Supporting Information

Indolo[3,2-b]indole donor based D-π-A dyes for DSCs: Investigating the role of π-spacers towards recombination

P. V. Santhini,[ac§] Jayadev V,[bc§] Sourava C. Pradhan,[bc] Sivasankaran Lingamoorthy,[bc] Nitha P. R.,[ac] Chaithanya M. V.,[a] Rakesh K. Mishra,[e] Narayanan Unni K. N,*[bcd] Jubi John*[ac] and Suraj Soman*[bcd]

[a]Organic Chemistry Section, Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology (CSIR-NIIST), Thiruvananthapuram 695019, India. [b]Photosciences and Photonics Section, Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology (CSIR-NIIST), Thiruvananthapuram 695019, India. [c]Academy of Scientific and Innovative Research (AcSIR), CSIR-NIIST Campus, Thiruvananthapuram 695019, India. [d]CSIR-Network of Institutes for Solar Energy (CSIR-NISE), India. [e]Department of Sciences & Humanities, NIT, Uttarakhand

E-mail: unni@niist.res.in; jubijohn@niist.res.in; suraj@niist.res.in;

[§]Both authors contributed equally to this work

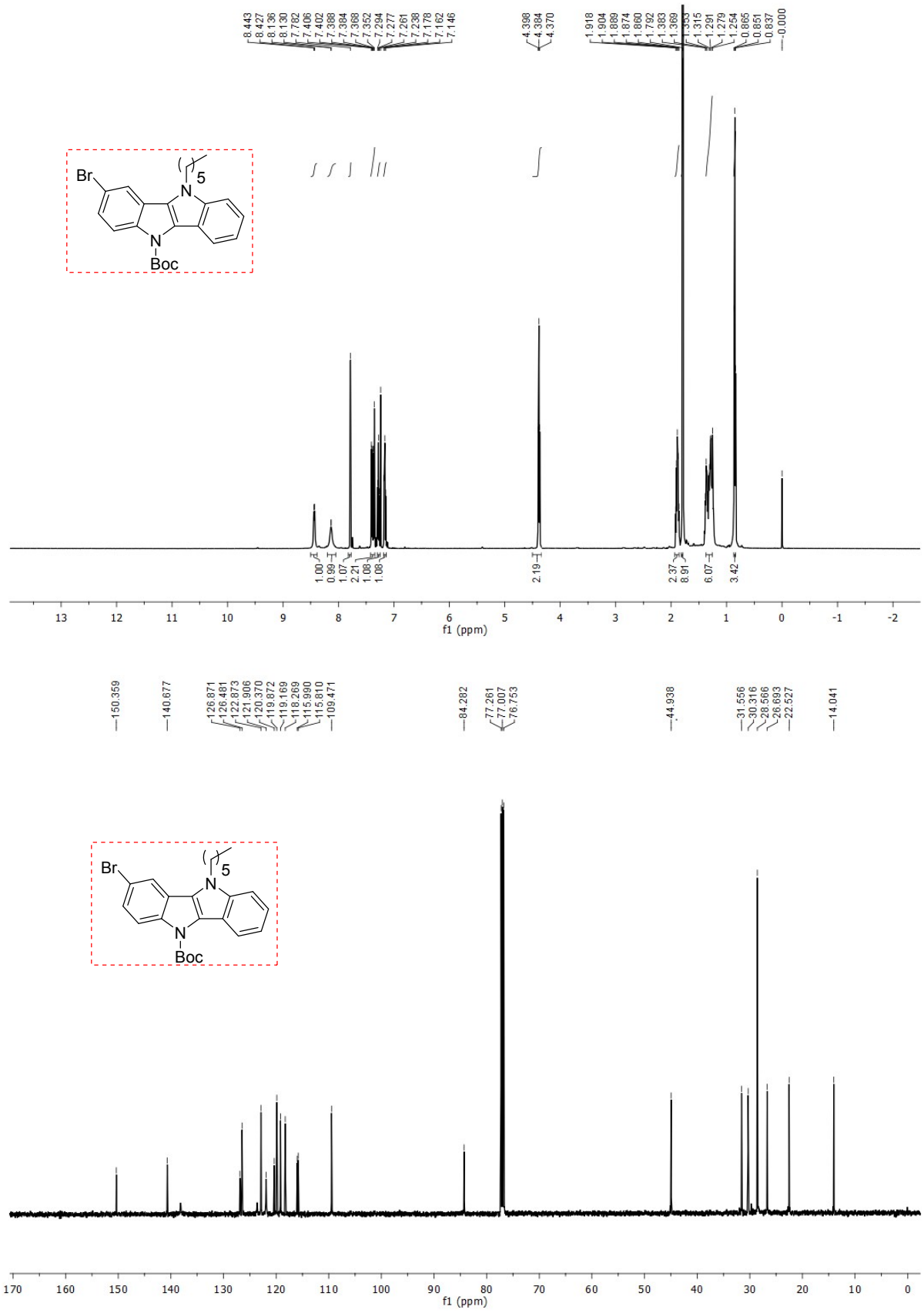

Fig. S1 ^{1}H NMR (500 MHz) & ^{13}C (125 MHz) Spectra of **4**.

