Electronic Supplementary Information

Photoinduced energy and charge transfer in bis(triphenylamine)-BODIPY-C_{60} artificial photosynthetic system

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Beate Röder and Eugeny A. Ermilov*

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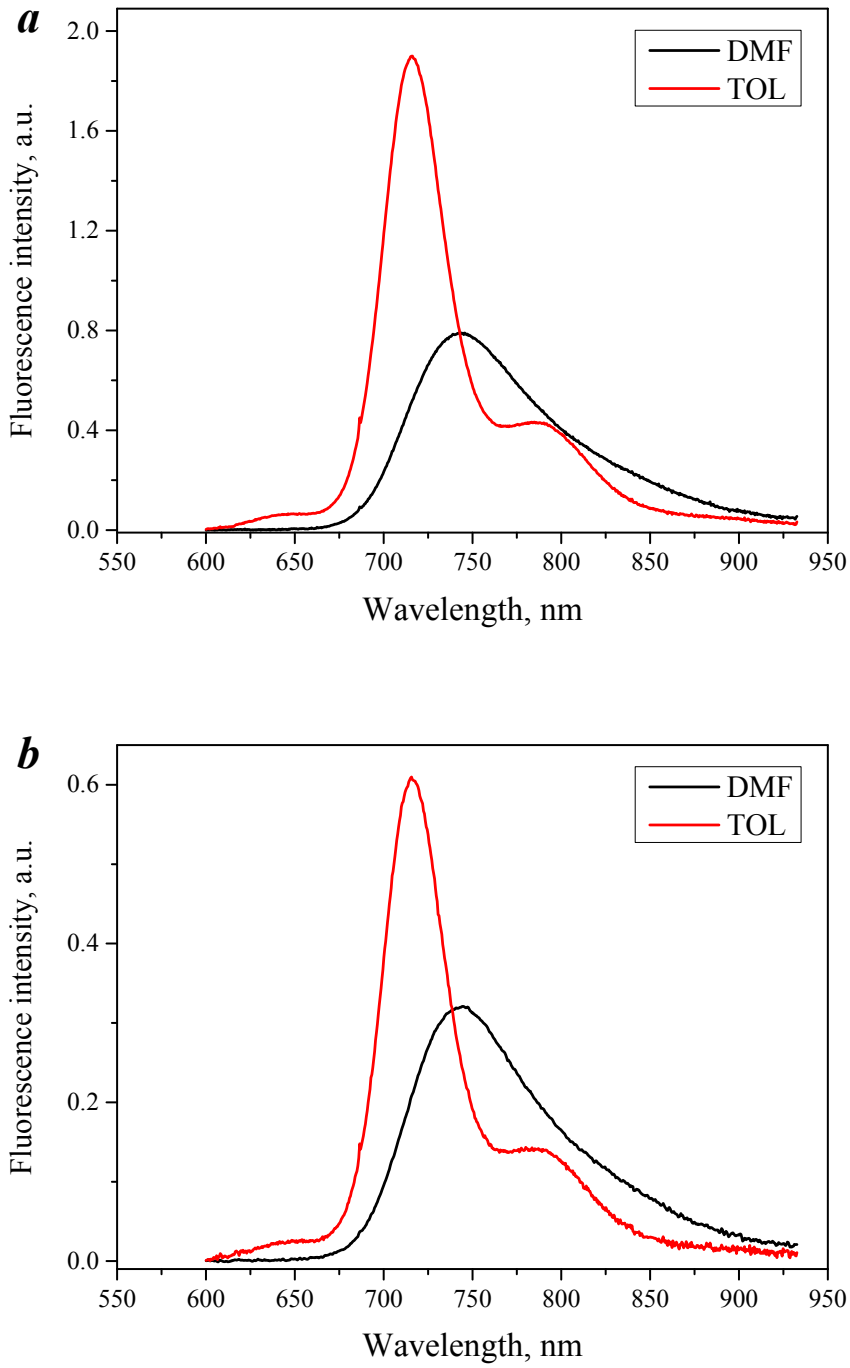

Fig. S1 Fluorescence spectra of triad **4** (***a***) and tetrad **6** (***b***) in polar DMF and nonpolar TOL upon excitation at 613 nm (BODIPY-part excitation). Optical density of the samples was adjusted to 0.1 at the BODIPY absorption maximum

