

Electronic Supplementary Information

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

Xiongrong Song,^a Weiwei Zhang,^a Xin Li,^b Huiyun Jiang,^a Chao Shen^a and Wei-Hong Zhu^{*a}

^aShanghai Key Laboratory of Functional Materials Chemistry, Key Laboratory for Advanced Materials and Institute of Fine Chemicals, Collaborative Innovation Center for Coal Based Energy (i-CCE), School of Chemistry and Molecular Engineering, East China University of Science and Technology, Shanghai 200237, P. R. China. *E-mail: whzhu@ecust.edu.cn.

^bDivision of Theoretical Chemistry and Biology, School of Biotechnology, KTH Royal Institute of Technology, SE-10691 Stockholm, Sweden.

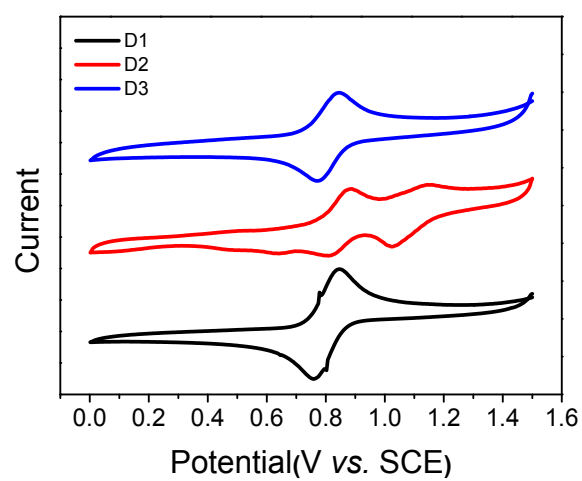


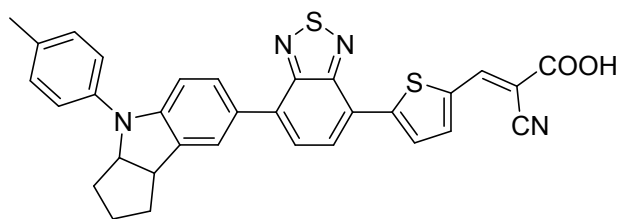
Fig. S1 Cyclic voltammograms of dyes **D1**, **D2** and **D3** obtained in CH_2Cl_2 .

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**.

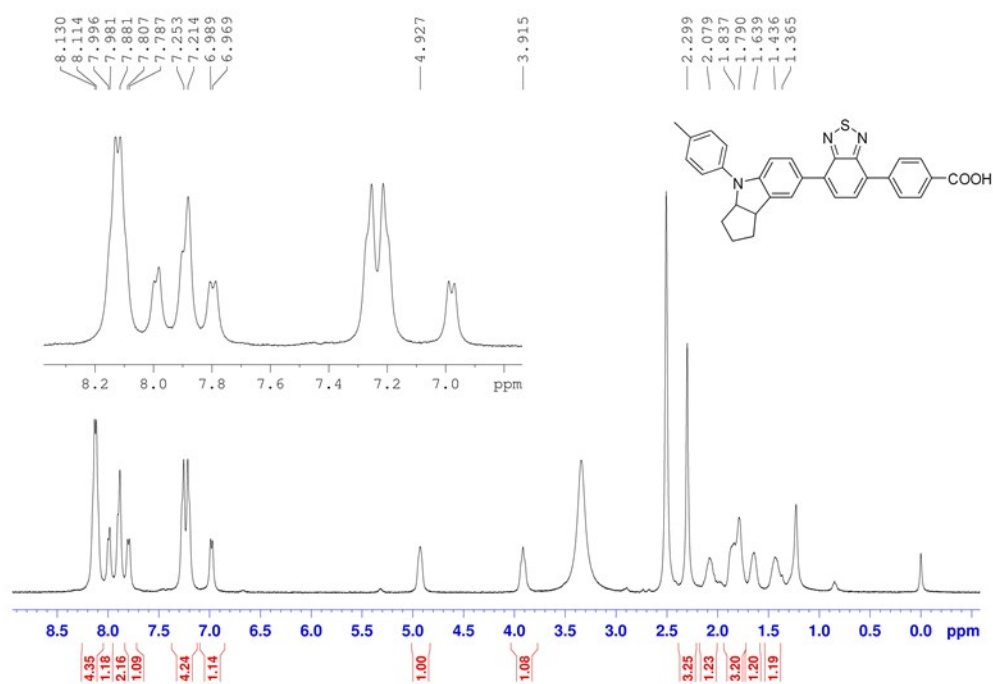


Fig. S3 ¹H NMR of **D1** in DMSO.

