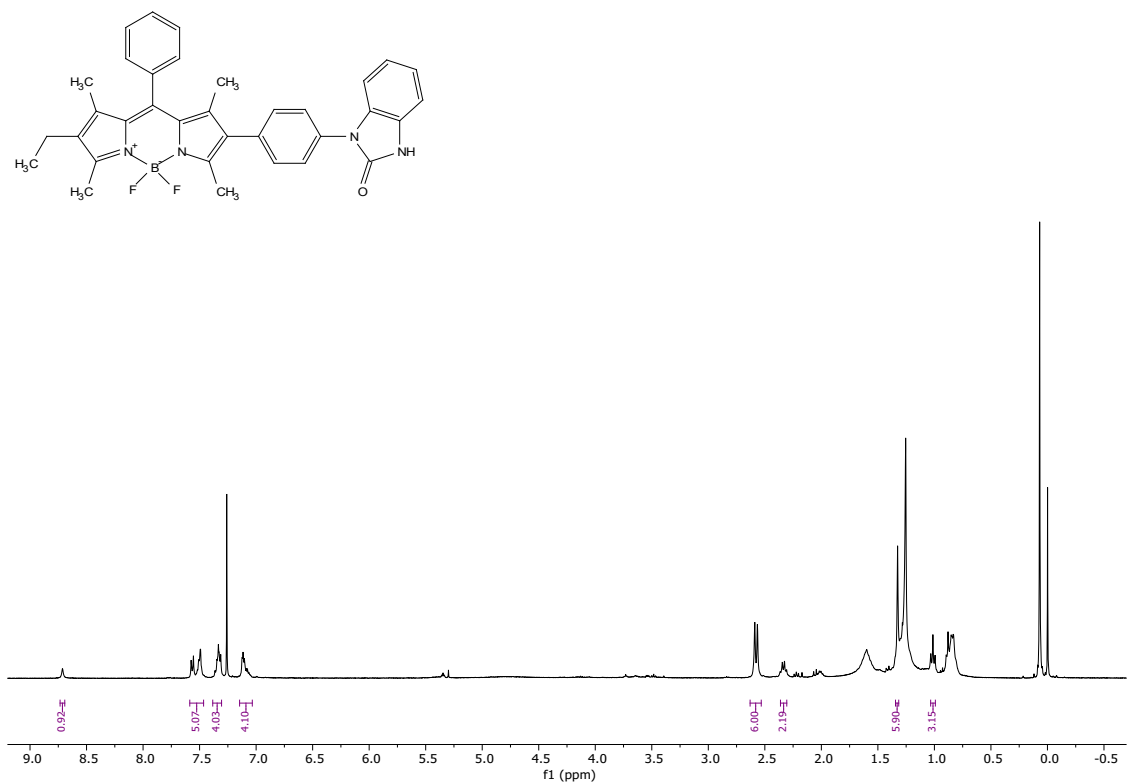


Figure S6. ^1H NMR and ^{13}C NMR Spectra of BOPD-PHOS

BOBA

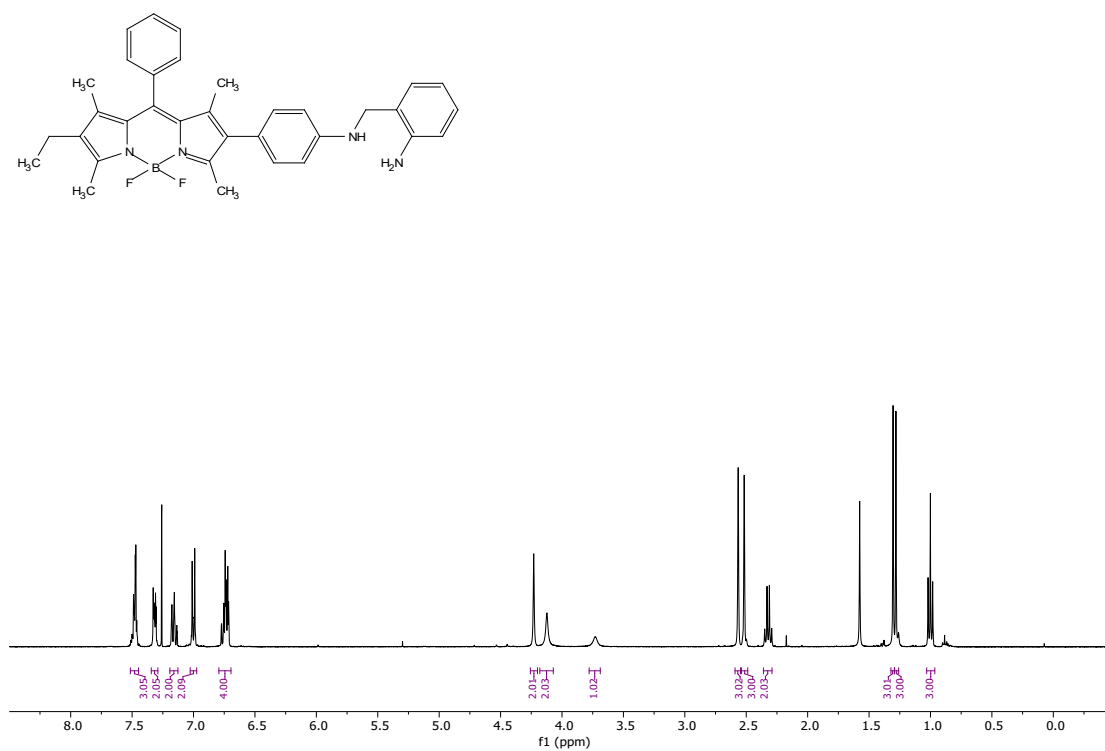