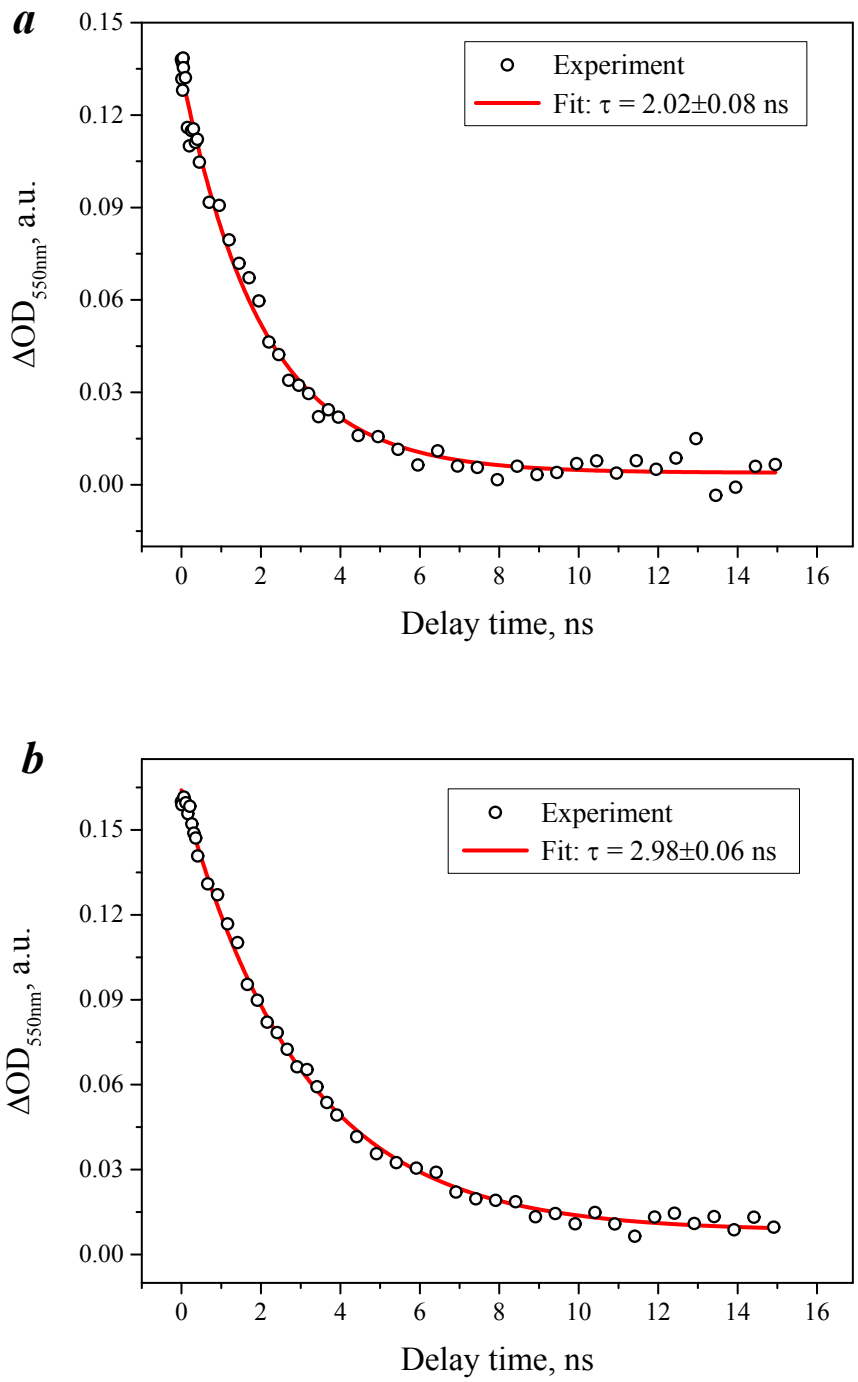

Fig. S2 Fit of the ΔOD signal at 550 nm of triad **4** solved in DMF (***a***) and TOL (***b***)

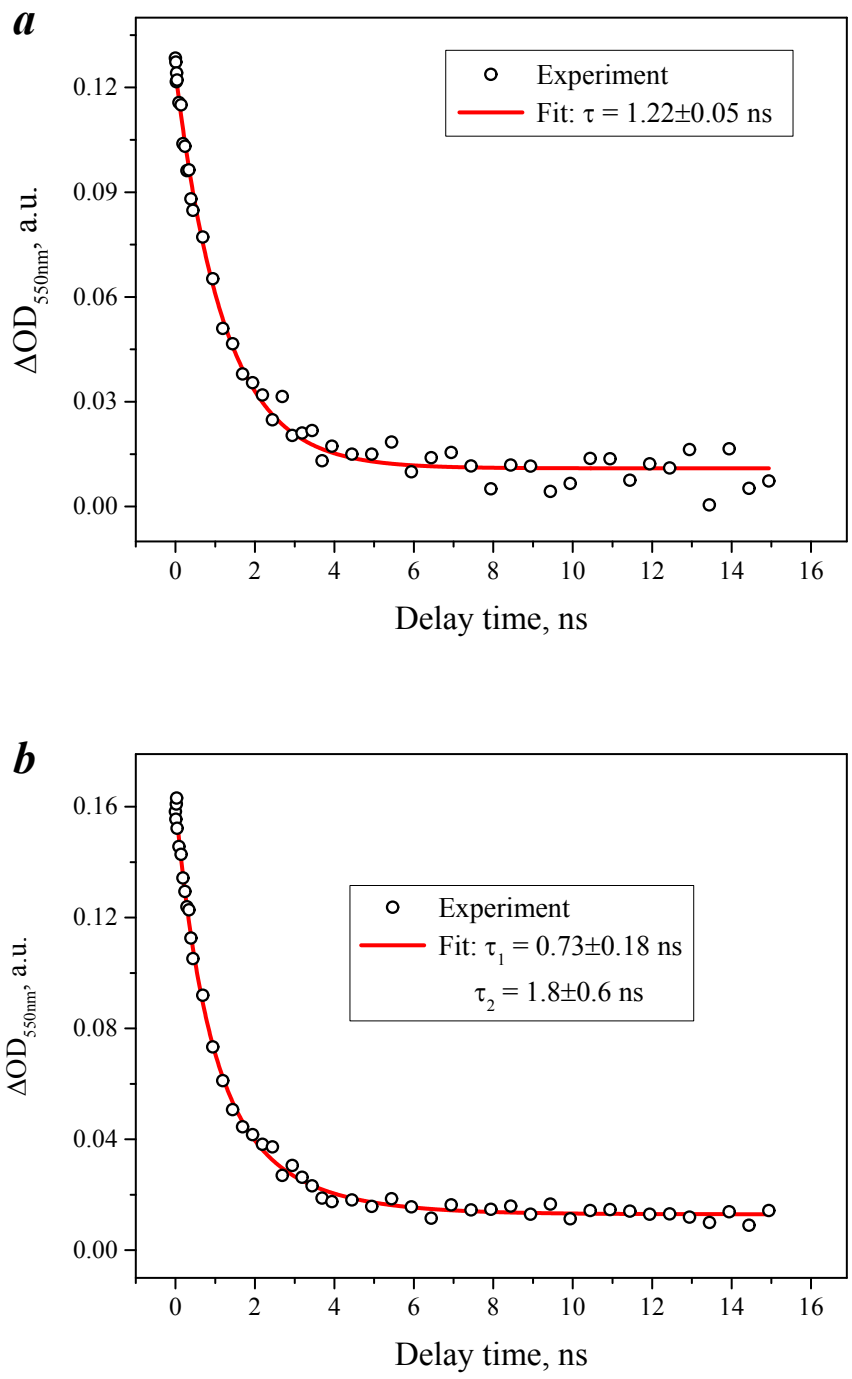

Fig. S3 Fit of the ΔOD signal at 550 nm of tetrad **6** solved in DMF (***a***) and TOL (***b***)

