Electronic Supplementary Information

Effect of Structural Manipulation in Hetero-tri-aryl Amine Donor Based D-A'-π-A sensitizers in Dye Sensitized Solar Cells

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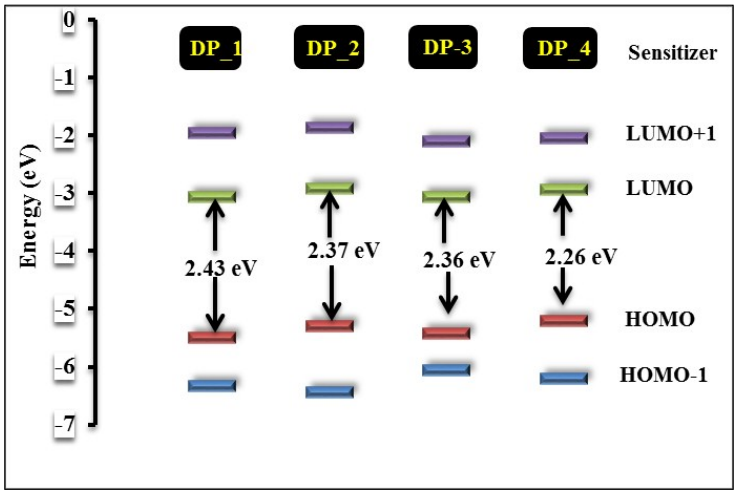

Figure S1. HOMO LUMO energy representation of the all sensitizer, parameters obtained at the B3LYP/6-31G(d) level in vacuum.

