Theoretical and experimental characterization of a novel pyridine benzimidazole: Suitability for fluorescence staining in cells and antimicrobial properties.†

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Supporting Information

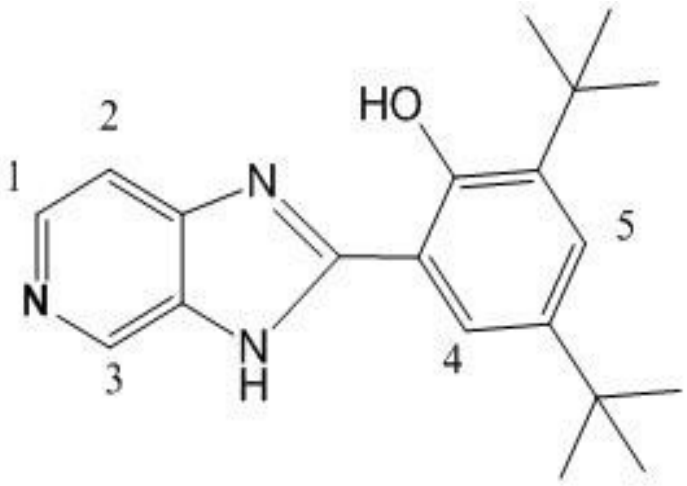

Figure S1. Numbering of protons for **B2**.

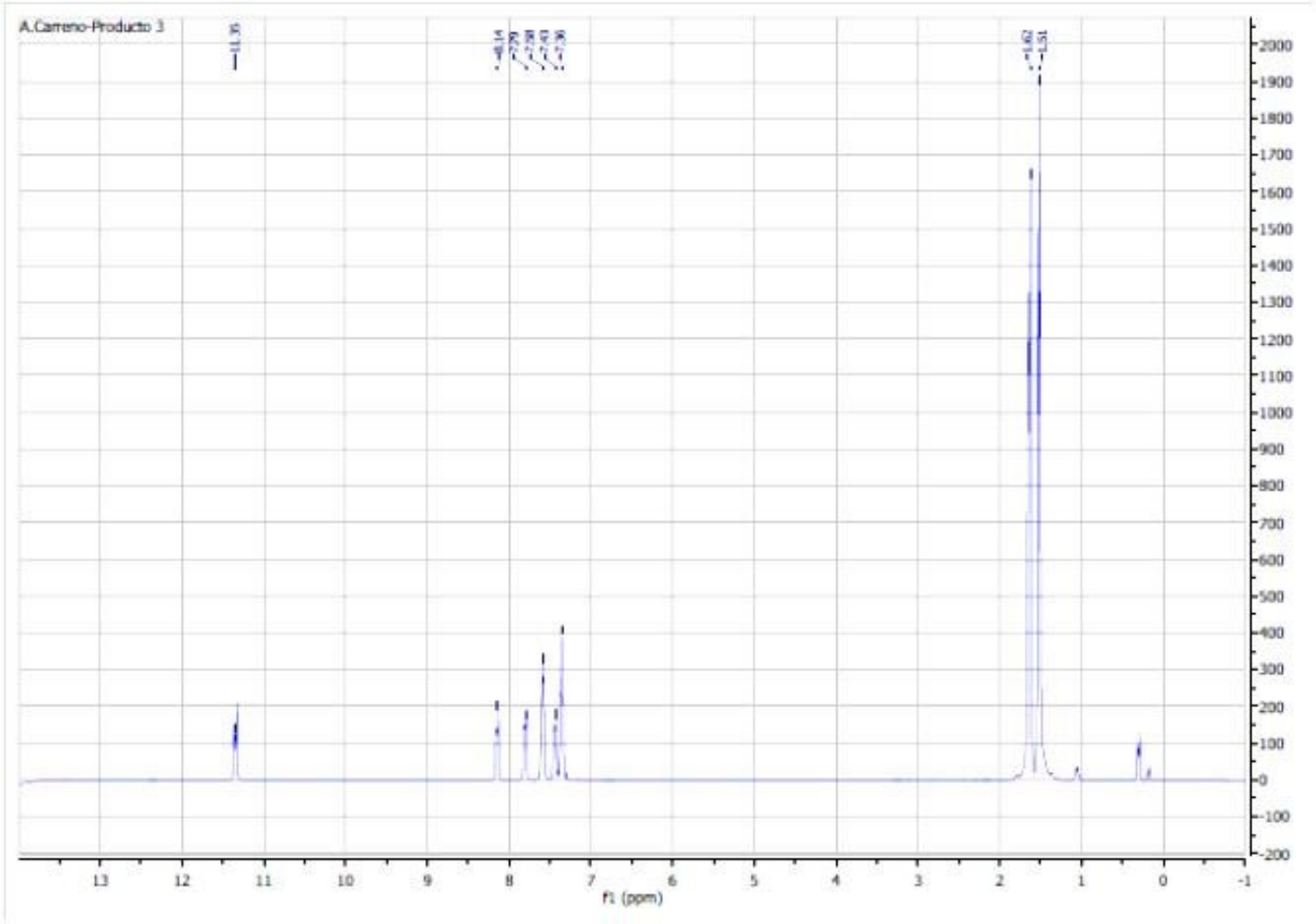

Figure S2. ^{1}HNMR of **B1** in $CDCl_3$.