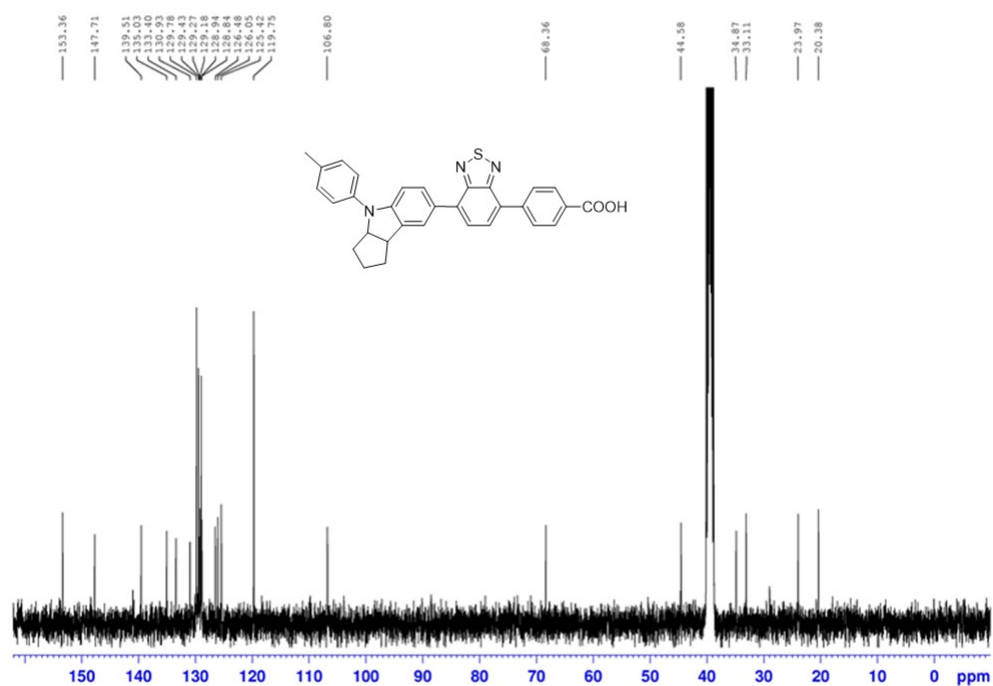


Fig. S4 ¹³C NMR of **D1** in DMSO.

Elemental Composition Report

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Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

22 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-31 H: 0-26 N: 0-3 O: 0-2 S: 0-2

WH-ZHU

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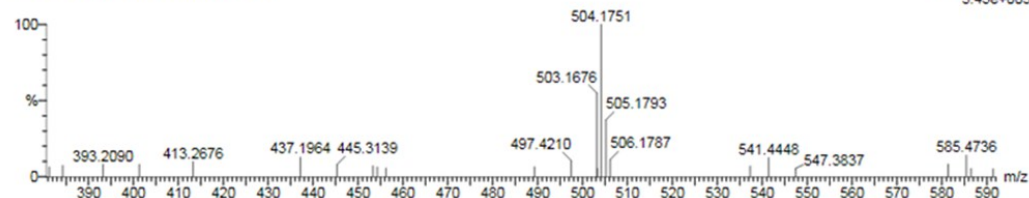
ZW-SXR-001 122 (0.846) Cm (119:124)

12-Jun-2016

13:30:46

1: TOF MS ES+

5.43e+003



Minimum: 300.0 50.0 -1.5
Maximum: 300.0 50.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
504.1751	504.1746	0.5	1.0	20.5	7.1	0.0	C31 H26 N3 O2 S

Fig. S5 HRMS of D1.

