Supporting Information for "New BODIPY Derivatives as OFF-ON Fluorescent Chemosensor and Fluorescent Chemodosimeter for Cu^{2+}: Cooperative Selectivity Enhancement towards Cu^{2+}"

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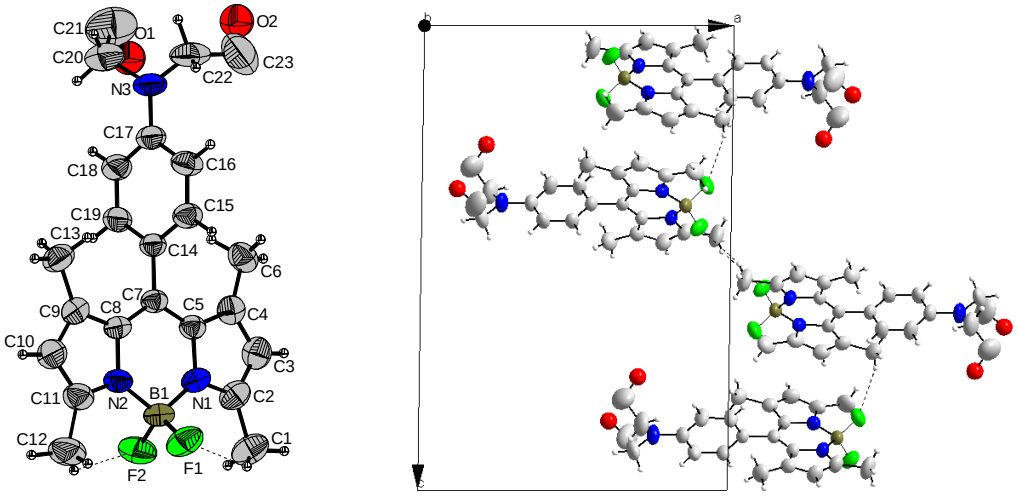
Experimental Section

General methods. Unless otherwise noted, materials were obtained from commercial suppliers and were used without further purification. Flash chromatography was carried out on silica gel (230-400 mesh). Melting points were measured, and are uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded using 250 MHz or 500 MHz NMR. Chemical shifts were expressed in ppm and coupling constants (*J*) in Hz. Electrospray ionization mass (ESI MS) was taken by infusing samples directly into the source at 20ul/min using a syringe pump. The spray voltage was set at 3KV and the capillary temperature at 150 ^{o}C.



S-Figure 1. X-ray crystal structures of the compound **1** and the packing of the compound **1** in the unit cell.

S-Table 1. Hydrogen-bonding geometry (Å, º) for **2**

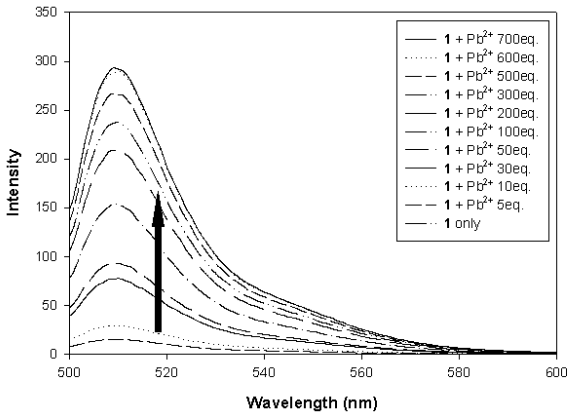
D-H…A	D-H	H…A	D…A	D-H…A
C15-H15C…F1^{i}	0.96	2.45	3.293(4)	146
C1-H1A…F1	0.96	2.61	3.122(3)	114
C1-H1C…F1^{ii}	0.96	2.70	3.145(6)	109

Symmetry code: (i) 0.5+x, 1.5-y, 0.5+z; (ii) 2-x, y, 1.5-z.

