

Electronic Supplementary Information for

Molecular Rotors of BOSCHIBAs as Endoplasmic Reticulum fluorescent probe in HeLa and human umbilical vein endothelial cells

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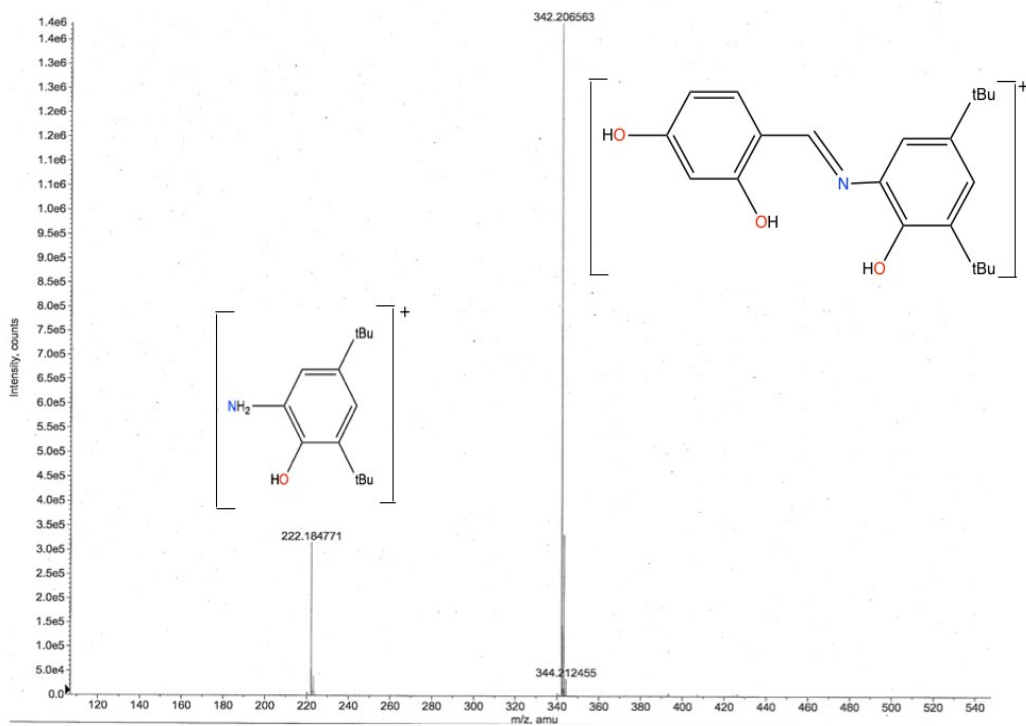


Figure S1. High resolution mass spectrum of **1**.

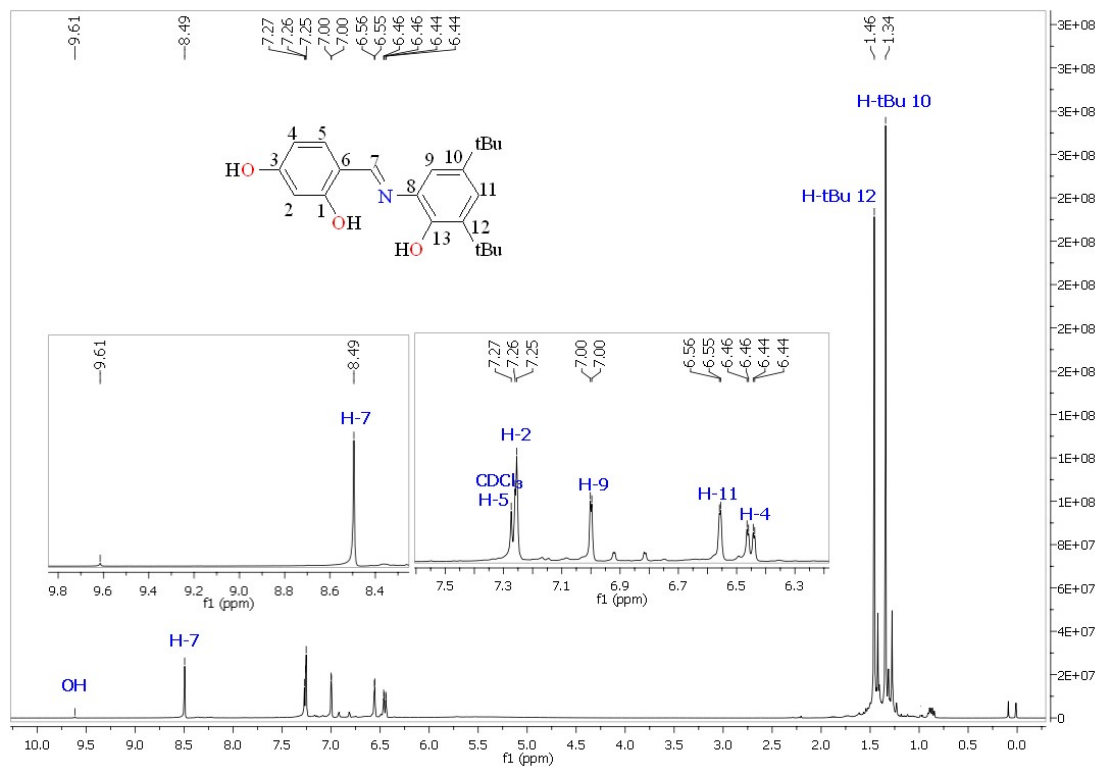


Figure S2. ^1H NMR (400 MHz, CDCl_3) spectrum of **1**.

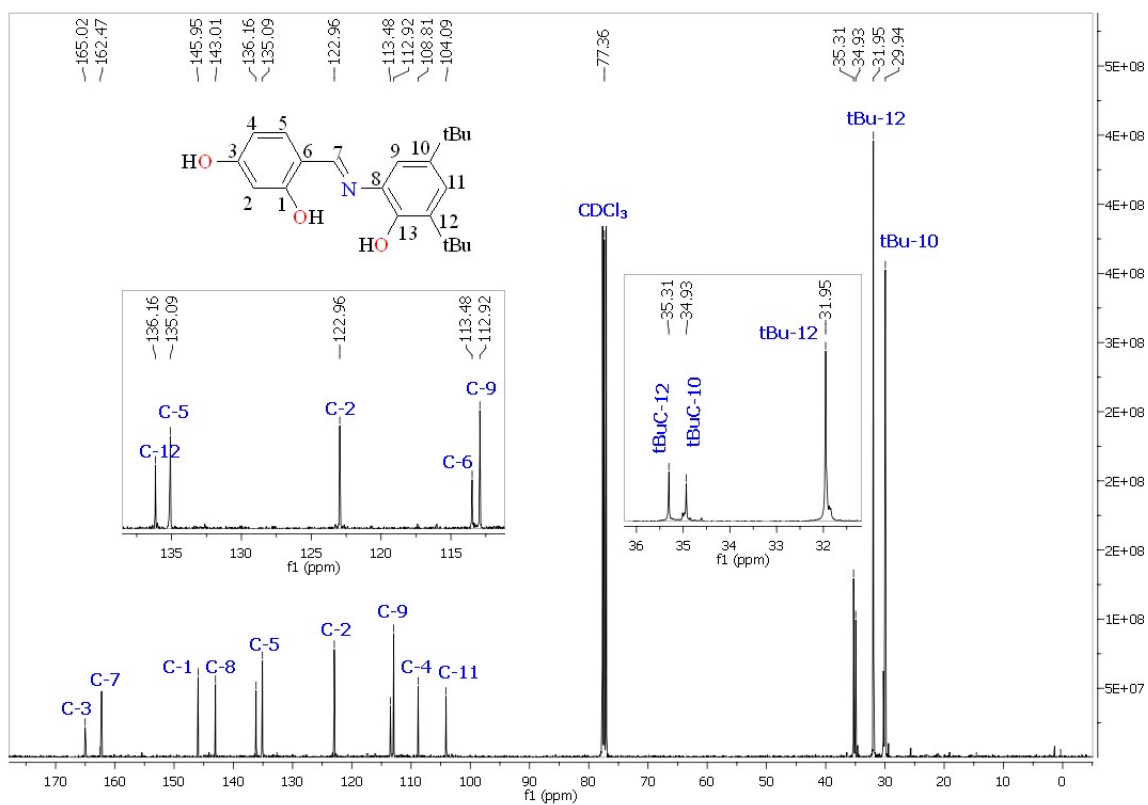


Figure S3. ¹³C NMR (CDCl₃) spectrum of 1.