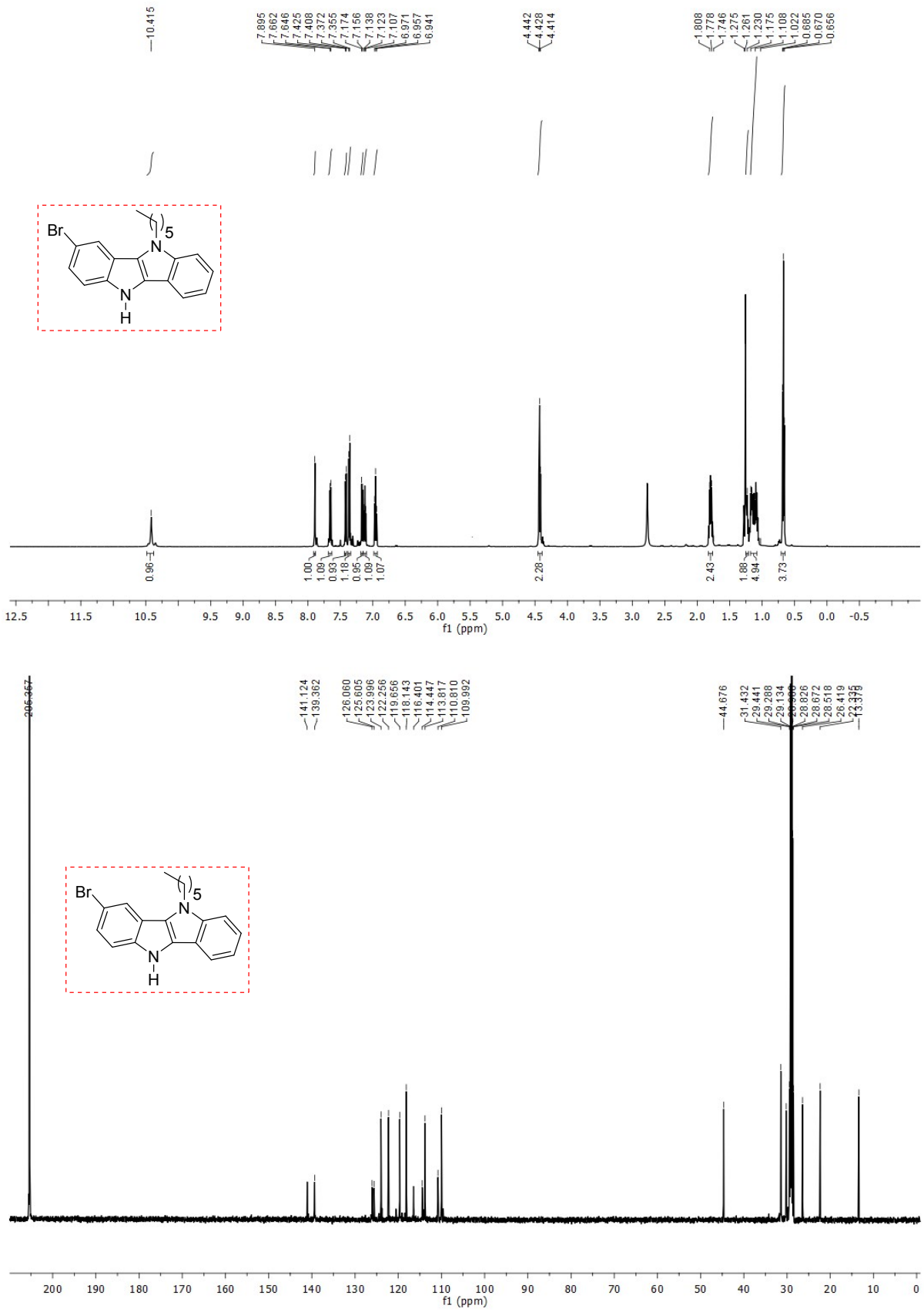

Fig. S2 ^{1}H NMR (500 MHz) & ^{13}C (125 MHz) Spectra of **5**.

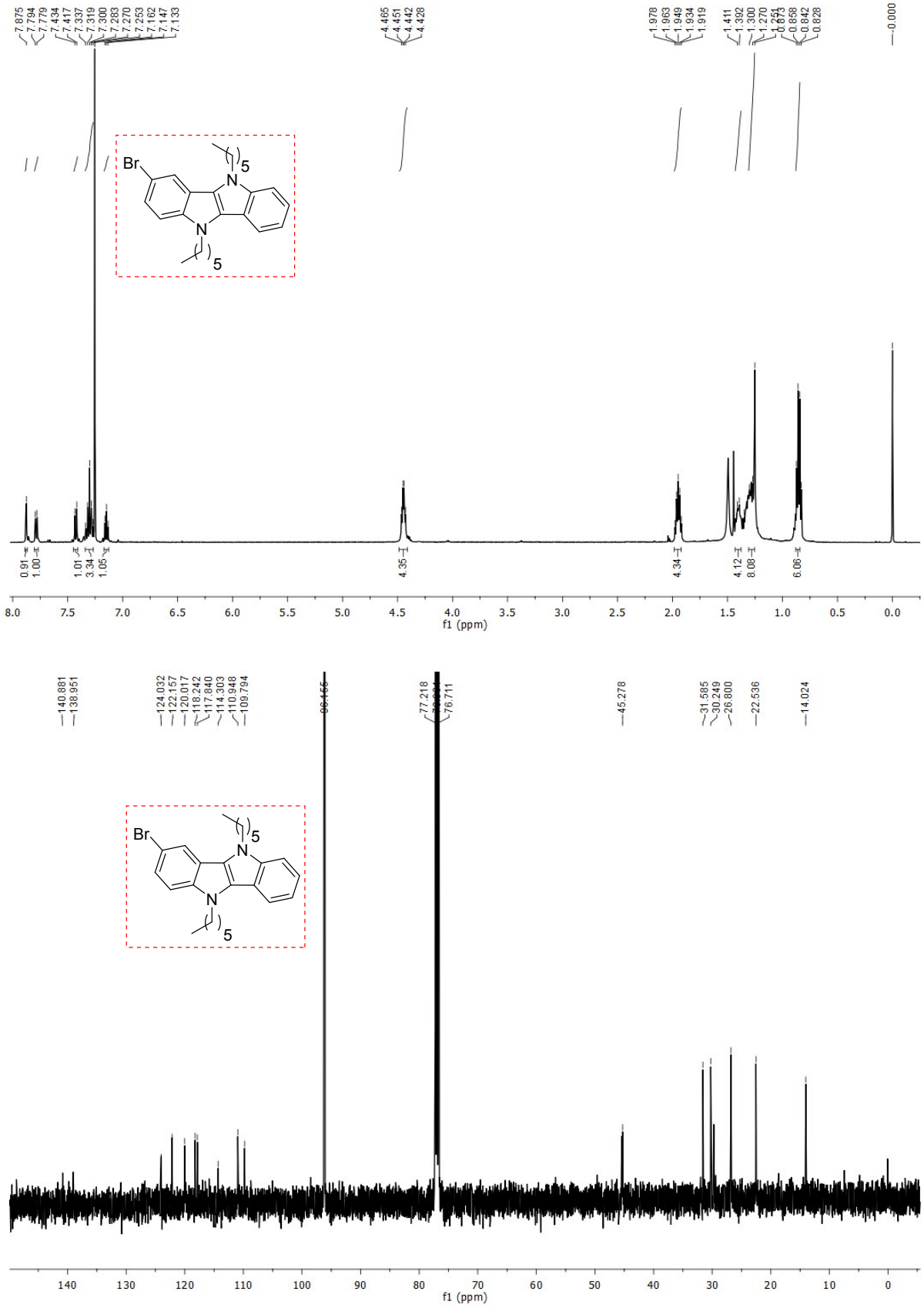

Fig. S3 ^{1}H NMR (500 MHz) & ^{13}C (125 MHz) Spectra of **6**.

