Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Direct and Water-Mediated Excited State Intramolecular Proton Transfer (ESIPT) from Phenol OH to Carbon Atoms of Extended *ortho*-Substituted Biaryl Systems

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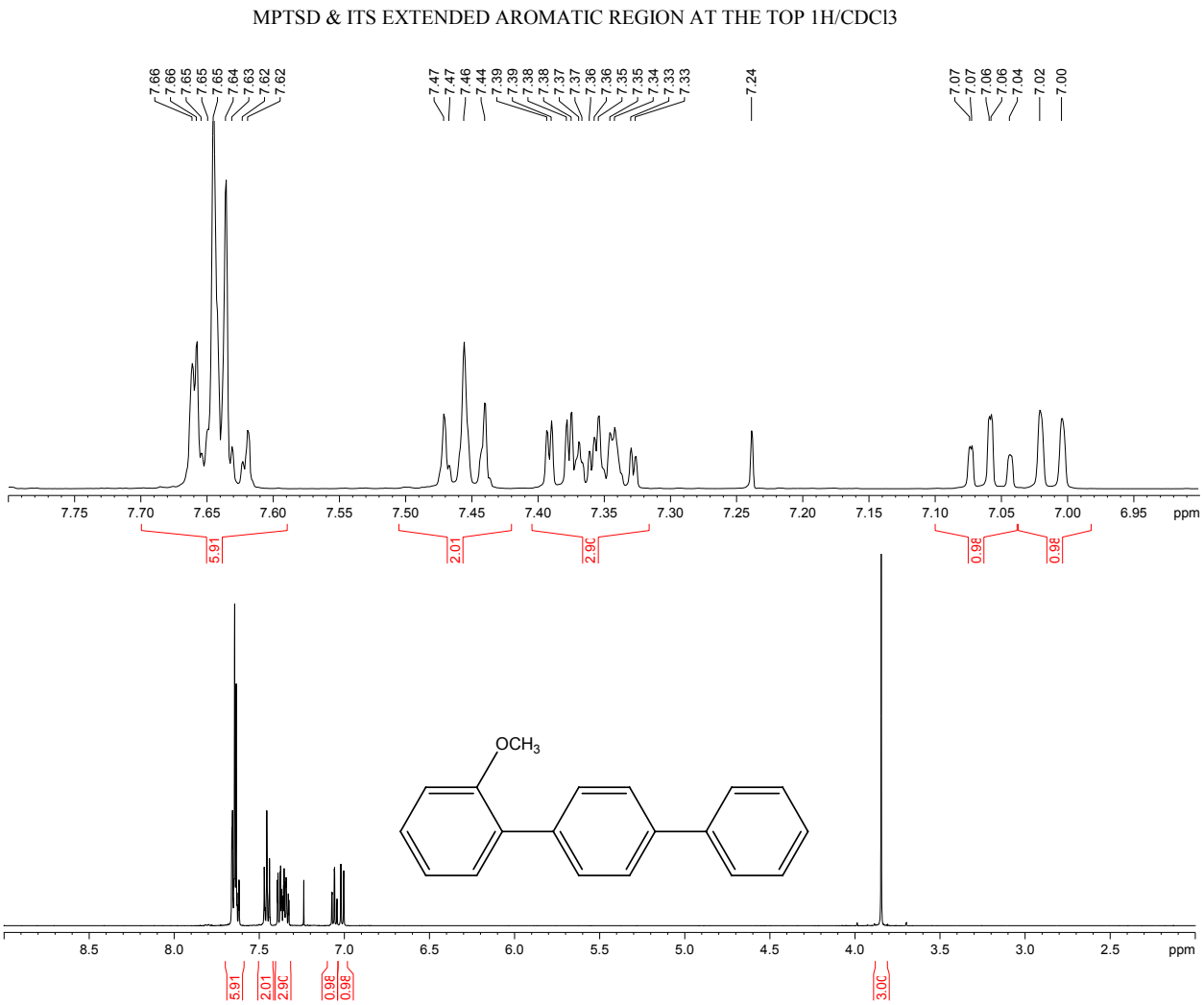