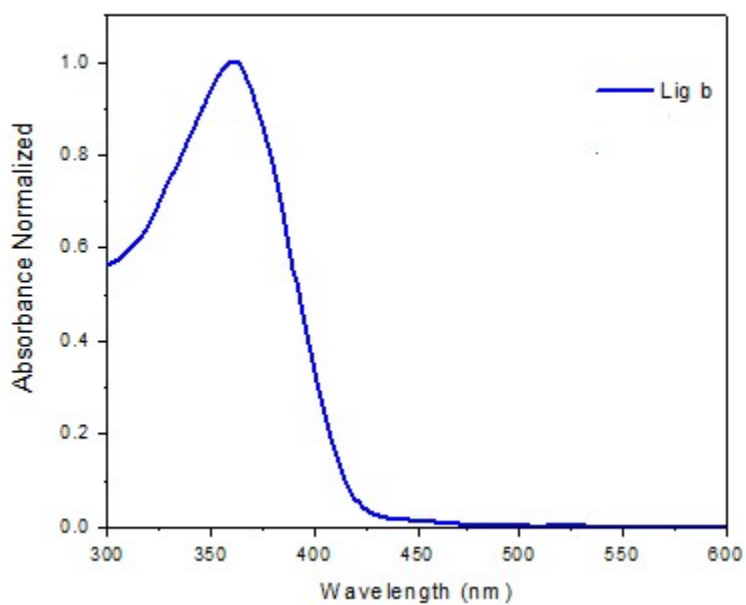


Figure S4. Absorbance of 1 in CHCl₃.

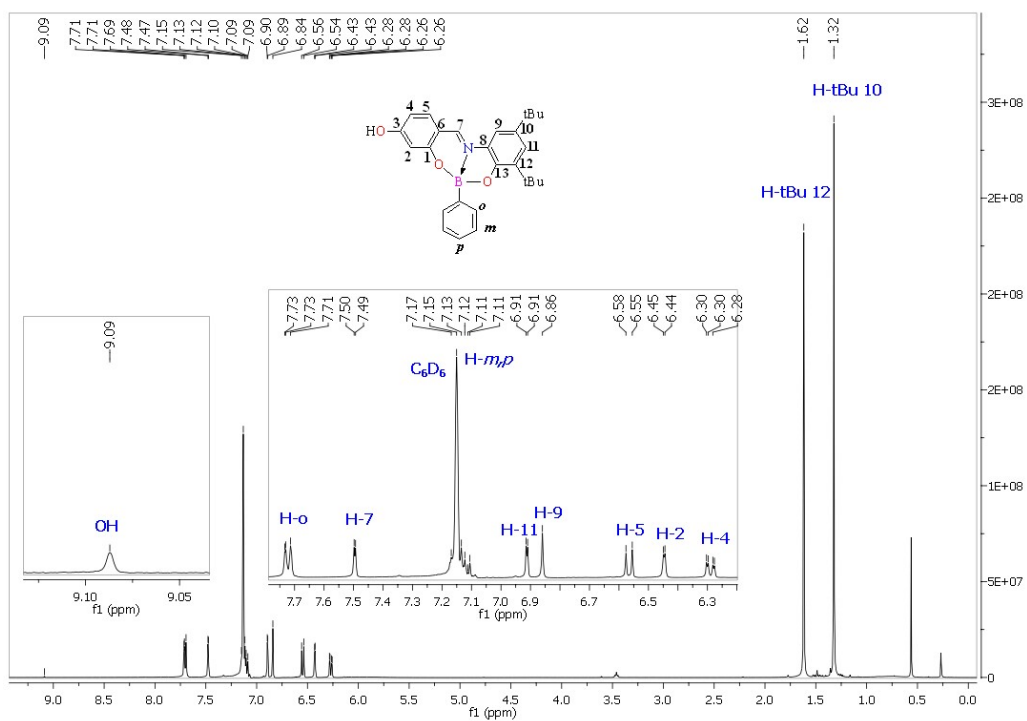


Figure S5. ^1H NMR (C_6D_6) spectrum of **2**.

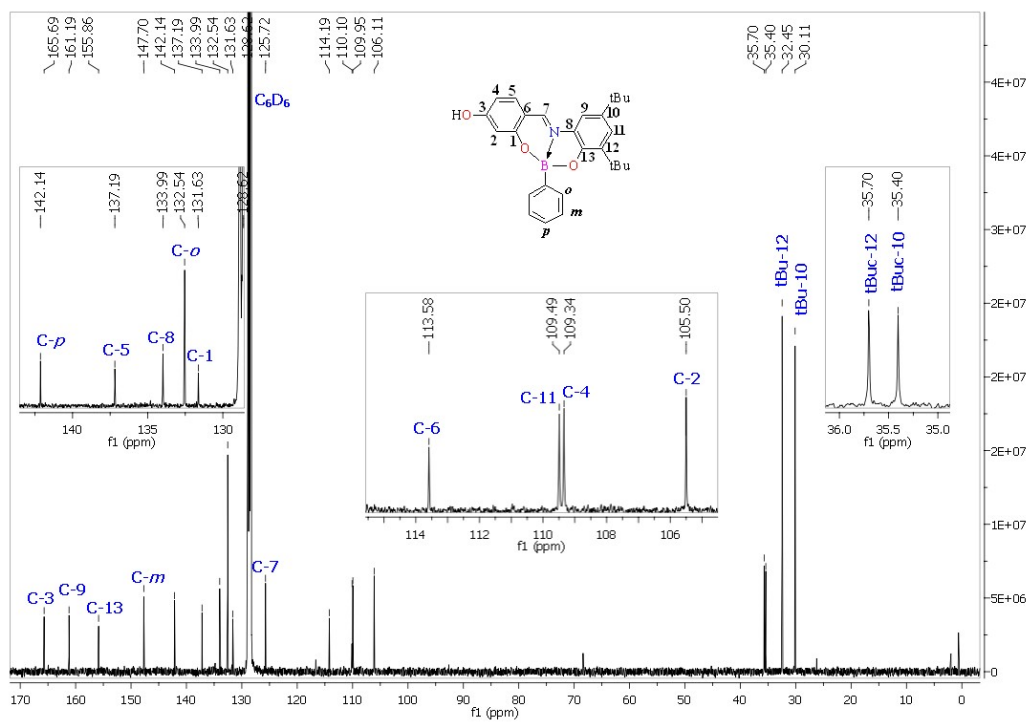


Figure S6. ^{13}C NMR (C_6D_6) spectrum of **2**.