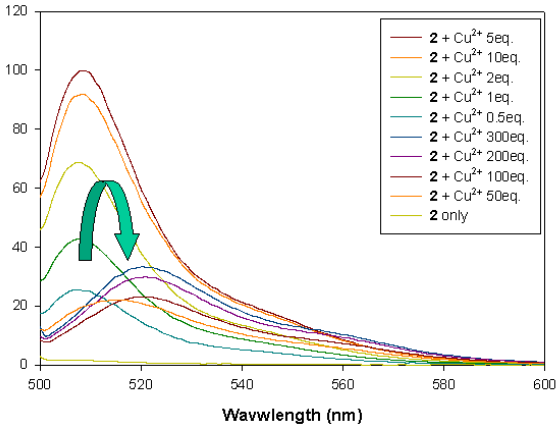
S-Table 2. Hydrogen-bonding geometry (Å, º) for **1**

D-H…A	D-H	H…A	D…A	D-H…A
C6-H6C...F2^{i}	0.96	2.646(1)	3.525(1)	152
C12-H12C…F1^{ii}	0.96	2.545(3)	3.356(3)	142
C1-H1A…F1	0.96	2.581(2)	3.224(2)	125
C12-H12A…F2	0.96	2.415(2)	3.082(4)	126

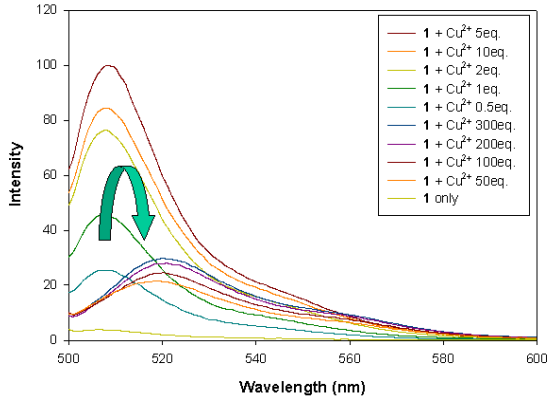
Symmetry code: (i) -0.5-x, 0.5+y, 0.5-z; (ii) -1-x, 1-y, -z.



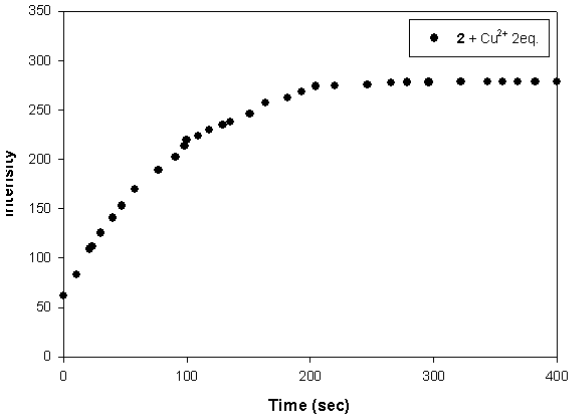
S-Figure 2. Fluorescent titrations of **1** (1 μM) upon addition of Pb^{2+} in acetonitrile (excitation at 504 nm).