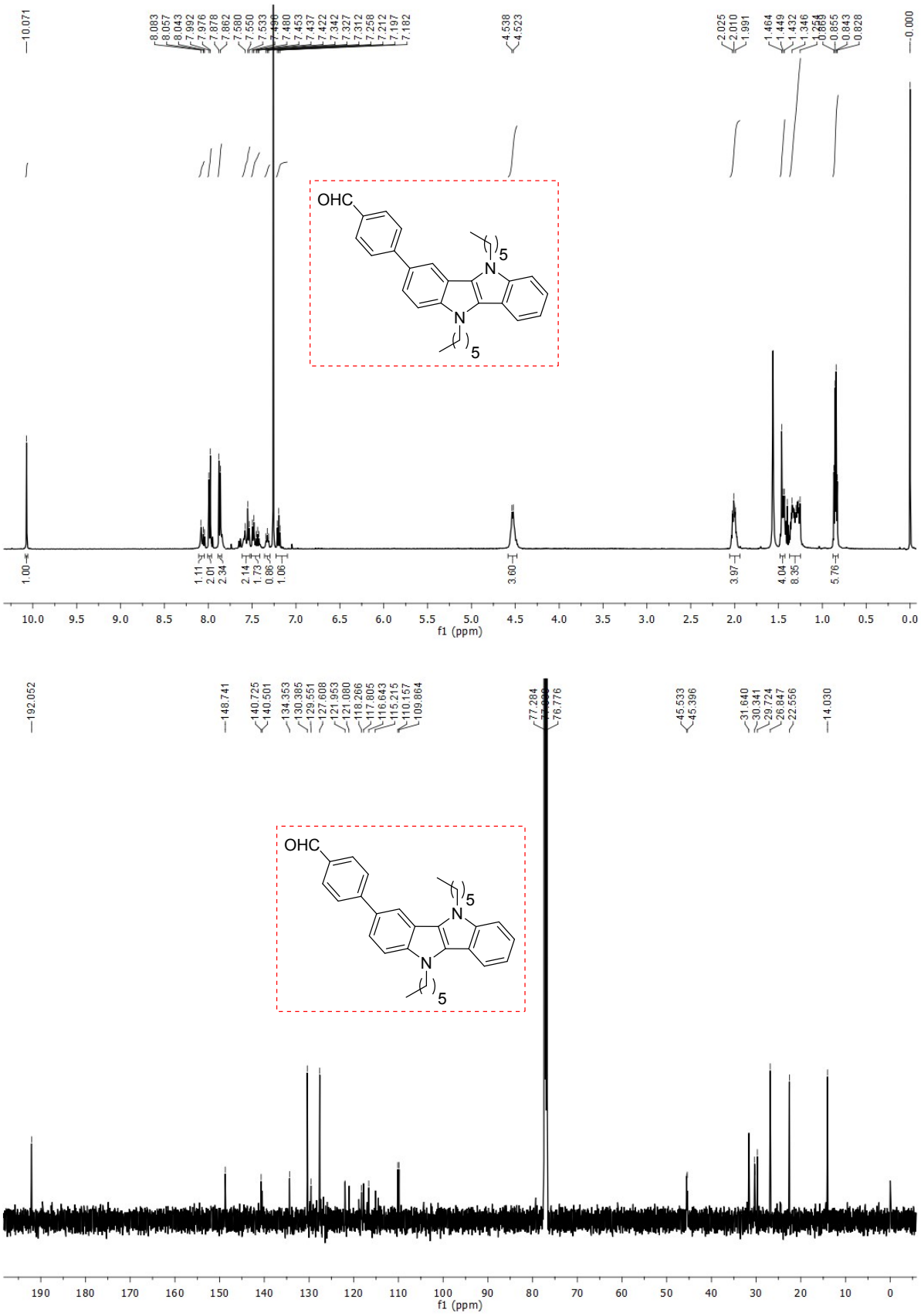

Fig. S4 ^{1}H NMR (500 MHz) & ^{13}C (125 MHz) Spectra of **7**.