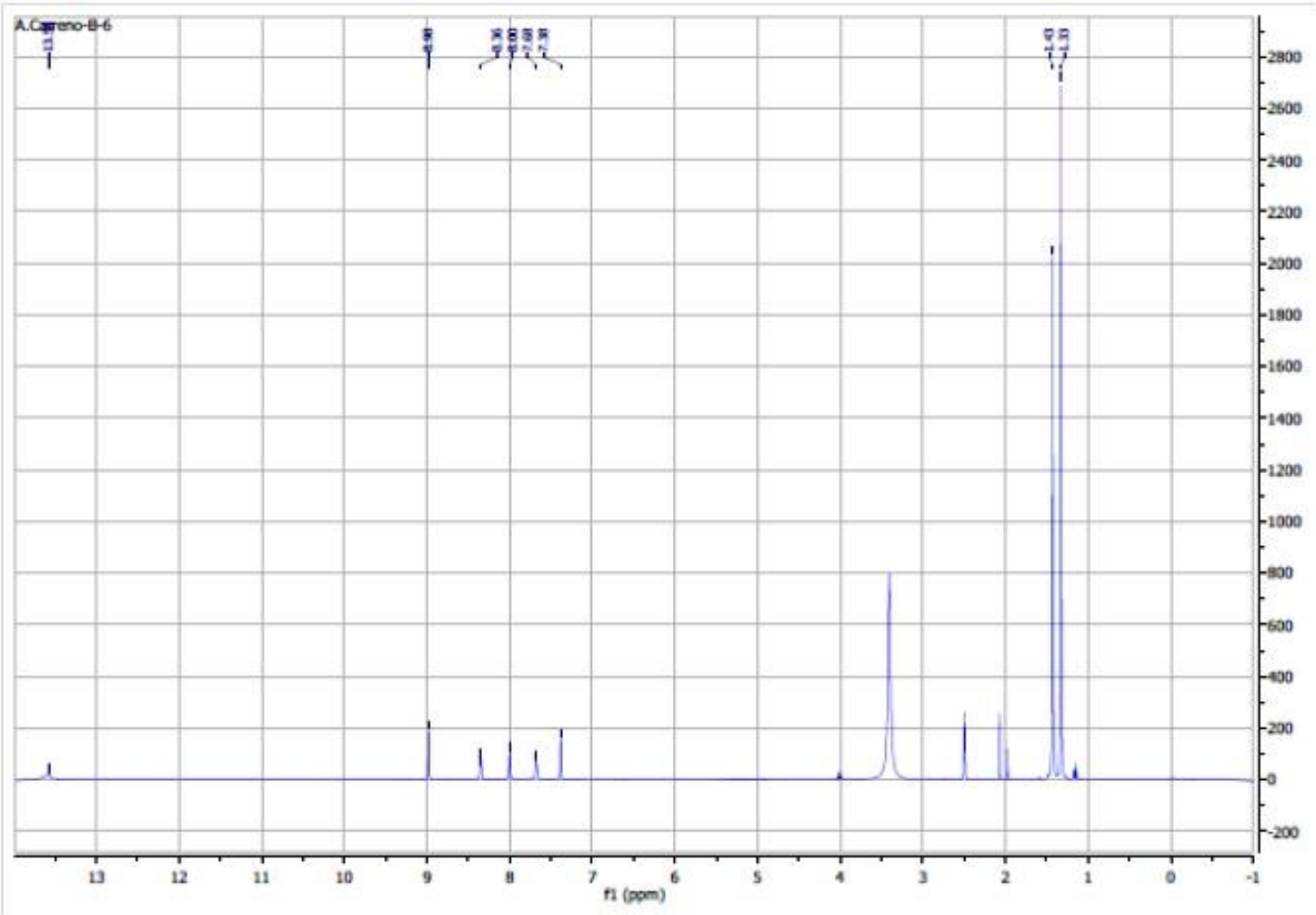

Figure S3. [1]HNMR of **B2** in DMSO-d6.