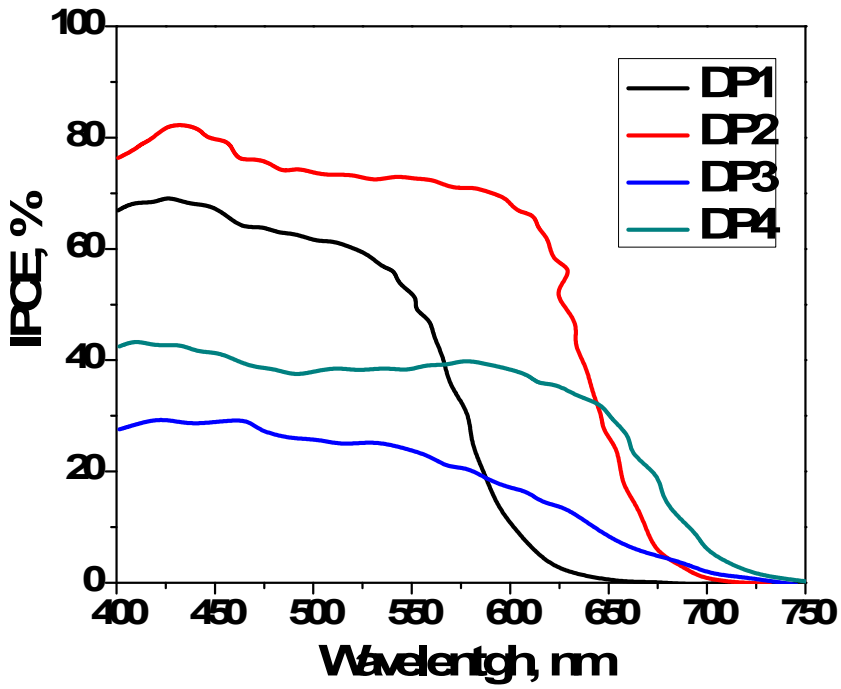

Figure S2. IPCE characteristics of DP devices

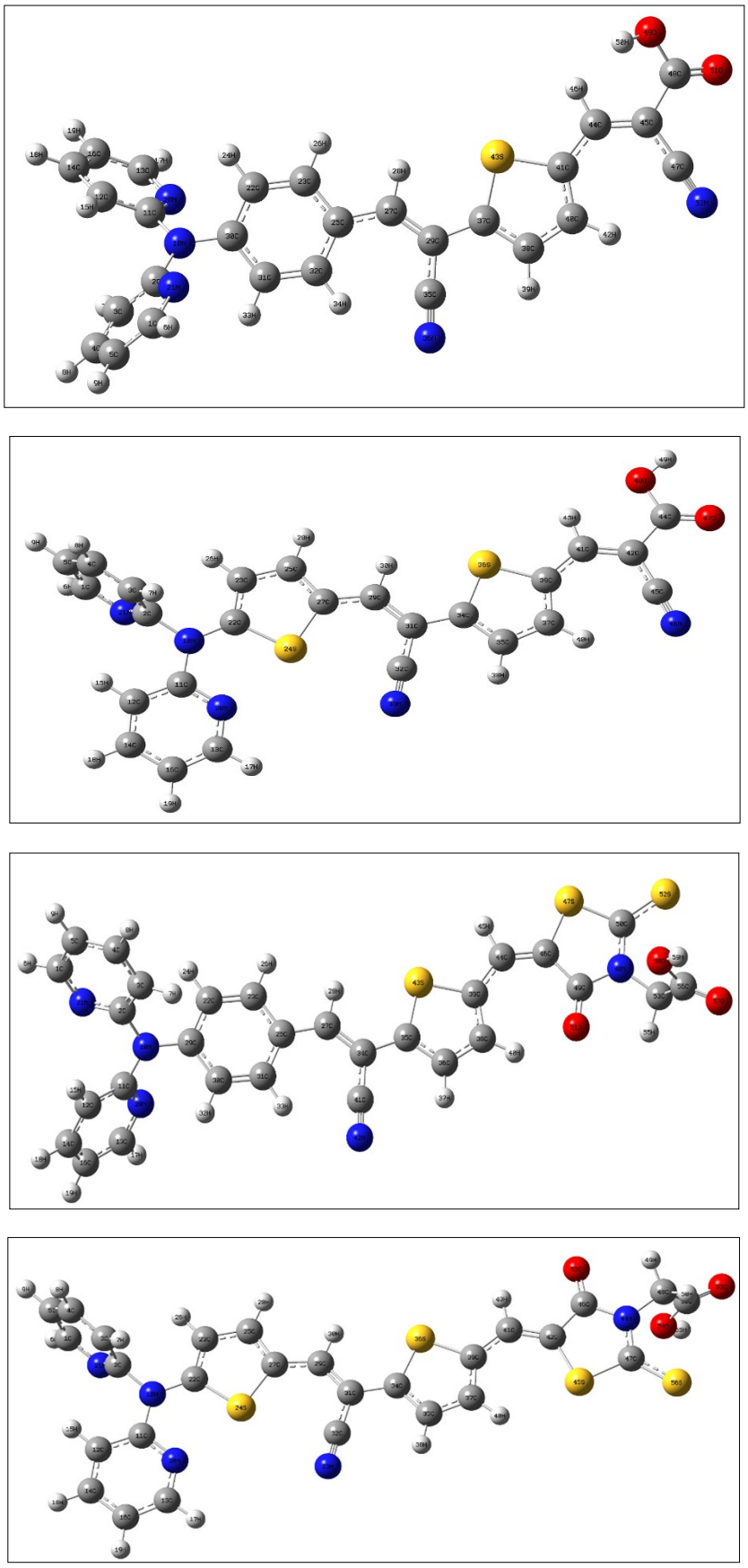

Figure S3. The optimized geometries of the DP1, DP2, DP3 and DP4 sensitizers, obtained at the B3LYP/6-31G(d) level in vacuum.