Figure S7. ¹H NMR Spectrum of BOBA

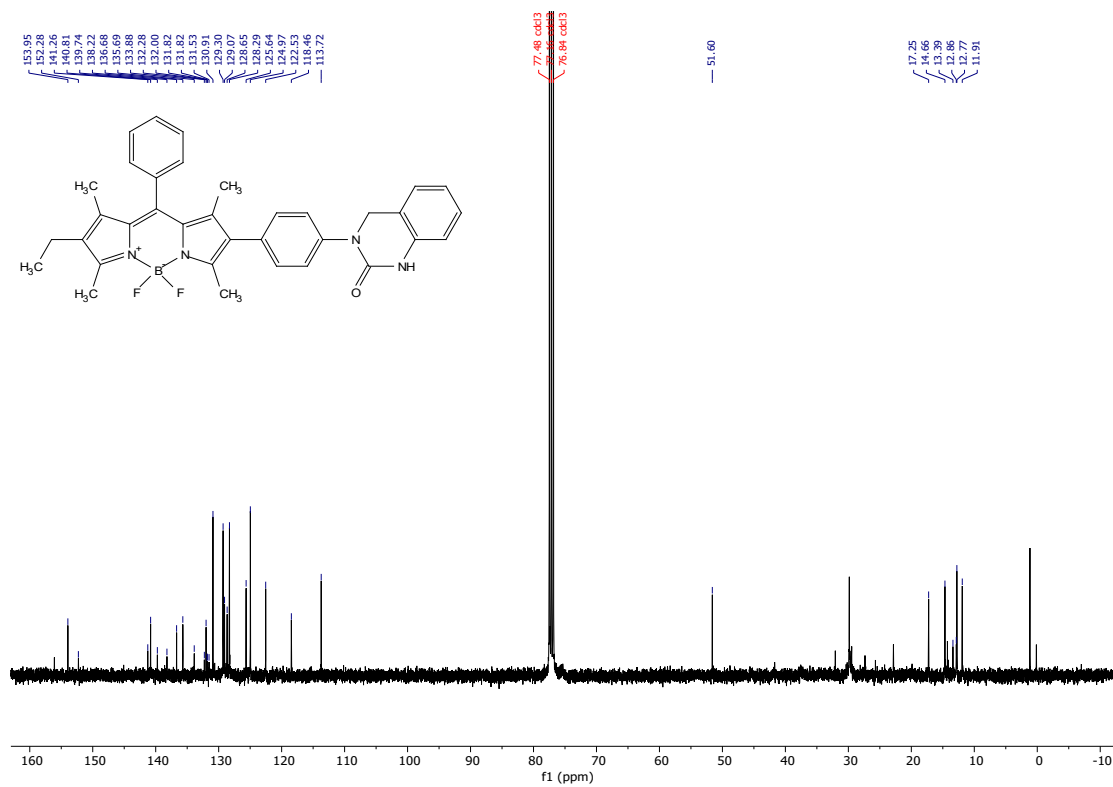
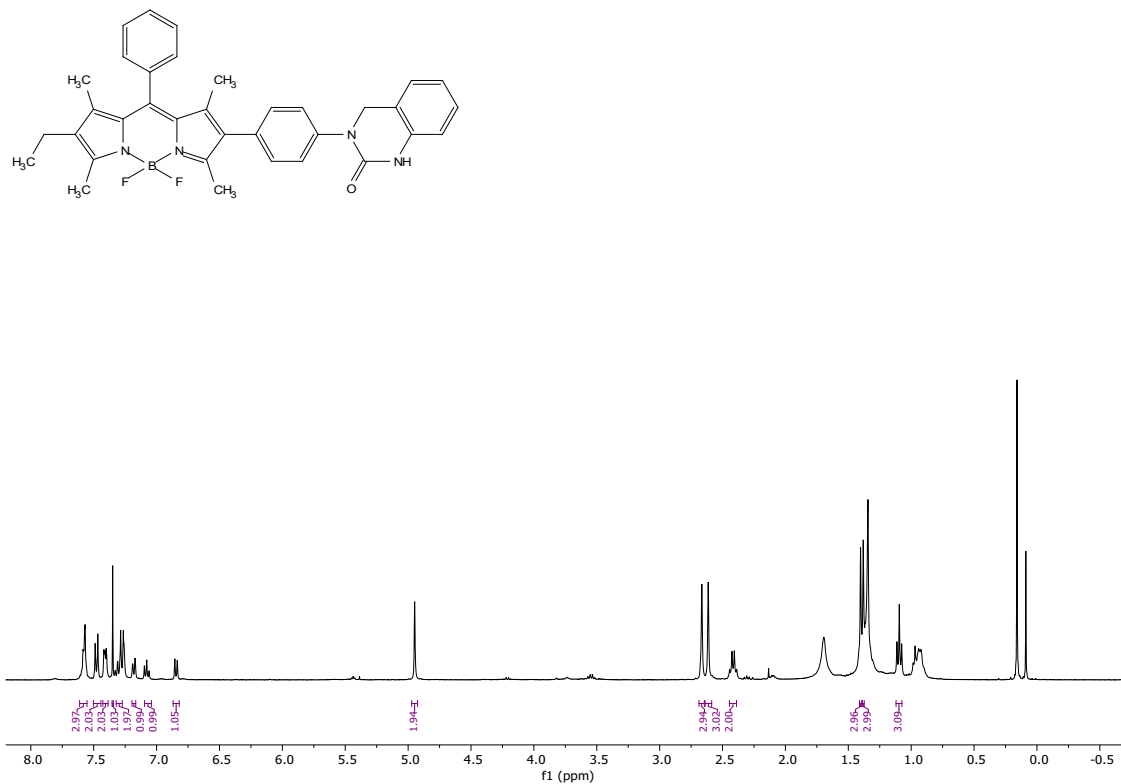