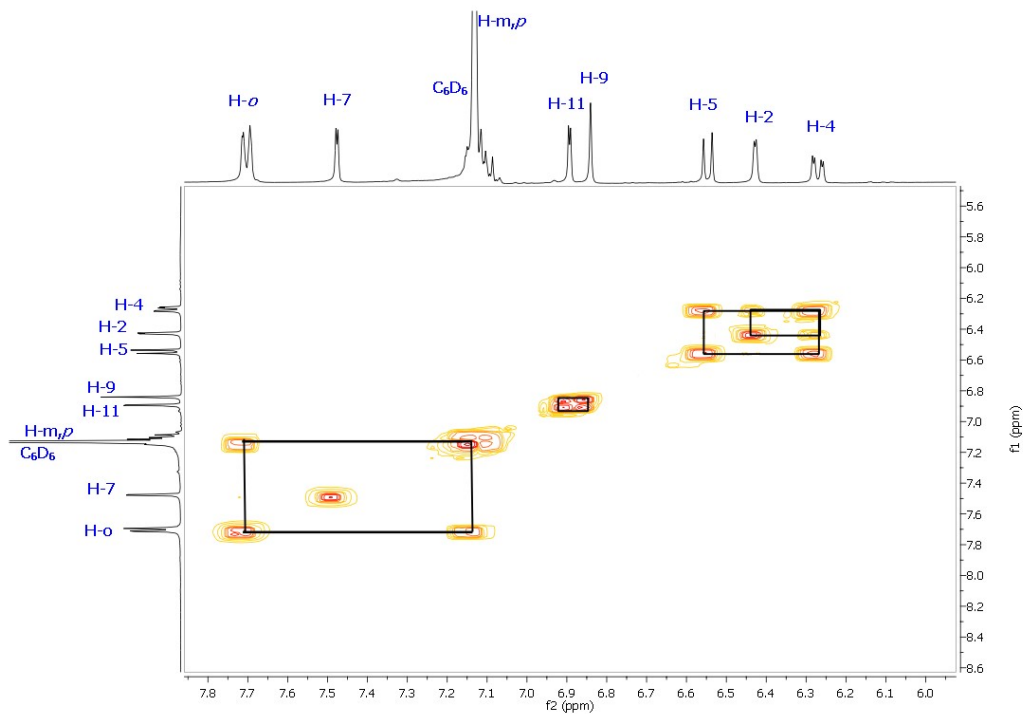


Figure S7. COSY spectra in C_6D_6 of **2**.

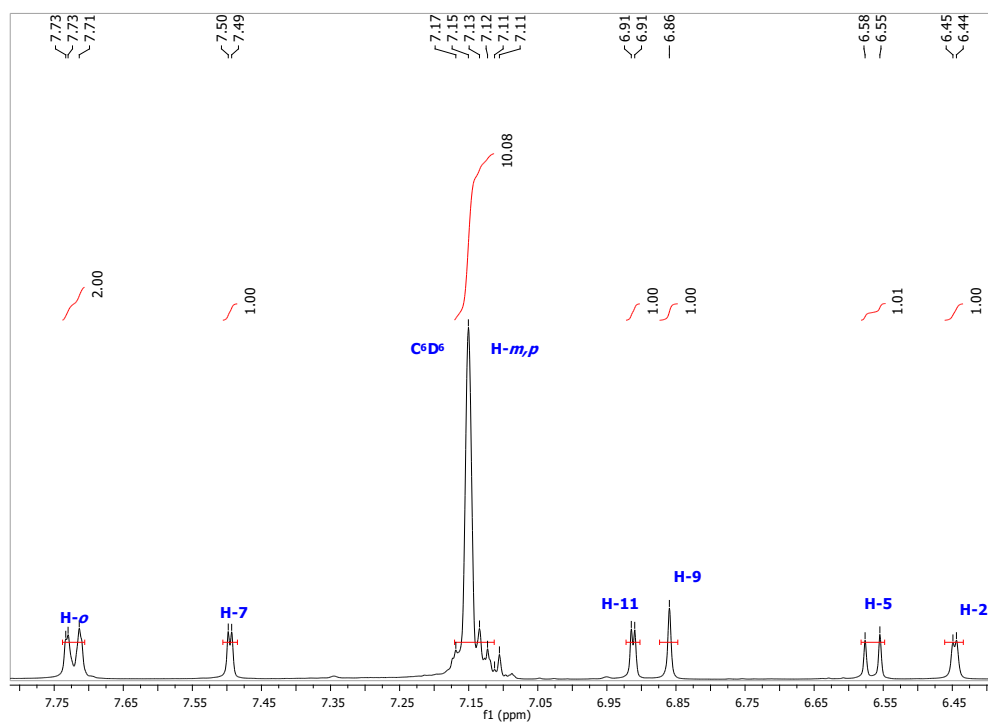


Figure S8. Integration spectra in C_6D_6 of **2**.

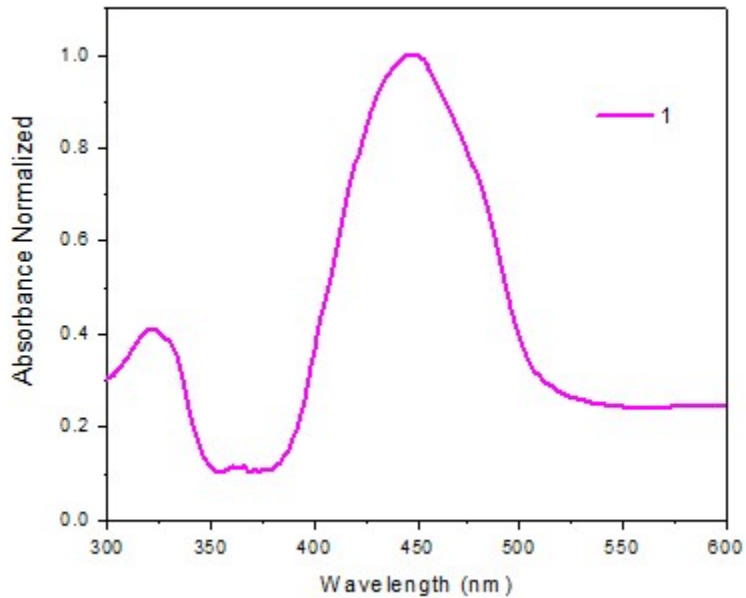


Figure S9. Absorbance of **2** in CHCl_3 .

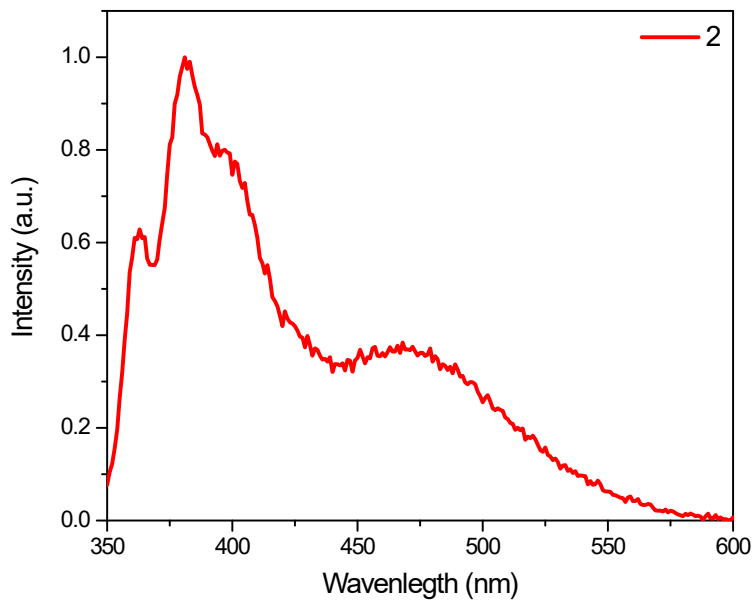


Figure S10. Emission of **2** in CHCl_3 .