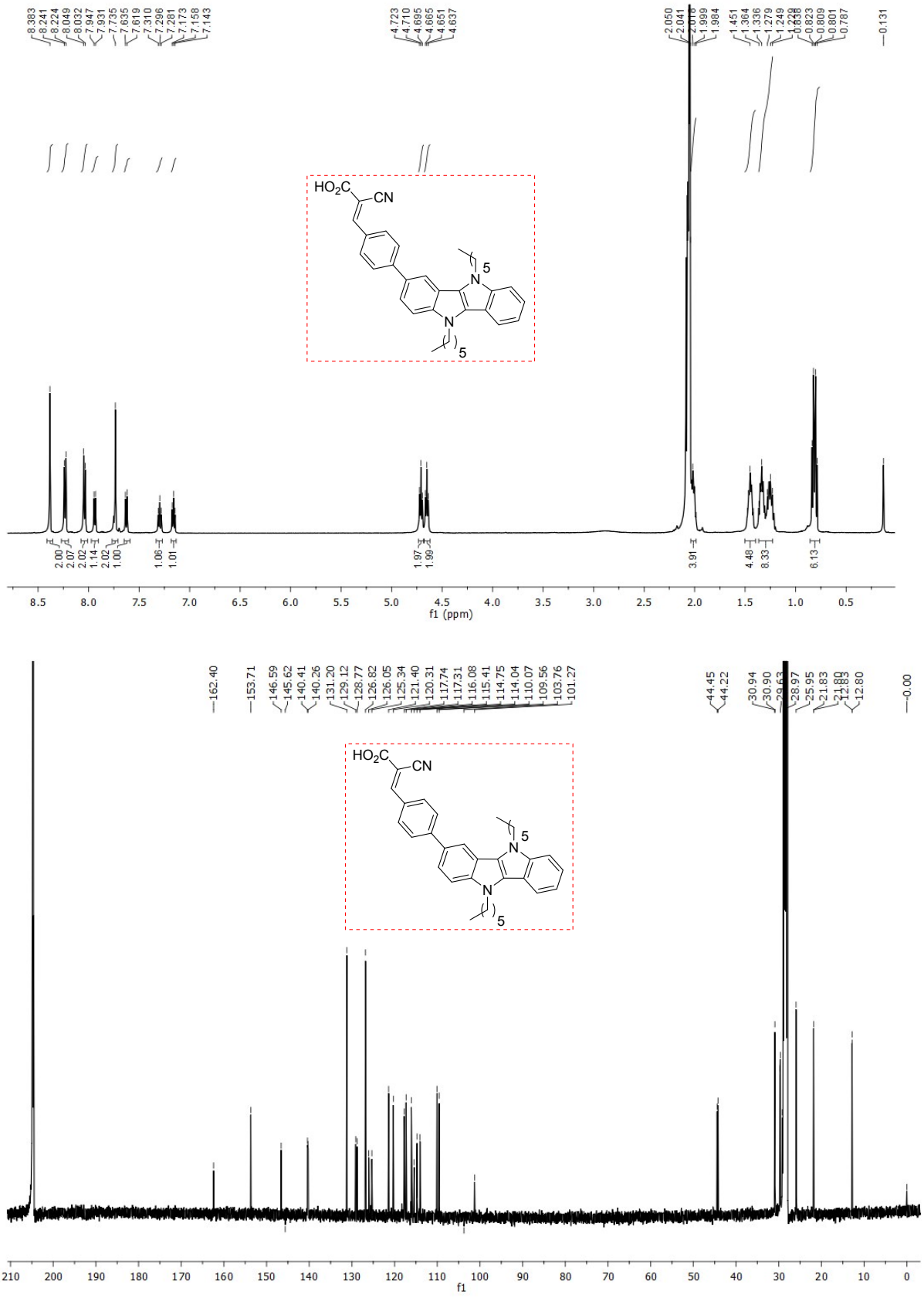

Fig. S5 ^{1}H NMR (500 MHz) & ^{13}C (125 MHz) Spectra of **IID-1**.

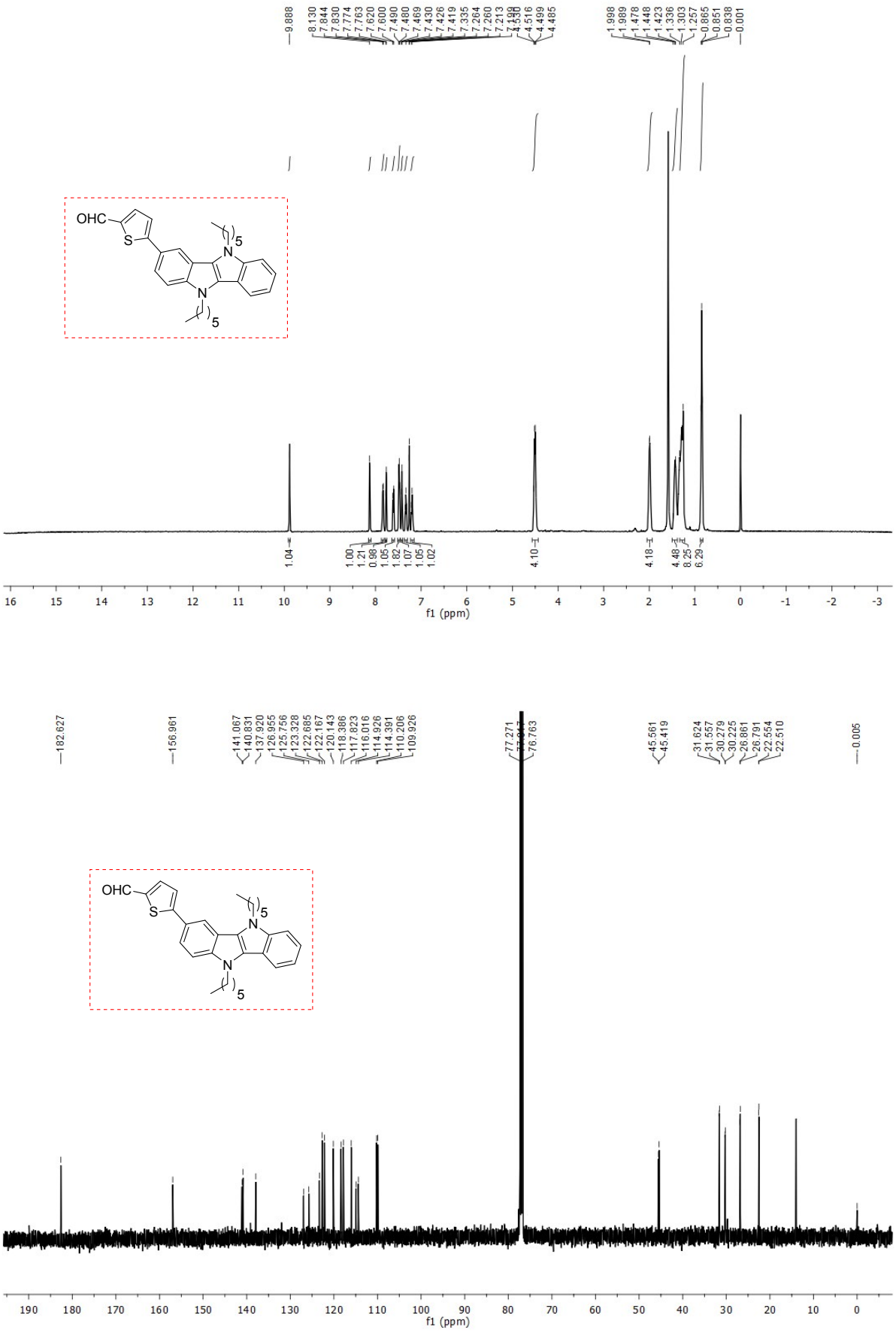

Fig. S6 ^{1}H NMR (500 MHz) & ^{13}C (125 MHz) Spectra of **8**.

