Electronic Supplementary Information

Influence of ethynyl position on benzothiadiazole based D-A-π-A dye-sensitized solar cells: spectral response and photovoltage performance†

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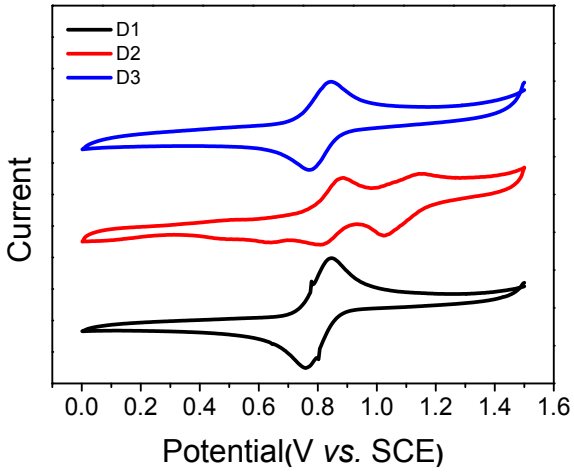


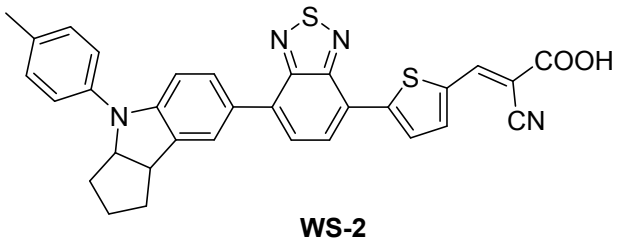
Fig. S1 Cyclic voltammograms of dyes **D1, D2** and **D3** obtained in CH_2Cl_2.

Table S1. Energy levels (in eV) of frontier molecular orbitals.

Compound	E(HOMO)	E(LUMO)	Gap
D1	-5.07	-2.51	2.56
D2	-5.06	-2.67	2.39
D3	-5.07	-2.66	2.41

Table S2. Computed excitation energy, absorption wavelength, oscillator strength and molecular orbital composition for the lowest excited state.

Compound	Excited state	Excitation energy	Oscillator strength	MO composition
D1	S_1	2.87 eV, 432 nm	0.705	H-1 → L (13%)
				H → L (82%)
D2	S_1	2.74 eV, 452 nm	1.165	H-1 → L (17%)
				H → L (77%)
D3	S_1	2.68 eV, 462 nm	1.054	H-1 → L (12%)
				H → L (82%)