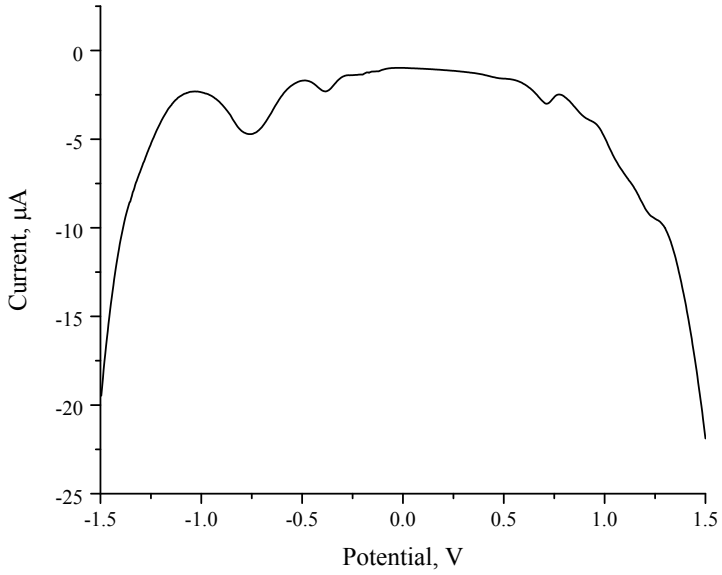

Fig. S4 Differential pulse voltammetry of tetrad **6** in deaerated DMF in the presence of 0.1 M [*n*-Bu_4N][ClO_4]. Scan rate = 20 mV s^{-1}

Table S1 Vertical transition wavelengths λ_{max} (nm), transition energies ΔE (eV) and transition contributions calculated at TD-DFT B3LYP/(cc-pVDZ) level

Compound	λ_{max} (nm)	ΔE (eV)	Transitions (contribution)
2	535	2.32	HOMO → LUMO (100%)
	387	3.20	HOMO-3 → LUMO (63%)
			HOMO-1 → LUMO (36%)
4	708	1.75	HOMO → LUMO (99%)
	561	2.21	HOMO-1 → LUMO (96%)
	405	3.06	HOMO → LUMO+1 (71%)
			HOMO-3 → LUMO (25%)
	371	3.34	HOMO-3 → LUMO (41%)
			HOMO-4 → LUMO (17%)
			HOMO → LUMO+1 (16%)
	353	3.51	HOMO → LUMO+3 (38%)
6	712	1.74	HOMO → LUMO+3 (92%)
	568	2.18	HOMO-1 → LUMO+3 (95%)

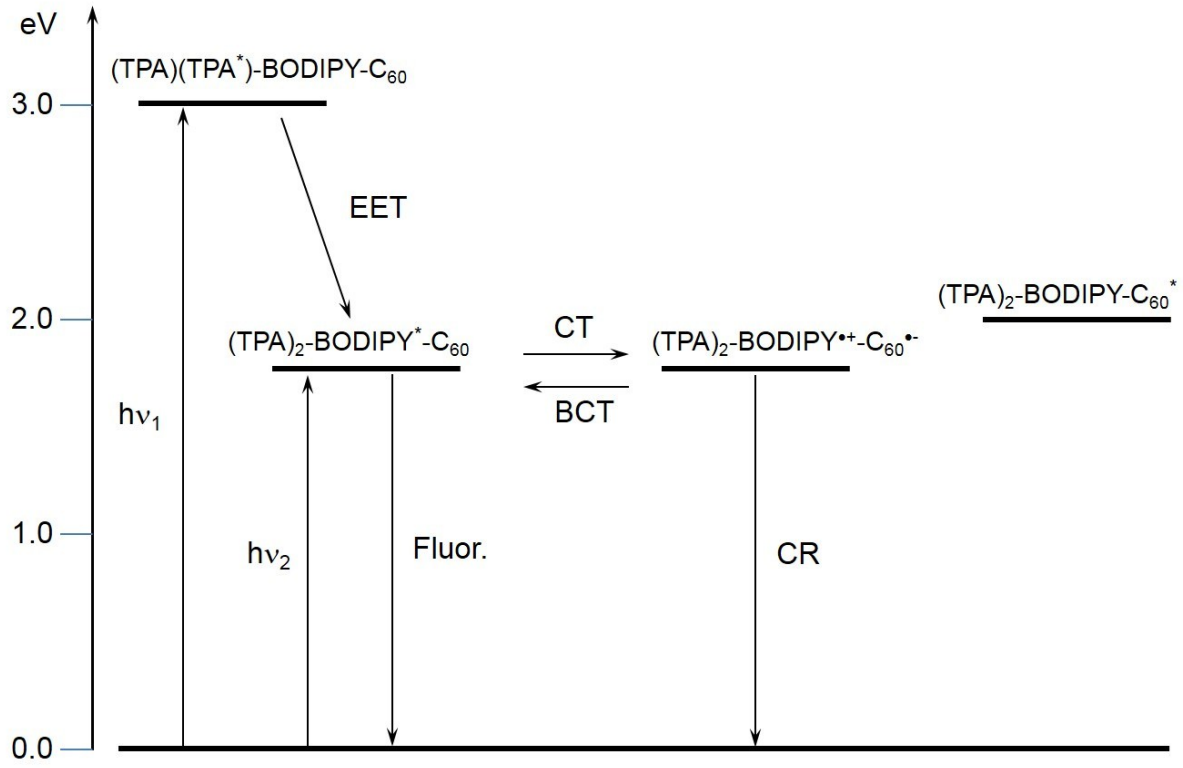

Fig. S5 Energy level diagram showing the different photophysical events of tetrad **6** in TOL

In all of the following spectra, the residual solvent signals are marked with asterisks