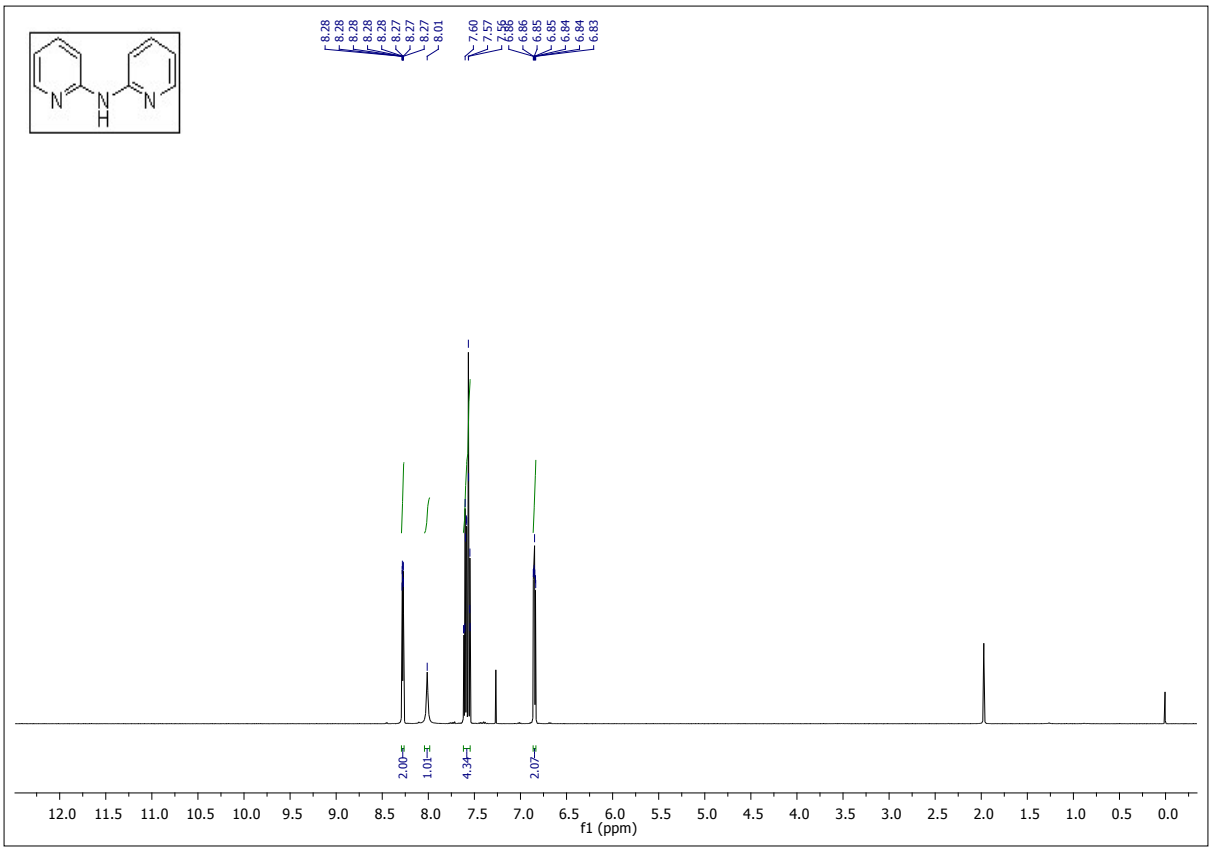

Figure S4: ^{1}H NMR spectrum of compound 1

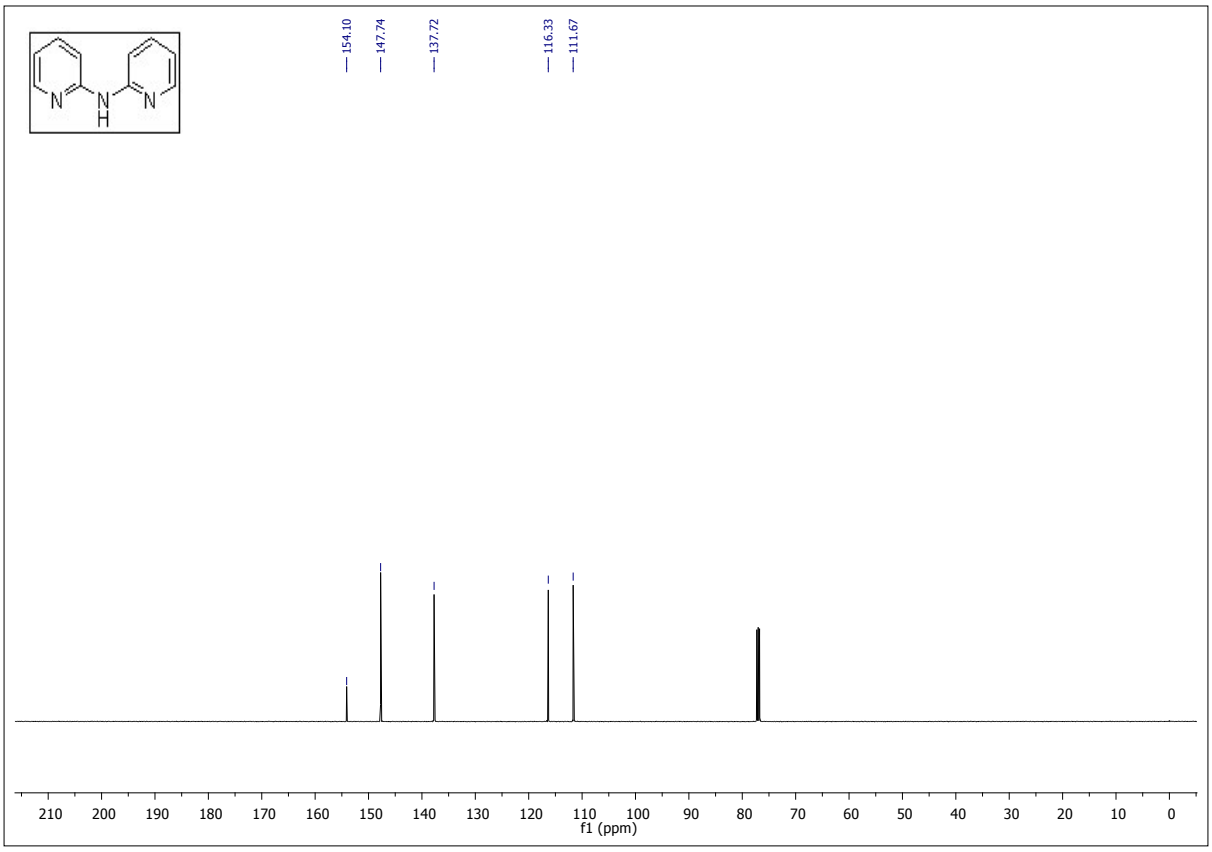

Figure S5: ^{13}C NMR spectrum of compound 1