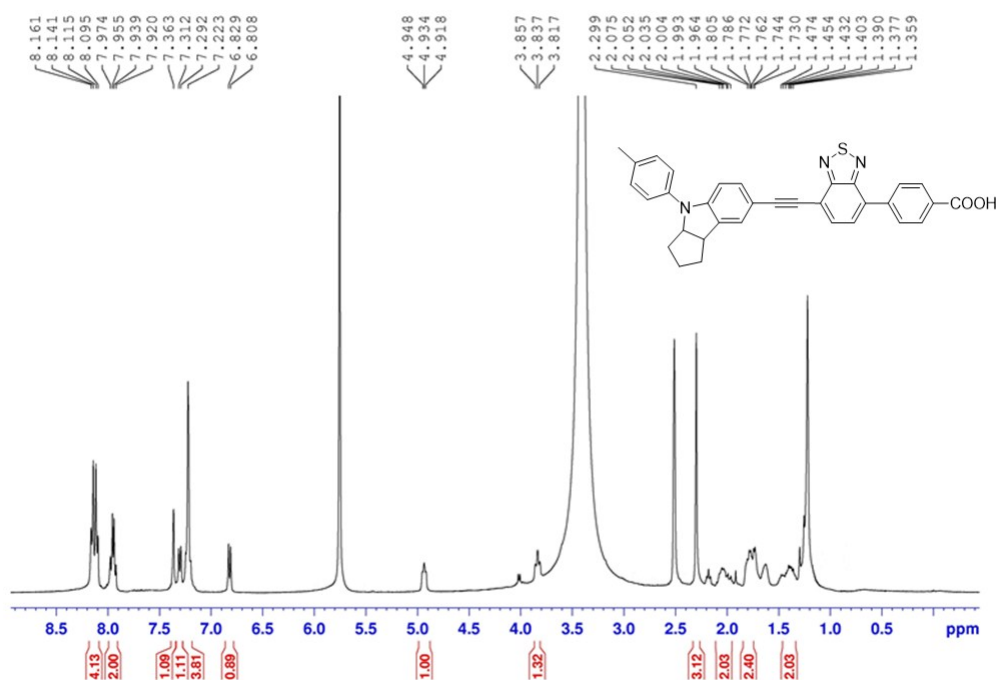


Fig. S6 ¹H NMR of D2 in DMSO.