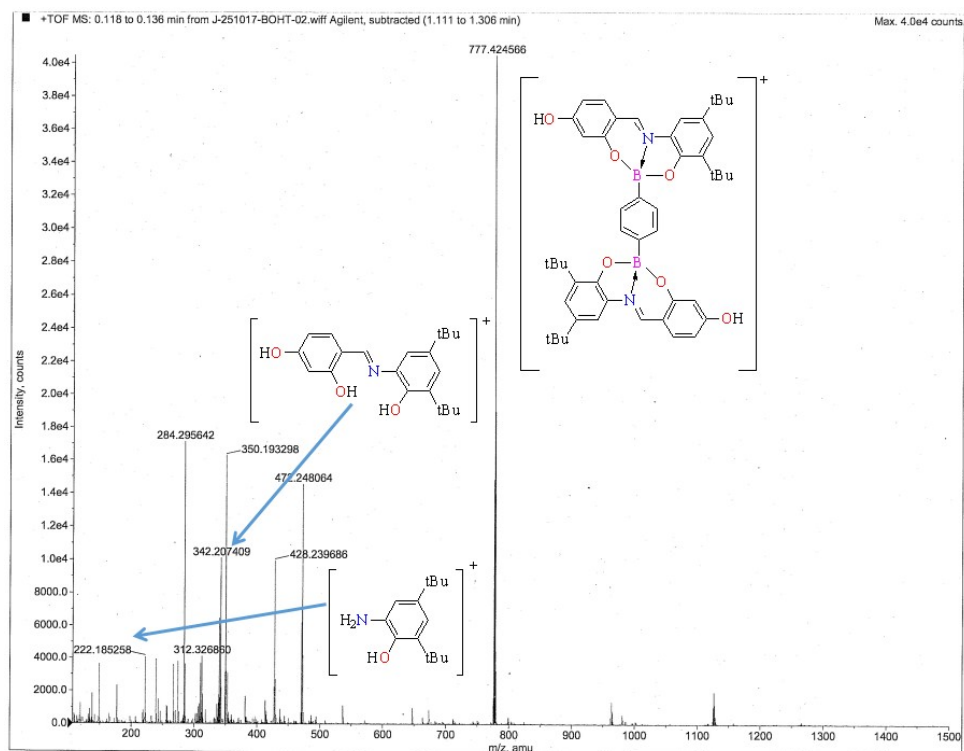


Figure S11. High resolution mass spectrum of **3**.

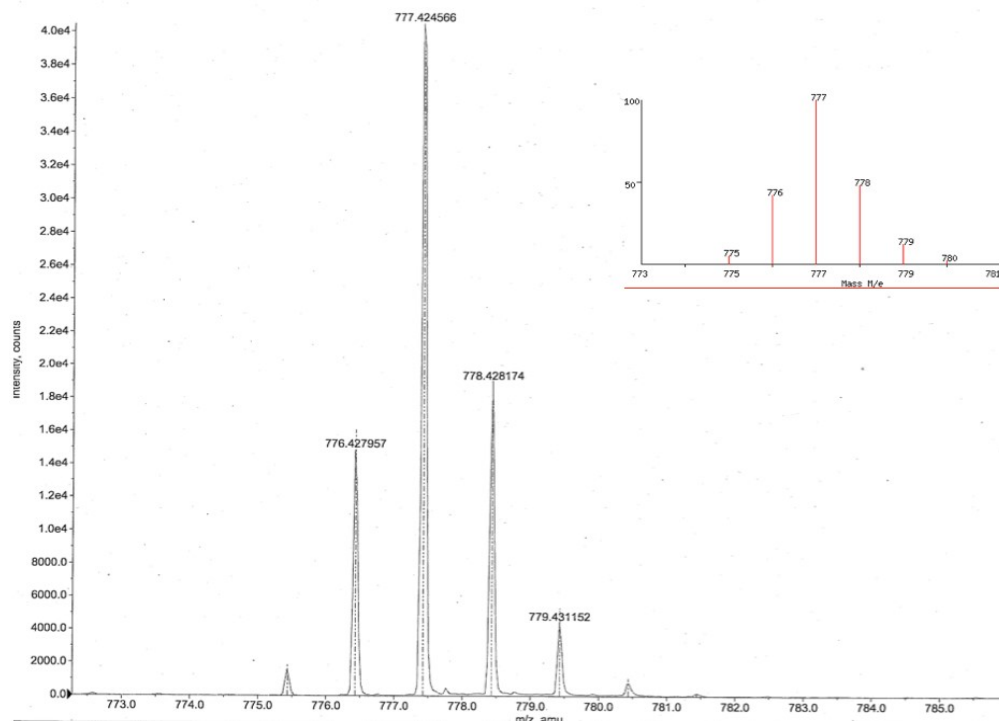


Figure S12. Comparison of theoretical and experimental isotopic distributions of spectra of the $[M+H]^+$ of compound **3**, the spectrum clearly indicates the presence of two boron atoms.

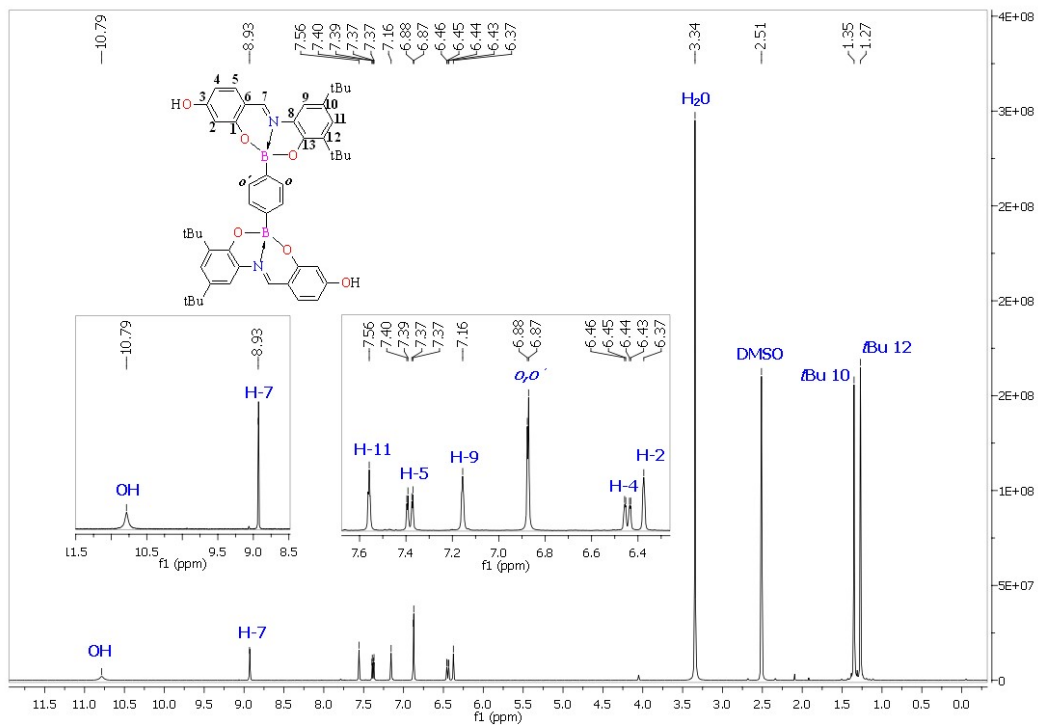


Figure S13. ^1H NMR ($\text{DMSO}-d_6$) spectrum of **3**.