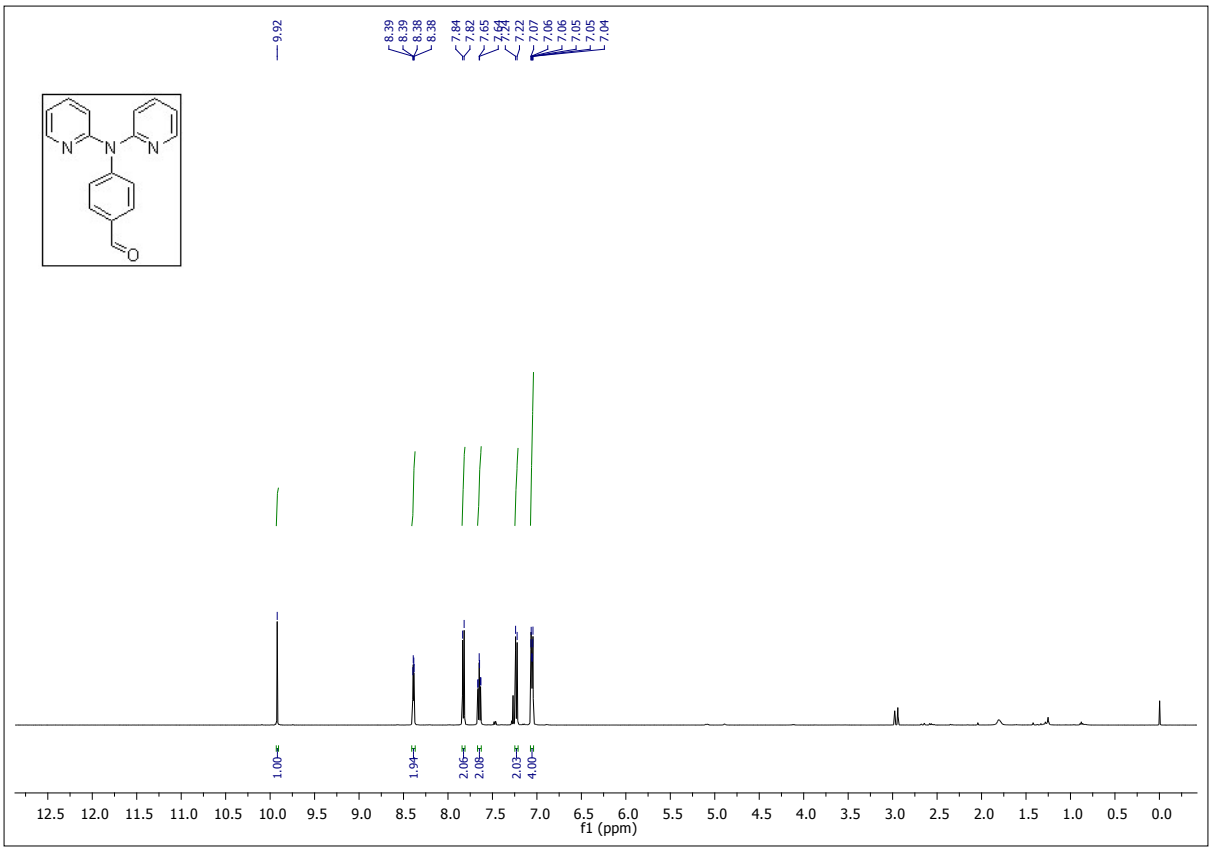

Figure S6: ^{1}H NMR spectrum of compound 2a

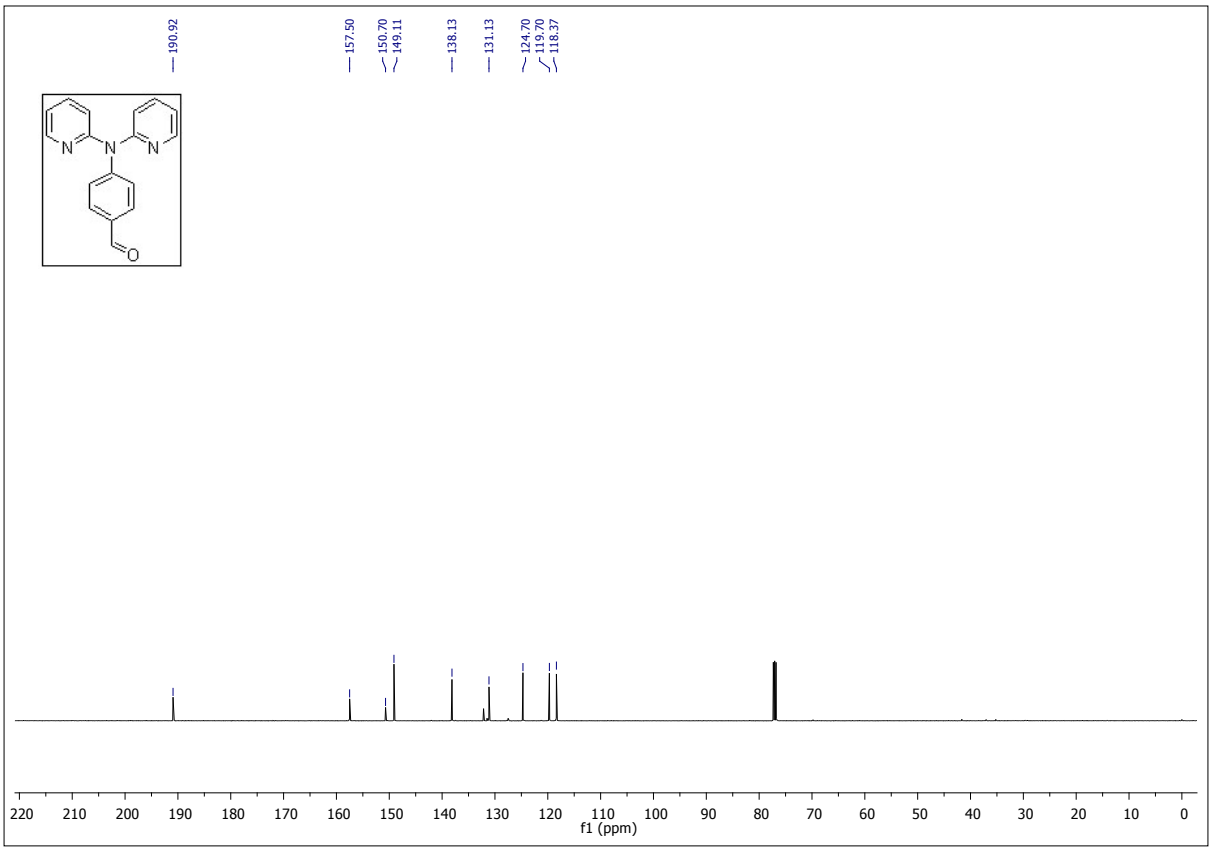