WS-2

Fig. S2 Chemical structure of dye **WS-2.**

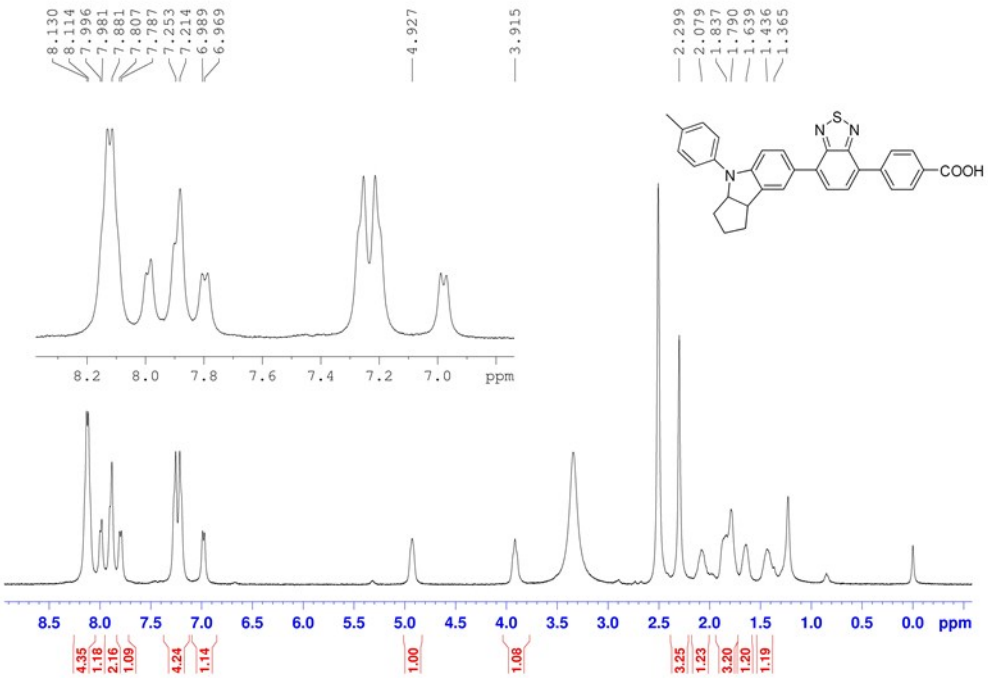


Fig. S3 ^{1}H NMR of **D1** in DMSO.

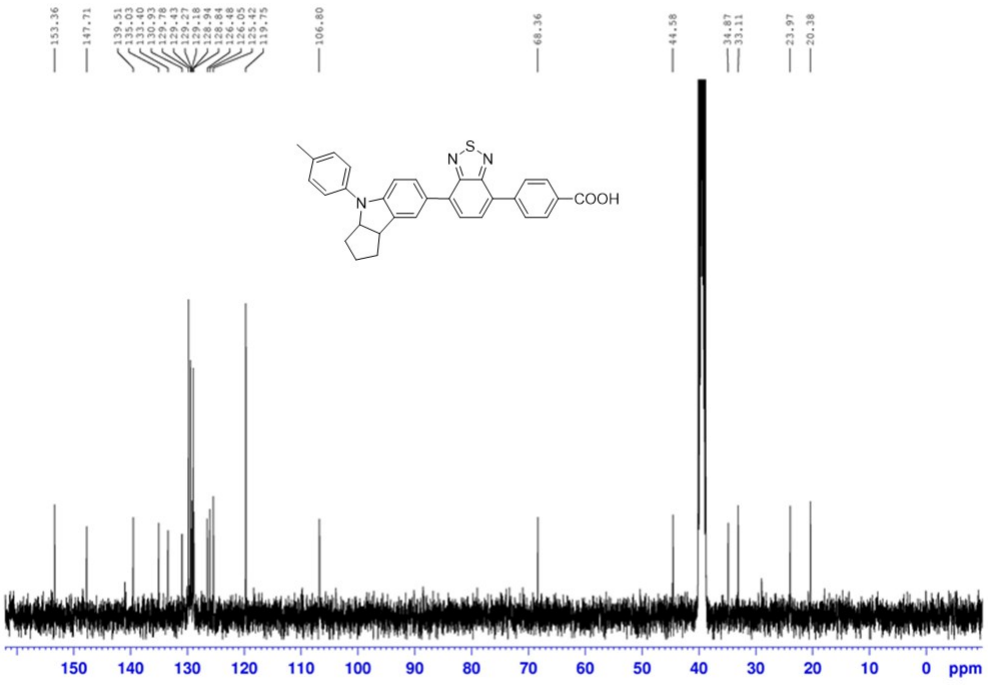


Fig. S4 ^{13}C NMR of **D1** in DMSO.