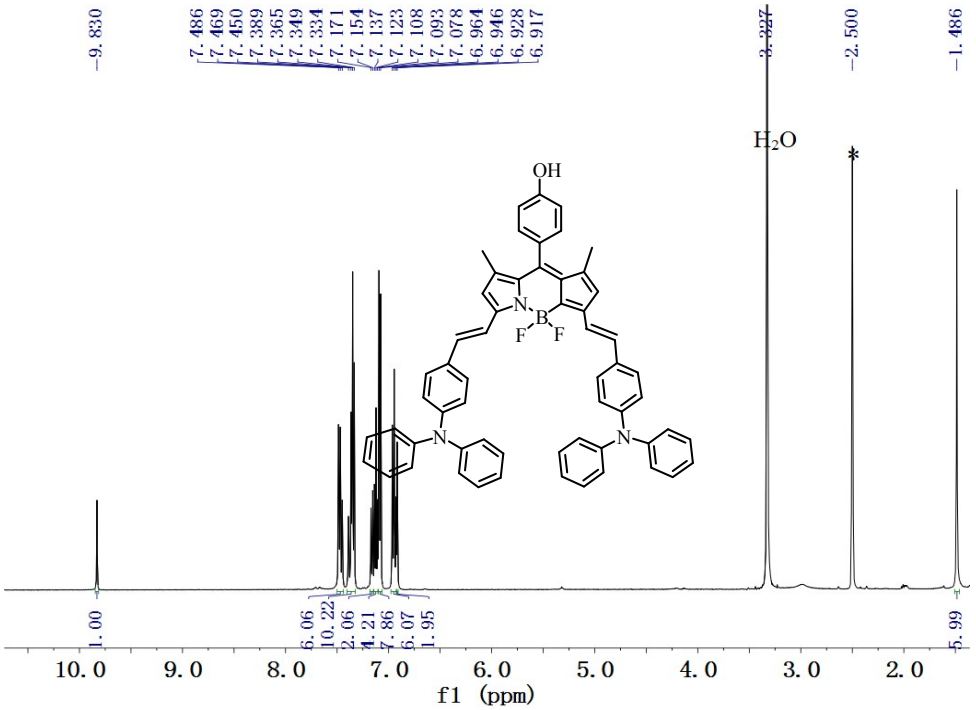

Fig. S6 ^{1}H NMR spectrum of **3**

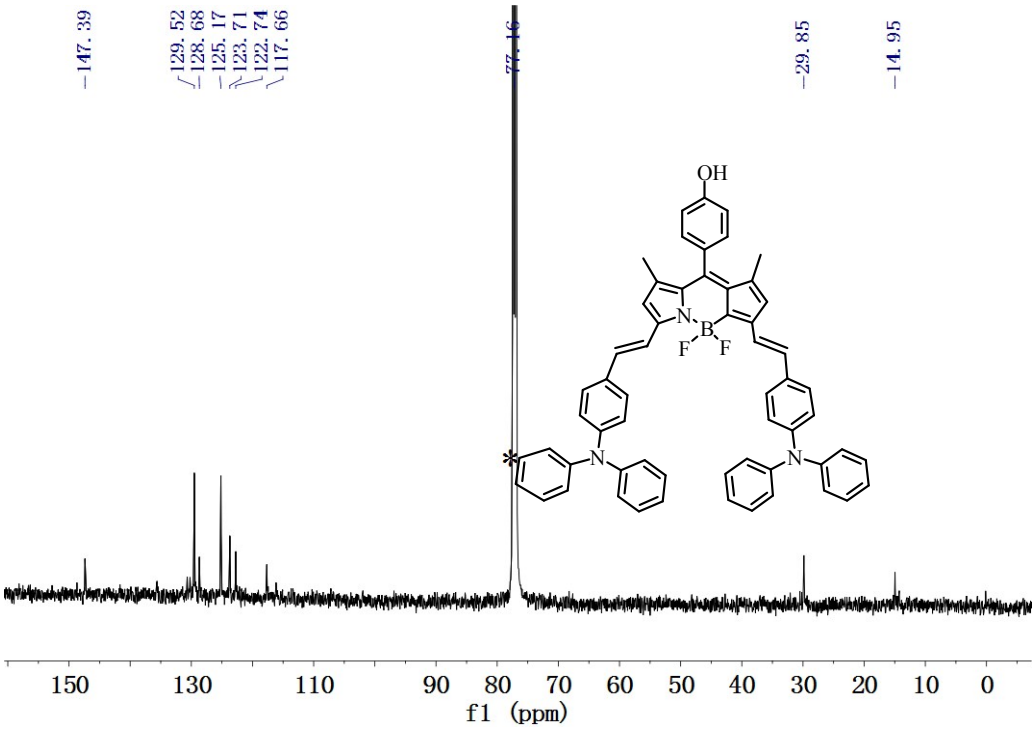

Fig. S7 $^{13}C\{^{1}H\}$ NMR spectrum of **3**

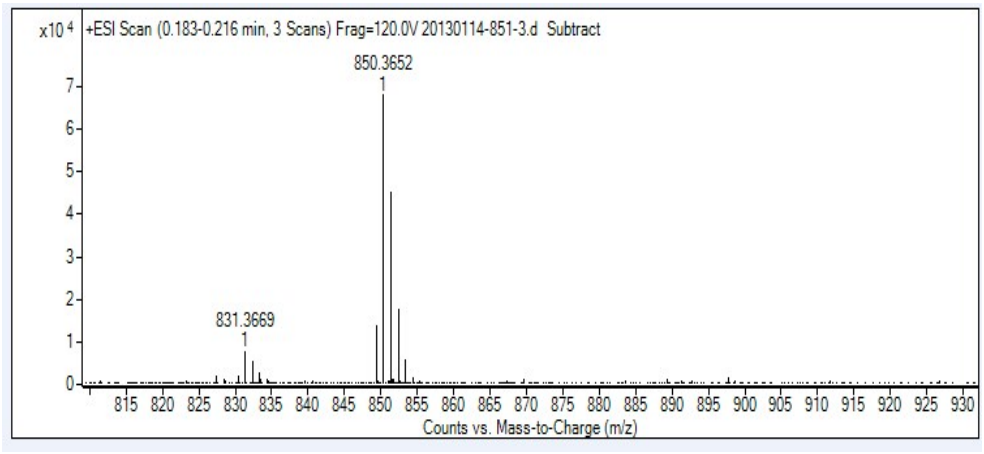