Figure S1: ^{1}H-nmr/$CDCl_3$ Spectra of **6.**

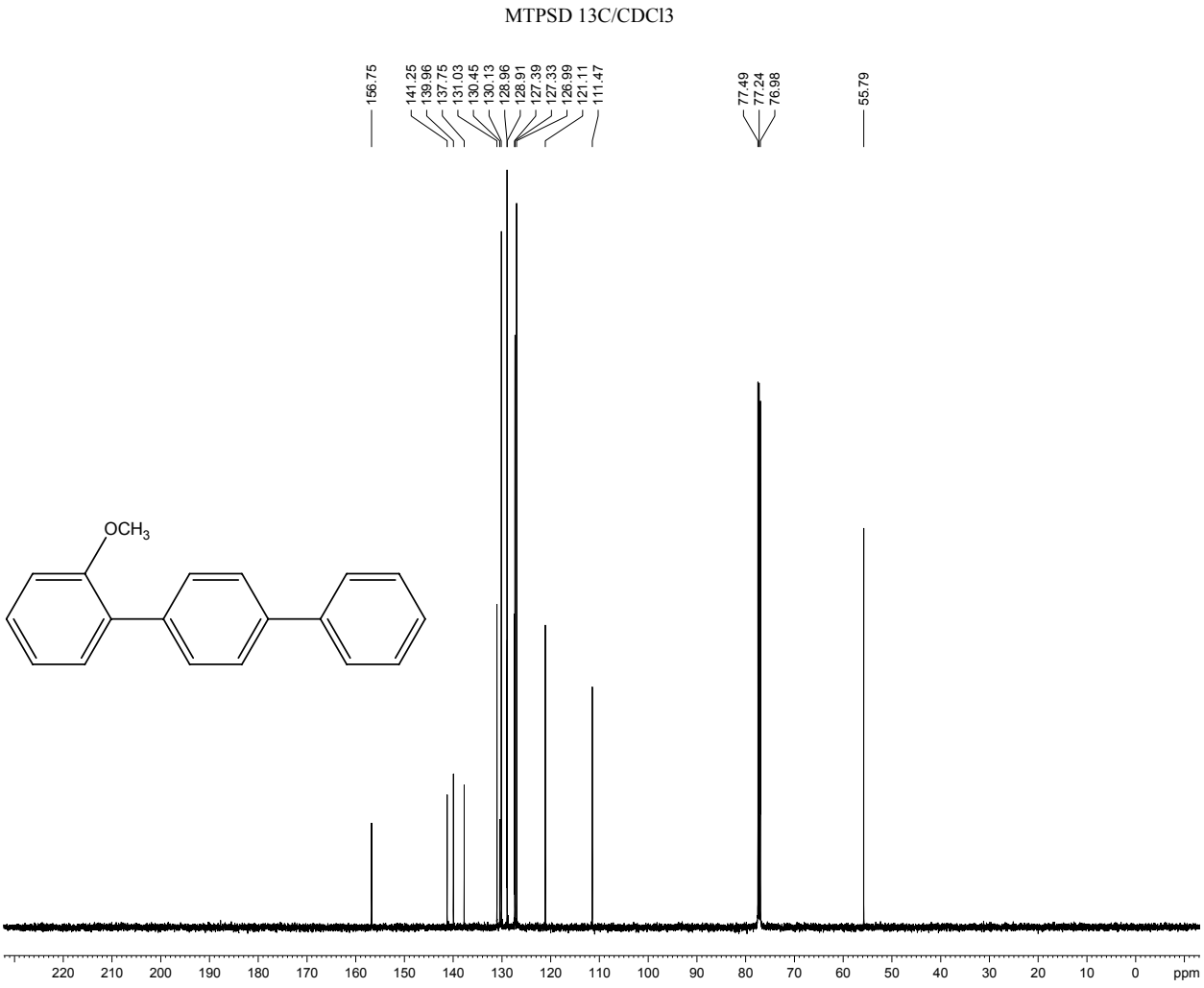


Figure S2: ^{13}C-nmr/$CDCl_3$ Spectra of **6.**

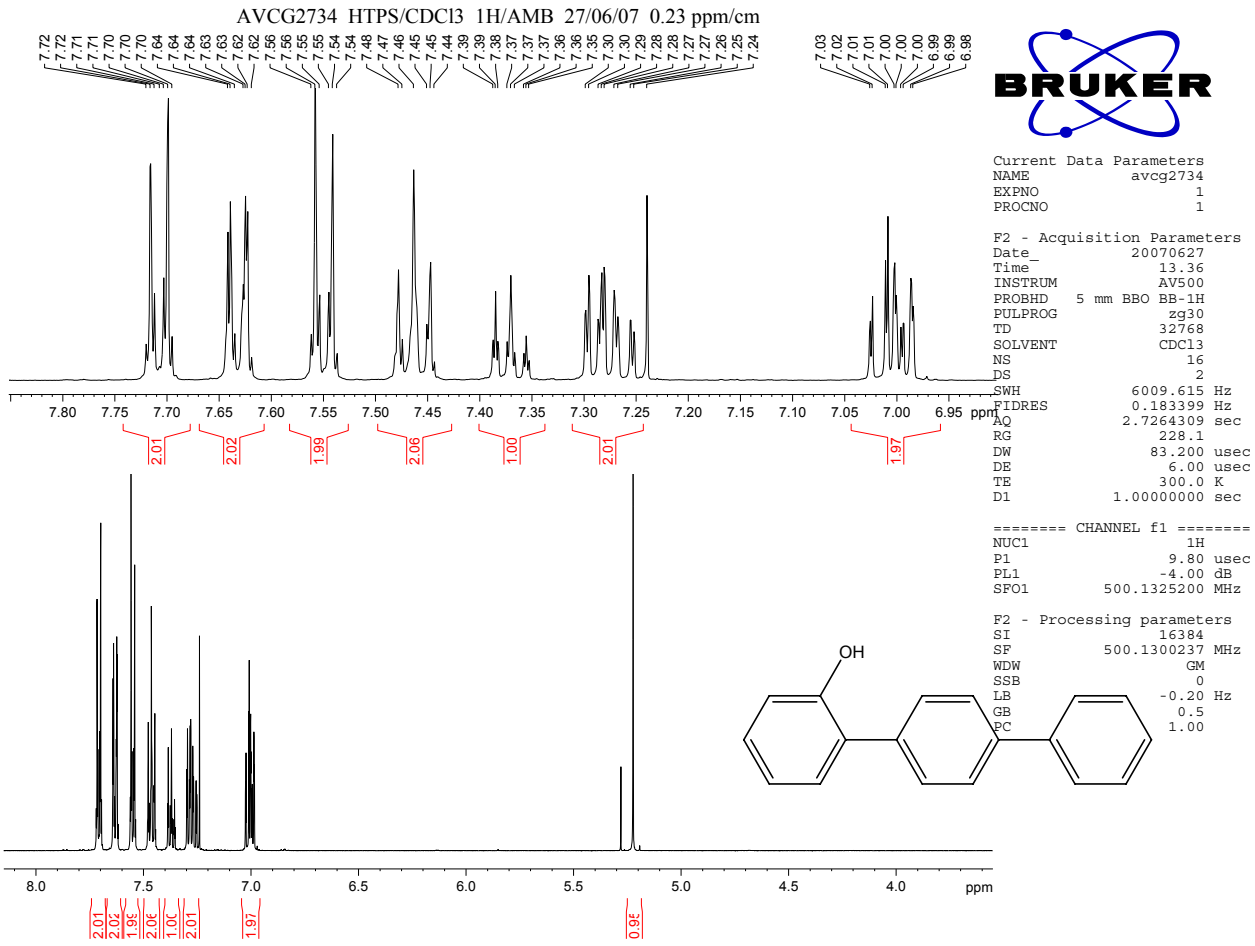


Figure S3: ^{1}H-nmr/$CDCl_3$ Spectra of **3.**

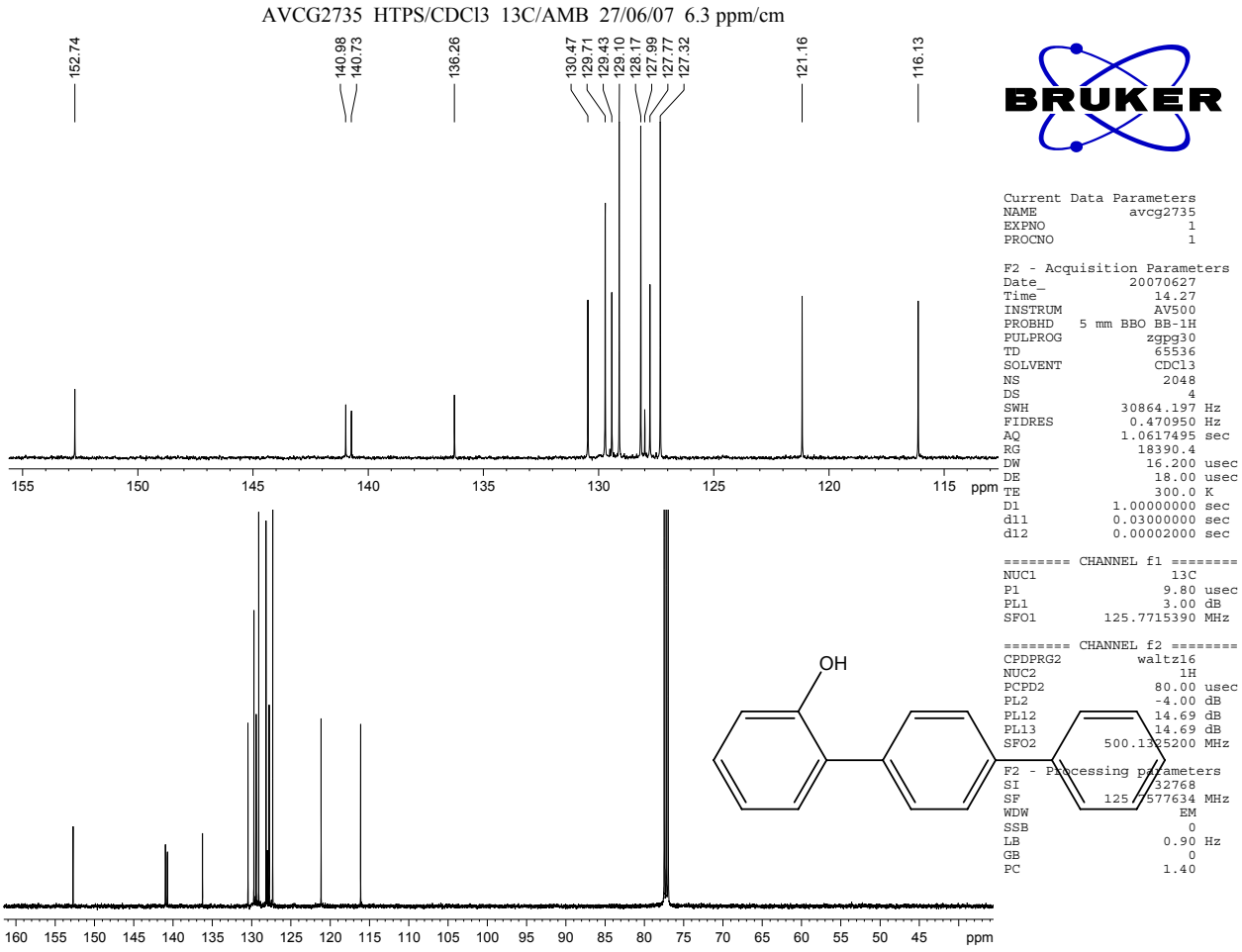


Figure S4: ^{13}C-nmr/$CDCl_3$ Spectra of **3.**

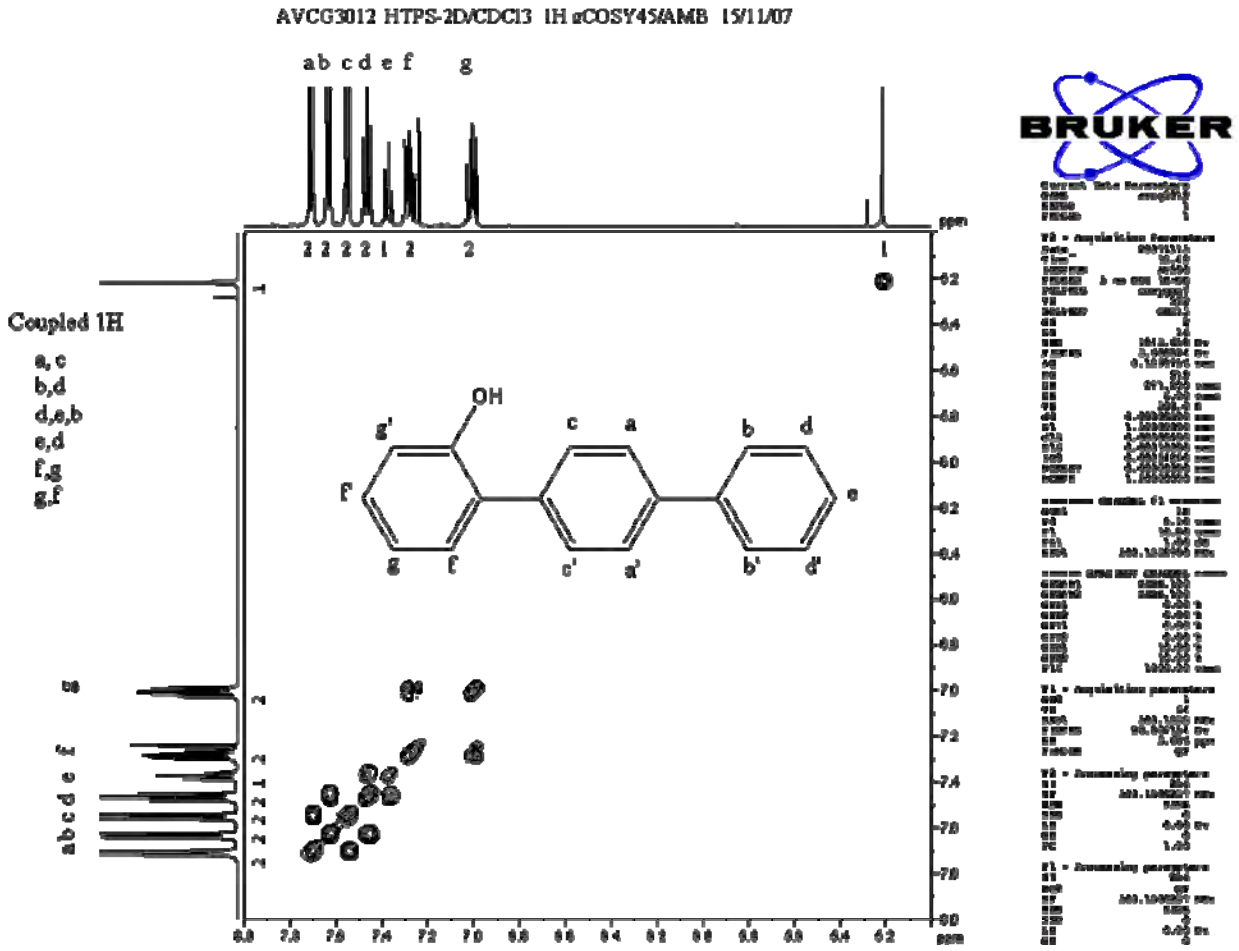


Figure S5: 2D COSY ^{1}H-nmr/$CDCl_3$ Spectra of **3.**

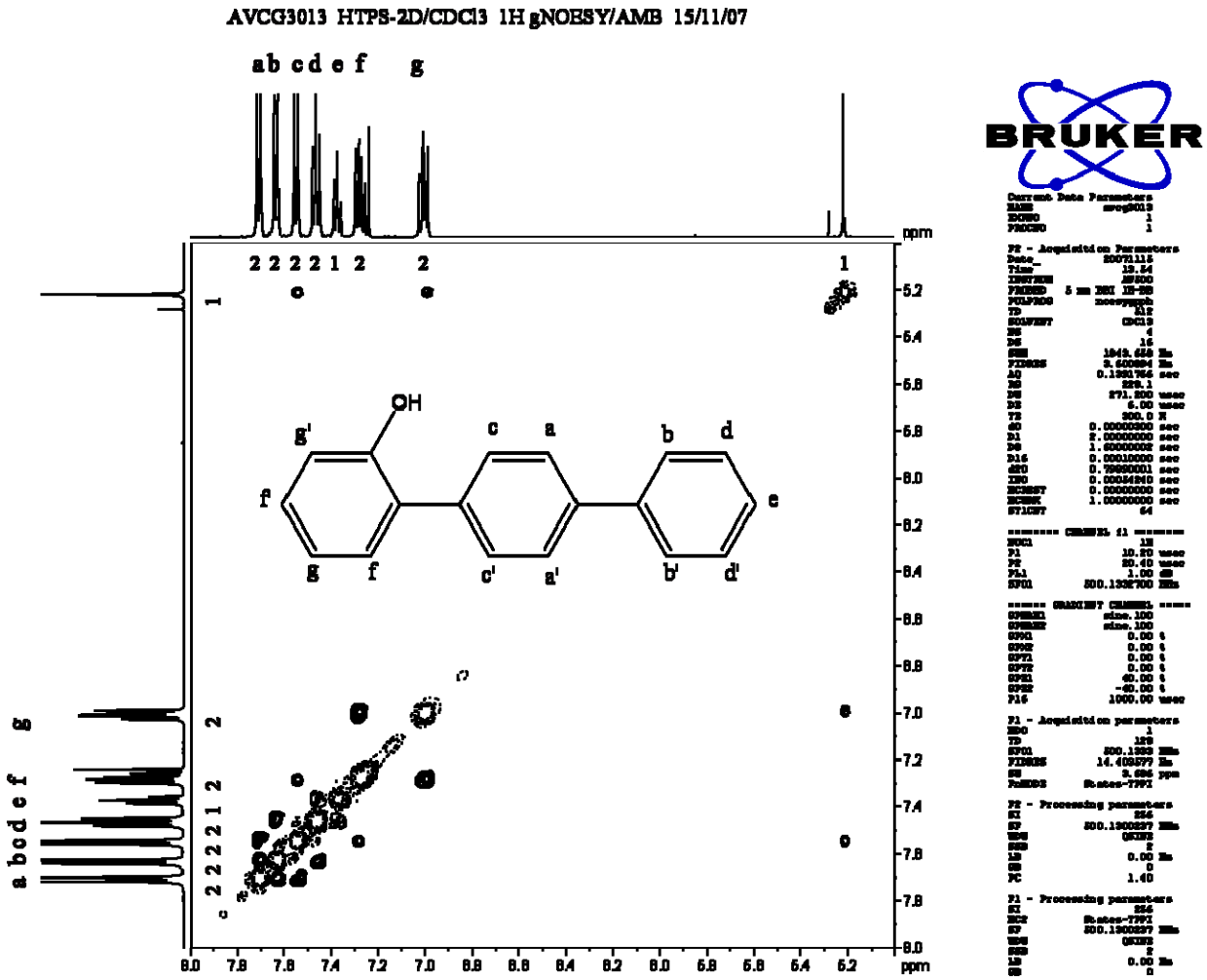


Figure S6: 2D NOESY ^{1}H-nmr/$CDCl_3$ Spectra of **3.**

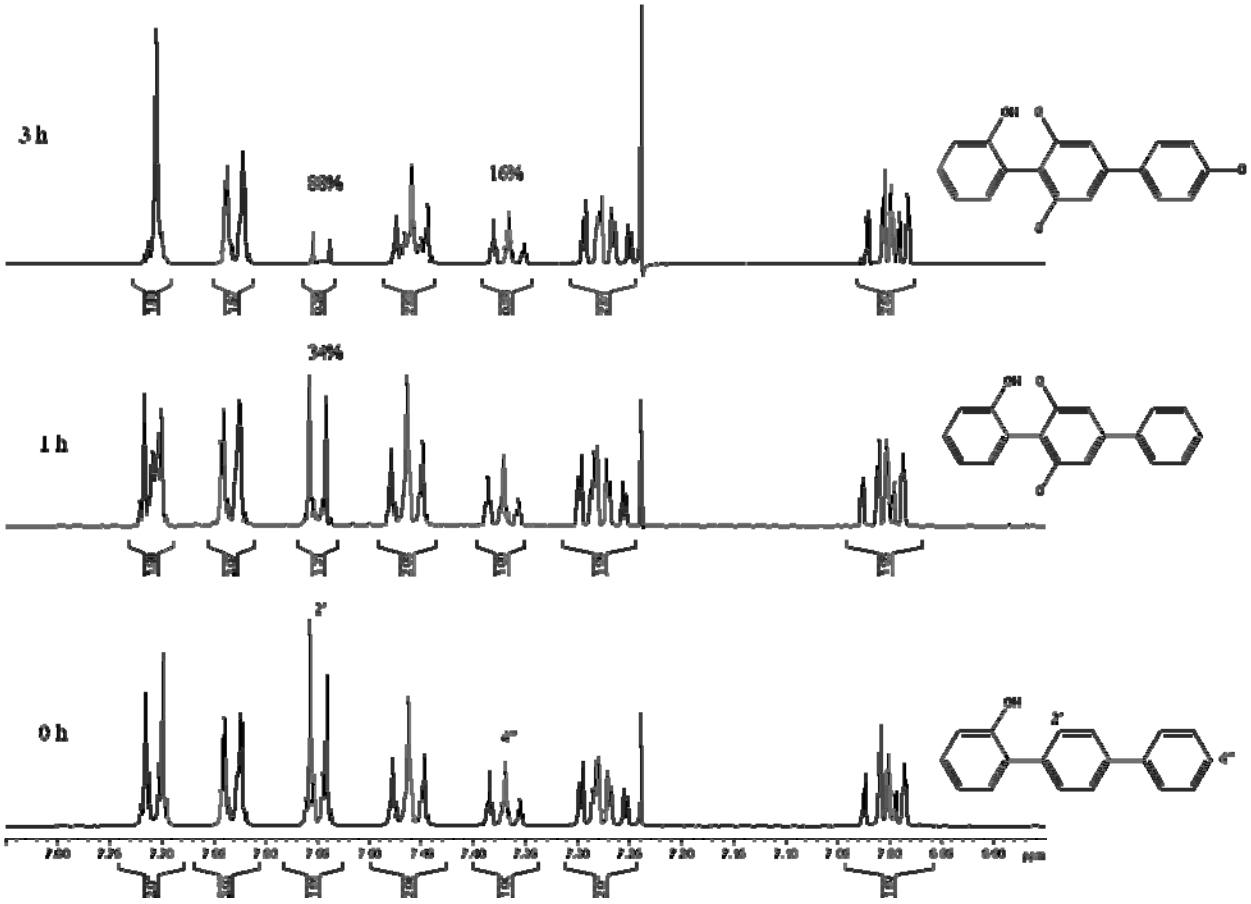


Figure S7: ^{1}H-nmr/$CDCl_3$ Spectra of expanded aromatic region of **3** before and after irradiating with 1:3 D_2O-CH_3CN at different photolysis time.

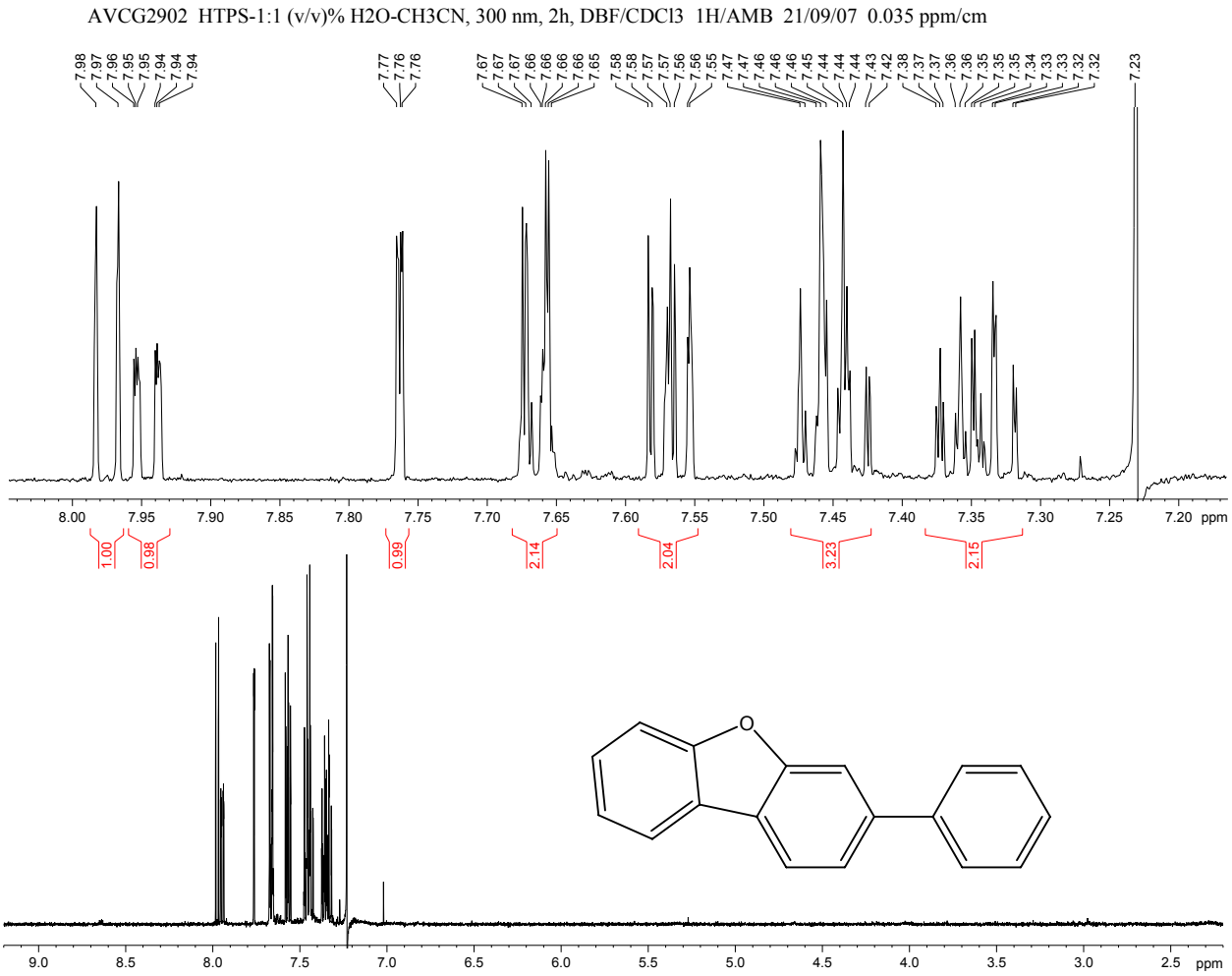


Figure S8: ^{1}H-nmr/$CDCl_3$ Spectra of **9**.