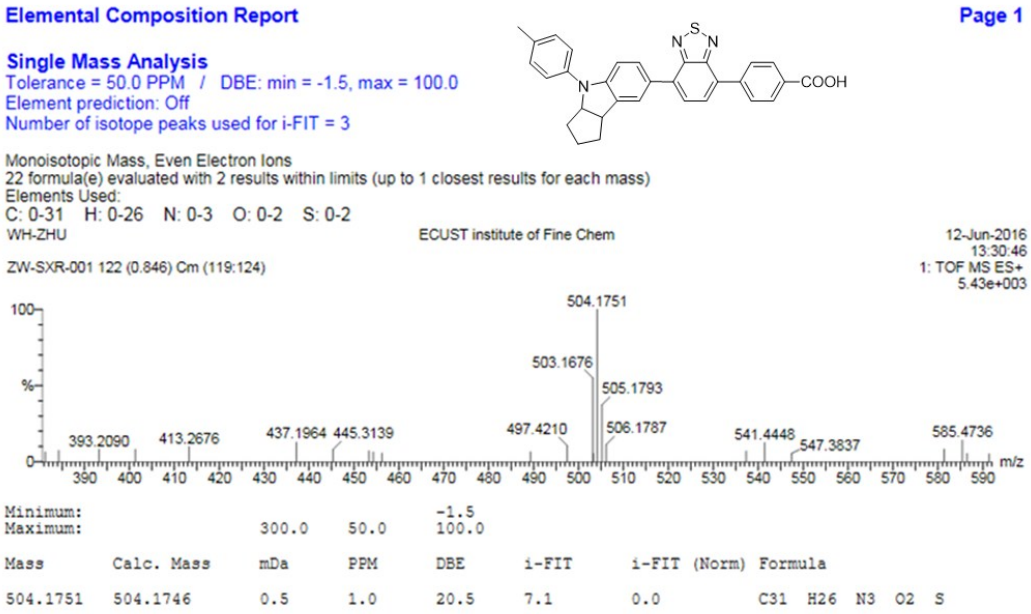


Fig. S5 HRMS of **D1**.

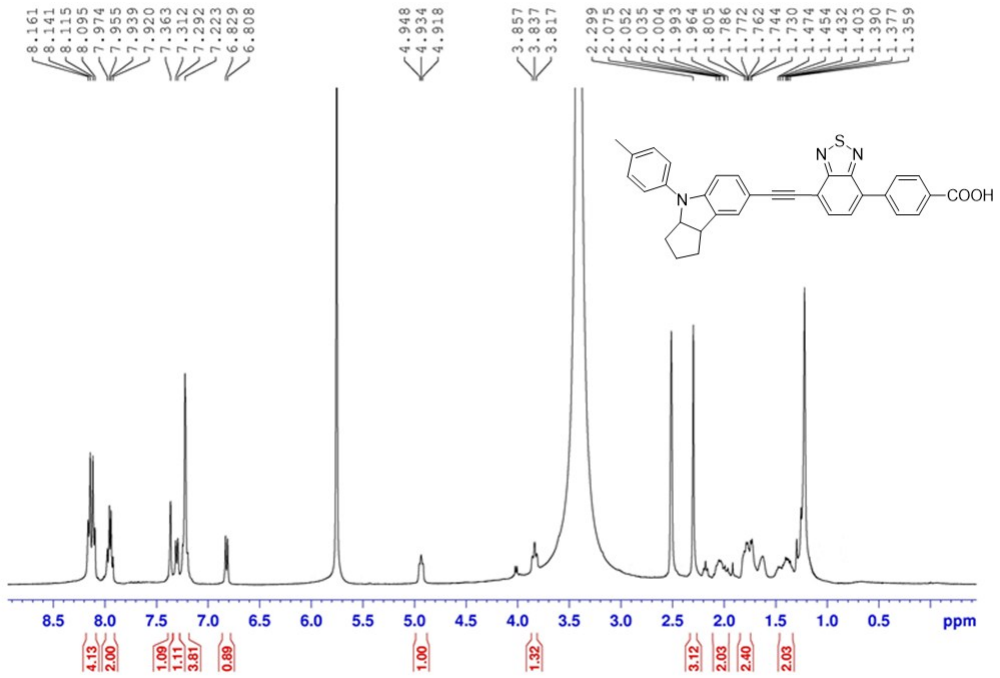


Fig. S6 ^{1}H NMR of **D2** in DMSO.