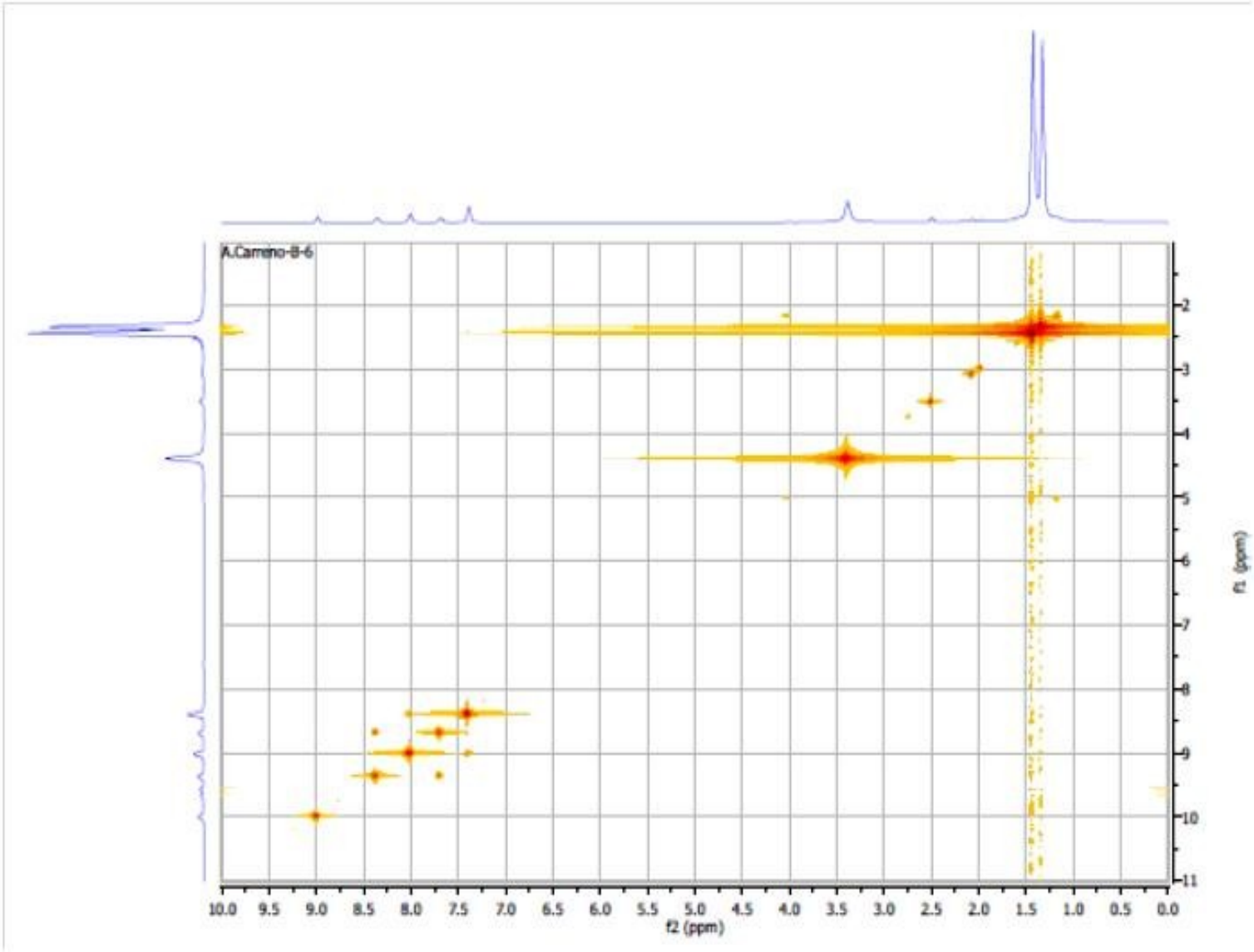

Figure S4. HHCOSY of **B2** in DMSO-d6.

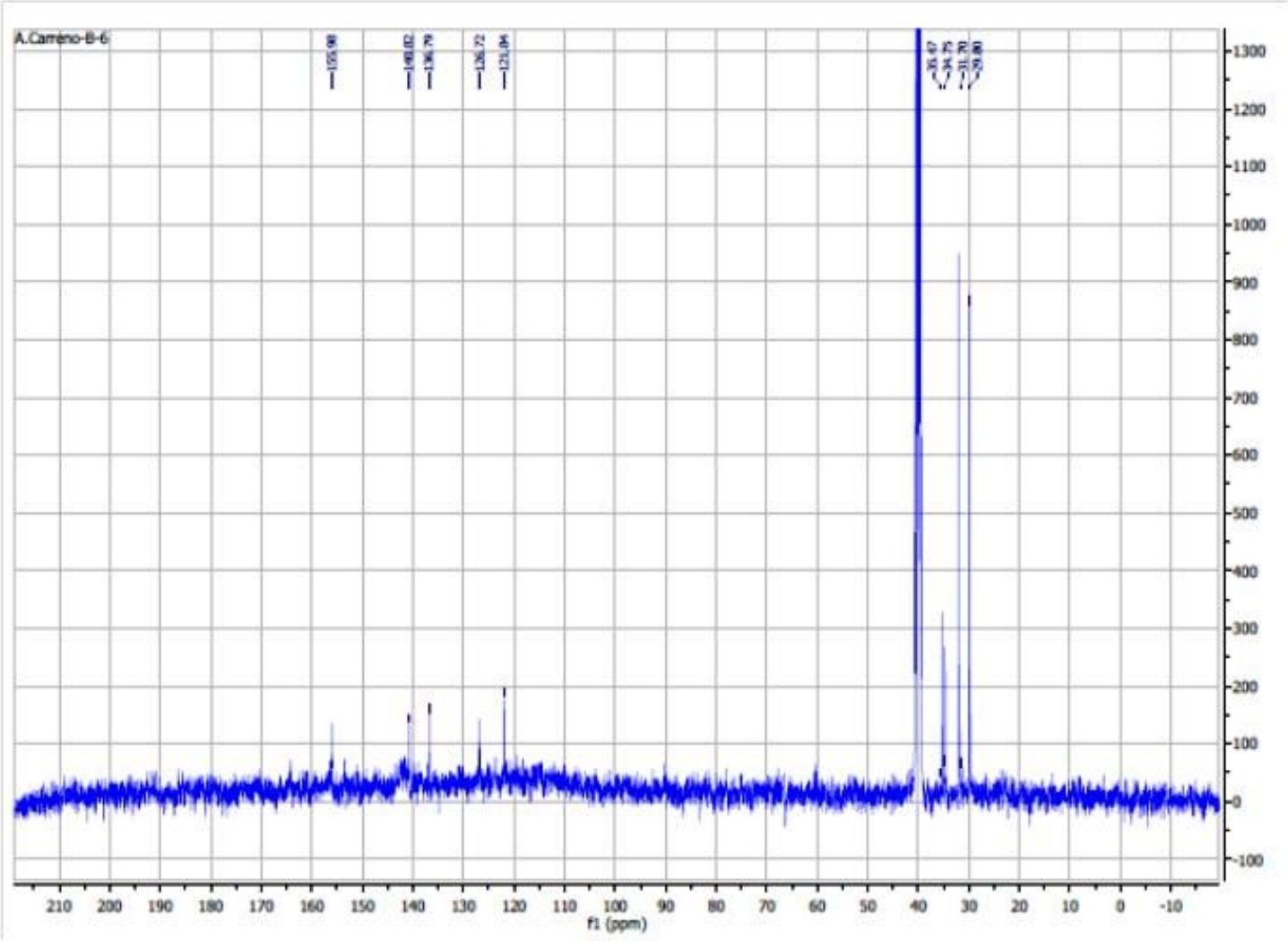

Figure S5. ^{13}CNMR of **B2** in DMSO-d6.