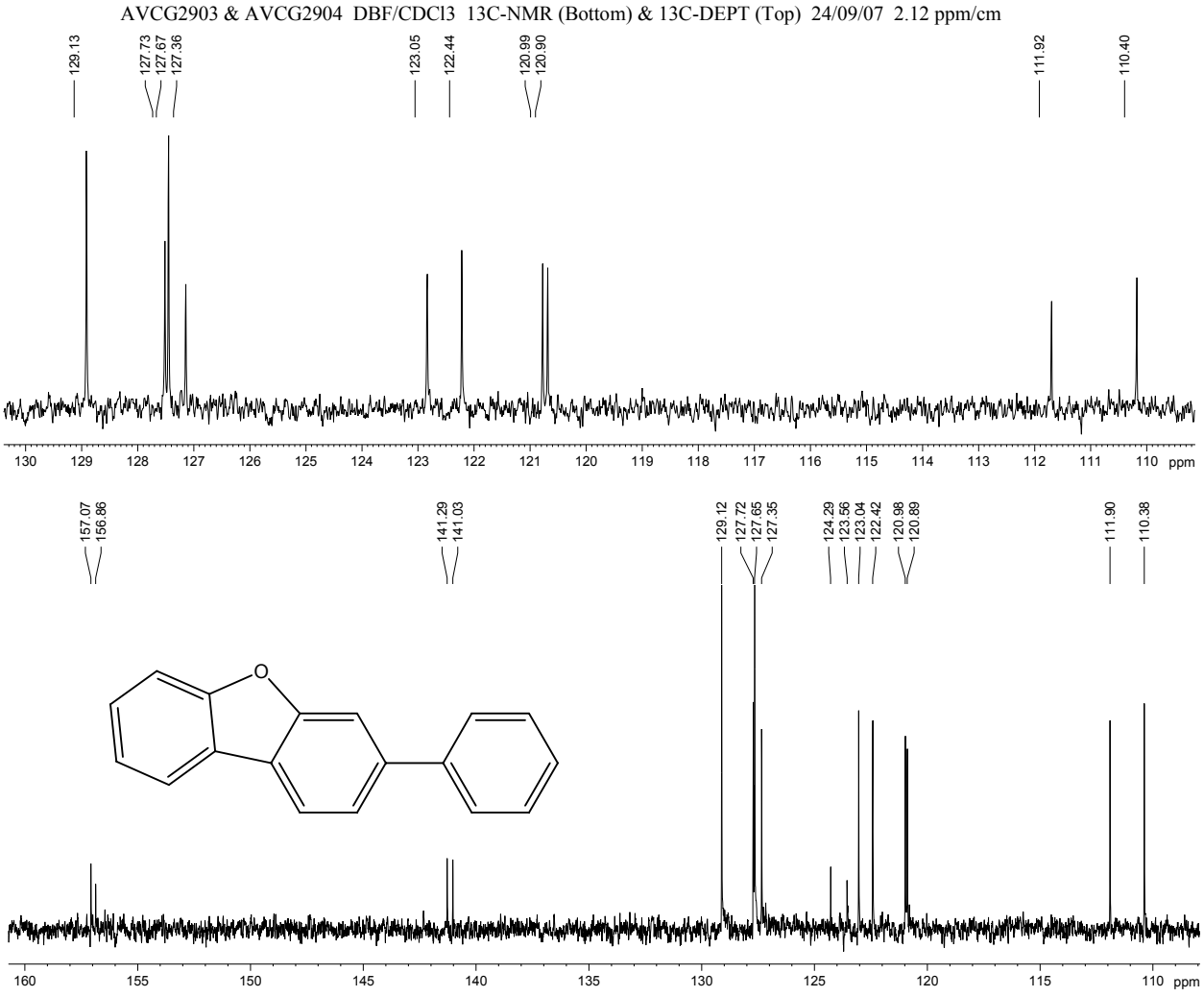


Figure S9: ^{13}C-nmr/$CDCl_3$ Spectra of **9.**

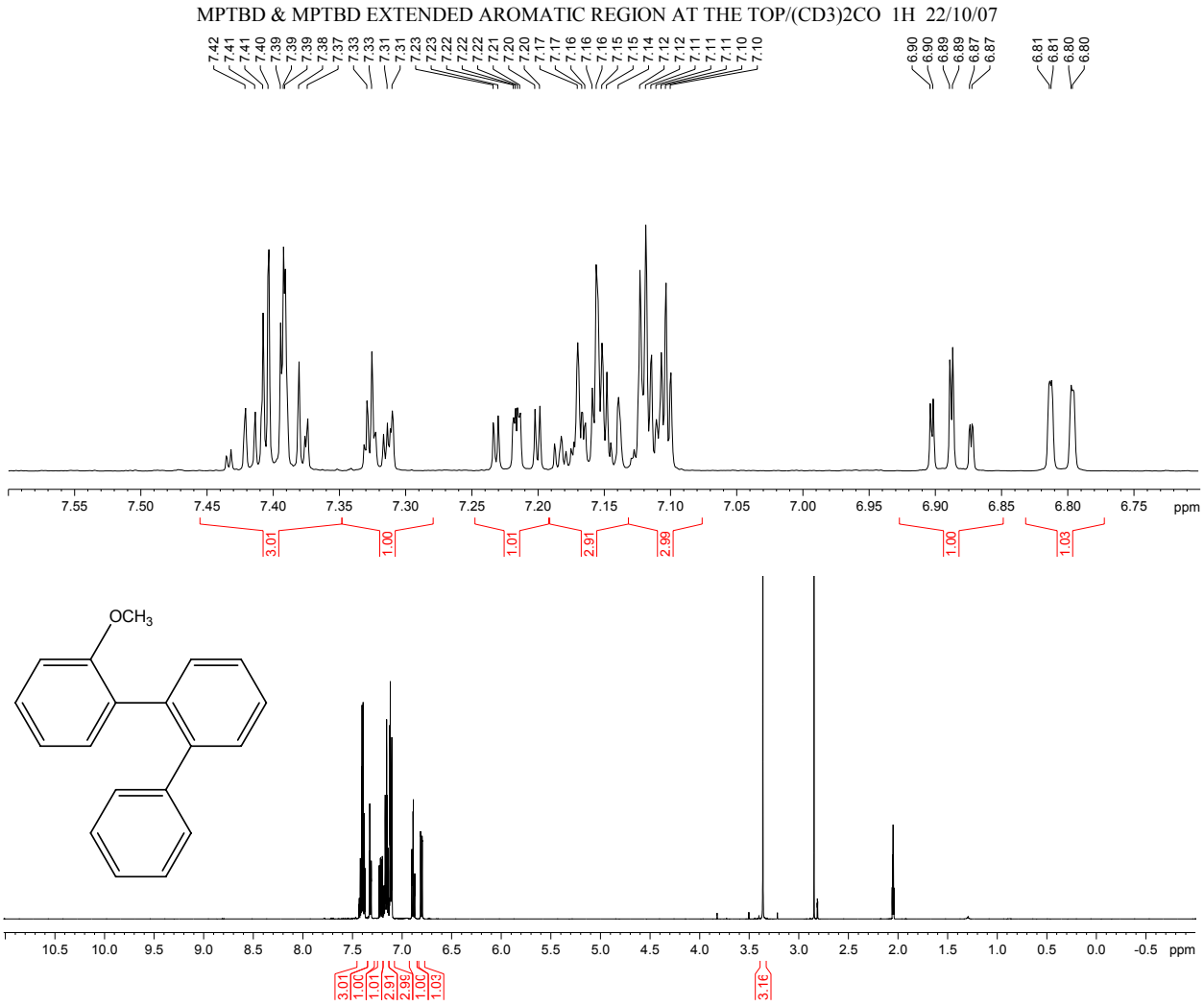


Figure S10: ^{1}H-nmr/$(CD_3)_2CO$ Spectra of **7.**

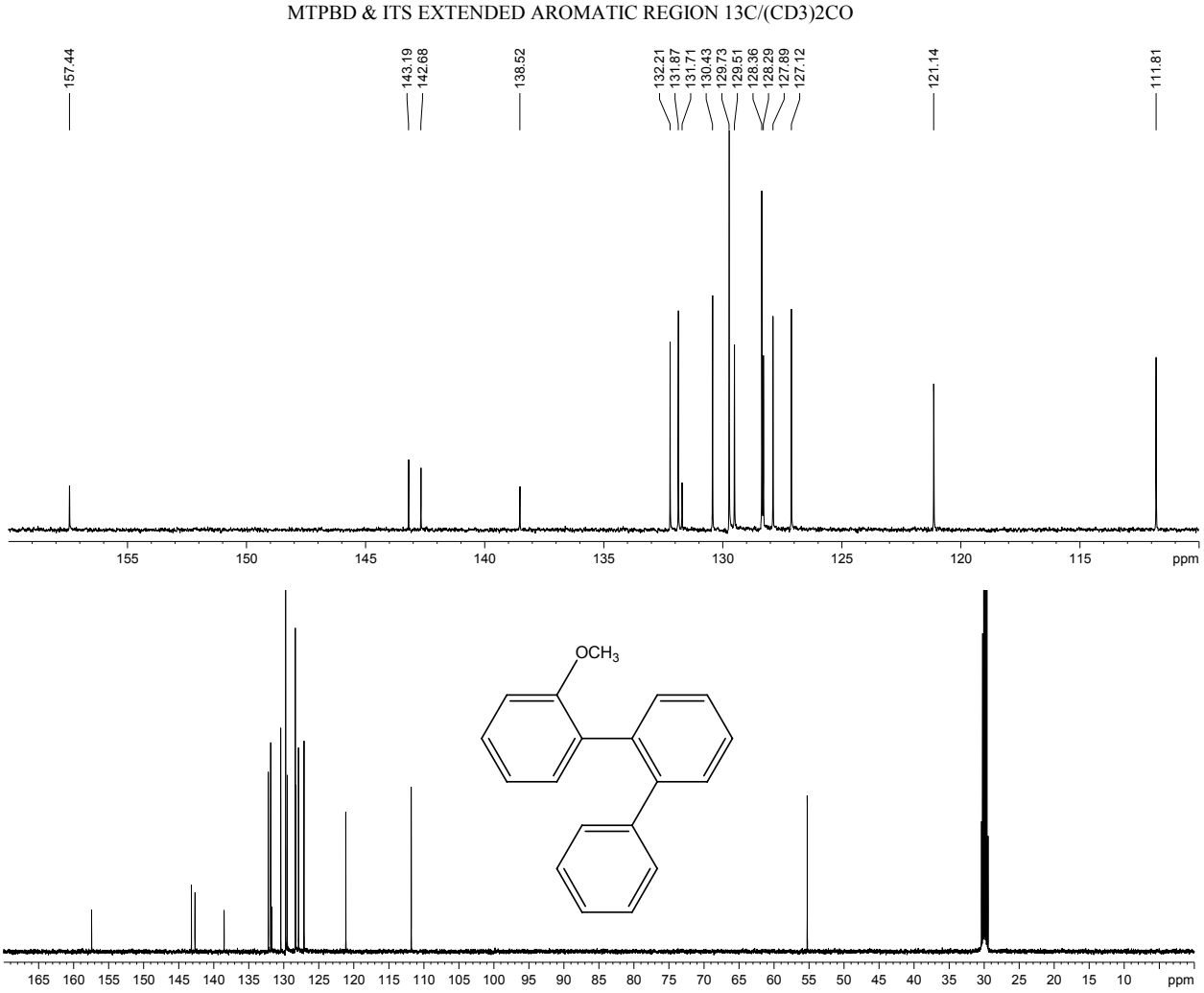


Figure S11: ^{13}C-nmr/$(CD_3)_2CO$ Spectra of **7.**

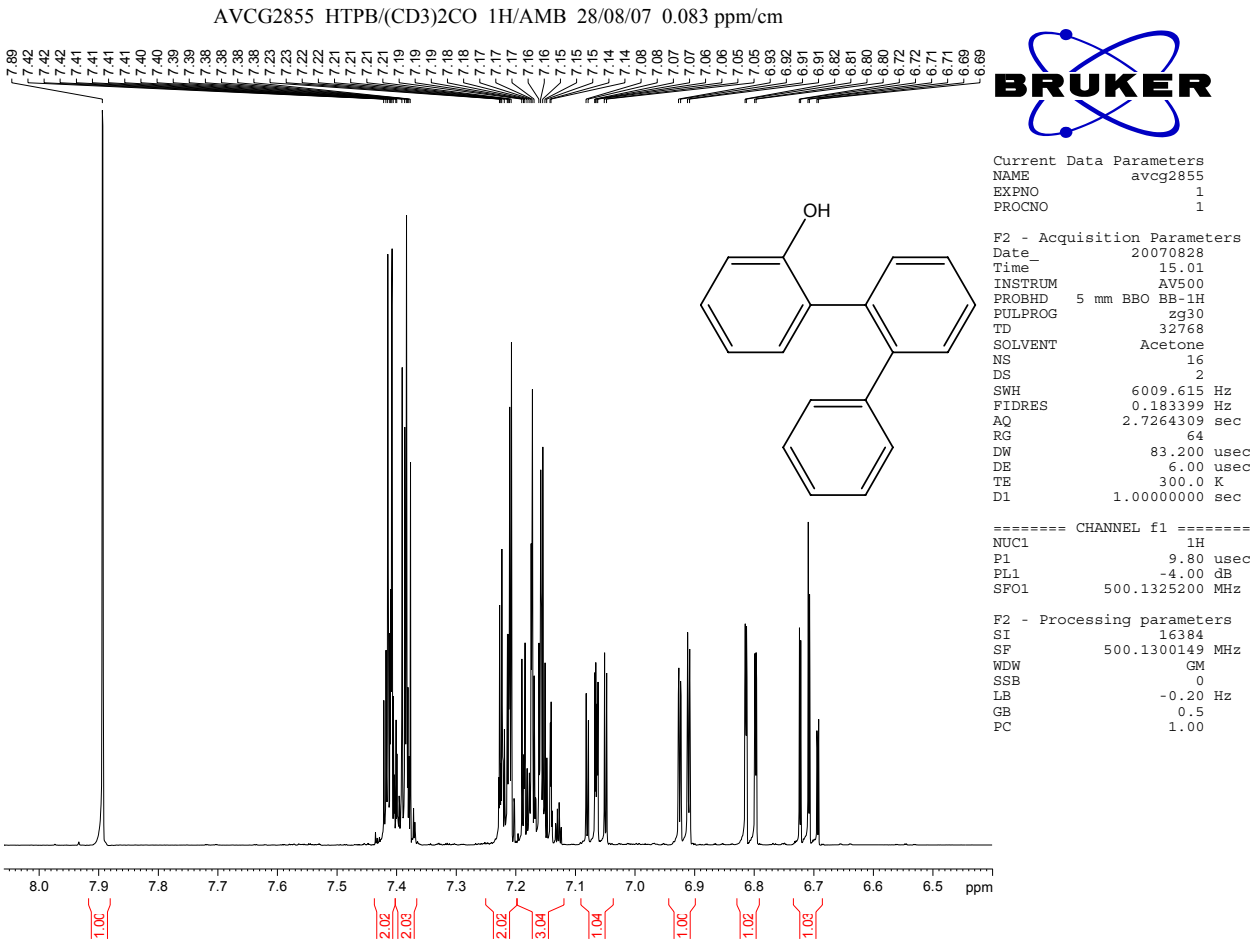


Figure S12: ^{1}H-nmr/$(CD_3)_2CO$ Spectra of **4.**

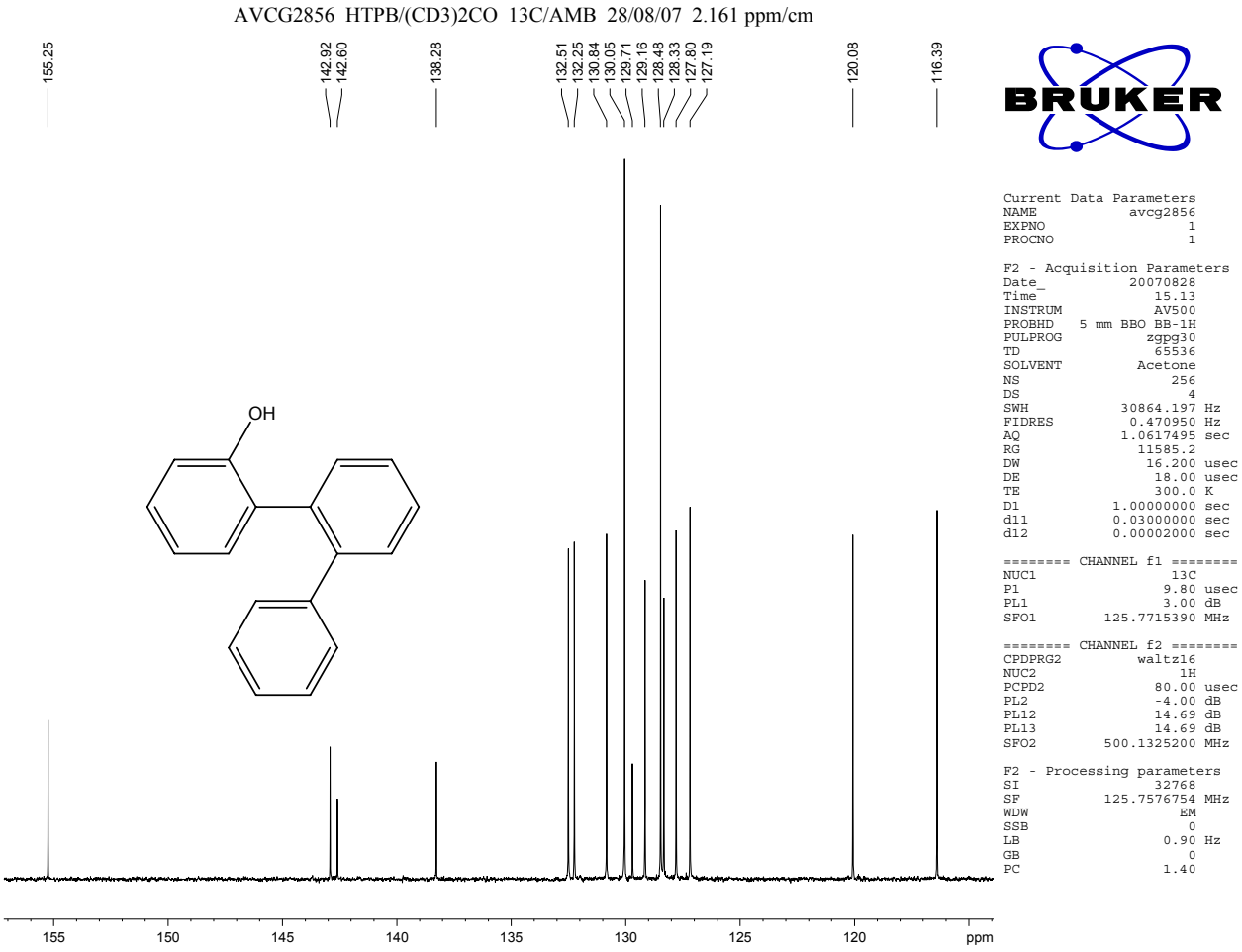