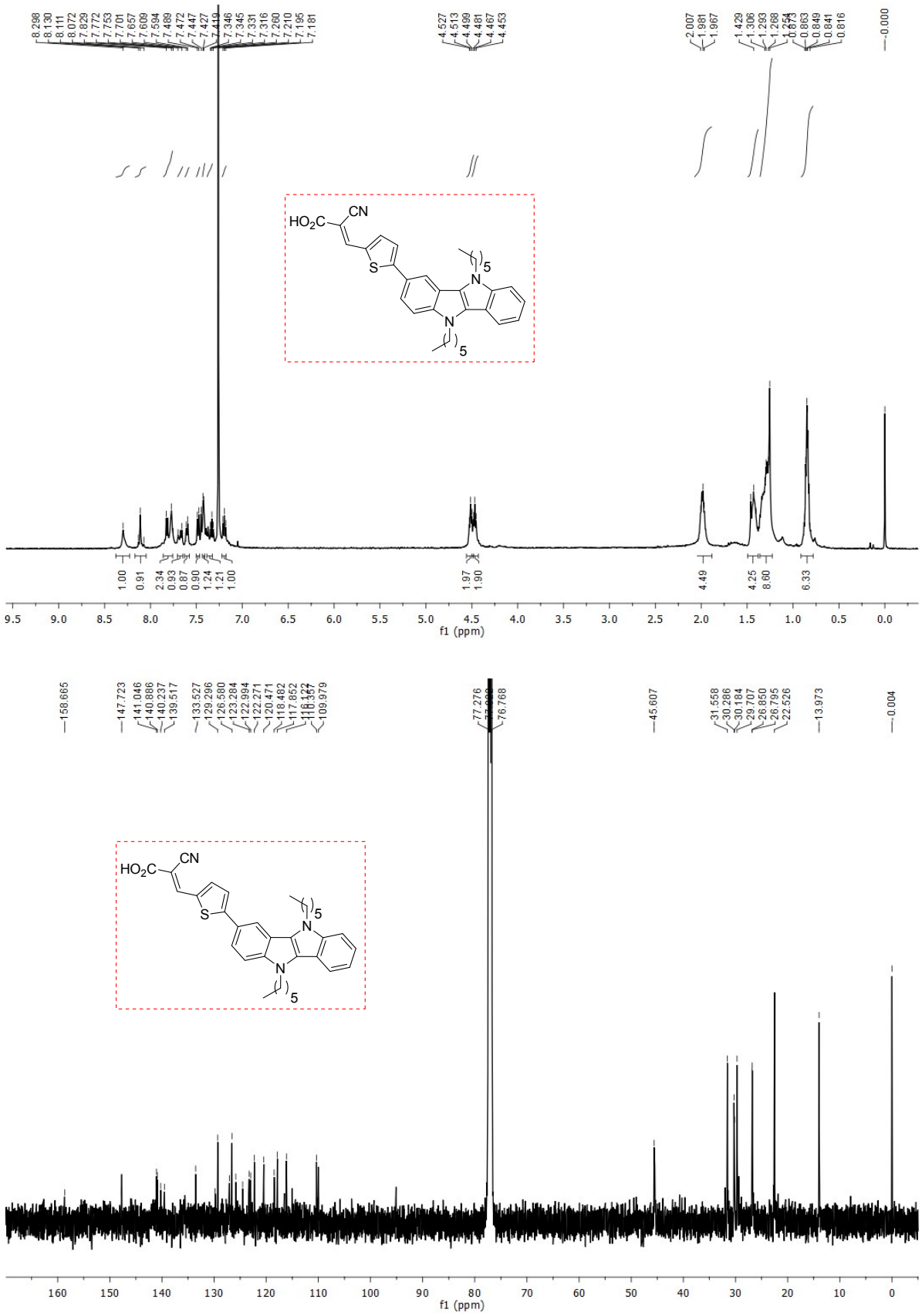

Fig. S7 ^{1}H NMR (500 MHz) & ^{13}C (125 MHz) Spectra of **IID-2**.