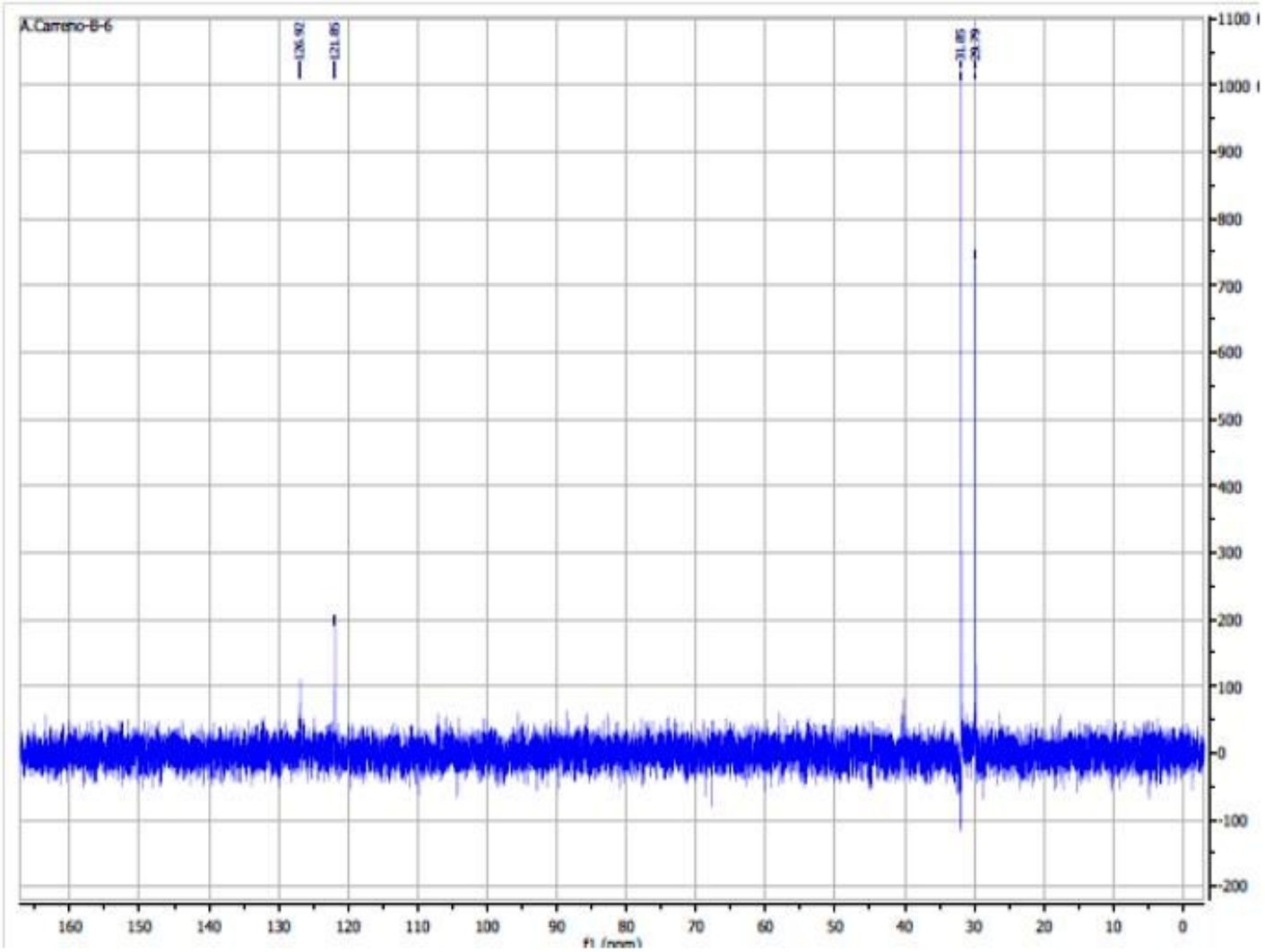

Figure S6. DEPT of **B2** in DMSO-d6.