Figure S13: ^{13}C-nmr/$(CD_3)_2CO$ Spectra of **4.**

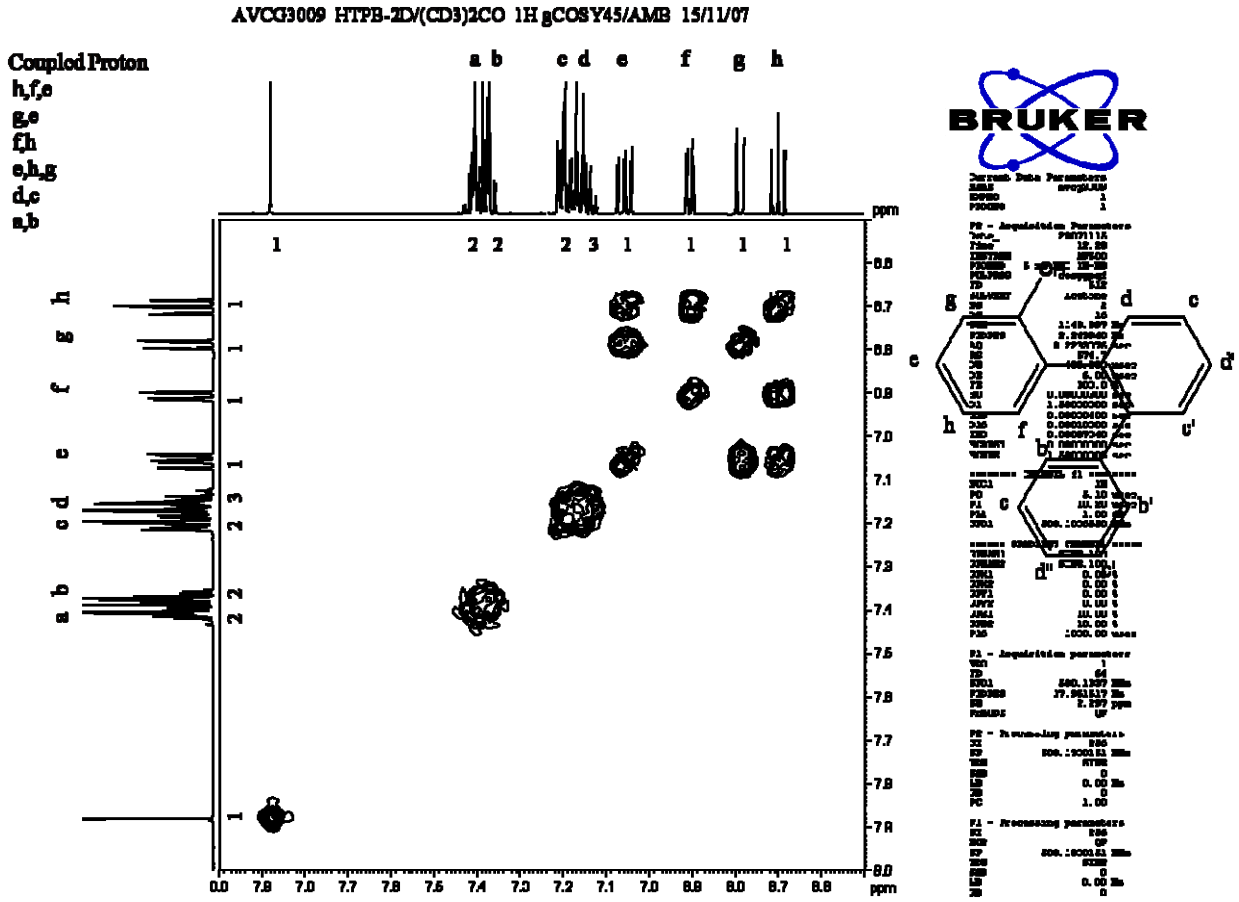


Figure S14: 2D COSY ^{1}H-nmr/$(CD_3)_2CO$ Spectra of **4.**

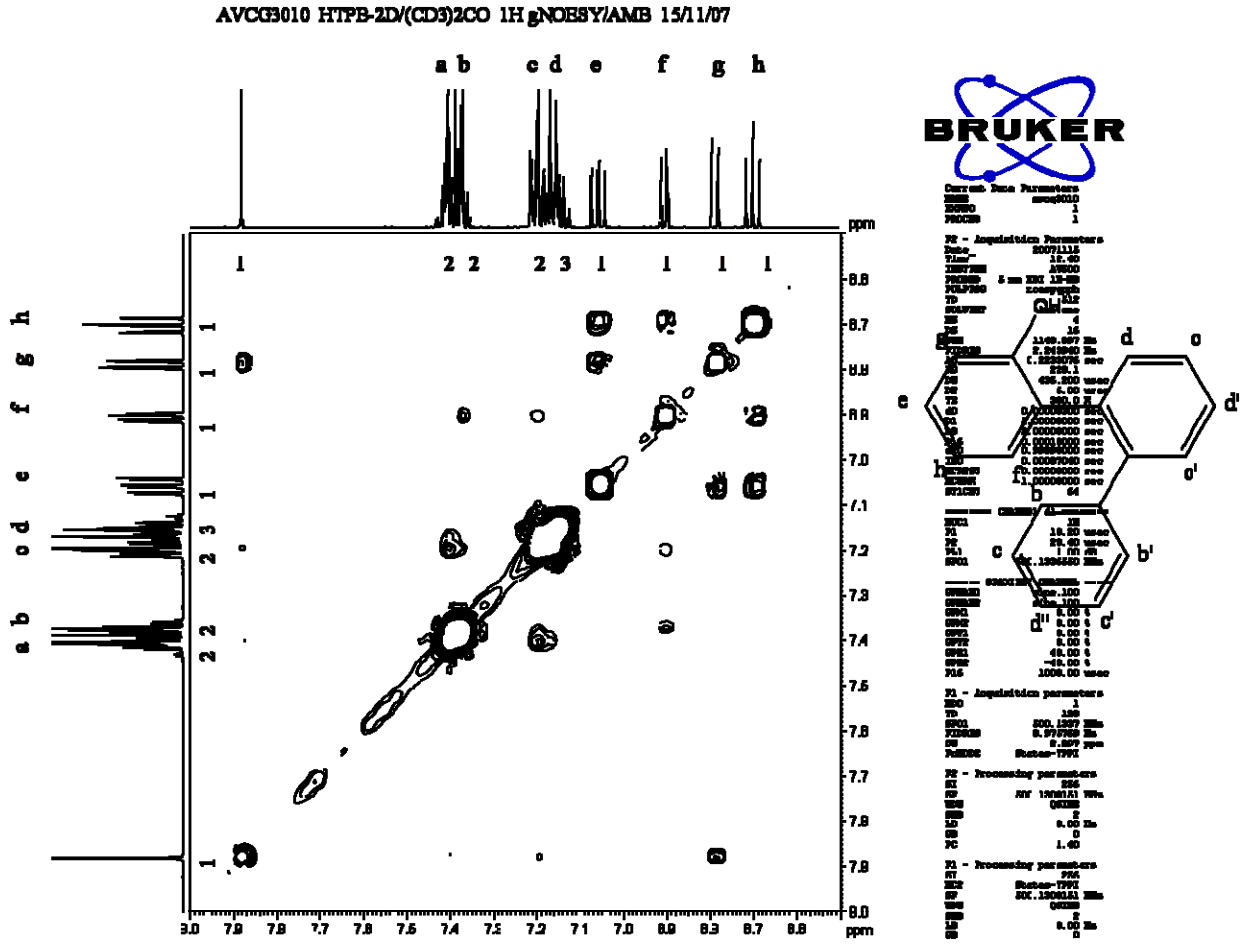


Figure S15: 2D NOESY ^{1}H-nmr/$(CD_3)_2CO$ Spectra of **4.**

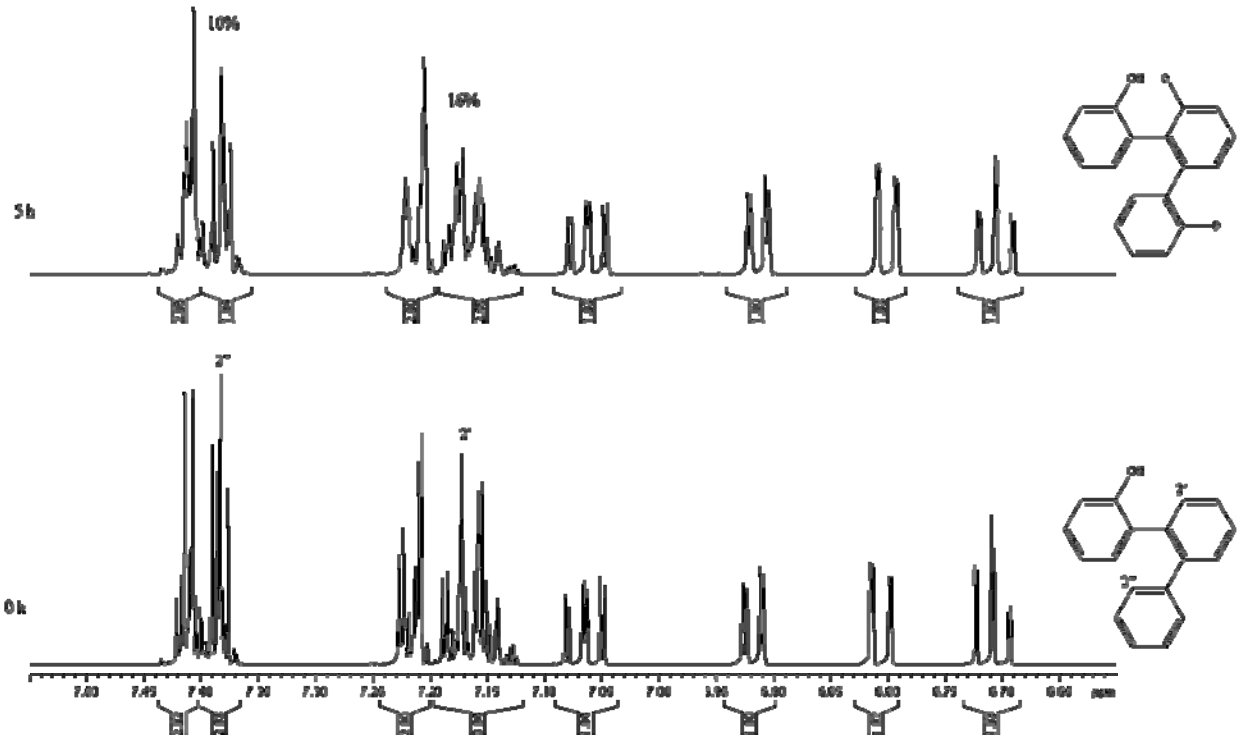


Figure S16: ^{1}H-nmr/$(CD_3)_2CO$ Spectra of expanded aromatic region of **4** before and after 5 h irradiation with 1:2 D_2O-CH_3CN, 254 nm.