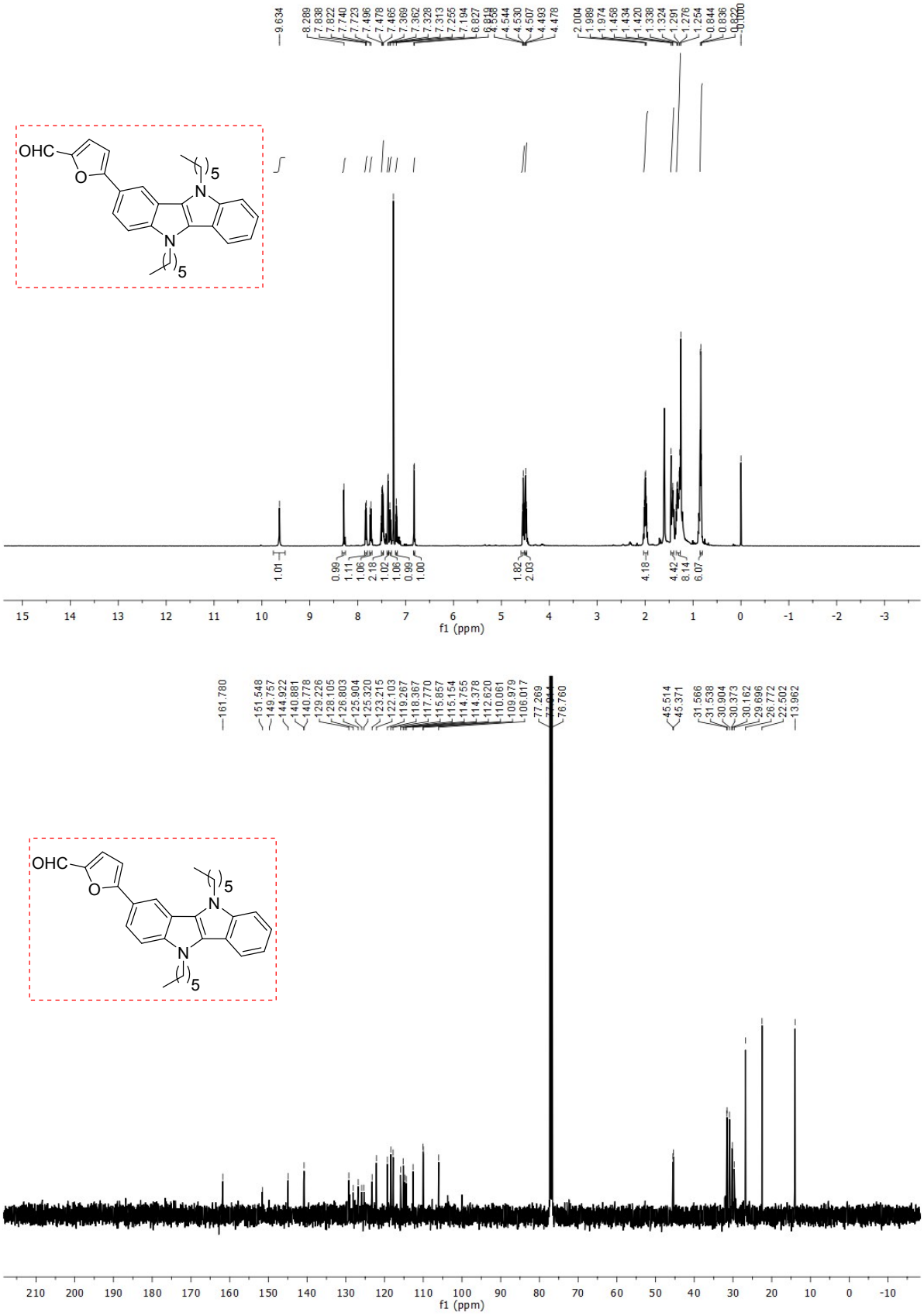

Fig. S8 ^{1}H NMR (500 MHz) & ^{13}C (125 MHz) Spectra of **9**.

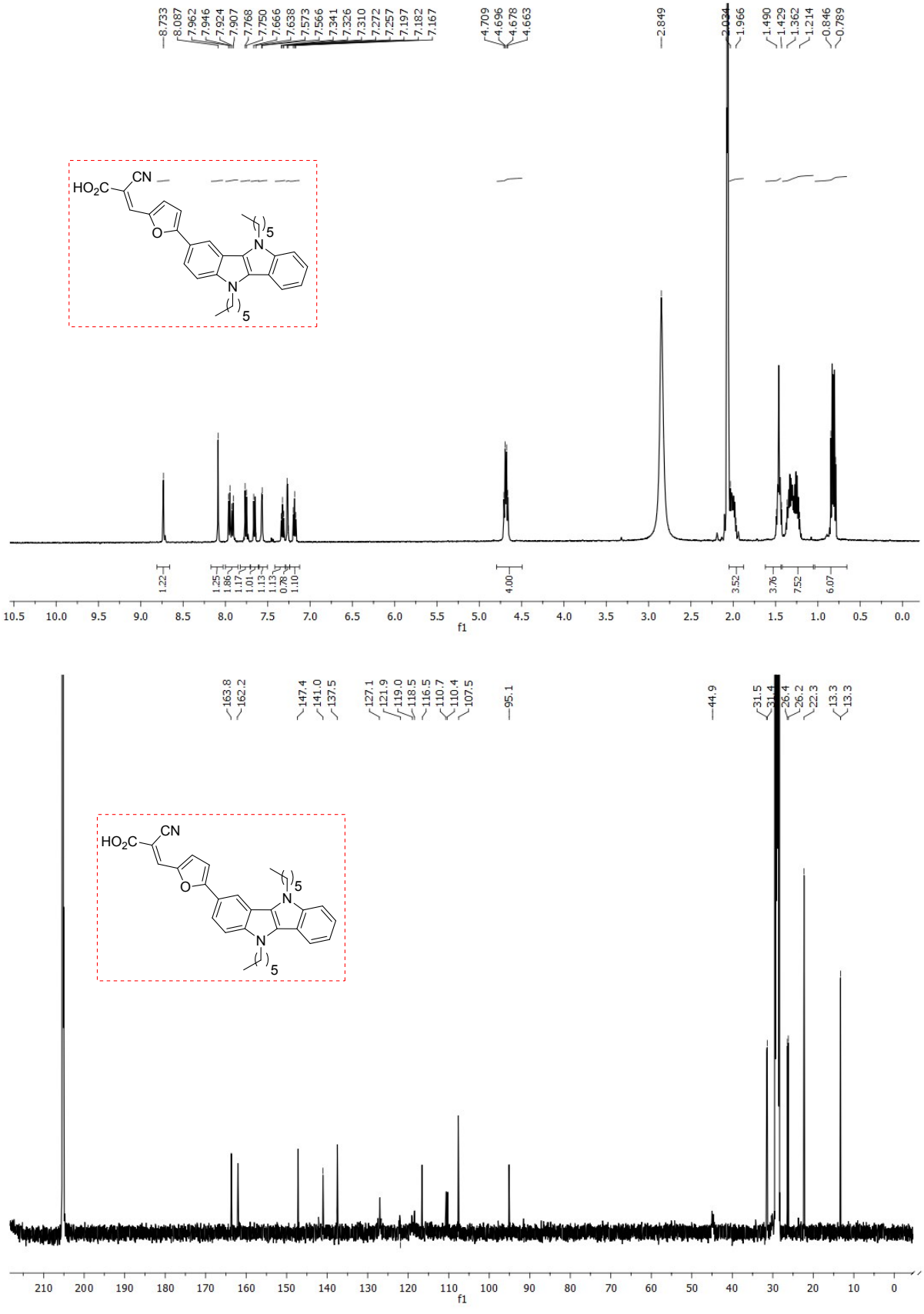

Fig. S9 ^{1}H NMR (500 MHz) & ^{13}C (125 MHz) Spectra of **IID-3**.