Fig. S8 HRMS spectrum of **3**

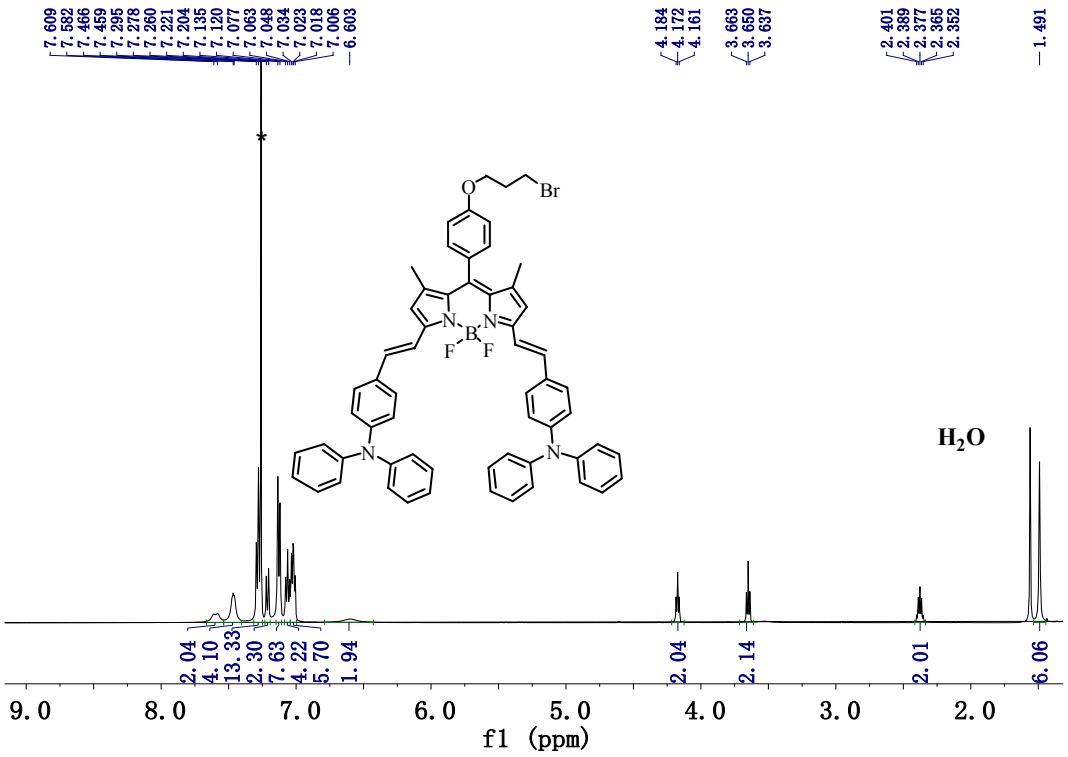

Fig. S9 ^{1}H NMR spectrum of **4**

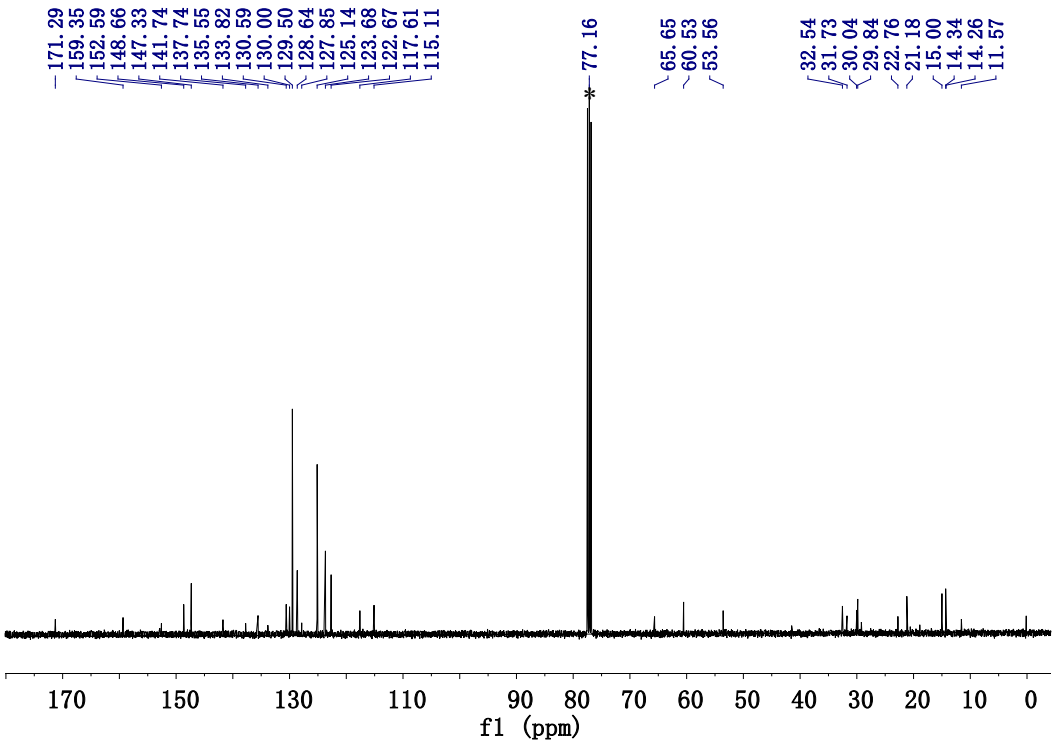

Fig. S10 $^{13}C\{^{1}H\}$ NMR spectrum of **4**