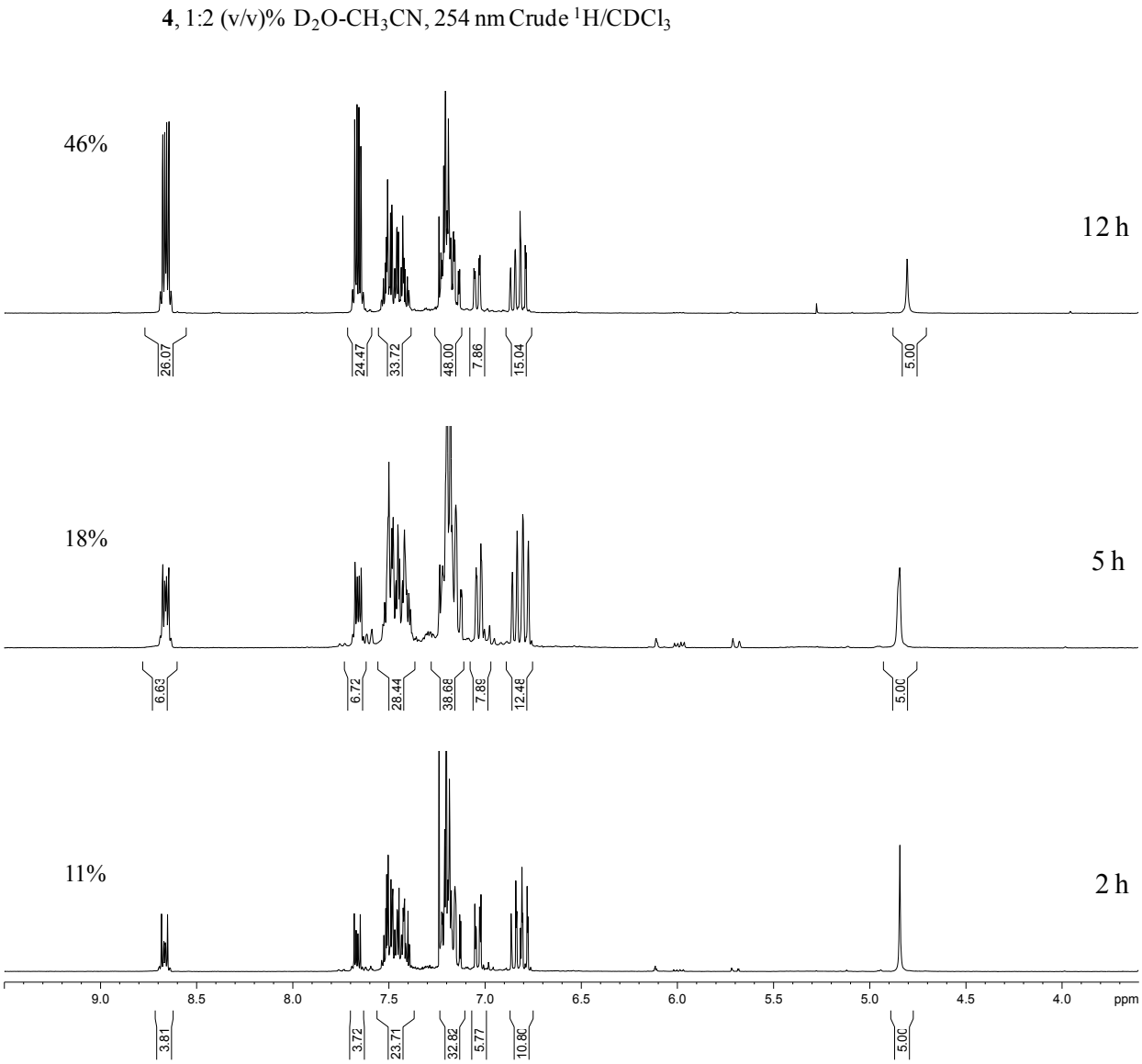


Figure S17: Crude ^{1}H-nmr/$CDCl_3$ Spectra of sample **4** after irradiating with 1:2 D_2O-CH_3CN at 254 nm and varying photolysis time from 2-12 h.

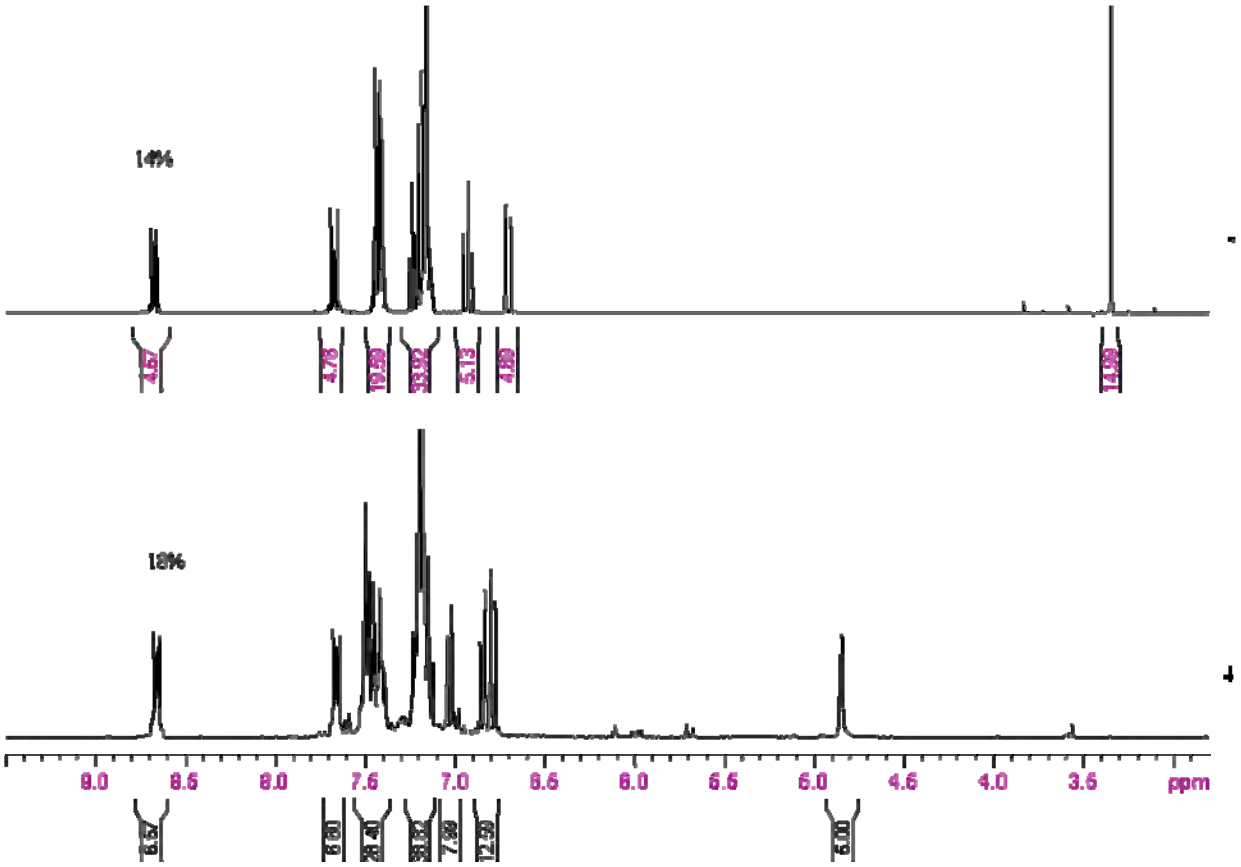


Figure S18: Crude ^{1}H-nmr/$CDCl_3$ Spectra of sample **7** (top) and **4** (bottom) after irradiating 5 h with 1:2 D_2O-CH_3CN at 254 nm.

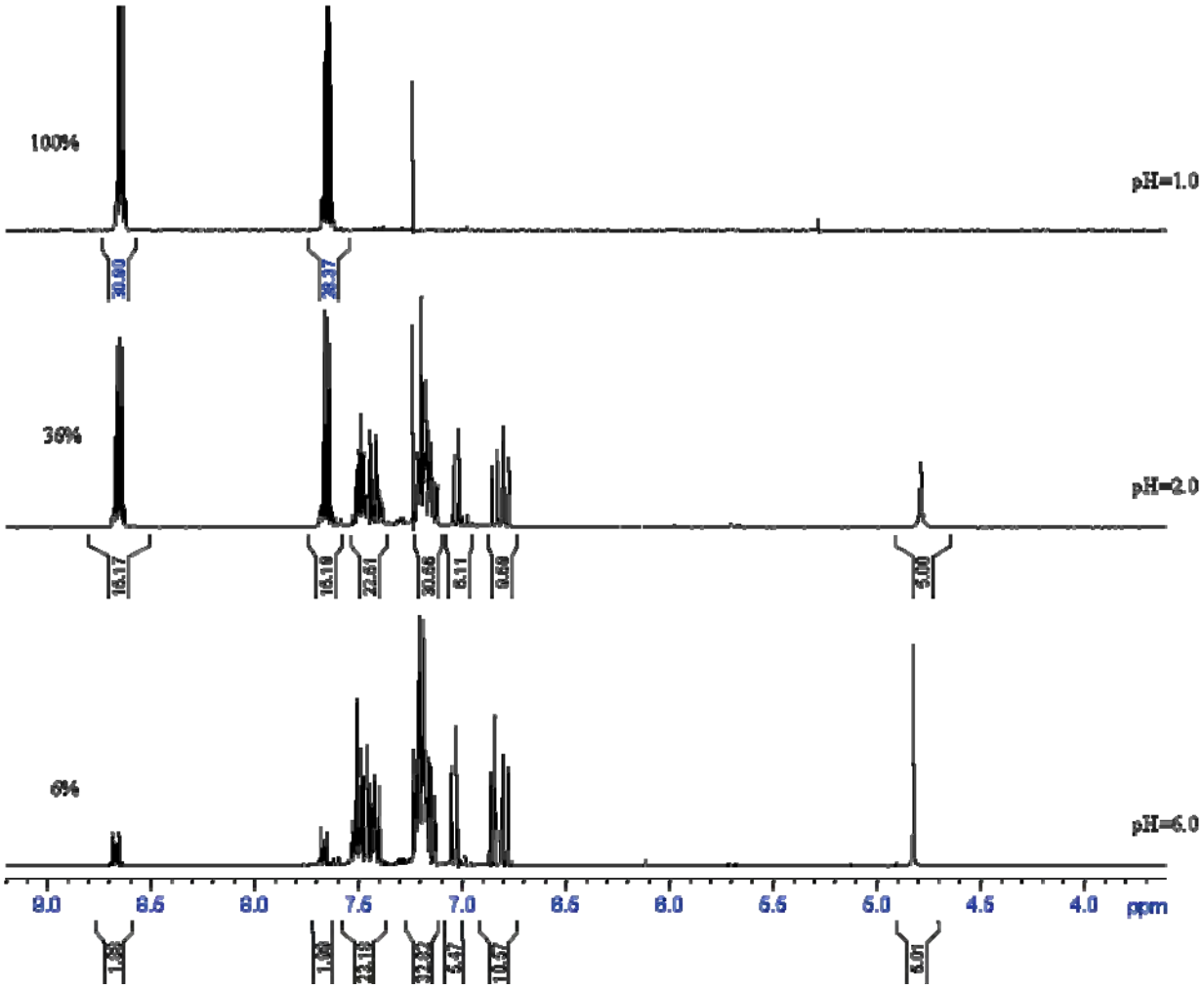


Figure S19: Crude ^{1}H-nmr/$CDCl_3$ Spectra of sample **4** after irradiating 2 h with 1:1 H_2O-CH_3CN at 254 nm, by varying the pH of aqueous solution from 7.0 to 1.0.