Figure S8. ¹H NMR and ¹³C NMR Spectra of BOBA-PHOS

6. HRMS Results for the BOBA and BOPD

User Spectra

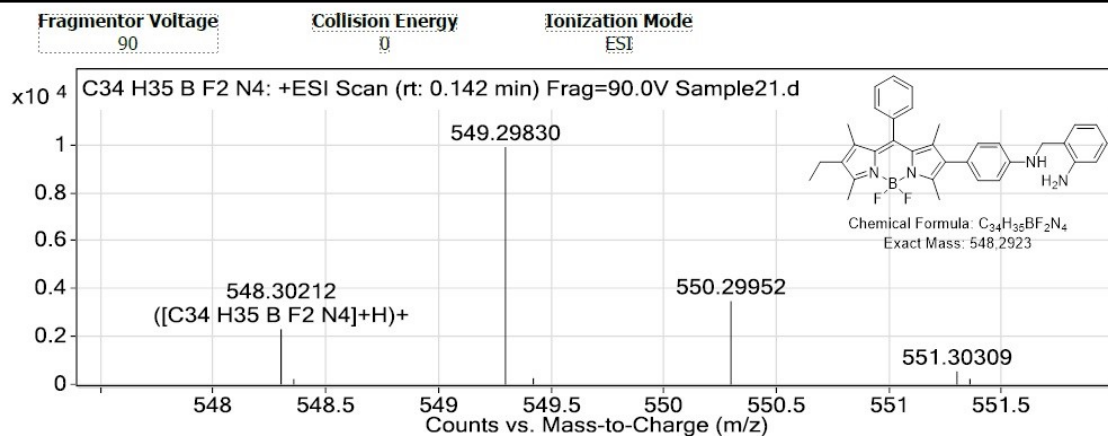


Figure S9. HRMS Spectrum of BOBA

User Spectra

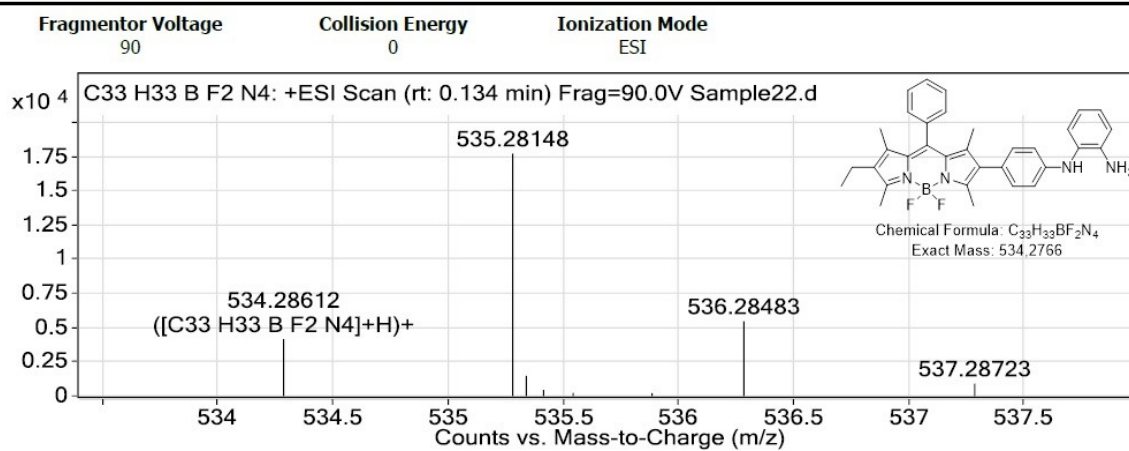
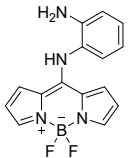
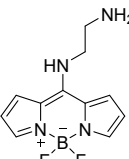
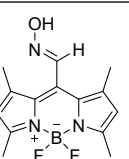
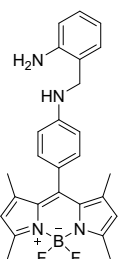
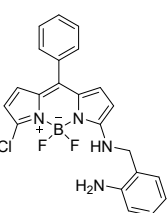
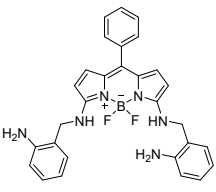
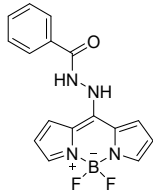
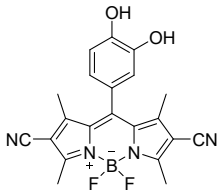
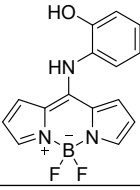
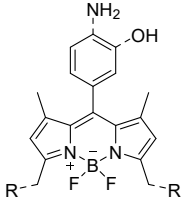
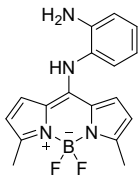
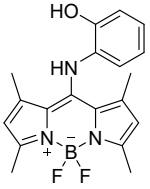
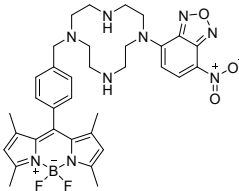
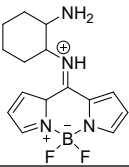
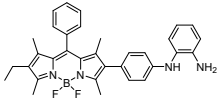


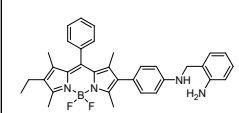
Figure S10. HRMS Spectrum of BOPD