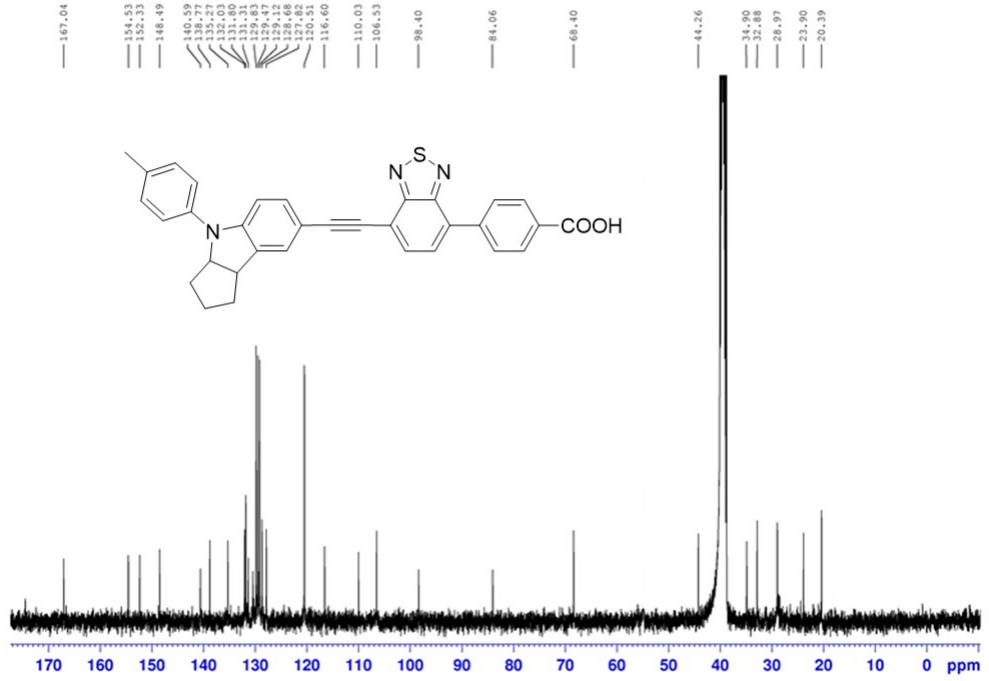


Fig. S7 ^{13}C NMR of **D2** in DMSO.