Figure S7: ^{13}C NMR spectrum of compound 2a

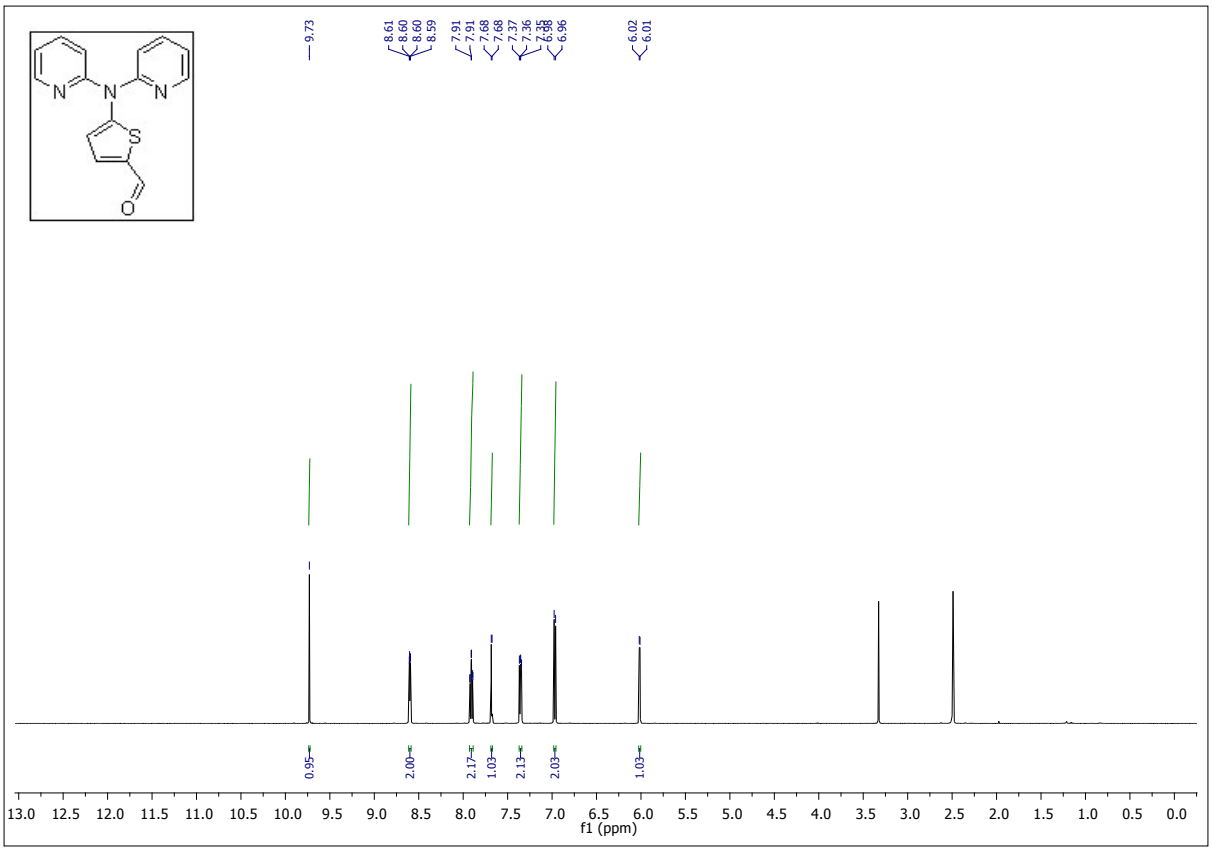

Figure S8: ^{1}H NMR spectrum of compound 2b

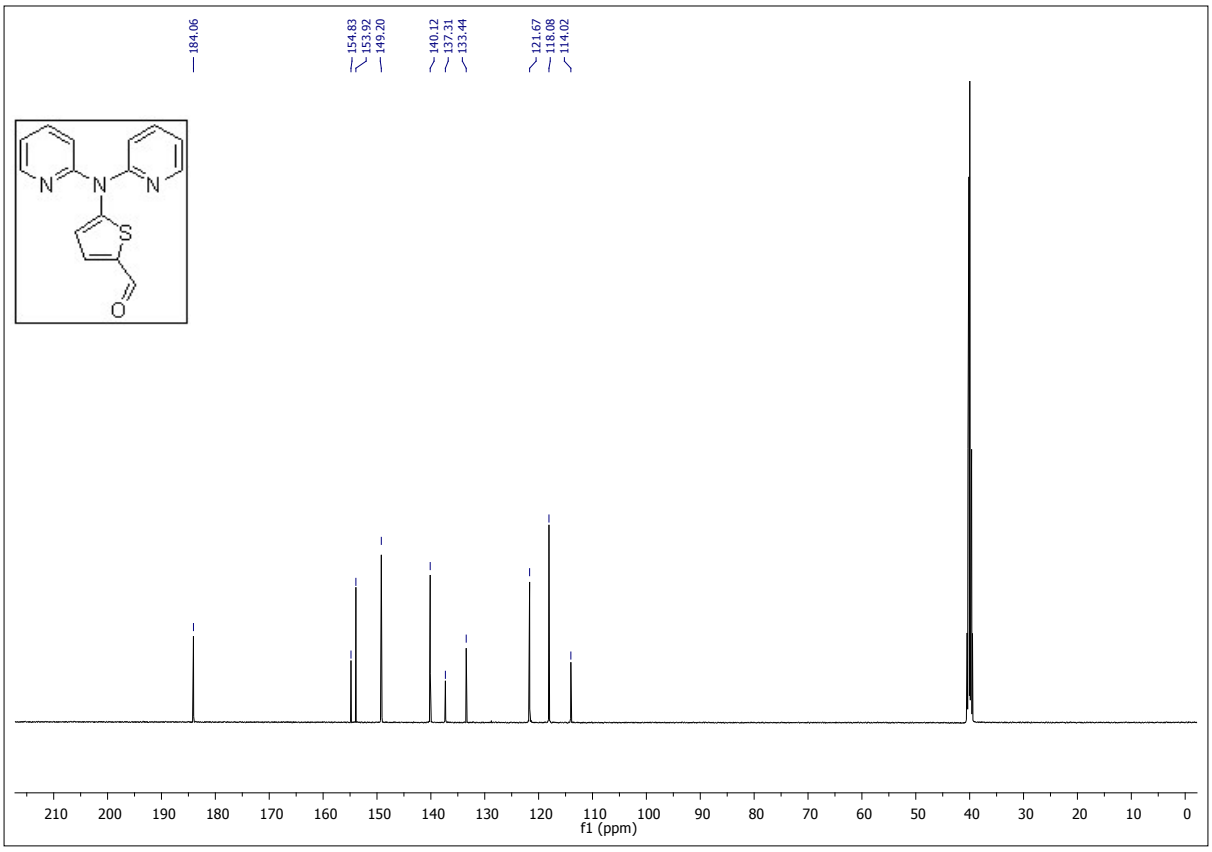