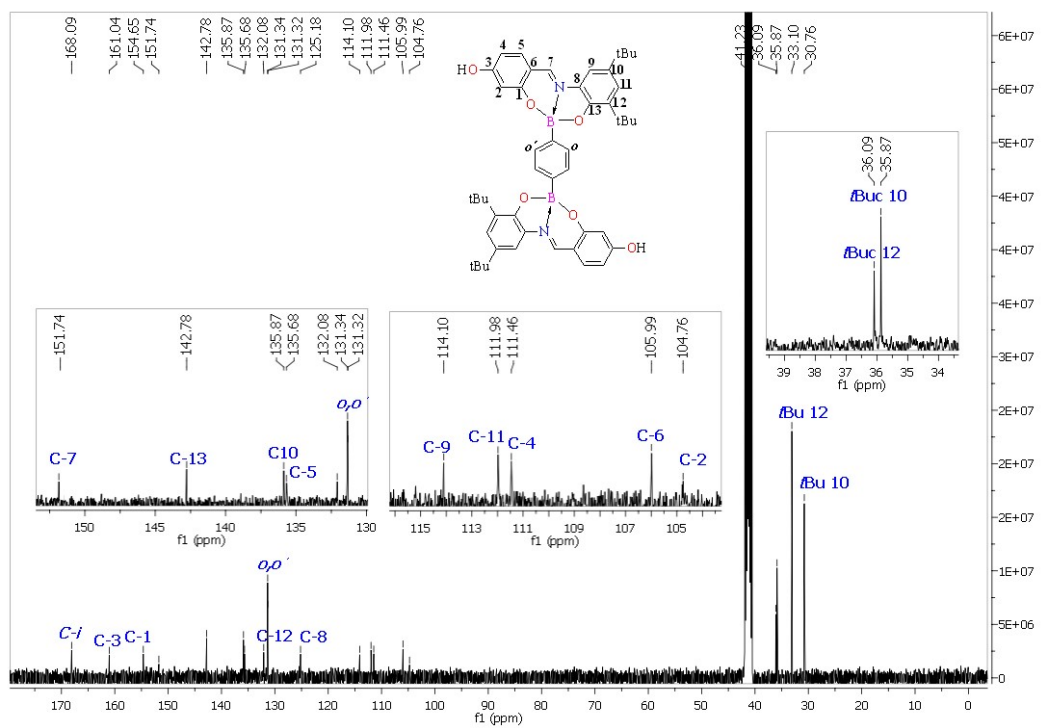


Figure S14. ^{13}C NMR ($\text{DMSO}-d_6$) spectrum of **3**.

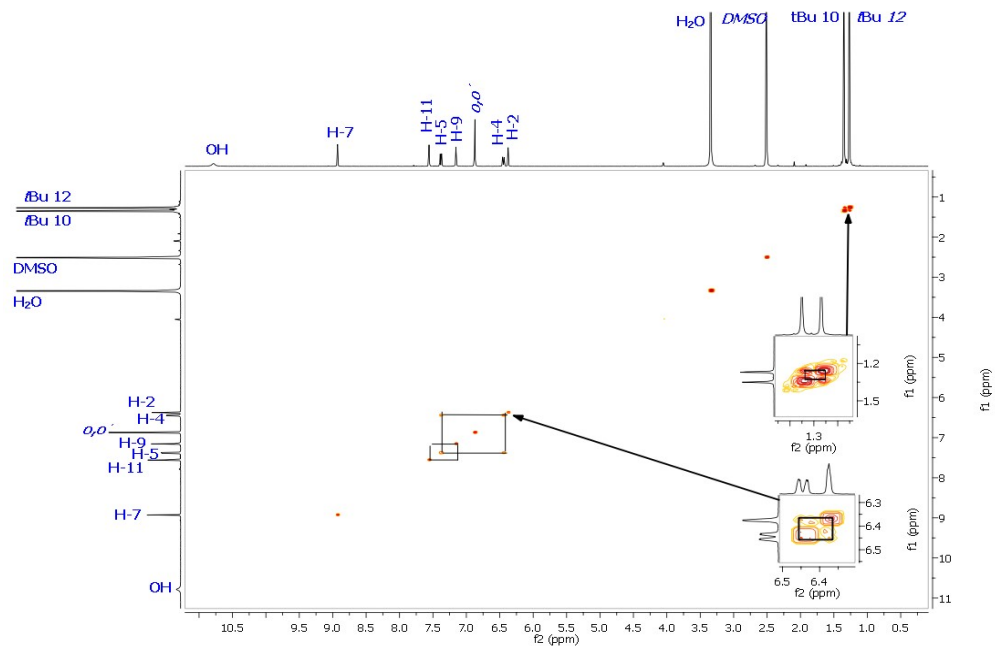


Figure S15. COSY spectra in DMSO- d_6 of **3**.

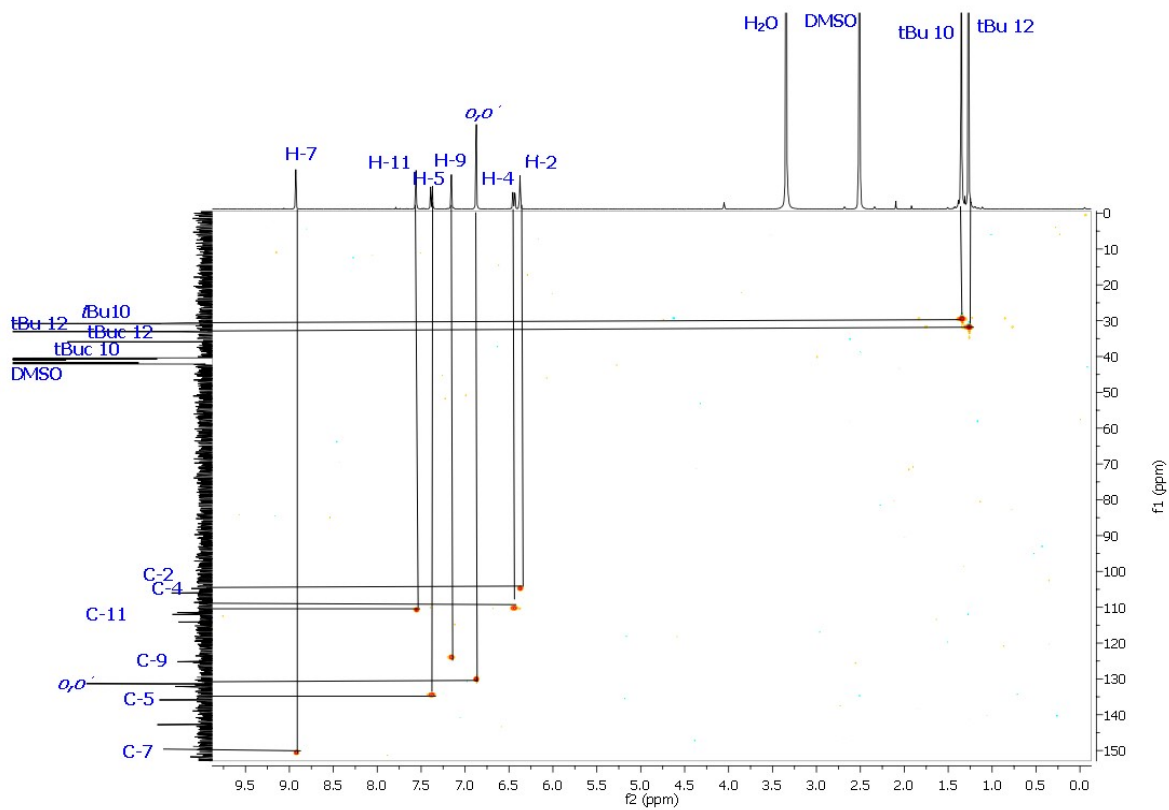


Figure S16. HSQC spectra in DMSO- d_6 of **3**.