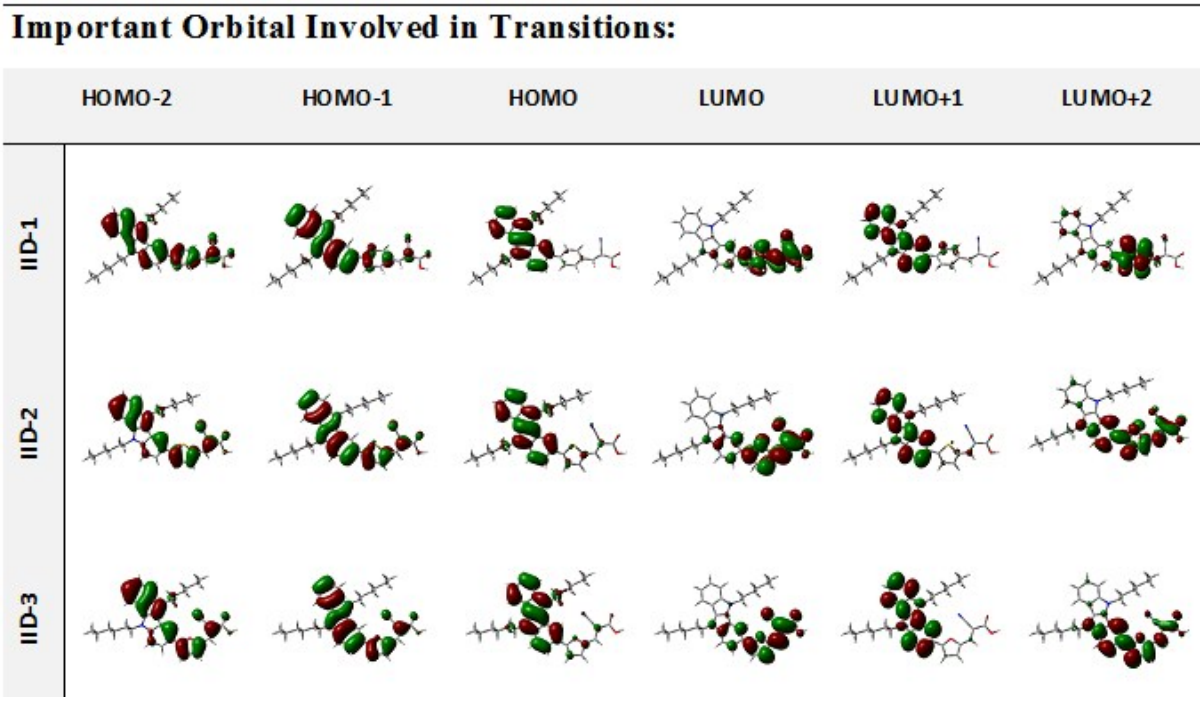

Fig. S10 Molecular orbital contributions for IID dyes obtained from **TD-DFT** analysis.

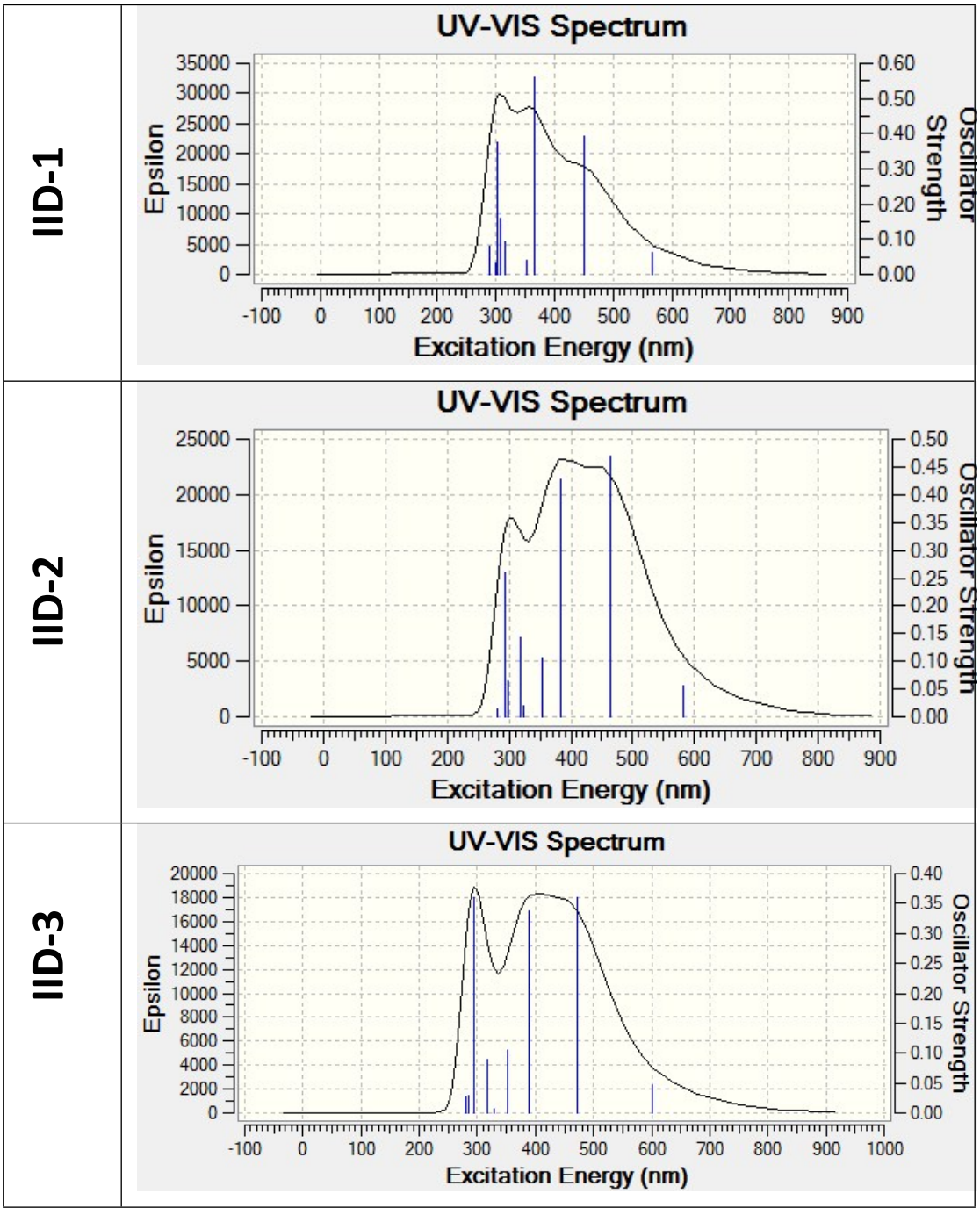

Fig. S11 Simulated absorption spectra of IID dyes obtained from TD-DFT analysis.