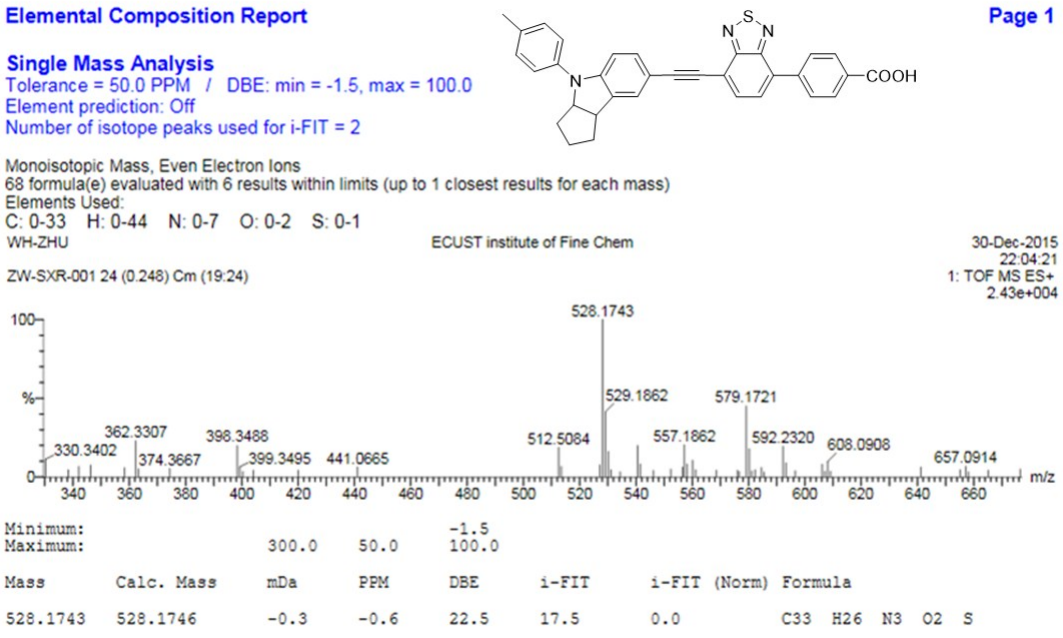


Fig. S8 HRMS of **D2**.

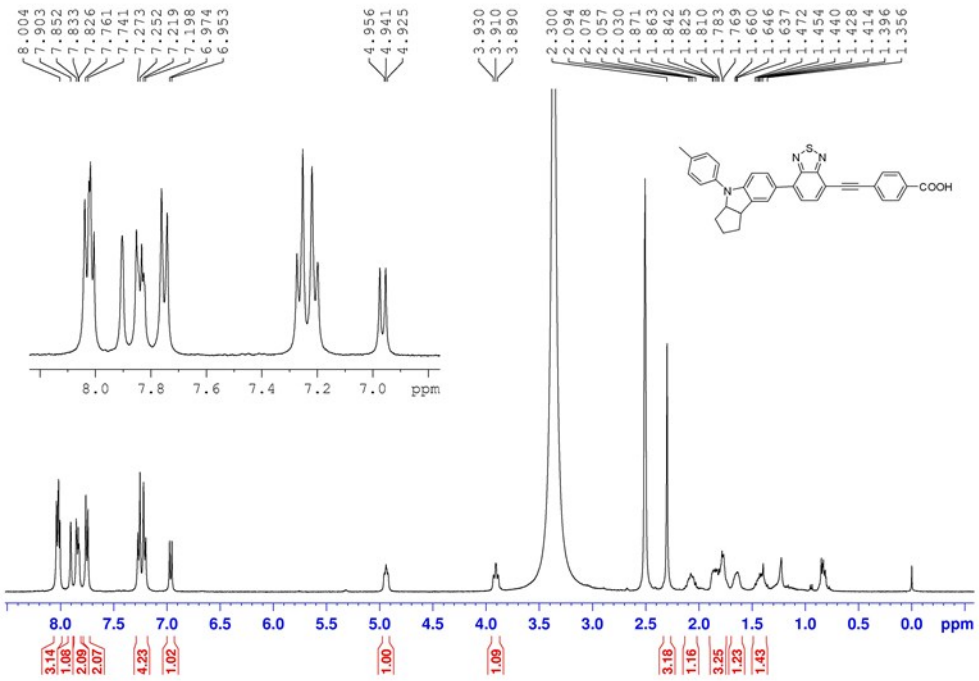


Fig. S9 ^{1}H NMR of **D3** in DMSO.