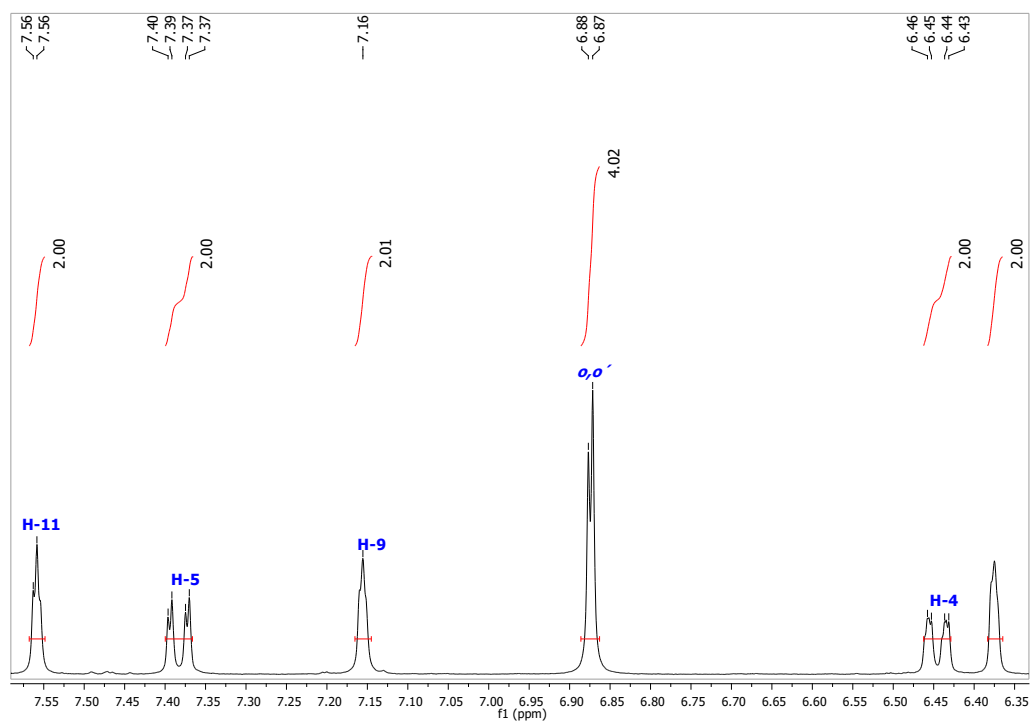


Figure S17. Integration spectra in DMSO- d_6 of **3**.

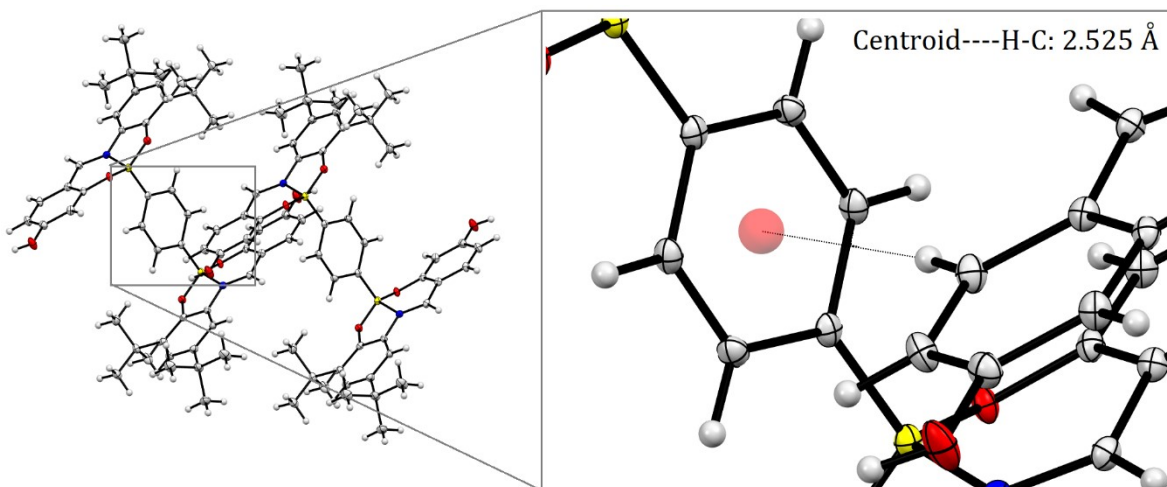


Figure S18. Intermolecular interactions of compound **3**.

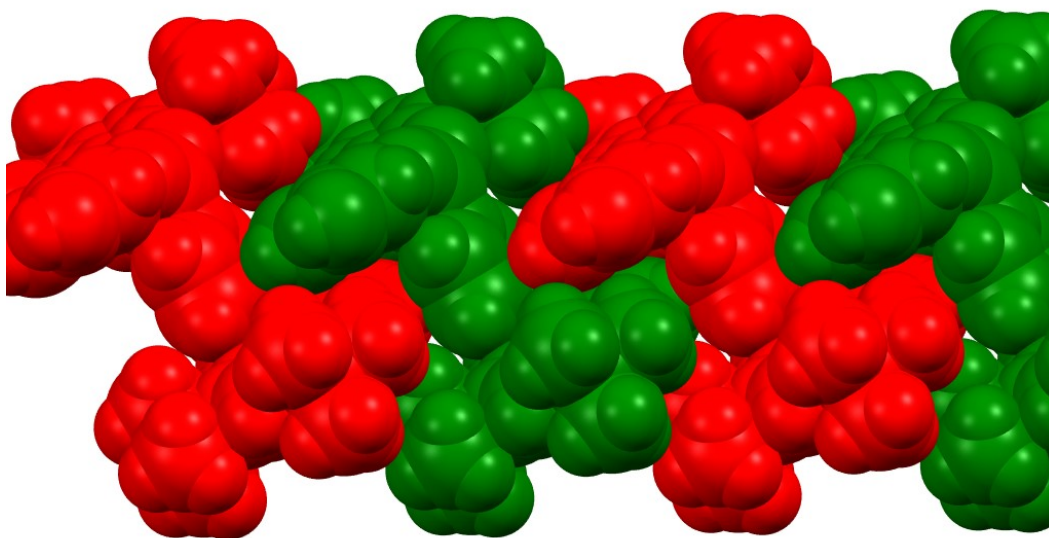


Figure S19. Space fill of compound **3**.