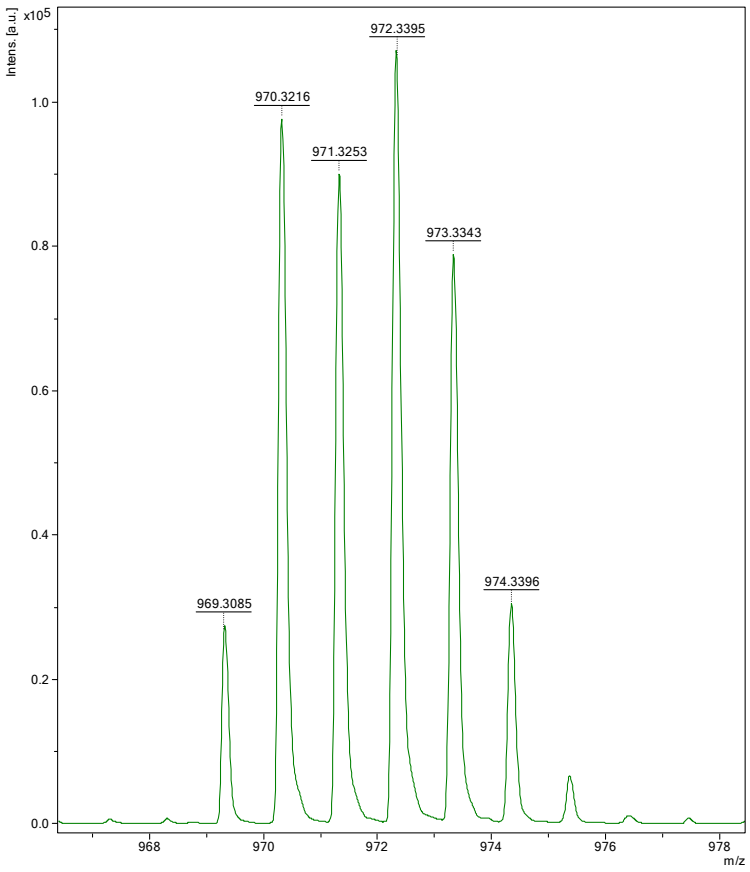

Fig. S11 HRMS spectrum of **4**

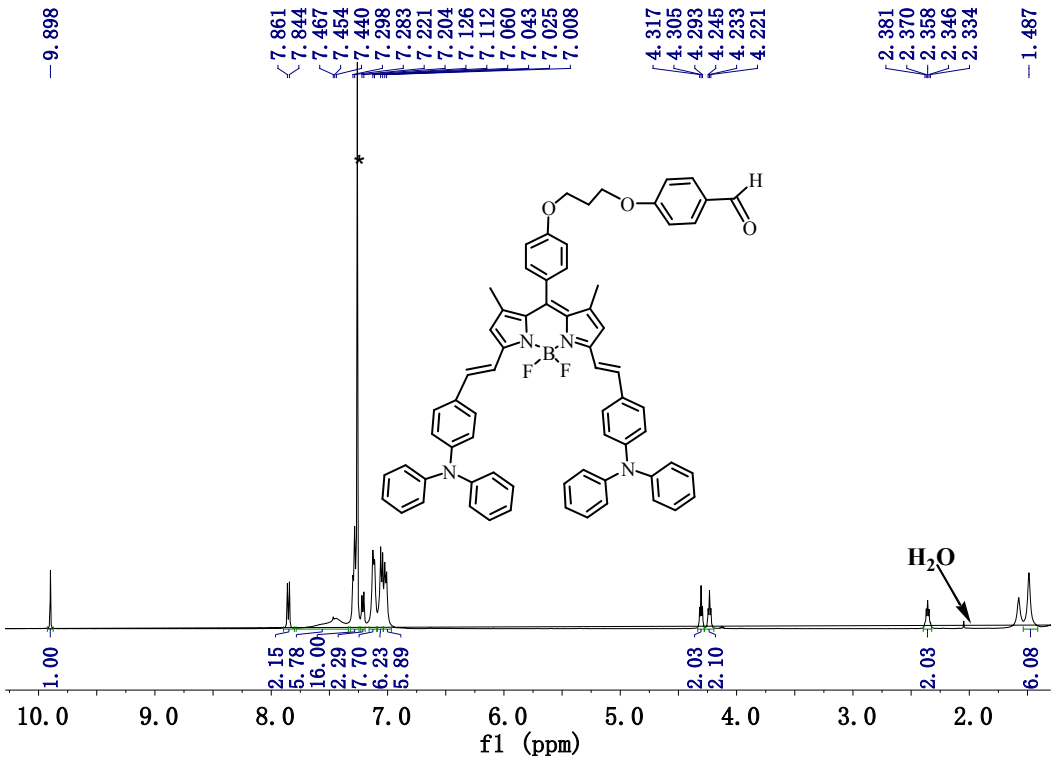

Fig. S12 ^{1}H NMR spectrum of **5**

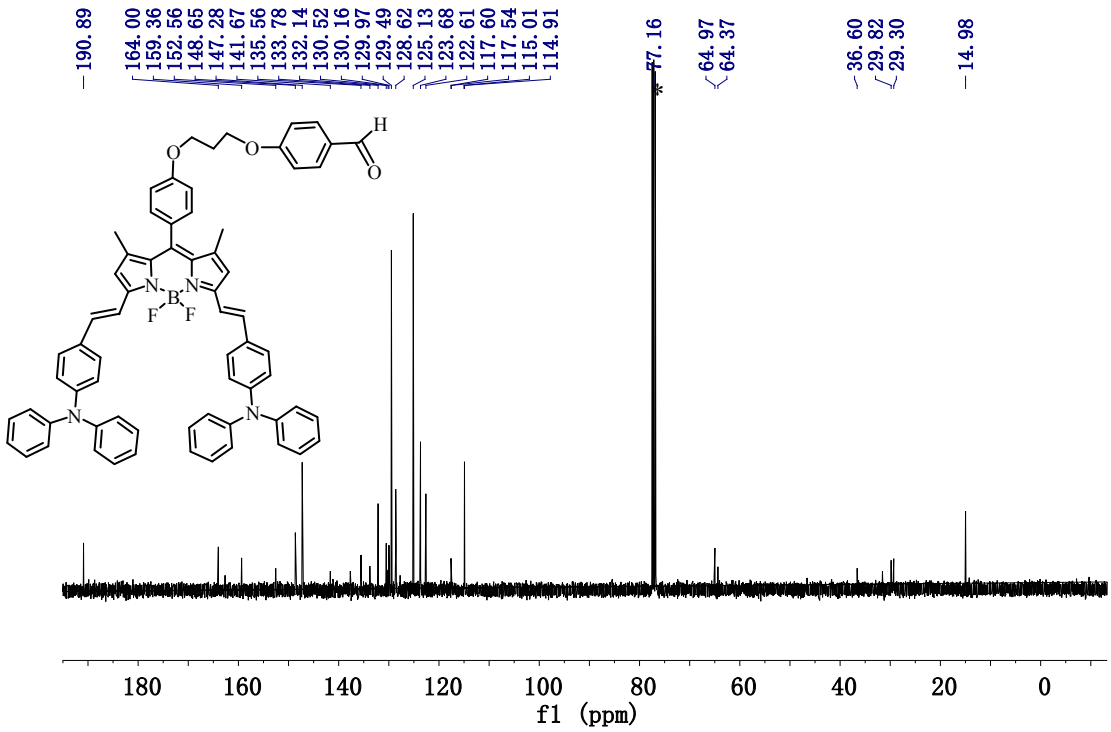