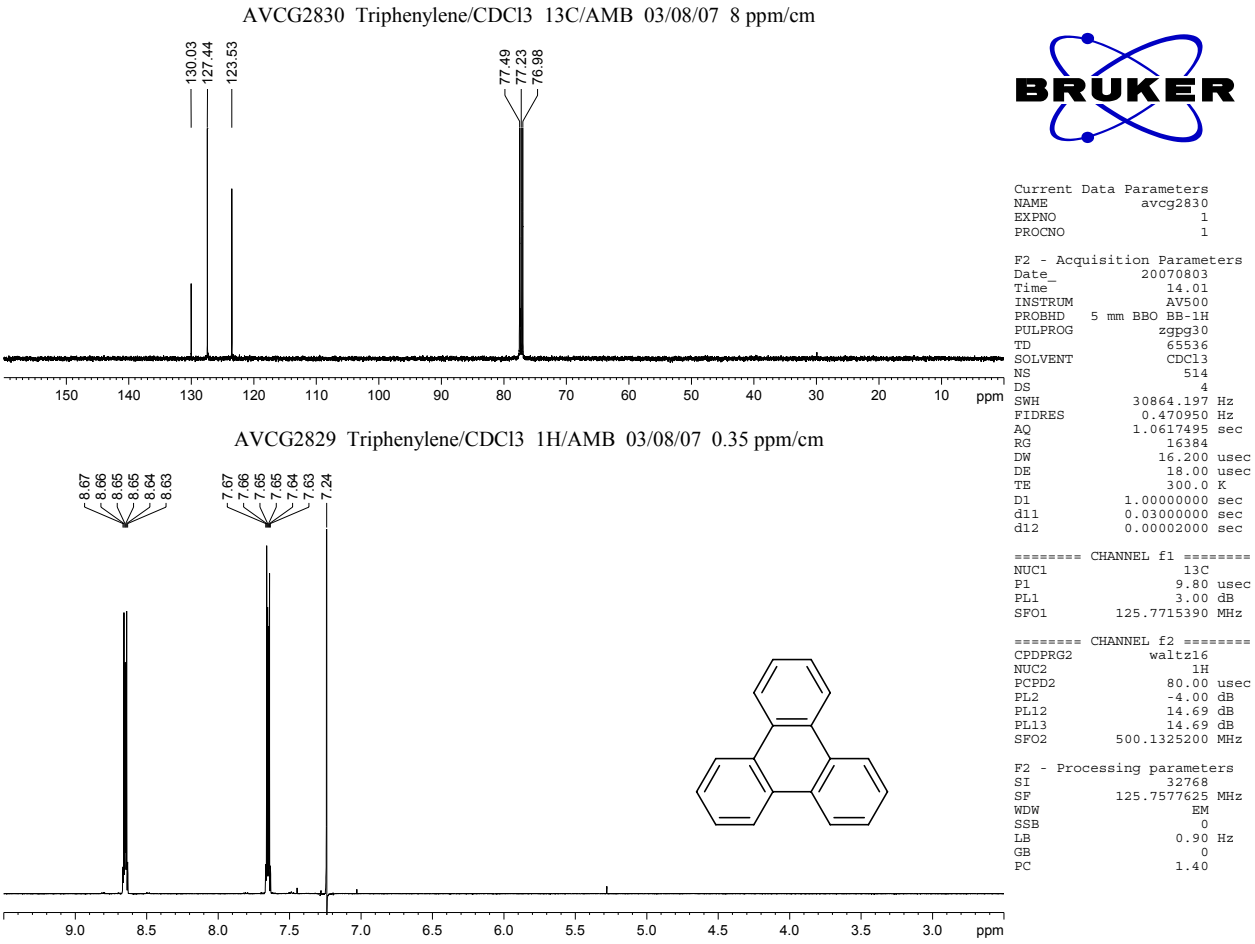


Figure S20: ^{1}H & ^{13}C-nmr/($CDCl_3$) Spectra of triphenylene (**10).**

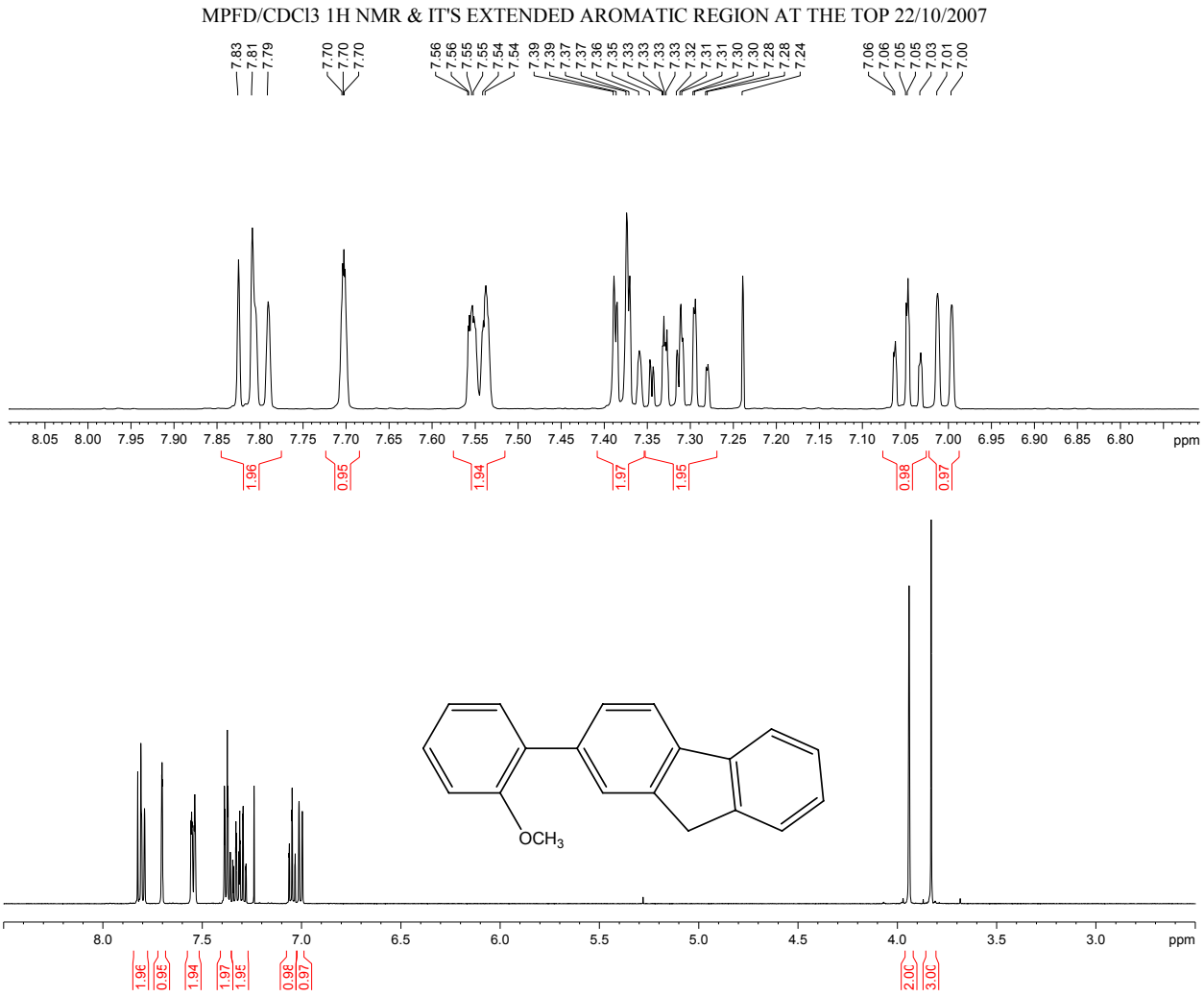


Figure S21: ^{1}H-nmr/$CDCl_3$ Spectra of **8.**

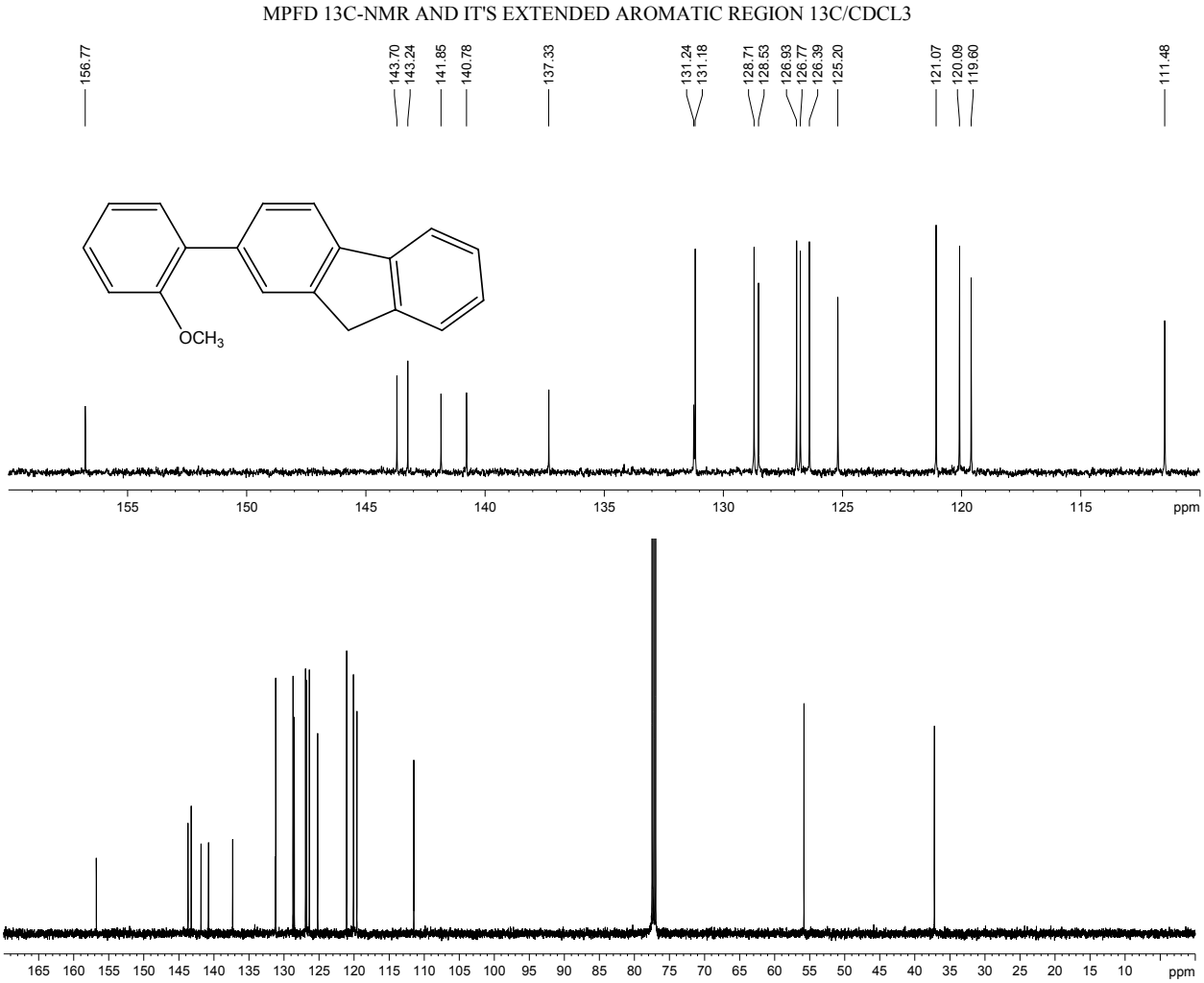


Figure S22: ^{13}C-nmr/$CDCl_3$ Spectra of **8.**

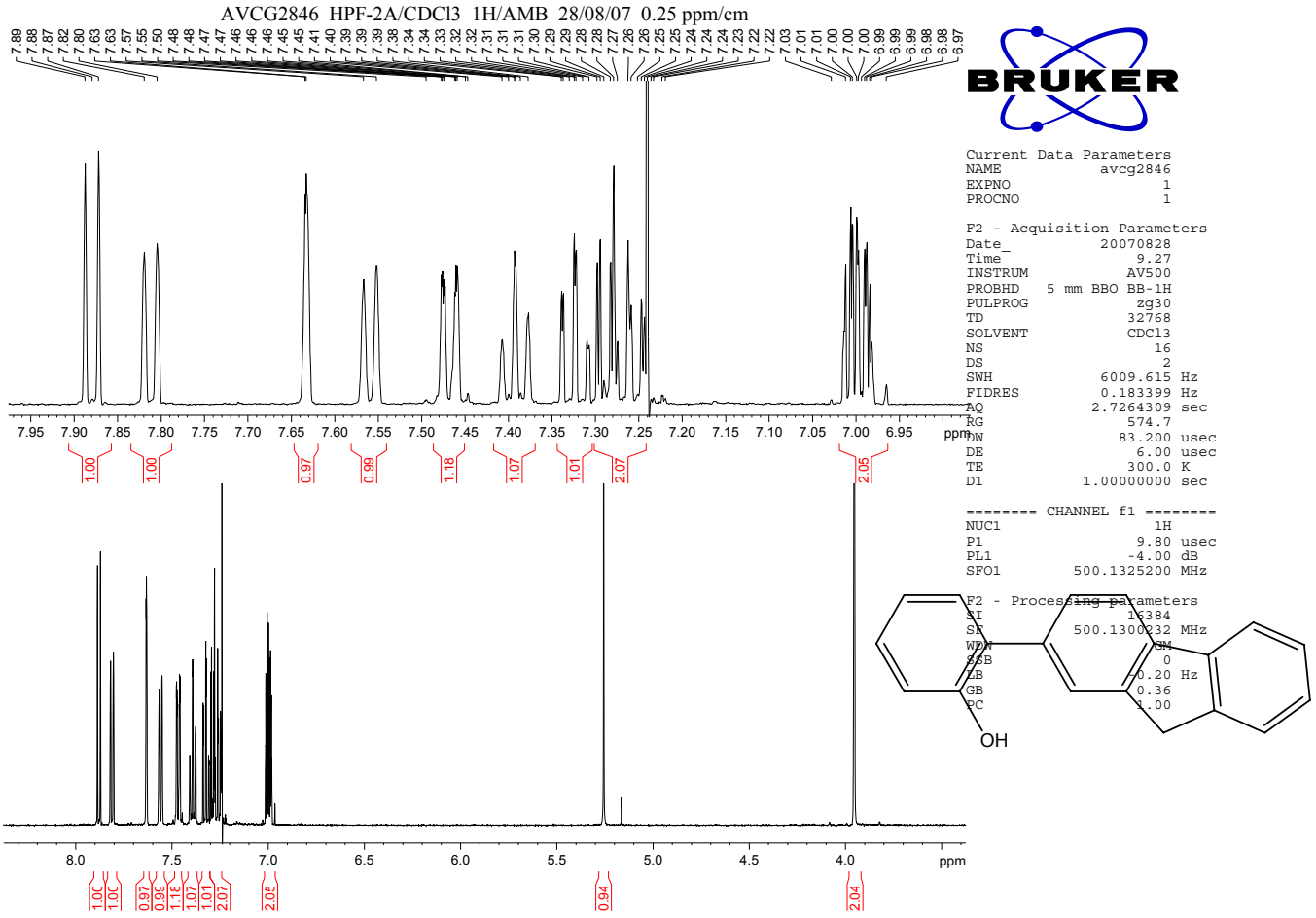


Figure S23: ^{1}H-nmr/$CDCl_3$ Spectra of **5.**

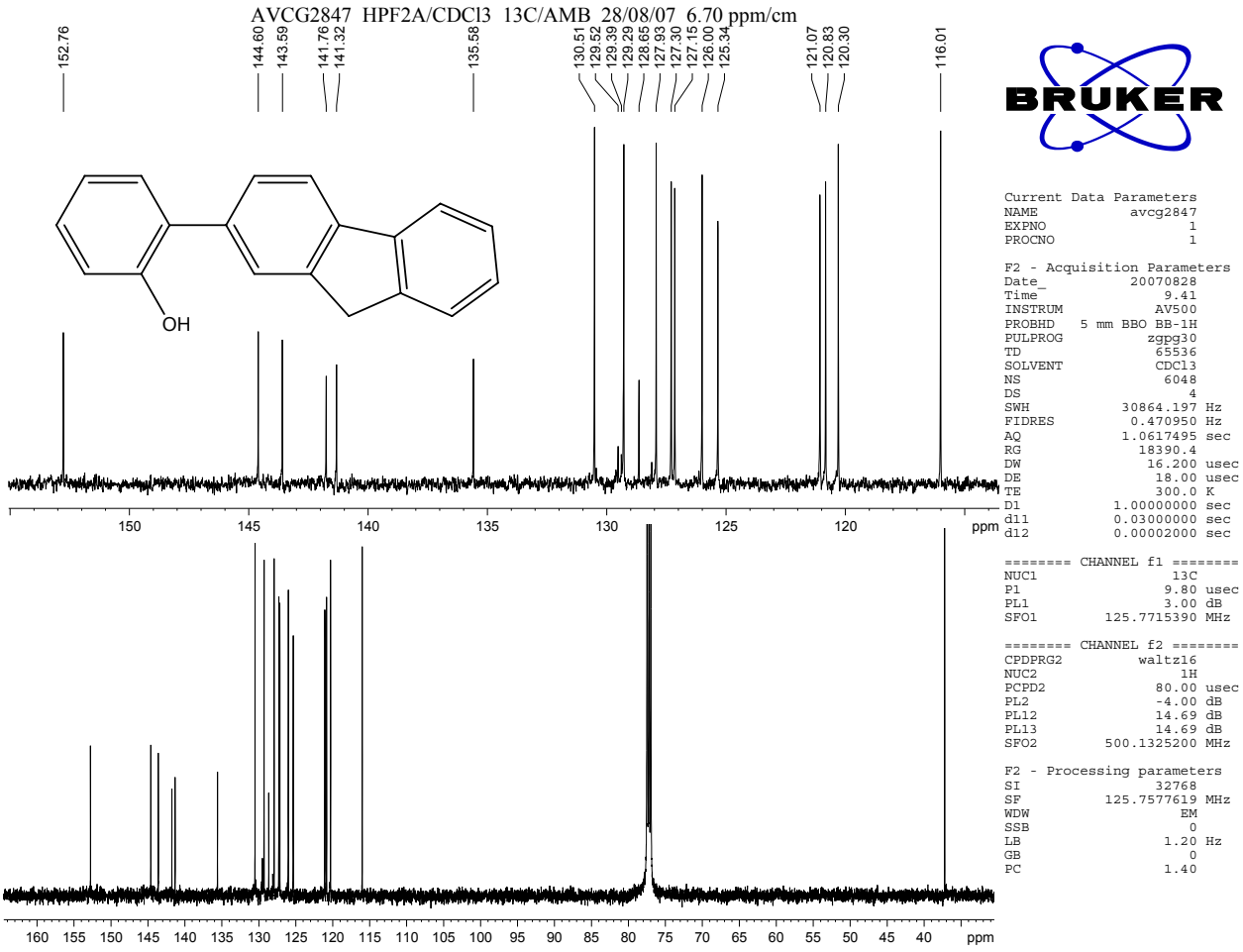


Figure S24: ^{13}C-nmr/$CDCl_3$ Spectra of **5.**

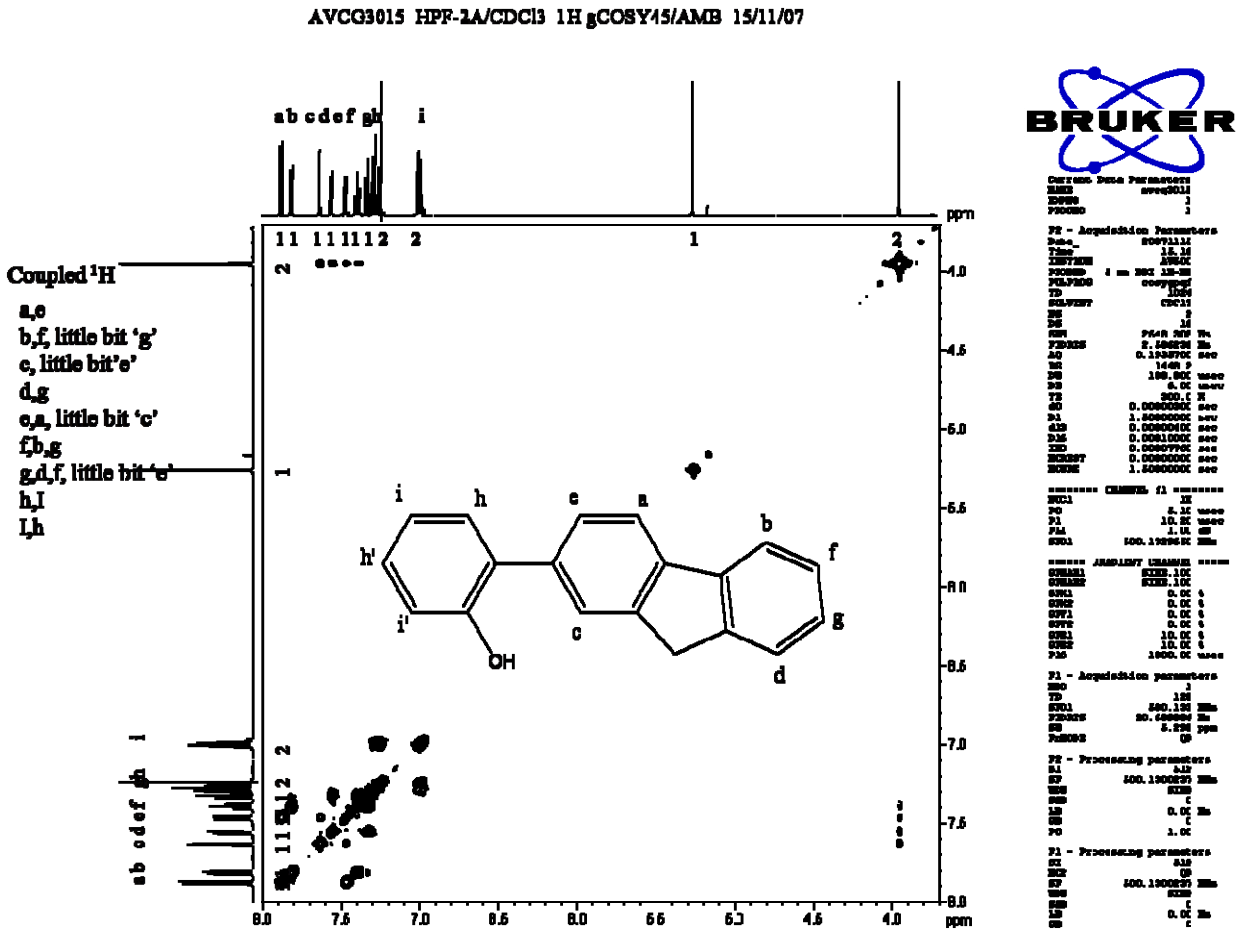


Figure S25: 2D COSY ^{1}H-nmr/$CDCl_3$ Spectra of **5.**

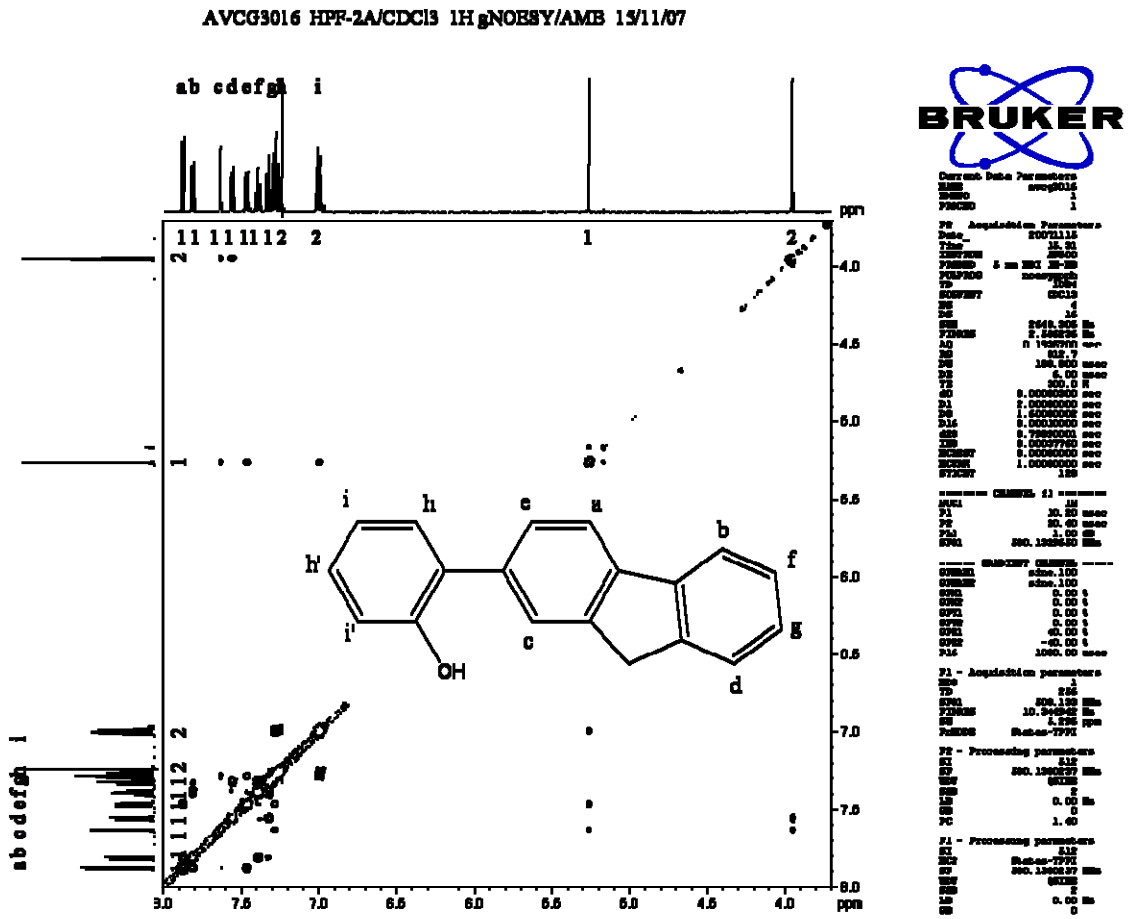
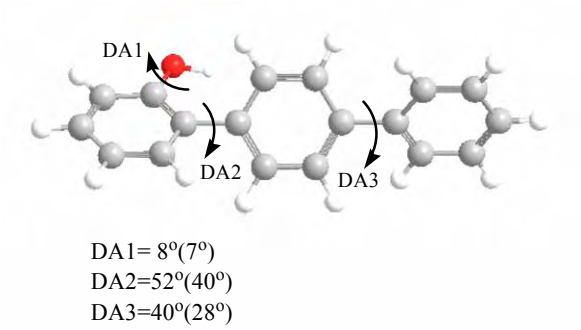
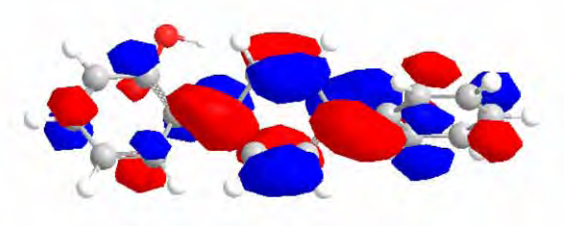


Figure S26: 2D NOESY ^{1}H-nmr/$CDCl_3$ Spectra of **5.**



LUMO



HOMO

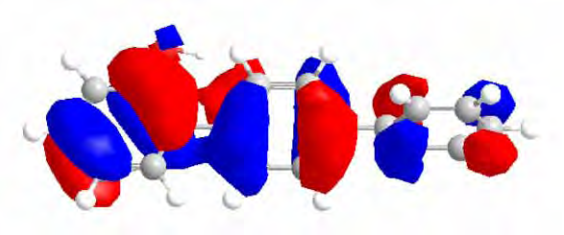
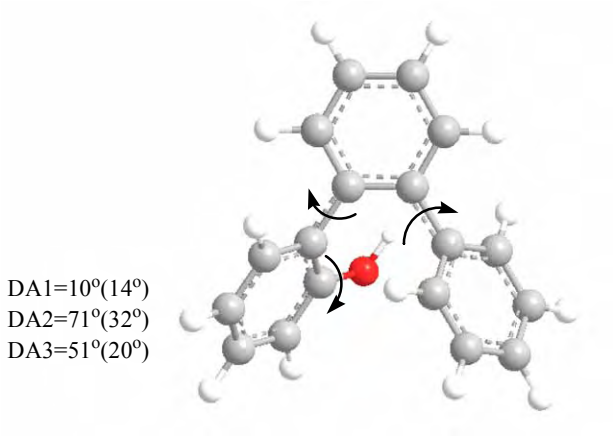
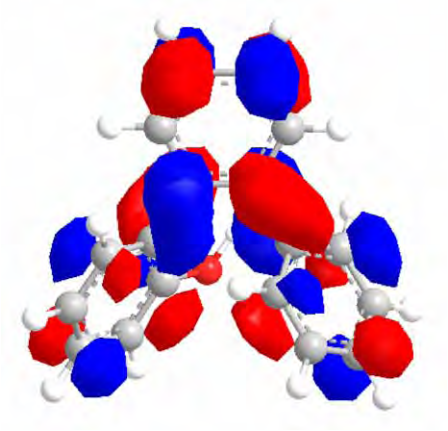