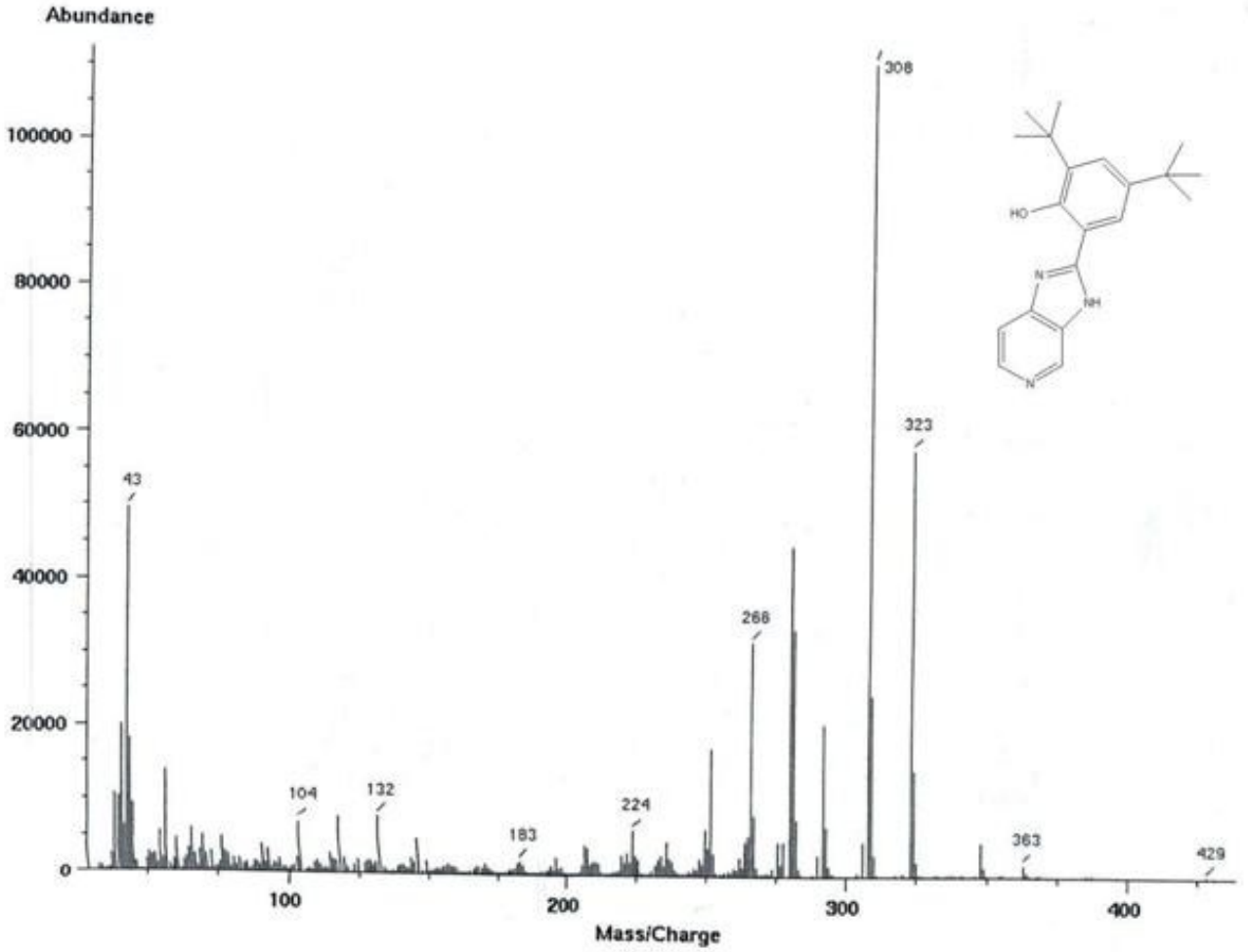

Figure S7. Mass spectra of **B2**.

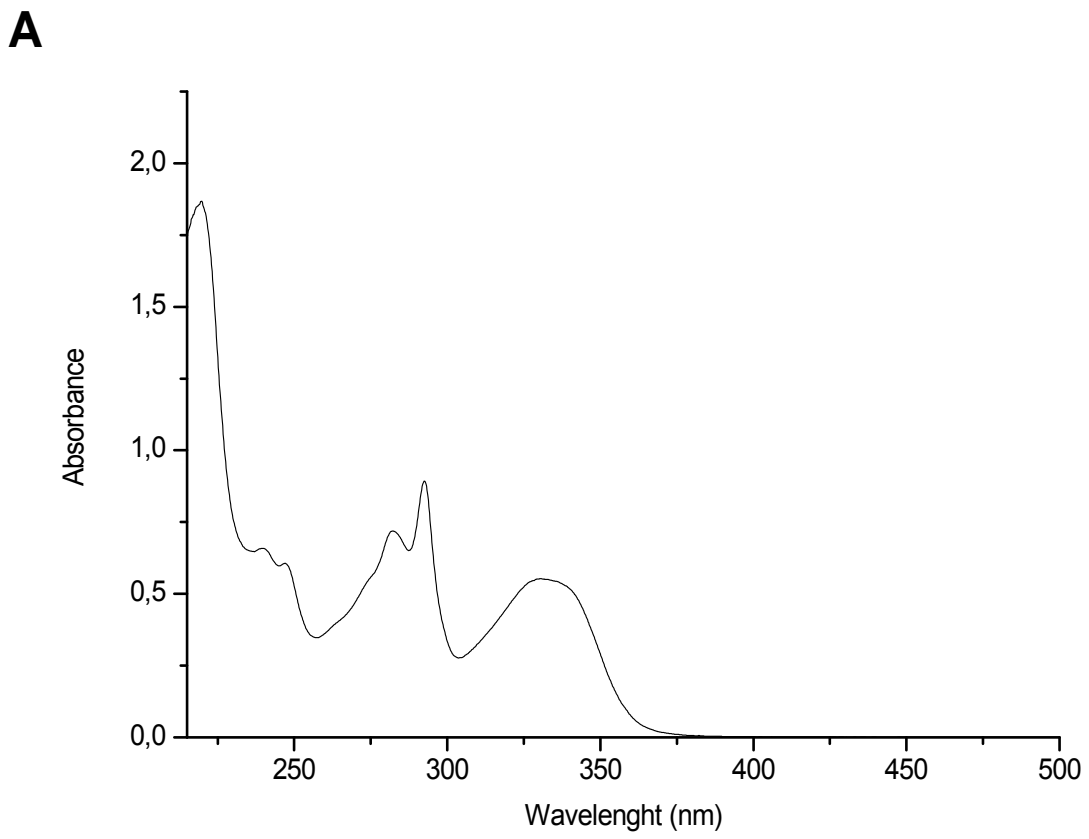

Figure S8. Absorption spectra for **B2** in ethanol solutions.