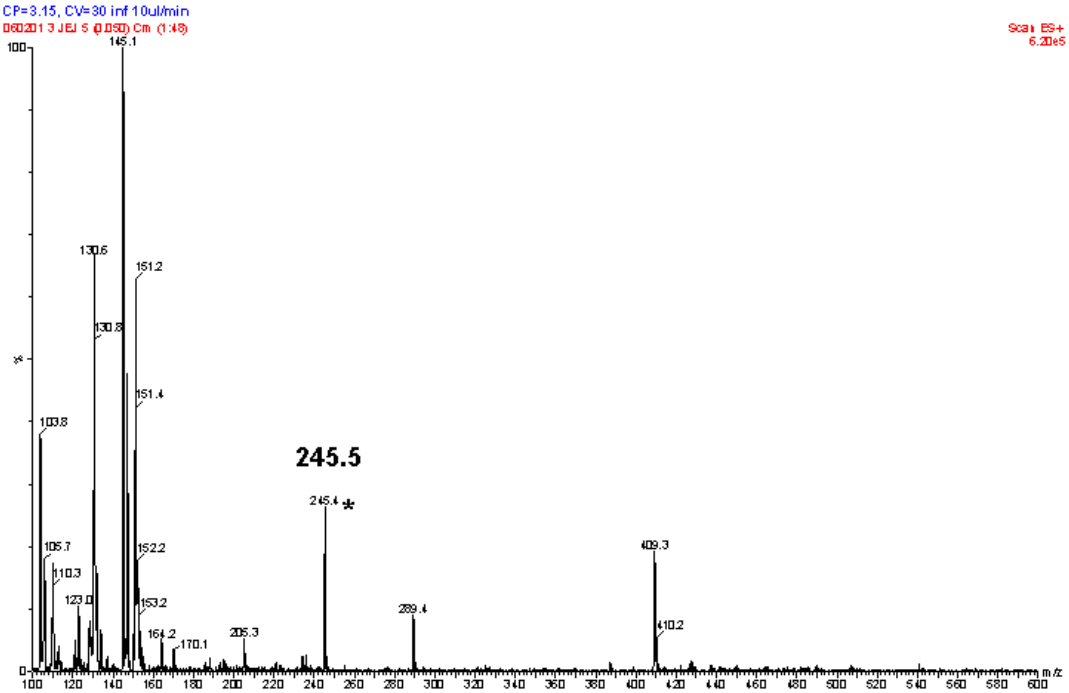
S-Figure 3. Fluorescent titrations of **2** (1 μM) upon addition of Cu^{2+} in acetonitrile (containing 0.5 % water) (excitation at 504 nm).



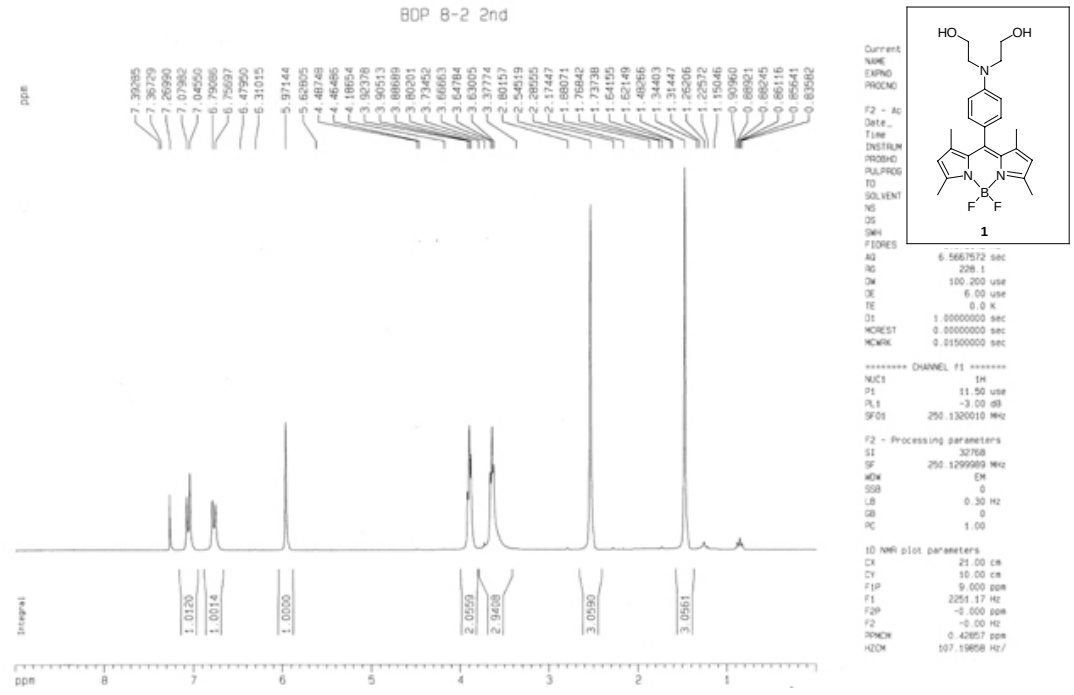
S-Figure 4. Fluorescent titrations of **1** (1 μM) upon addition of Cu^{2+} in acetonitrile (containing 0.5 % water) (excitation at 504 nm).