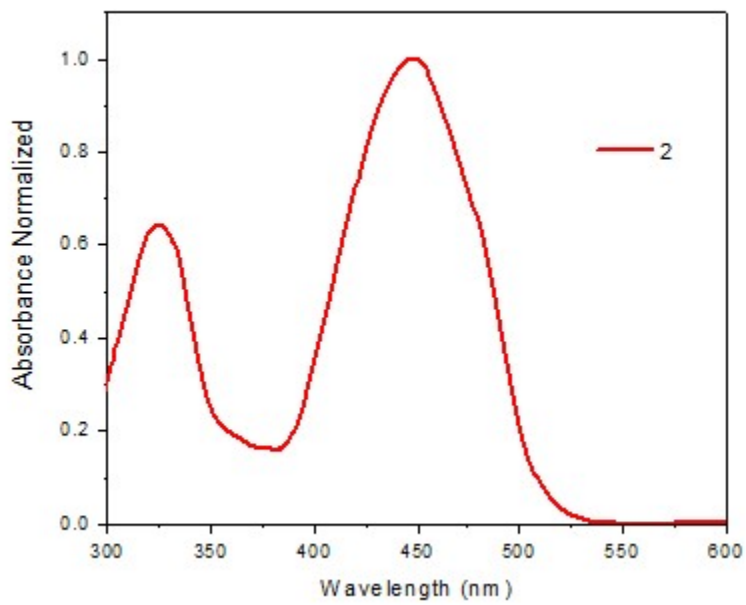


Figure S20. Absorbance of **3** in CHCl₃.

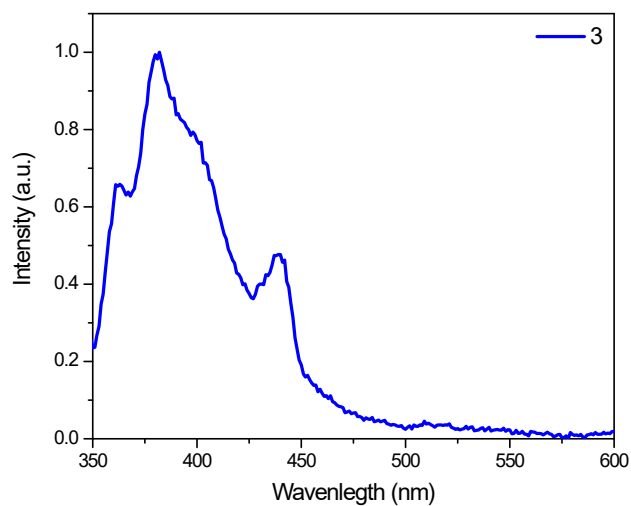


Figure S21. Emission spectra of **3** in CHCl_3 .

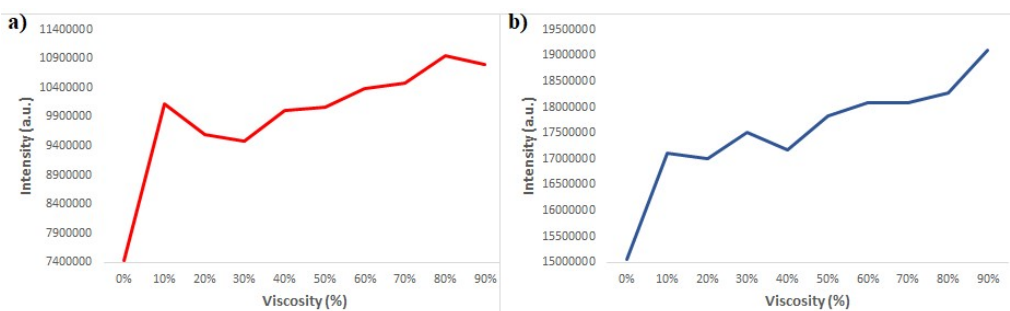


Figure S22. Emission spectra of **2**(a) and **3**(b) in mixtures of methanol/glycerol.

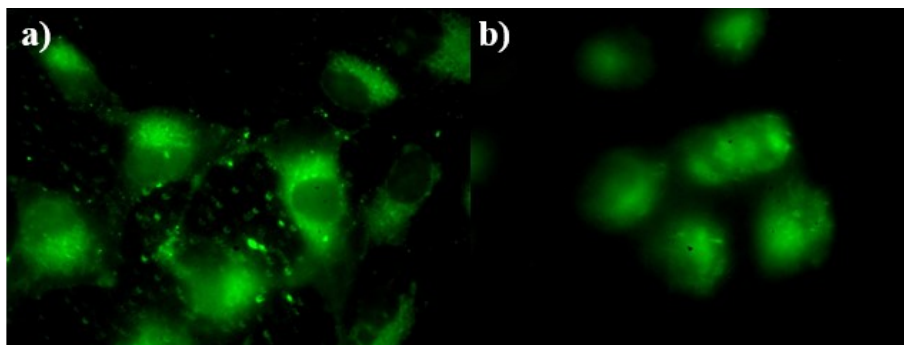


Figure S23. Fluorescence microscopy at 100X of magnification of **3** compound on HUVEC(a) and HeLa(b) cells.

Table S1. Computed structure of **2** calculated with the b3lyp/6-31g(d,p) functionals.

Atomic				
Number		X	Y	X
6	-4.907028000	-2.723404000	-0.222048000	
6	-3.642360000	-2.726607000	0.325053000	
6	-5.258890000	-1.689427000	-1.116253000	
6	-4.359583000	-0.675314000	-1.439728000	
6	-3.087582000	-0.649507000	-0.855743000	
6	-2.708772000	-1.705985000	0.036314000	
6	-1.337849000	-1.799610000	0.426920000	
7	-0.548812000	-0.783061000	0.216245000	
8	-2.243944000	0.324720000	-1.191159000	
8	0.052315000	1.170525000	-0.967063000	
5	-1.135132000	0.620223000	-0.258926000	
6	-1.608438000	1.546263000	0.973604000	
6	-2.567643000	2.551448000	0.758935000	
6	-2.968829000	3.413543000	1.780212000	
6	-2.417268000	3.288395000	3.056541000	
6	-1.465022000	2.297405000	3.297936000	
6	-1.070206000	1.441959000	2.267405000	
1	-0.932414000	-2.738321000	0.802725000	
1	-3.713038000	4.180924000	1.582436000	
1	-1.031639000	2.189514000	4.289054000	
1	-0.326498000	0.677627000	2.481788000	
1	-3.010441000	2.655638000	-0.228612000	
1	-3.345950000	-3.530723000	0.993379000	
8	-6.512158000	-1.737262000	-1.634372000	
6	0.849353000	-0.693254000	0.140912000	
6	1.144411000	0.476974000	-0.586328000	
6	2.482789000	0.810979000	-0.874865000	

6	1.830590000	-1.567706000	0.603857000
6	3.166635000	-1.258702000	0.345609000
6	3.444327000	-0.081411000	-0.386582000
1	1.550013000	-2.454175000	1.160457000
1	4.484462000	0.148378000	-0.581337000
6	2.833792000	2.077734000	-1.672361000
6	2.171104000	2.003545000	-3.069741000
6	4.352686000	2.237757000	-1.870040000
6	2.310973000	3.322961000	-0.915466000
6	4.332390000	-2.140957000	0.831703000
6	3.839545000	-3.384829000	1.594903000
6	5.240052000	-1.323280000	1.781092000
6	5.162478000	-2.622360000	-0.382169000
1	2.400972000	2.909798000	-3.641697000
1	2.549420000	1.144137000	-3.634033000
1	1.086484000	1.913584000	-2.990534000
1	4.548452000	3.150820000	-2.441048000
1	4.885154000	2.326728000	-0.916987000
1	4.785512000	1.401581000	-2.429928000
1	2.541826000	4.230560000	-1.484849000
1	1.230921000	3.274962000	-0.767674000
1	2.788662000	3.410158000	0.066339000
1	4.696775000	-3.984508000	1.916944000
1	3.272415000	-3.115132000	2.492092000
1	3.208661000	-4.023928000	0.967856000
1	6.078188000	-1.936204000	2.131789000
1	5.657352000	-0.441373000	1.286367000
1	4.679898000	-0.979614000	2.656733000
1	5.996501000	-3.250793000	-0.049952000
1	4.545873000	-3.210774000	-1.069381000

1	5.583020000	-1.784969000	-0.946339000
1	-2.728543000	3.955425000	3.855978000
1	-5.633493000	-3.495479000	0.001626000
1	-4.628501000	0.122080000	-2.126344000
1	-6.642329000	-0.989120000	-2.233205000

Table S2. Computed structure of **3** calculated with the b3lyp/6-31g(d,p) functionals.