B

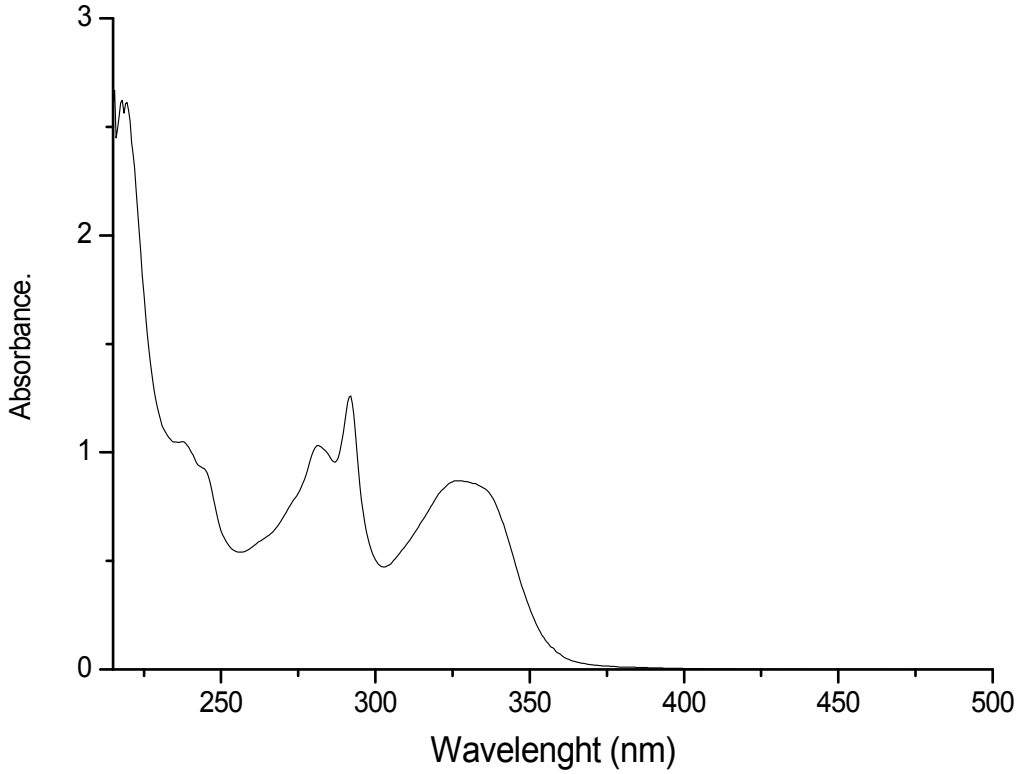

Figure S9. Absorption spectra for **B2** in dichlorometane solutions.

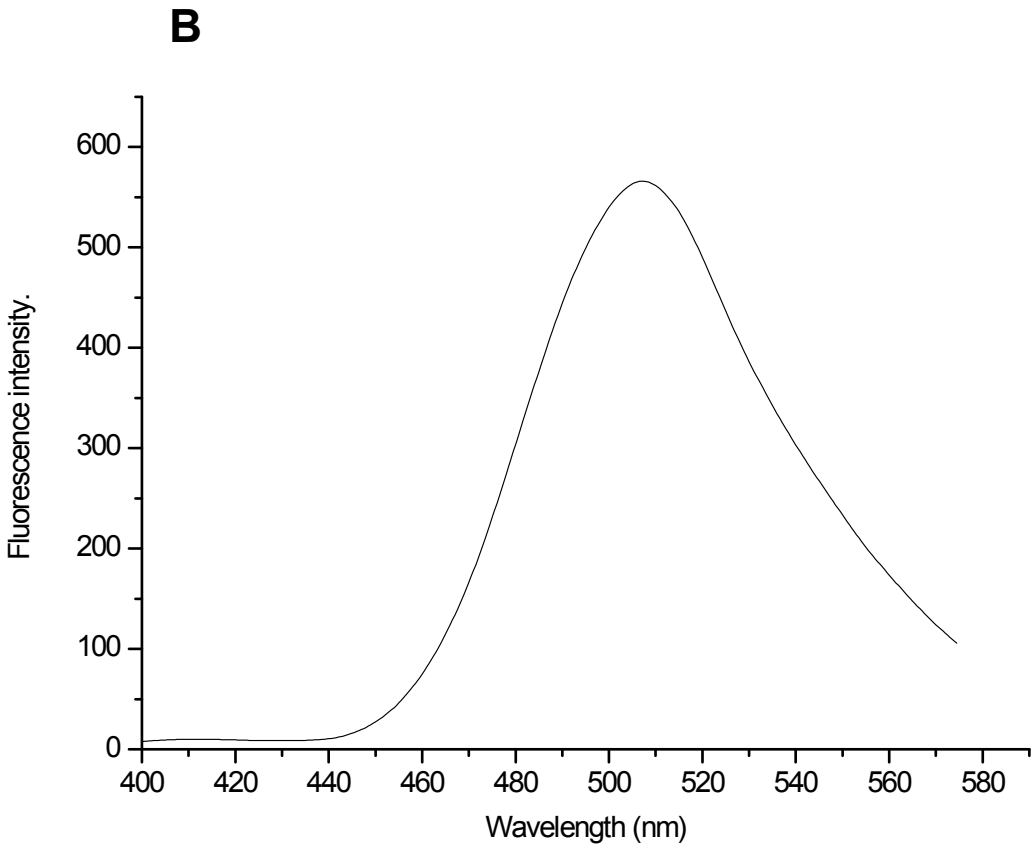

Figure S10. Emission spectra for **B2** in ethanol solutions.