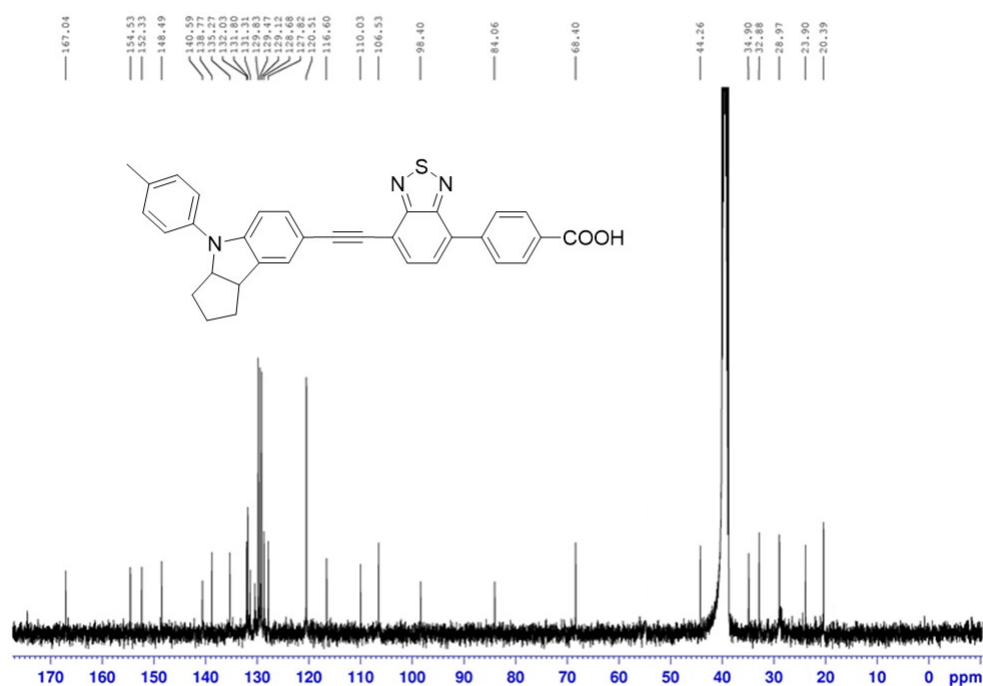


Fig. S7 ^{13}C NMR of **D2** in DMSO.

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

68 formula(e) evaluated with 6 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-33 H: 0-44 N: 0-7 O: 0-2 S: 0-1

WH-ZHU

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30-Dec-2015
22:04:21
1: TOF MS ES+
2.43e+004

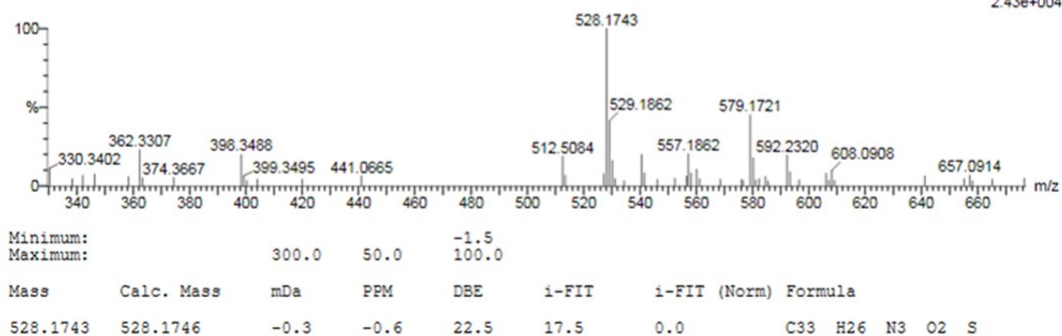


Fig. S8 HRMS of **D2**.

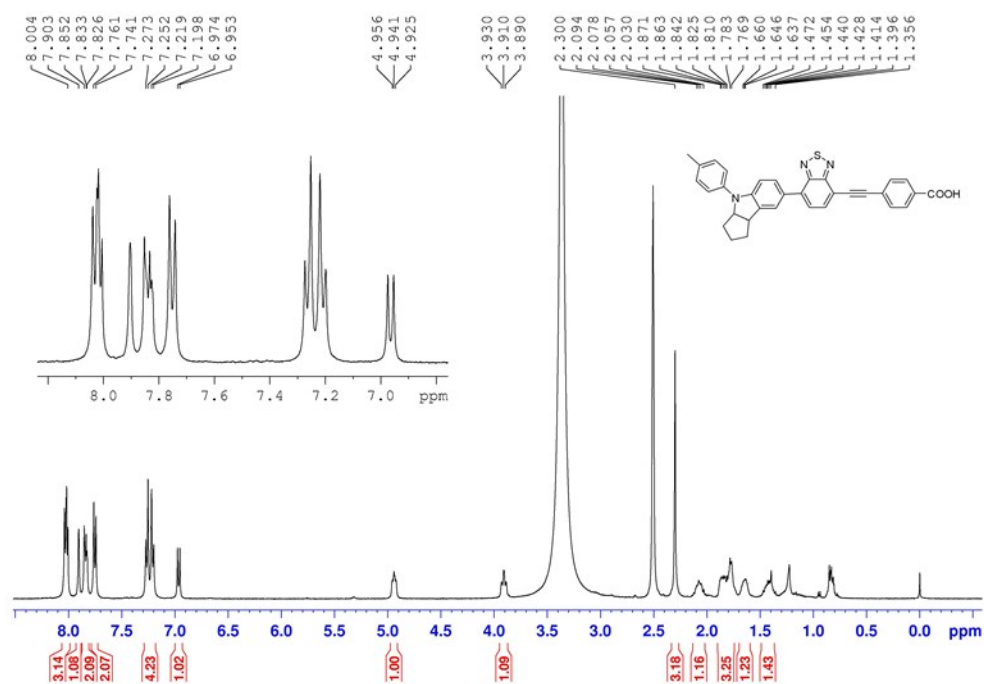


Fig. S9 ¹H NMR of **D3** in DMSO.