Fig. S13 $^{13}C\{^{1}H\}$ NMR spectrum of **5**

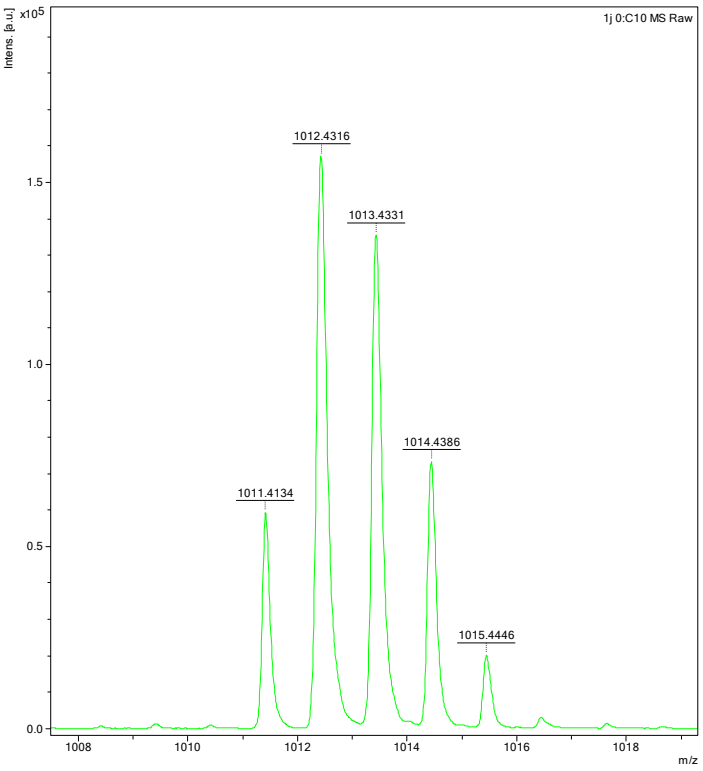

Fig. S14 HRMS spectrum of **5**

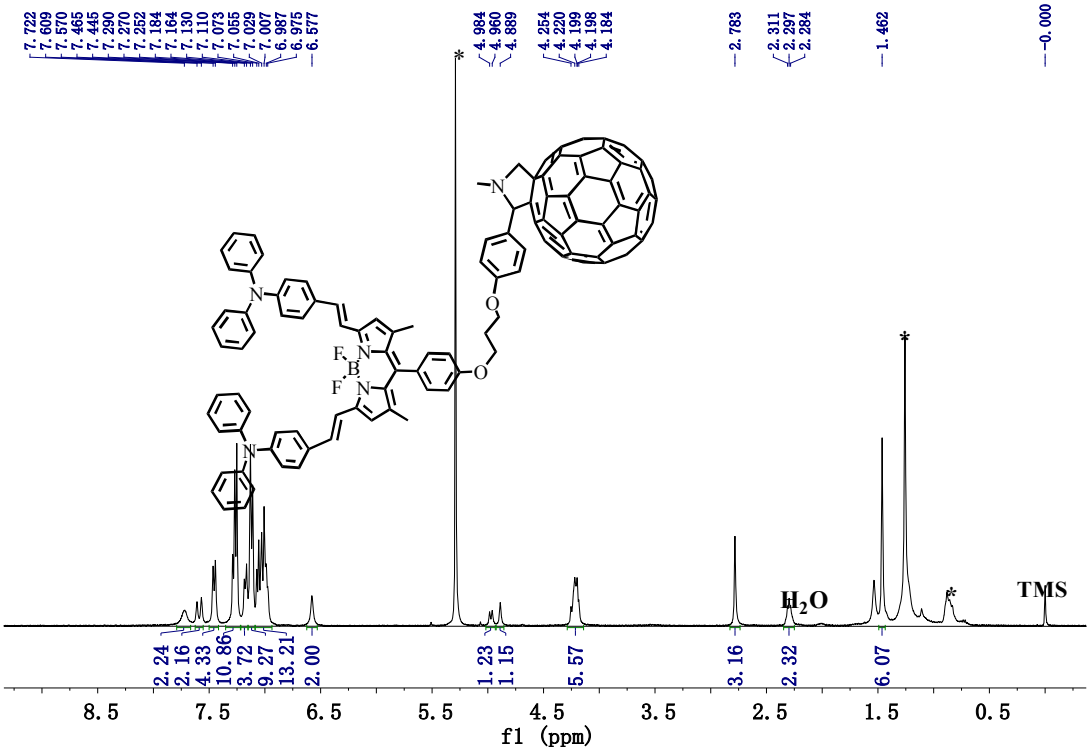

Fig. S15 ^{1}H NMR spectrum of **6**