Figure S27: Geometry Optimization and MO's Calculation in Ground and First Excited Singlet State (bracketed values) of **3** using AM1 Methodology.



LUMO



HOMO

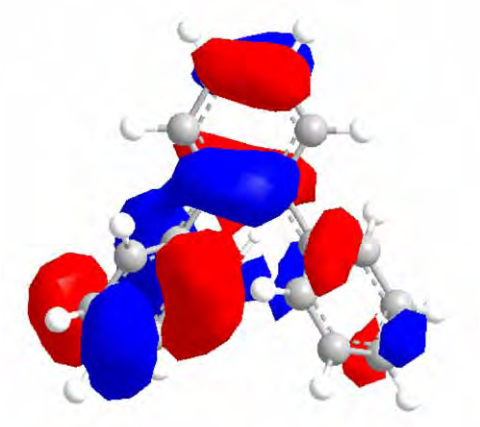
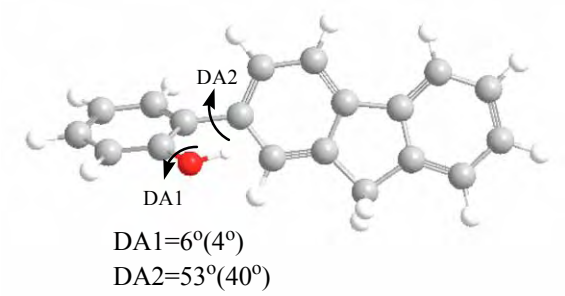
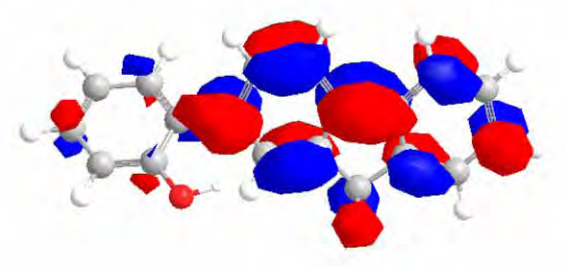


Figure S28: Geometry Optimization and MO's Calculation in Ground and First Excited Singlet State (bracketed values) of **4** using AM1 Methodology.



LUMO



HOMO

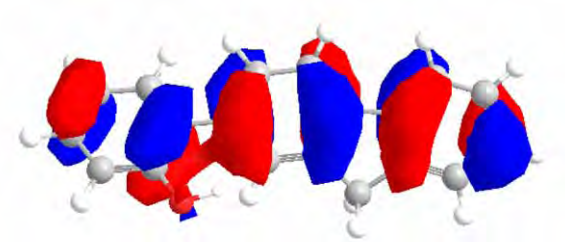


Figure S29: Geometry Optimization and MO's Calculation in Ground and First Excited Singlet State (bracketed values) of **5** using AM1 Methodology.

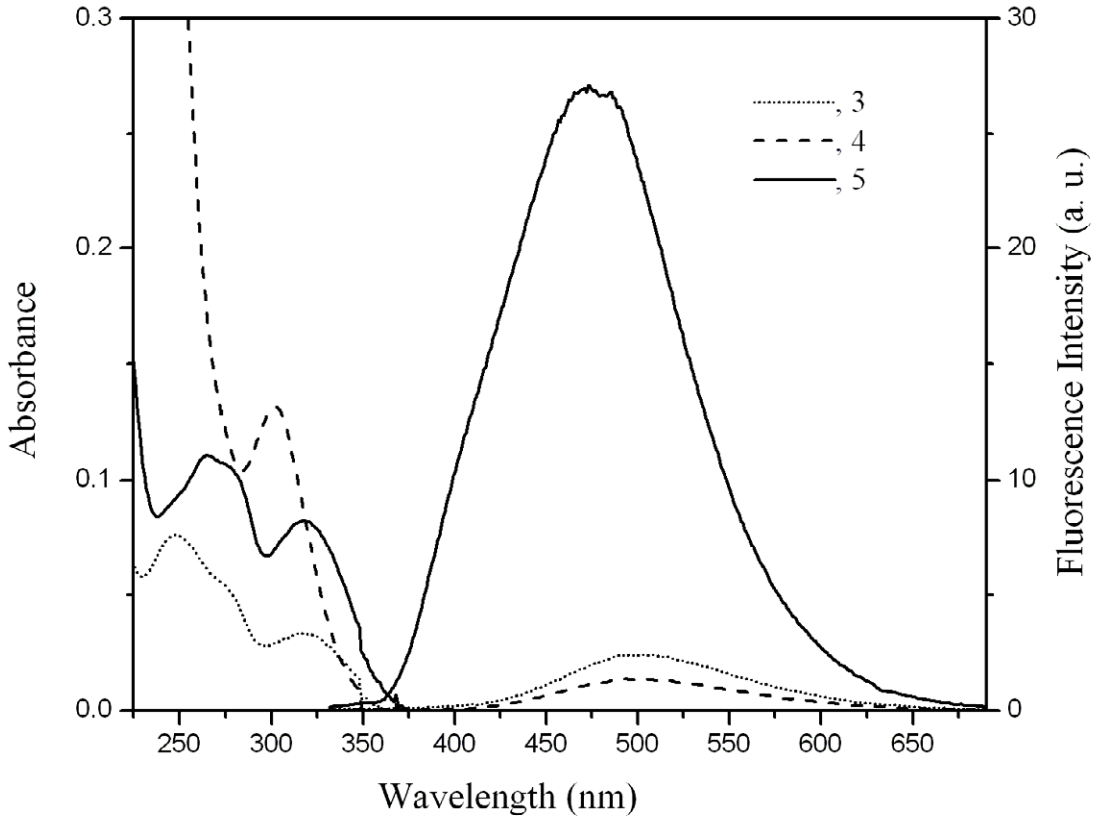


Figure S30: Absorption and Emission Spectra of Monoanions of **3**-**5** at pH 11.0.

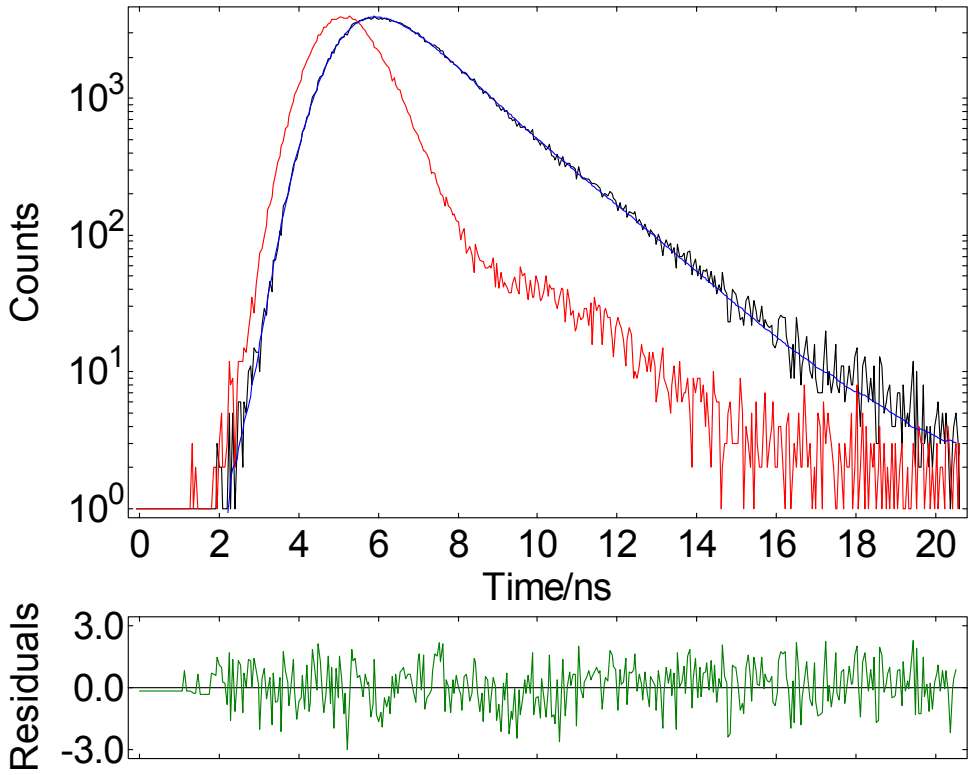


Figure S31: Fluorescence decay profile of **3** in CH_3CN.