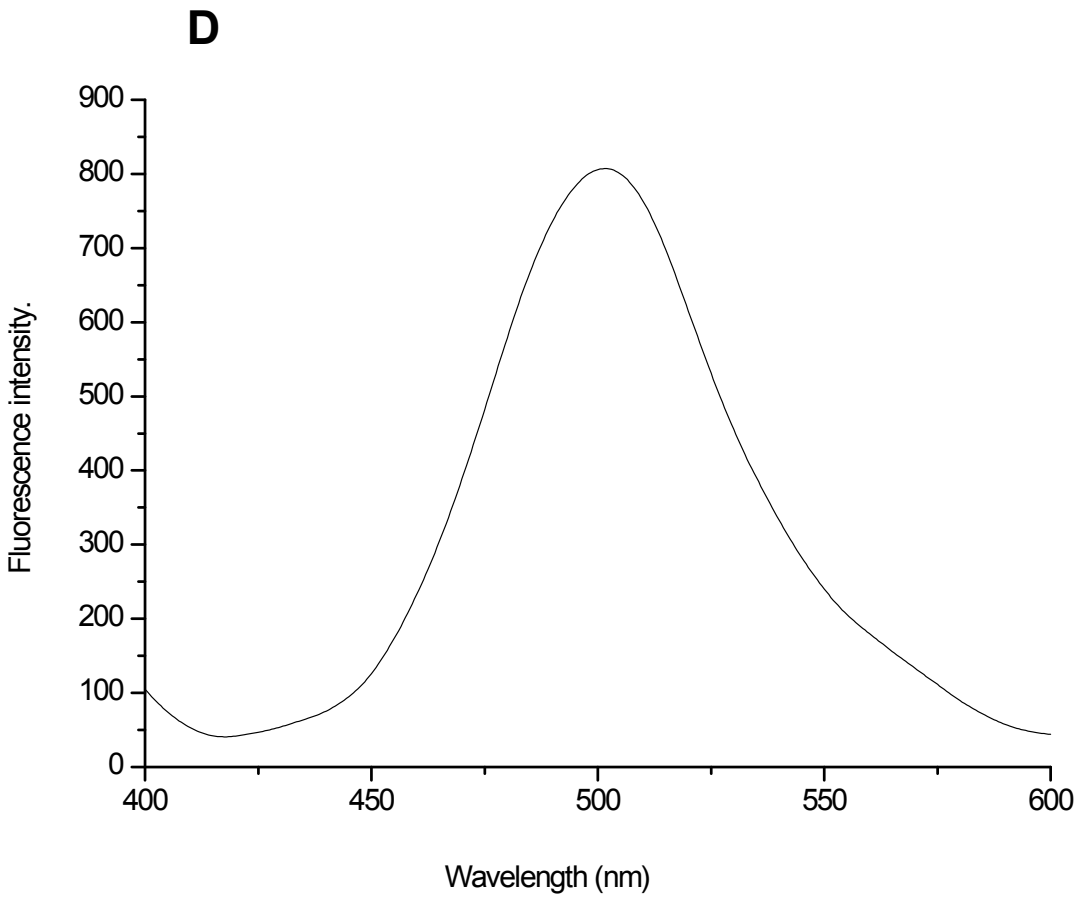

Figure S11. Emission spectra for **B2** in dichlorometane solutions.

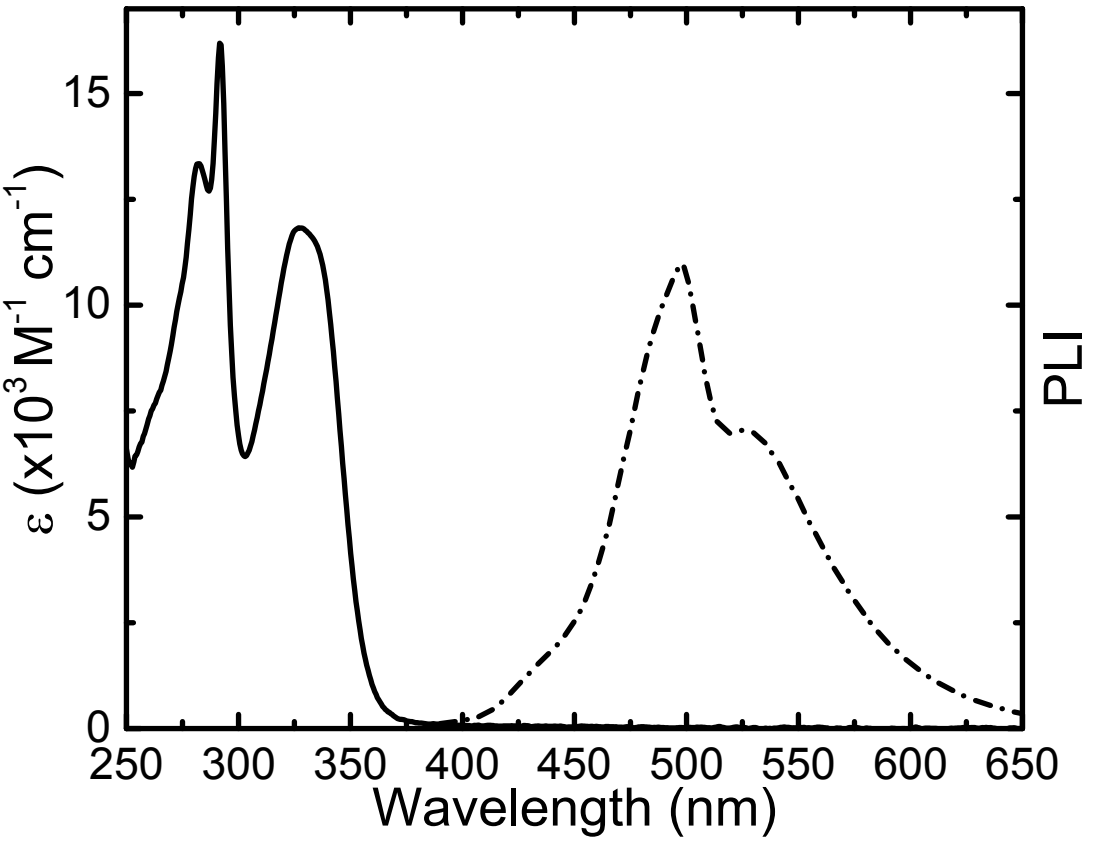

Figure S12. UV-visible absorption (solid line) and steady-state photoluminescence (dashed line) for **B2** in acetonitrile.