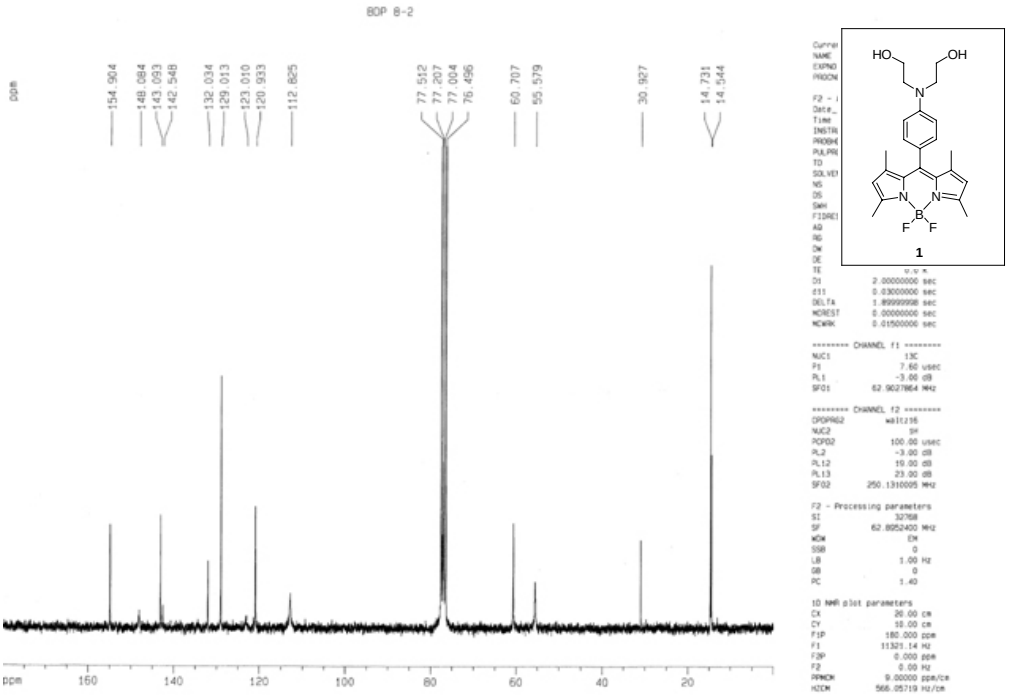
S-Figure 5. An assay of compound **2** (1 μM) for Cu^{2+}(2 eq.) in acetonitrile. (excitation at 504 nm, emission at 510 nm).



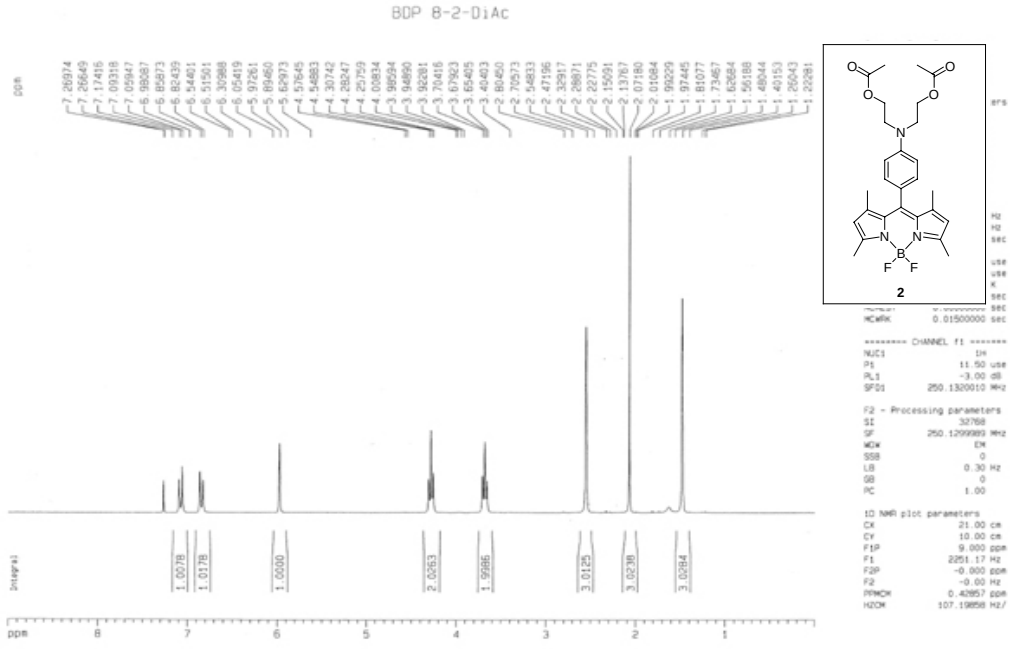
S-Figure 6. Electrospray ionization mass spectrum after hydrolysis of **2** in the presence of Cu2+ (10 eq.) in acetonitrile (containing 0.5 % water) (*m/z* 245.5corresponds to [**1** + Cu]$^{2+}$).