Atomic Number		X	Y	X
6	1.202986000	-6.100135000	-0.092719000	
6	1.927618000	-5.166608000	0.616387000	
6	0.853785000	-5.816233000	-1.430257000	
6	1.215155000	-4.613088000	-2.032944000	
6	1.913363000	-3.641941000	-1.304908000	
6	2.296764000	-3.927917000	0.046468000	
6	3.217573000	-3.042301000	0.686346000	
7	3.441110000	-1.872687000	0.156731000	
8	2.252484000	-2.504665000	-1.908161000	
8	3.515389000	-0.404575000	-1.692797000	
5	2.542764000	-1.334403000	-1.051494000	
6	1.205910000	-0.595590000	-0.543095000	
6	0.007889000	-0.696538000	-1.268075000	
6	-1.148411000	-0.019626000	-0.875039000	
6	-1.174412000	0.795418000	0.267731000	
6	0.025521000	0.898068000	0.993251000	
6	1.179812000	0.222030000	0.600943000	
1	3.799145000	-3.375297000	1.545301000	
1	-2.048248000	-0.134395000	-1.476754000	
1	0.053780000	1.524680000	1.882204000	

1	2.080677000	0.339295000	1.200550000
5	-2.493332000	1.548790000	0.798663000
8	-2.185596000	2.876402000	1.376683000
8	-3.302402000	0.716431000	1.733801000
6	-1.999851000	3.884246000	0.527226000
6	-1.279598000	5.006876000	0.952703000
6	-1.079370000	6.080754000	0.087802000
6	-1.616248000	6.080840000	-1.217491000
6	-2.361360000	4.997050000	-1.628937000
6	-2.569898000	3.880800000	-0.788556000
6	-3.498184000	2.845826000	-1.117641000
7	-3.569428000	1.793491000	-0.351362000
1	-4.204821000	2.975742000	-1.936573000
1	-0.018465000	-1.315650000	-2.161870000
1	2.229414000	-5.380808000	1.638241000
8	-0.360595000	7.174818000	0.447781000
1	-2.804367000	4.992726000	-2.621374000
1	-0.032972000	-6.472133000	-2.990261000
1	0.945676000	-4.392057000	-3.061676000
1	0.905460000	-7.048125000	0.339328000
1	-0.864786000	5.003059000	1.956456000
1	-1.440412000	6.936165000	-1.858865000
6	-4.575119000	0.829107000	-0.190574000
6	-4.373448000	0.236448000	1.071991000
6	-5.270706000	-0.742983000	1.543433000
6	-5.641919000	0.497675000	-1.023442000
6	-6.541408000	-0.477570000	-0.590533000
6	-6.324740000	-1.061079000	0.678989000
1	-5.750660000	0.983940000	-1.985940000
1	-7.029790000	-1.815581000	1.005645000

6	-5.079335000	-1.400926000	2.919649000
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6	-6.176474000	-2.436812000	3.226853000
6	-3.709607000	-2.121504000	2.957979000
6	-7.741996000	-0.935488000	-1.440209000
6	-7.618670000	-2.448244000	-1.740964000
6	-9.057056000	-0.672447000	-0.668500000
6	-7.820045000	-0.186920000	-2.784287000
6	4.508049000	-0.975722000	0.313289000
6	4.510579000	-0.142459000	-0.823084000
6	5.512161000	0.837043000	-0.978018000
6	5.467206000	-0.888993000	1.320141000
6	6.466459000	0.078092000	1.201716000
6	6.454295000	0.905365000	0.055334000
1	5.418694000	-1.553581000	2.174745000
1	7.234296000	1.652334000	-0.027195000
6	5.542058000	1.756155000	-2.210189000
6	5.685546000	0.894587000	-3.488600000
6	6.718533000	2.748700000	-2.166750000
6	4.226613000	2.569694000	-2.277571000
6	7.563192000	0.271174000	2.266219000
6	7.483817000	1.705315000	2.841342000
6	8.954604000	0.052573000	1.625805000
6	7.416110000	-0.720097000	3.436388000
1	-4.974031000	-0.767875000	5.004656000
1	-4.349015000	0.440421000	3.866812000
1	-6.097434000	0.192073000	4.027051000
1	-5.996048000	-2.872361000	4.214783000
1	-7.174793000	-1.986331000	3.244239000
1	-6.181771000	-3.258354000	2.502399000

1	-3.553251000	-2.575701000	3.943283000
1	-3.669886000	-2.919378000	2.208553000
1	-2.889872000	-1.428048000	2.763576000
1	-8.470073000	-2.790540000	-2.340279000
1	-6.701345000	-2.661746000	-2.299150000
1	-7.596486000	-3.044568000	-0.824365000
1	-9.919746000	-1.001514000	-1.259043000
1	-9.084227000	-1.207737000	0.284889000
1	-9.178084000	0.394611000	-0.455045000
1	-8.684665000	-0.539996000	-3.355237000
1	-7.938189000	0.892783000	-2.643249000
1	-6.929108000	-0.358221000	-3.397594000
1	5.688082000	1.538209000	-4.375765000
1	6.627006000	0.334518000	-3.476090000
1	4.862922000	0.183696000	-3.582267000
1	6.695370000	3.376459000	-3.063257000
1	6.663462000	3.414728000	-1.298804000
1	7.687789000	2.238605000	-2.148228000
1	4.230548000	3.214090000	-3.164245000
1	3.355604000	1.914762000	-2.330836000
1	4.120855000	3.210817000	-1.395739000
1	8.263639000	1.858916000	3.595991000
1	7.619254000	2.463571000	2.064789000
1	6.512679000	1.883238000	3.314552000
1	9.745704000	0.193396000	2.371113000
1	9.044140000	-0.961187000	1.222017000
1	9.141210000	0.753904000	0.807491000
1	8.213003000	-0.550908000	4.167613000
1	6.460857000	-0.596558000	3.957485000
1	7.493420000	-1.759981000	3.101373000

8	0.149007000	-6.771714000	-2.089024000
1	-0.043807000	7.066395000	1.354990000

Table S3. Electronic transitions for **2–3** calculated using the B3LYP/6-31G (d,p) method.

Comp.	Transition	MO Contribution	Energy gap [eV] ([nm])	Oscillator Strength(f)
2	S ₀ -S ₁	HOMO→LUMO	2.717 (456)	0.2753
3	S ₀ -S ₁	HOMO- 1→LUMO+1	2.670 (464)	0.0196
		HOMO→LUMO		
		HOMO→LUMO+1		