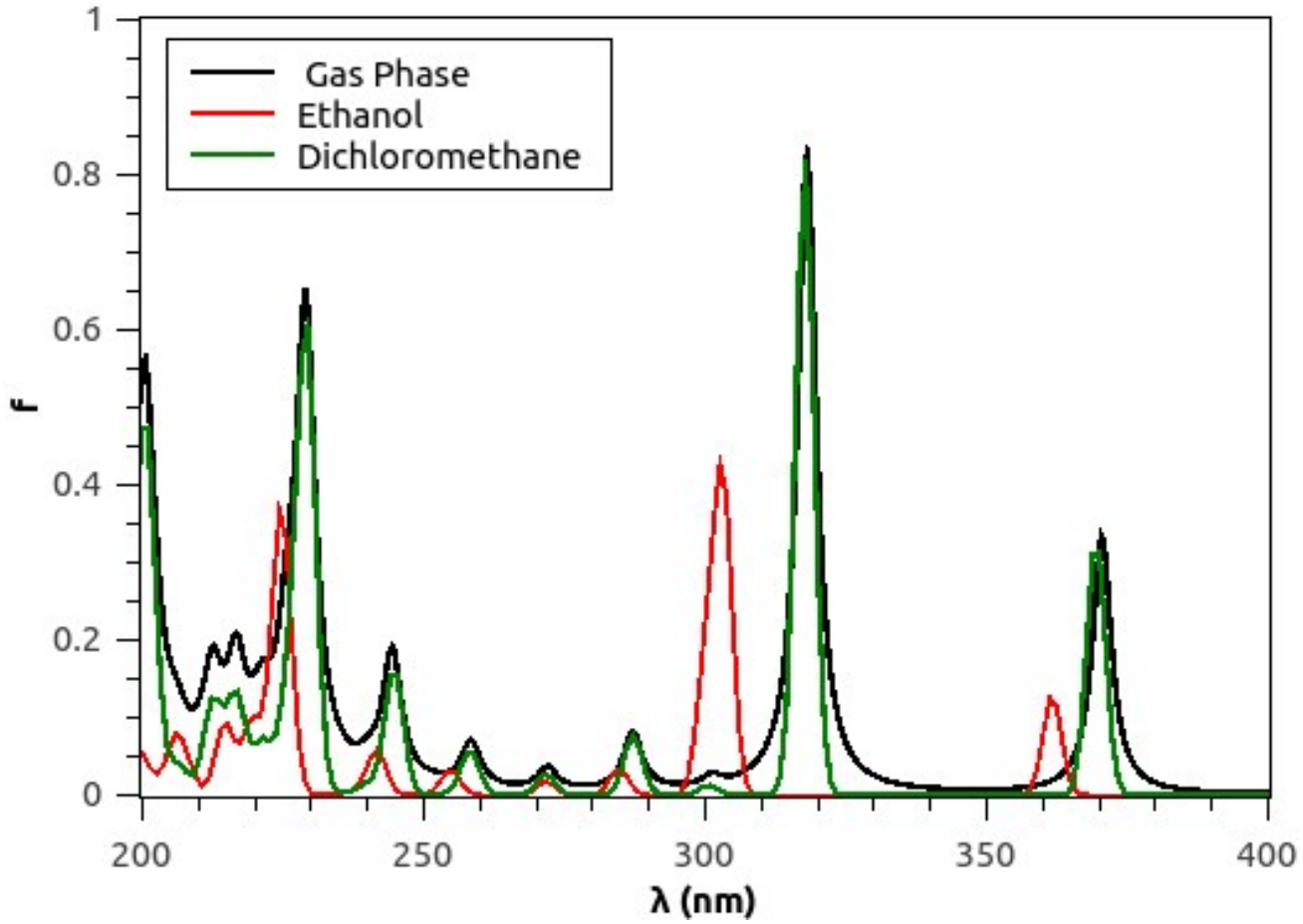

Figure S13. Calculated UV-vis absorption spectra for 2,4-di-*tert*-butyl-6-(3H-imidazo[4,5-c]pyridine-2-yl)phenol (**B2**) in different implicit solvents (ethanol and dichloromethane) and gas phase.

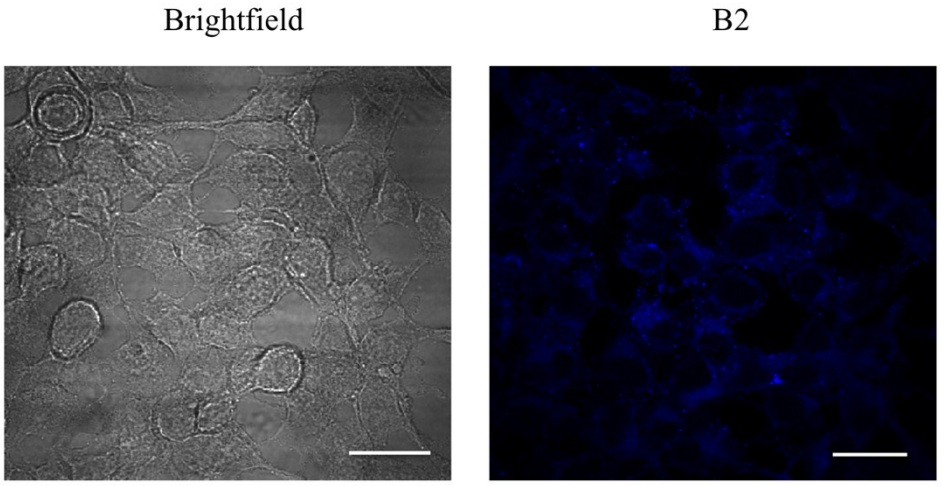

Figure S14. Intracellular staining of HEK293 cells using **B2**. Fluorescence confocal microscopy images showing HEK-293 cells (Human embryonic kidney cell line) fixed after treatment with 2,4-di-*tert*-butyl-6-(3H-imidazo[4,5-c]pyridine-2-yl)phenol (**B2),** 50 μM for 15 minutes. In all cases, cells were observed using a 100X objective. Compound emission was observed between 425-525 nm. White bars represent 10 μm.