Figure S9: ^{13}C NMR spectrum of compound 2b

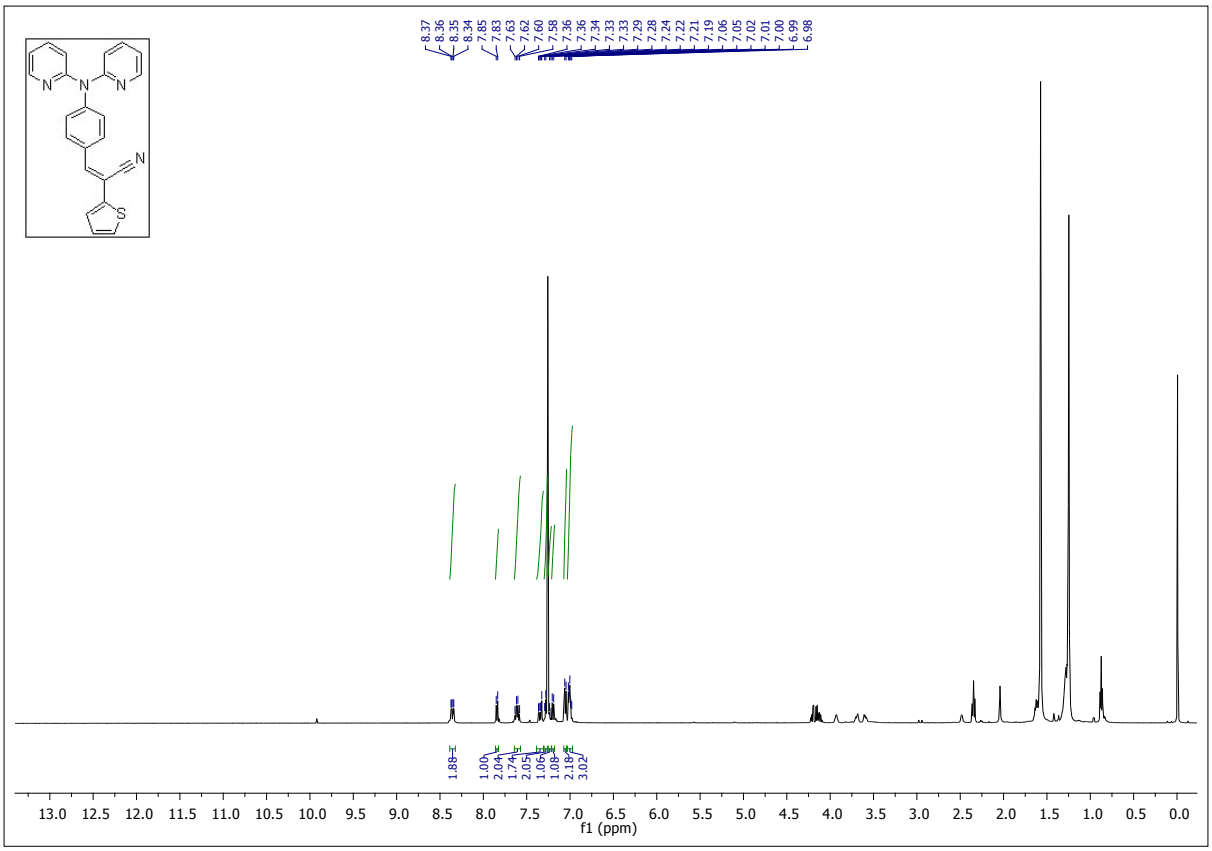

Figure S10: ^{1}H NMR spectrum of compound 3a

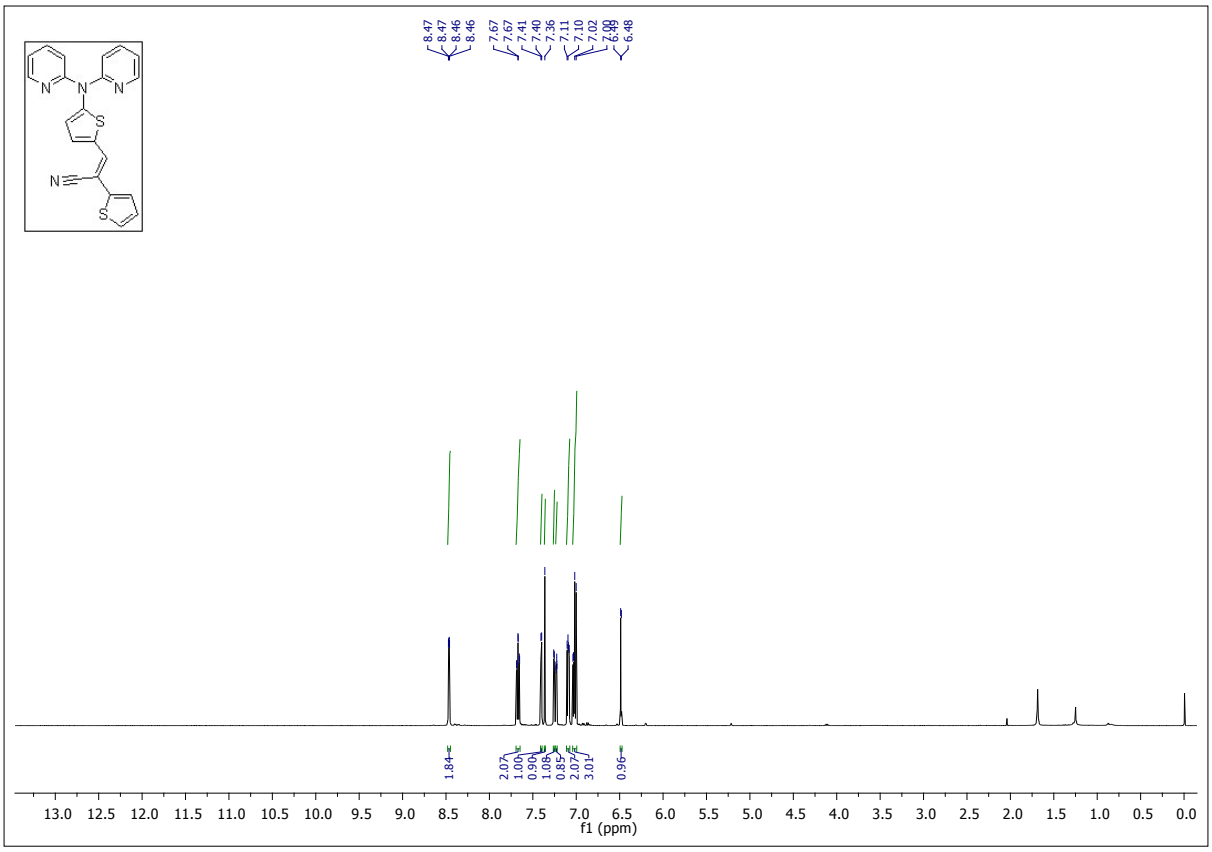