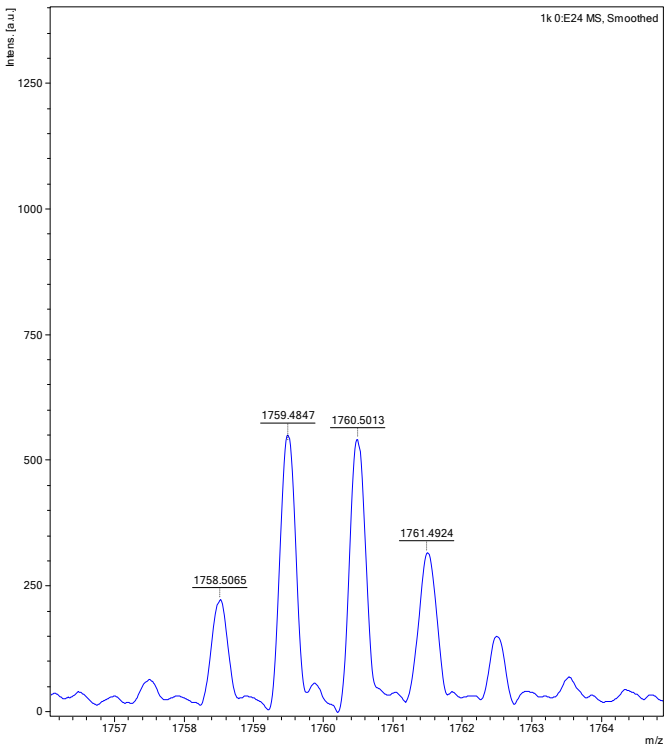

Fig. S16 HRMS spectrum of **6**

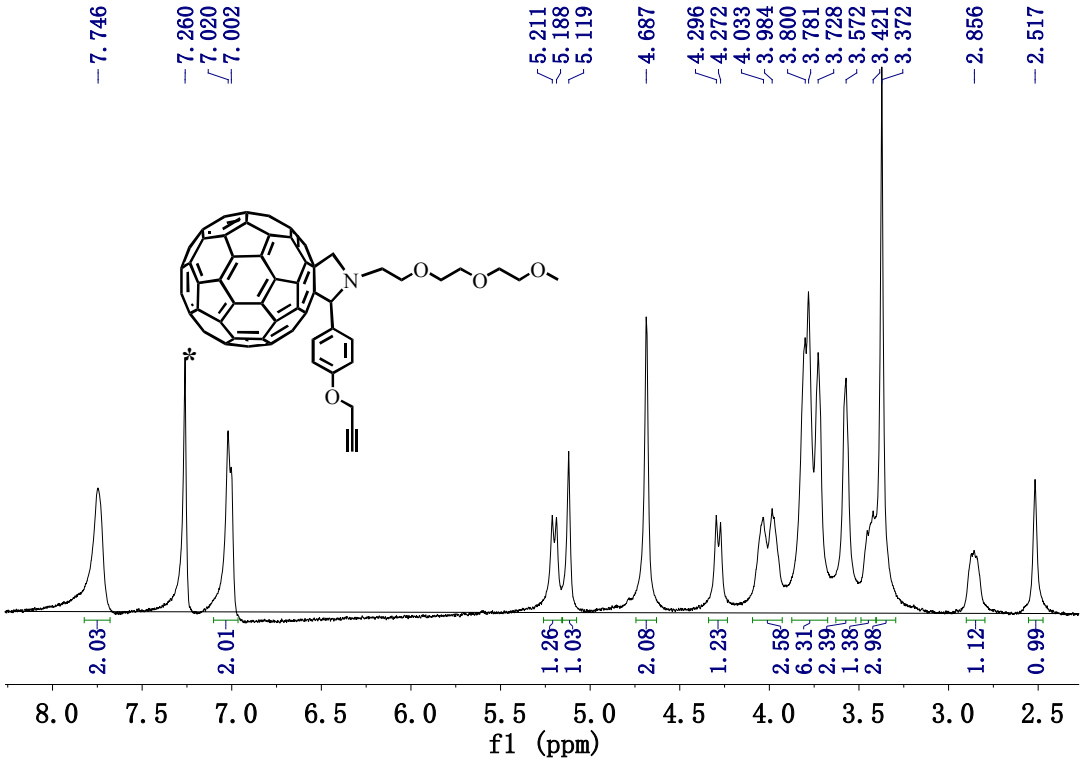

Fig. S17 ^{1}H NMR spectrum of **9**

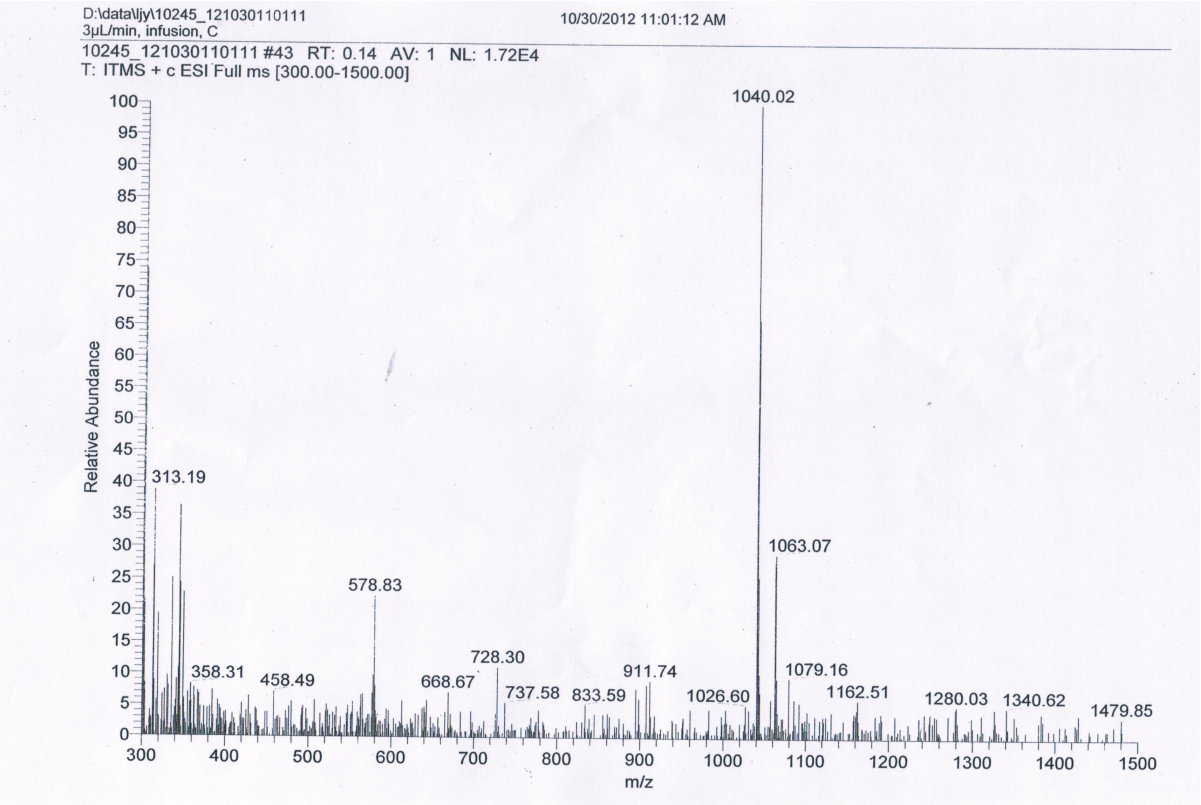

Fig. S18 MS spectrum of **9**