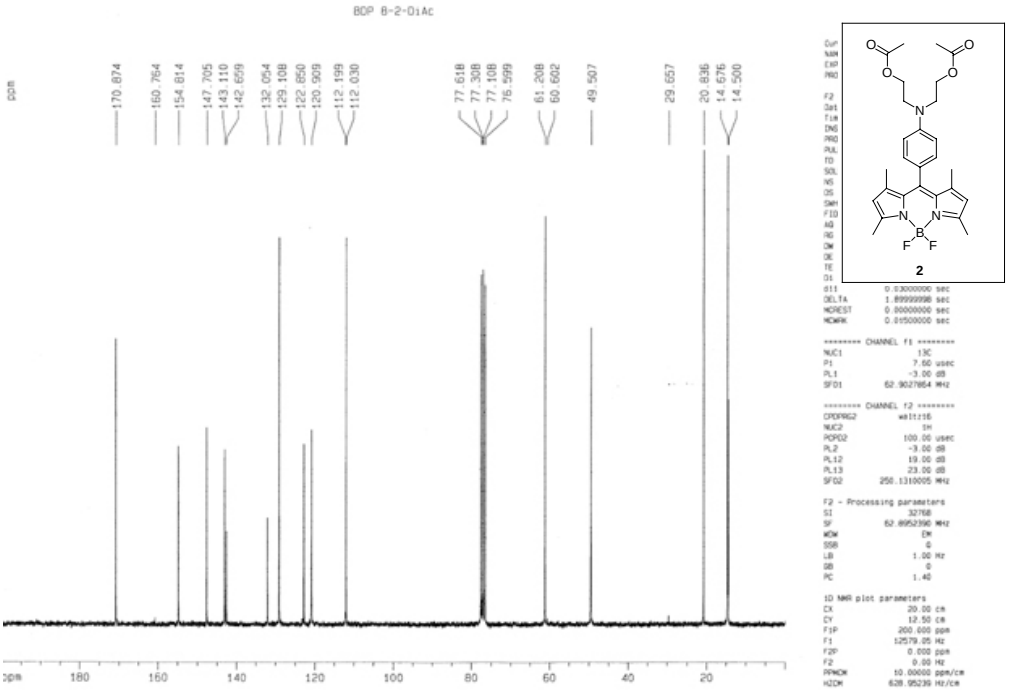
S-Figure 7. ^{1}H NMR (250 MHz) of compound **1** in $CDCl_3$.



S-Figure 8. ^{13}C NMR (62.5 MHz) of compound **1** in $CDCl_3$.



S-Figure 9. ^{1}H NMR (250 MHz) of compound **2** in $CDCl_3$.



S-Figure 10. ^{13}C NMR (62.5 MHz) of compound **2** in $CDCl_3$.