Figure S11: ^{1}H NMR spectrum of compound 3b

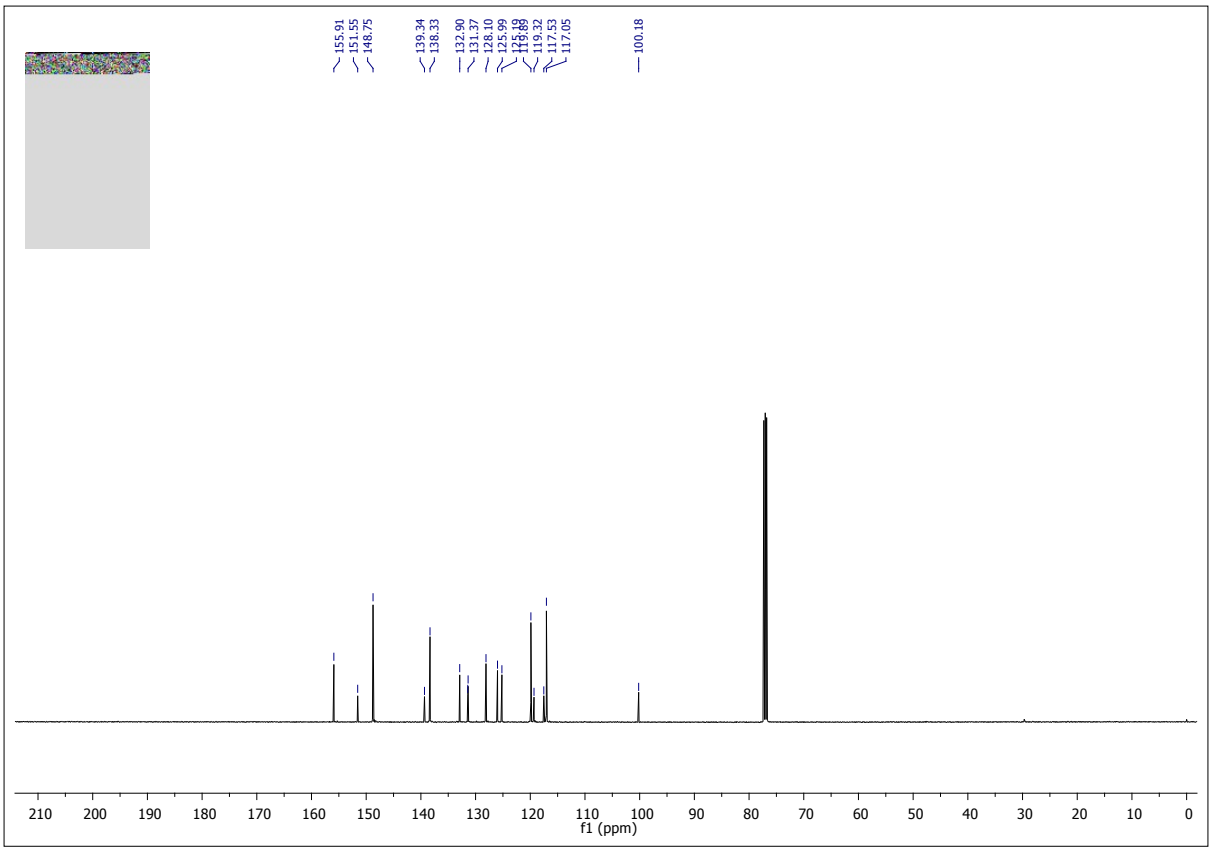

Figure S12: ^{13}C NMR spectrum of compound 3b