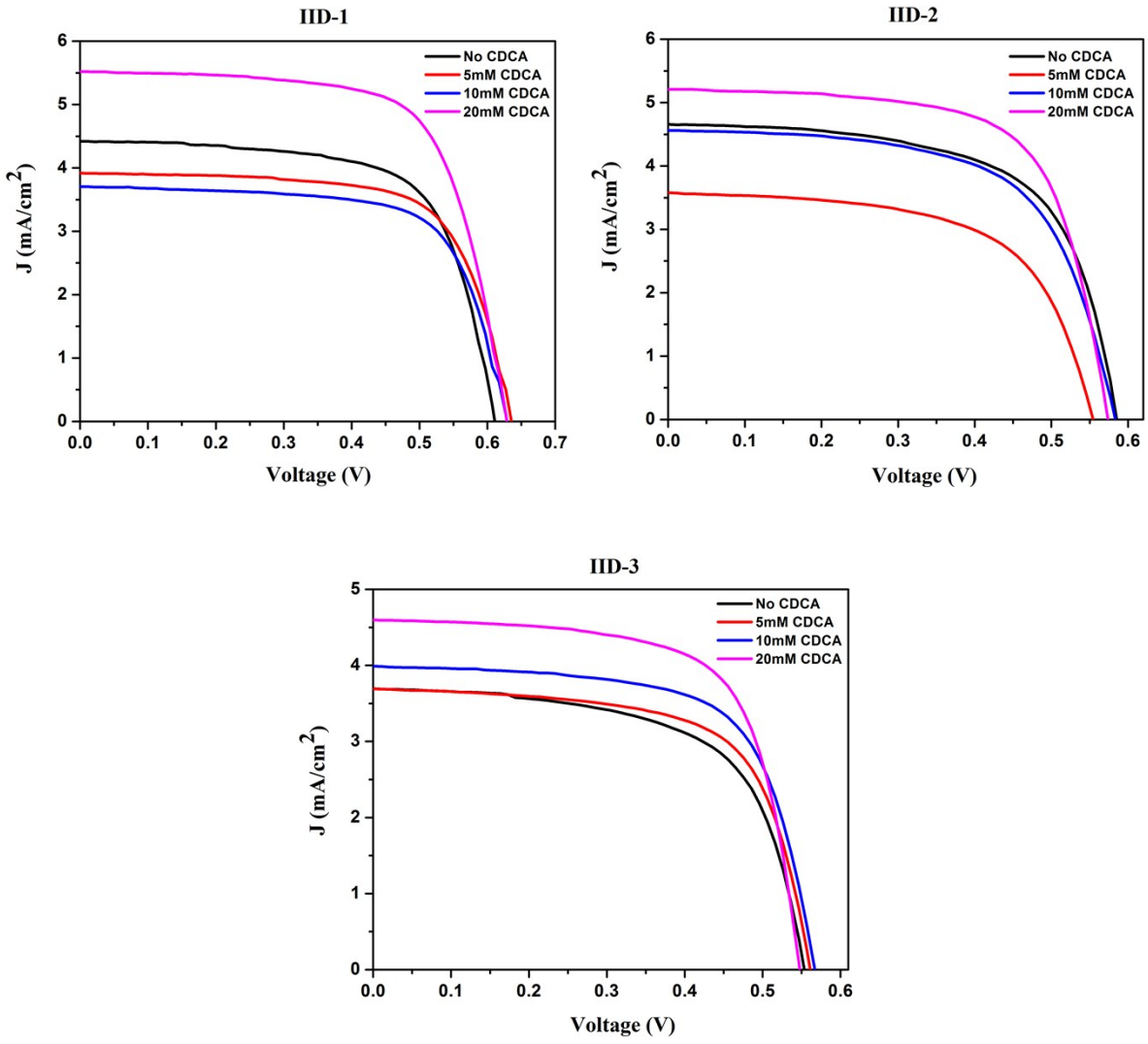

Fig. S12 *J-V* characteristic curves for the CDCA optimization carried out for DSSCs fabricated using **IID-1**, **IID-2** and **IID-3** at full sun condition.

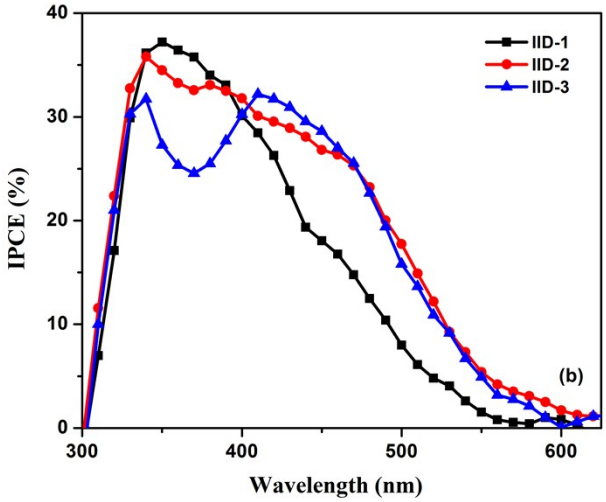

Fig. S13 Spectra of incident photon-to-current conversion efficiency (IPCE) for DSCs based on **IID-1**, **IID-2**, and **IID-3**.

Table S1 Solar Cell Characteristics of DSSCs for all three dyes (**IID-1**, **IID-2** and **IID-3**) without co-adsorbent (CDCA) and by varying the CDCA concentration.

IID-1	J_{sc} **(mAcm^{-2})**	V_{oc} **(V)**	***FF***	**Efficiency (%)**
No CDCA	4.42	0.6	0.68	1.82
5 mM	3.92	0.64	0.68	1.72
10 mM	3.70	0.63	0.69	1.61
20 mM	5.51	0.62	0.69	2.38

IID-2	J_{sc} **(mAcm^{-2})**	V_{oc} **(V)**	***FF***	**Efficiency (%)**
No CDCA	4.66	0.58	0.63	1.72
5 mM	3.57	0.55	0.61	1.21
10 mM	4.57	0.58	0.63	1.67
20 mM	5.22	0.57	0.67	2.00

IID-3	J_{sc} **(mAcm^{-2})**	V_{oc} **(V)**	***FF***	**Efficiency (%)**
No CDCA	3.69	0.55	0.63	1.27
5 mM	3.69	0.56	0.66	1.37
10 mM	3.99	0.57	0.66	1.51
20 mM	4.60	0.54	0.69	1.71