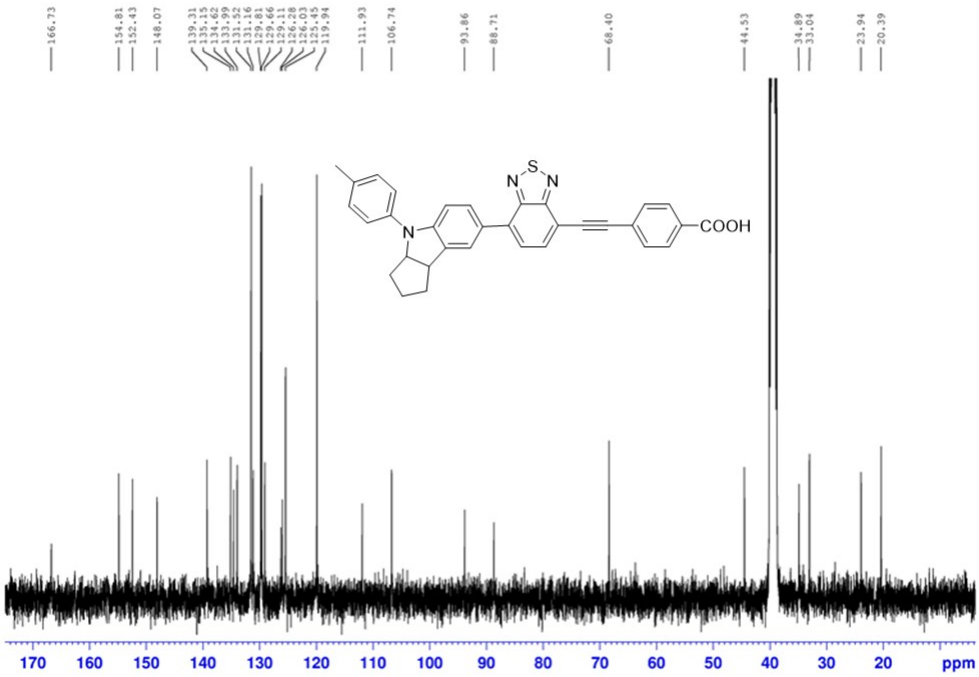


Fig. S10 ^{13}C NMR of **D2** in DMSO.

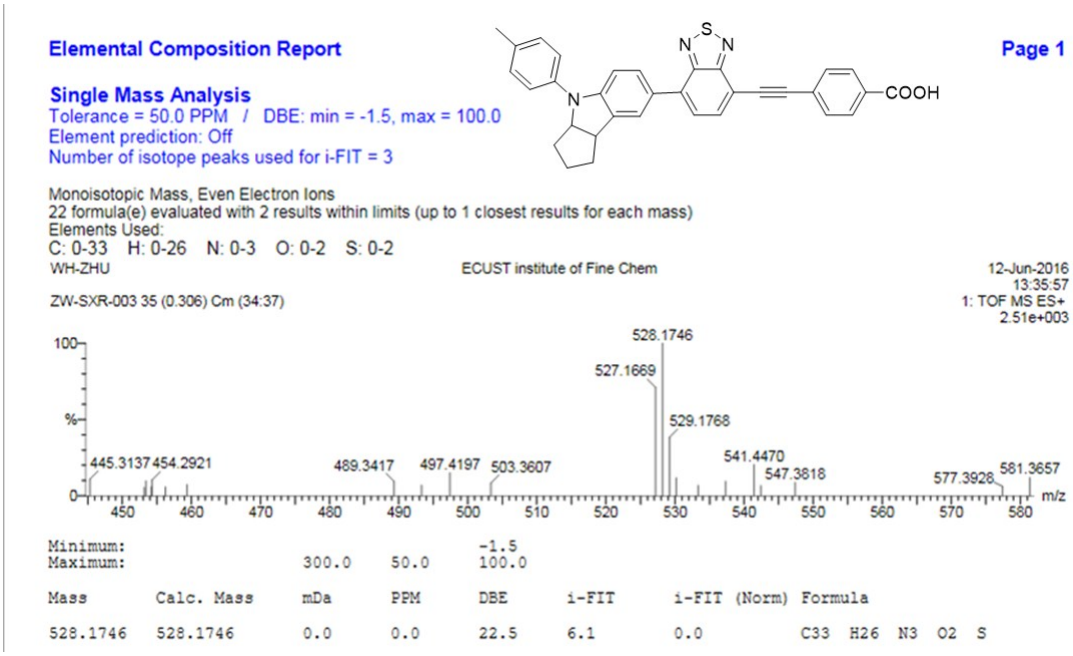


Fig. S11 HRMS of **D3**.