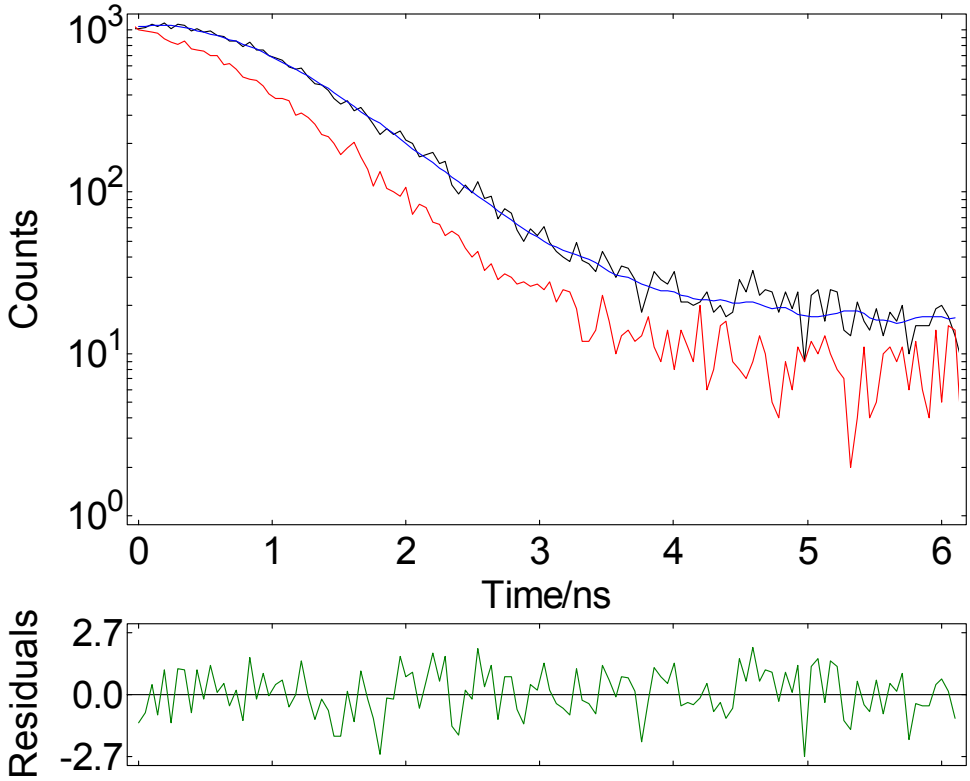


Figure S32: Fluorescence decay profile of **4** in CH_3CN.

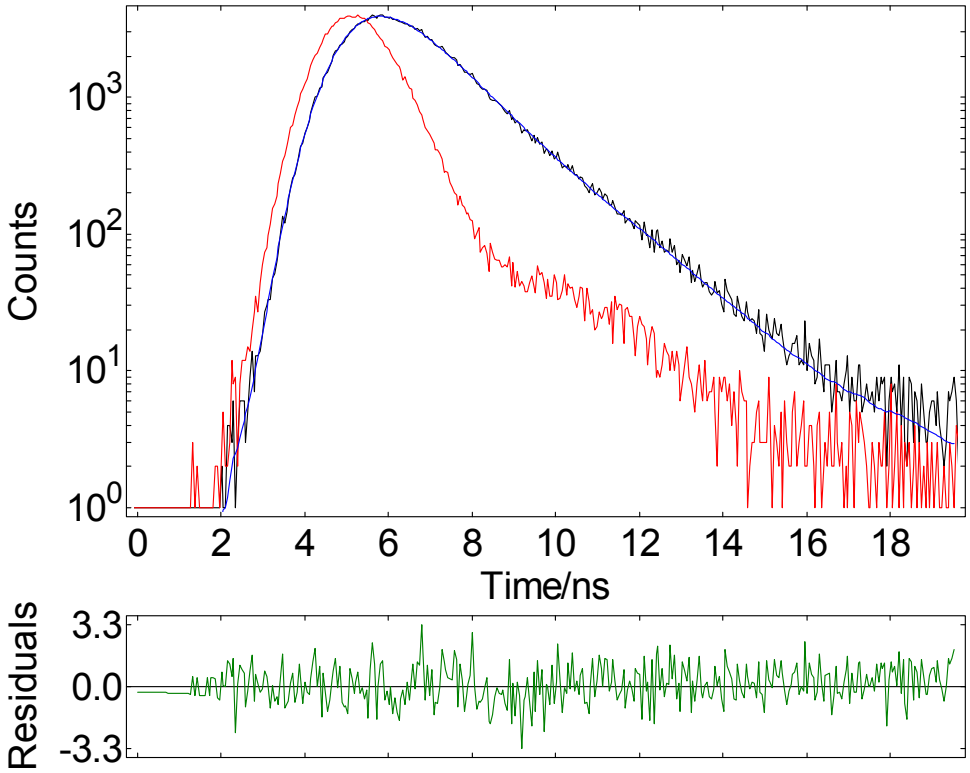


Figure S33: Fluorescence decay profile of **5** in CH_3CN.

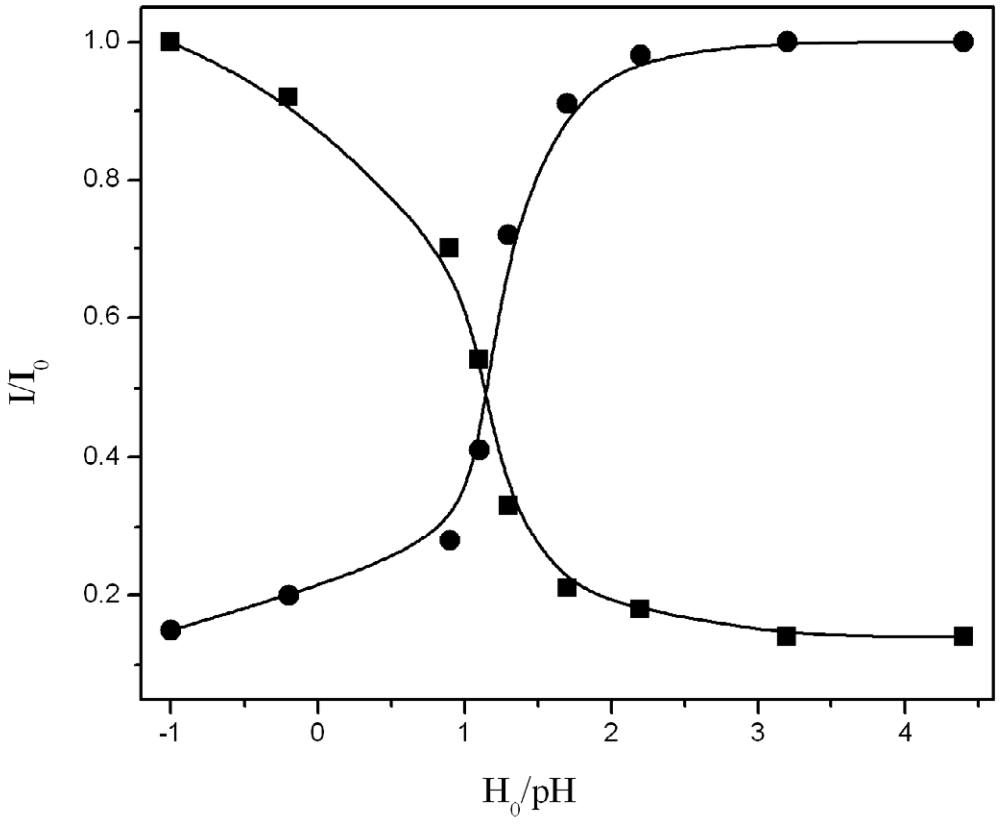


Figure S34: Plot of I/I_0 of **3** vs. H_0/pH of aqueous (5.0×10^{-6} M) solution containing 1% of CH_3CN and excited at isosbestic point at 305 nm: (■) neutral and (●) anion.

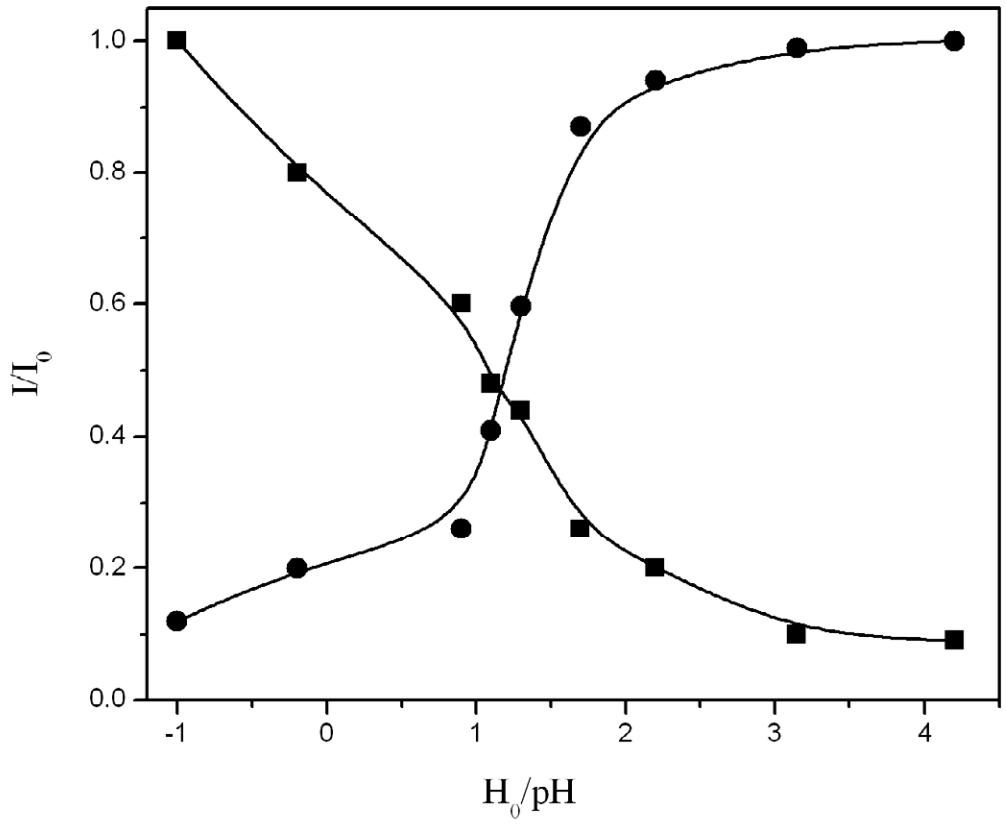


Figure S35: Plot of I/I_0 of **4** vs. H_0/pH of aqueous (2.4×10^{-5} M) solution containing 1% of CH_3CN and excited at isosbestic point at 285 nm: (■) neutral and (●) anion.

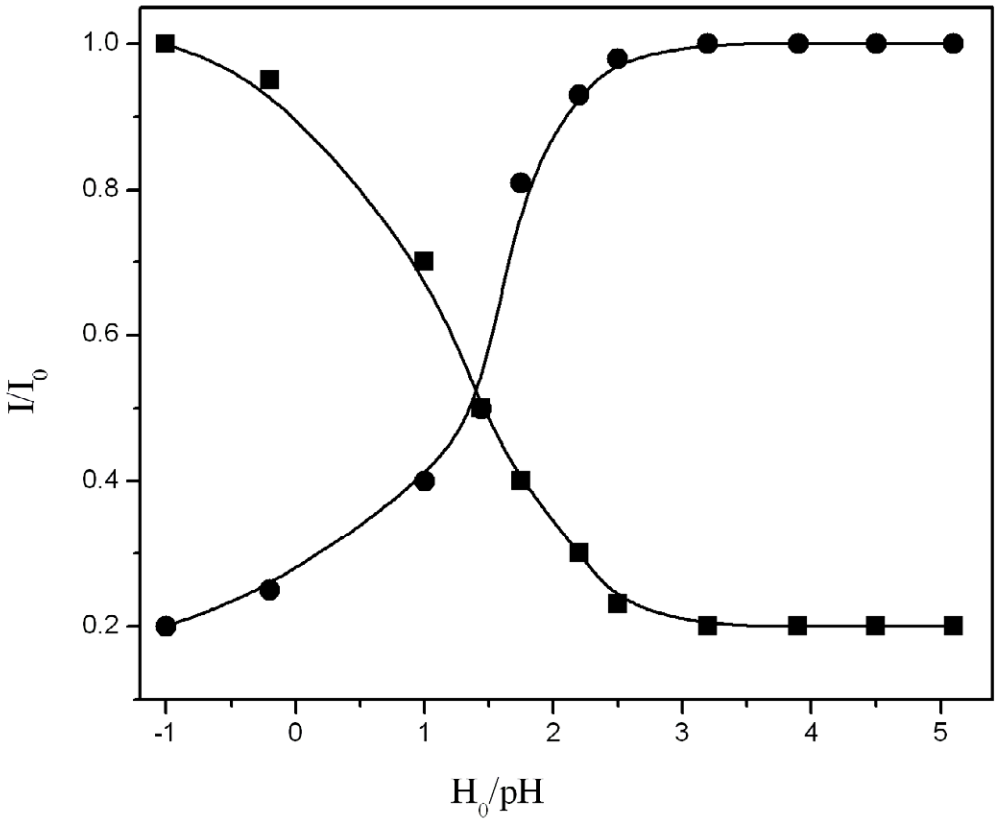


Figure S36: Plot of I/I_0 of **5** vs. H_0/pH of aqueous (5.0×10^{-5} M) solution containing 1% of CH_3CN and excited at isosbestic point at 314 nm: (■) neutral and (●) anion.

Table S1: Effects of Solvents on Photocyclization Reaction of **4** to Triphenylene (**10**).

[**4**]= ~ $1x10^{-3}$ M, 100 mL	% Triphenylene (**10**)
254 nm, 2h, 16 Lamp	
Cosolvents	
1:1 (v/v)% CH_3CN-H_2O	11
1:1 (v/v)% CH_3CN-D_2O	10
1:1 (v/v)% H_2O-MeOH	16
1:1 (v/v)% CH_3CN-MeOH	2
CH_3CN	0
1:1 (v/v)% CH_3CN-pH=7.0	3
1:1 (v/v)% CH_3CN-pH=5.5	6
1:1 (v/v)% CH_3CN-pH=4.0	13
1:1 (v/v)% CH_3CN-pH=3.0	24
1:1 (v/v)% CH_3CN-pH=2.0	36
1:1 (v/v)% CH_3CN-pH=1.0	100