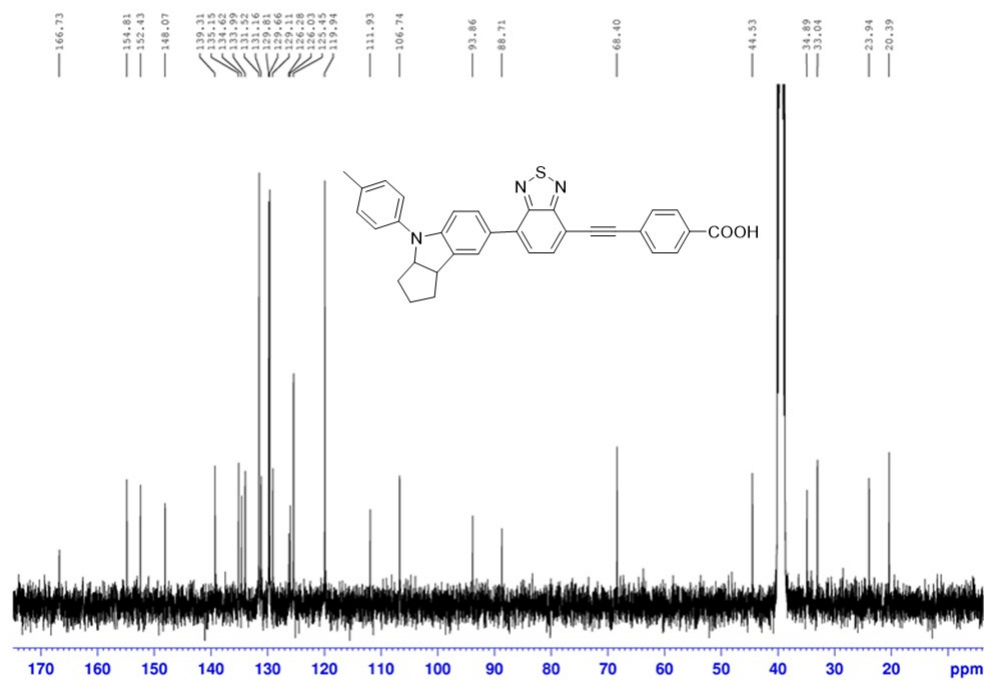


Fig. S10 ¹³C NMR of **D2** in DMSO.

Elemental Composition Report

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

22 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-33 H: 0-26 N: 0-3 O: 0-2 S: 0-2

WH-ZHU

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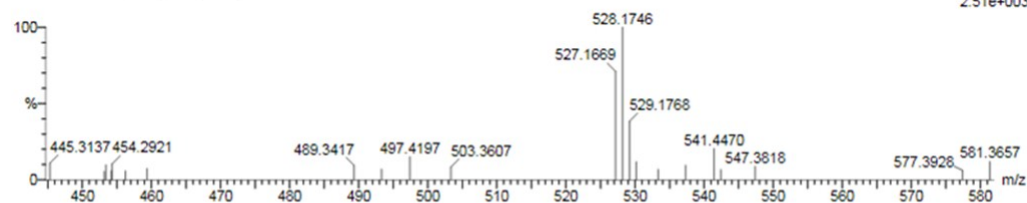
ZW-SXR-003 35 (0.306) Cm (34:37)

12-Jun-2016

13:35:57

1: TOF MS ES+

2.51e+003



Minimum:

Maximum:

300.0 50.0 -1.5
100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
528.1746	528.1746	0.0	0.0	22.5	6.1	0.0	C33 H26 N3 O2 S

Fig. S11 HRMS of D3.