7. Recently reported BODIPY-based phosgene responsive fluorescent probes

Table S1. Comparison of analytical performance of BODIPY-based phosgene probes

Probe	Structure	Sensing Mechanism	Detection Limit	Responsive time	Switching Mechanim	Ref. No
o-Pab		PET	2.7 nM	~15s	Turn-on	1
8-EBAB		ICT	0.12 nM	< 1.5s	Turn-on	2
1-oxime		No data	0.31 nM	< 10s	Turn-on	3
BOD-SYR		PET	179 nM	< 10s	Turn-on	4
1		ICT	0.81 nM	30s	Turn-on	5
2		ICT	2.36 nM	2 min	Ratiometric	5
Bohz		PET	0.15 nM	1.5s	Turn-on	6

1-CN		PET	24 pM	3s	Turn-on	7
BODIPY-OHA		PET	0.22 nM	2s	Turn-on	8
o-pha o-pah o-phac		TICT	0.34 nM 1.2 nM 0.88 nM	10s 200s 60s	Turn-on	9
BDY		PET	14 nM	9s	Turn-on	10
ONB		PET	1.2 nM	< 2s	Turn-on	11
F671		FRET	0.36 nM	6s	Turn-on	12
BODIPY-DCH BDP-CHD		PET	0.52 nM 51.4 ppt	< 3s	Ratiometric	13,14
BOPD		ICT	126 nM	< 10s	Turn-on	Our probe

BOBA		ICT	0.89 nM	< 30s	Turn-on	Our probe
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8. References

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