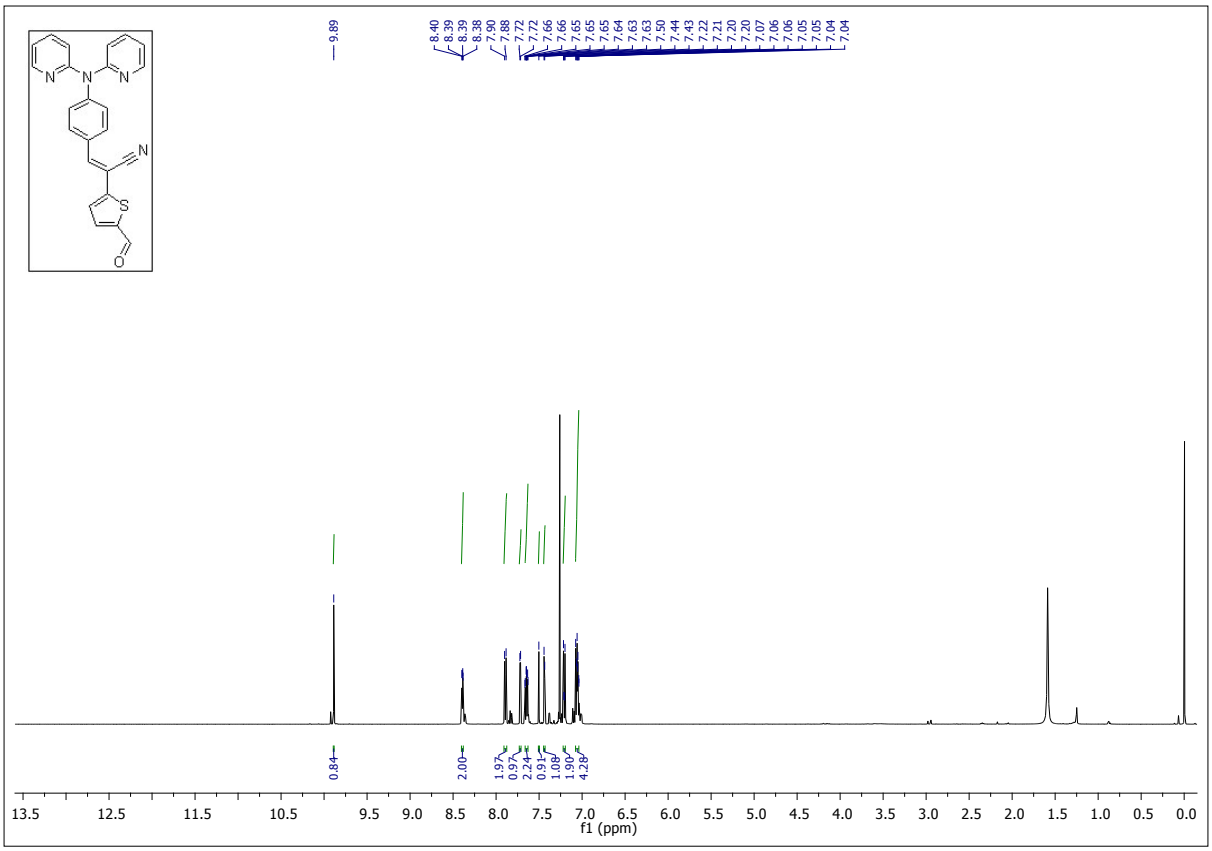

Figure S13: ^{1}H NMR spectrum of compound 4a

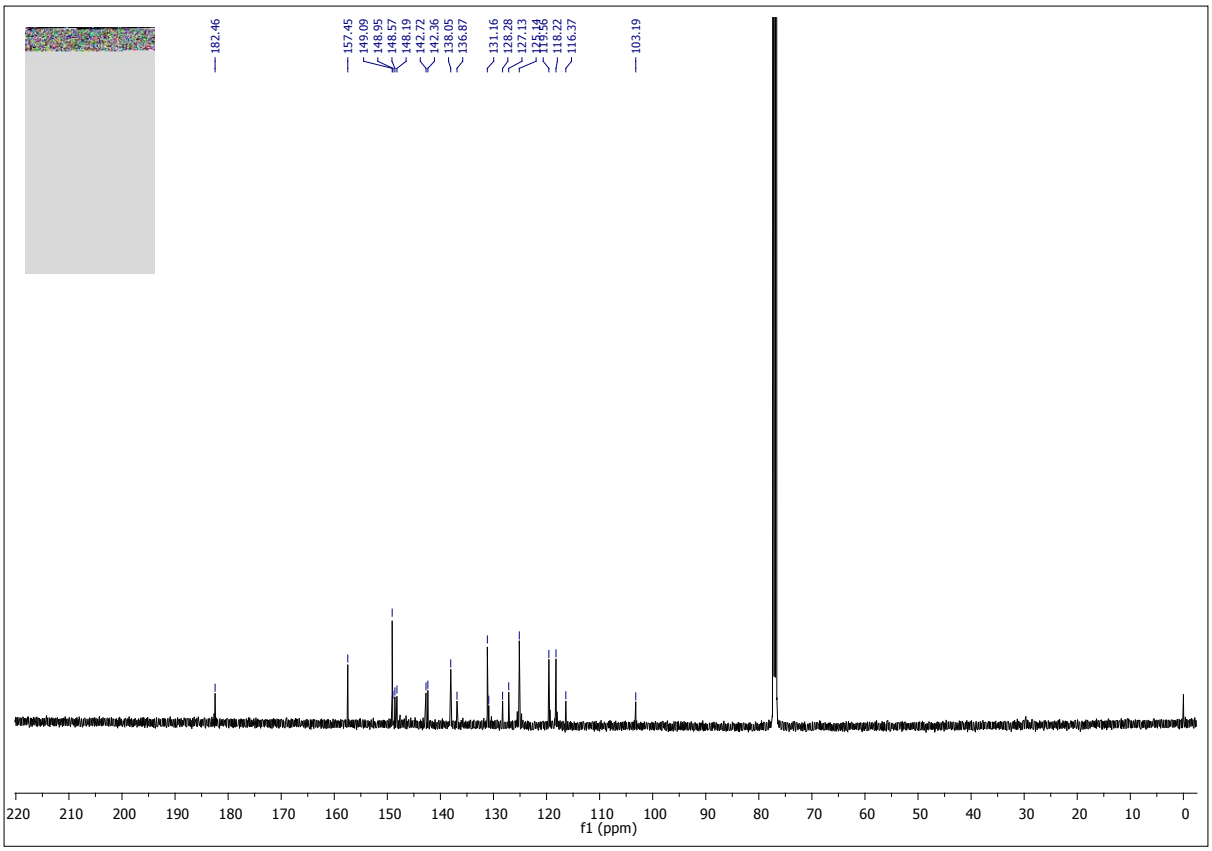

Figure S14: ^{13}C NMR spectrum of compound 4a

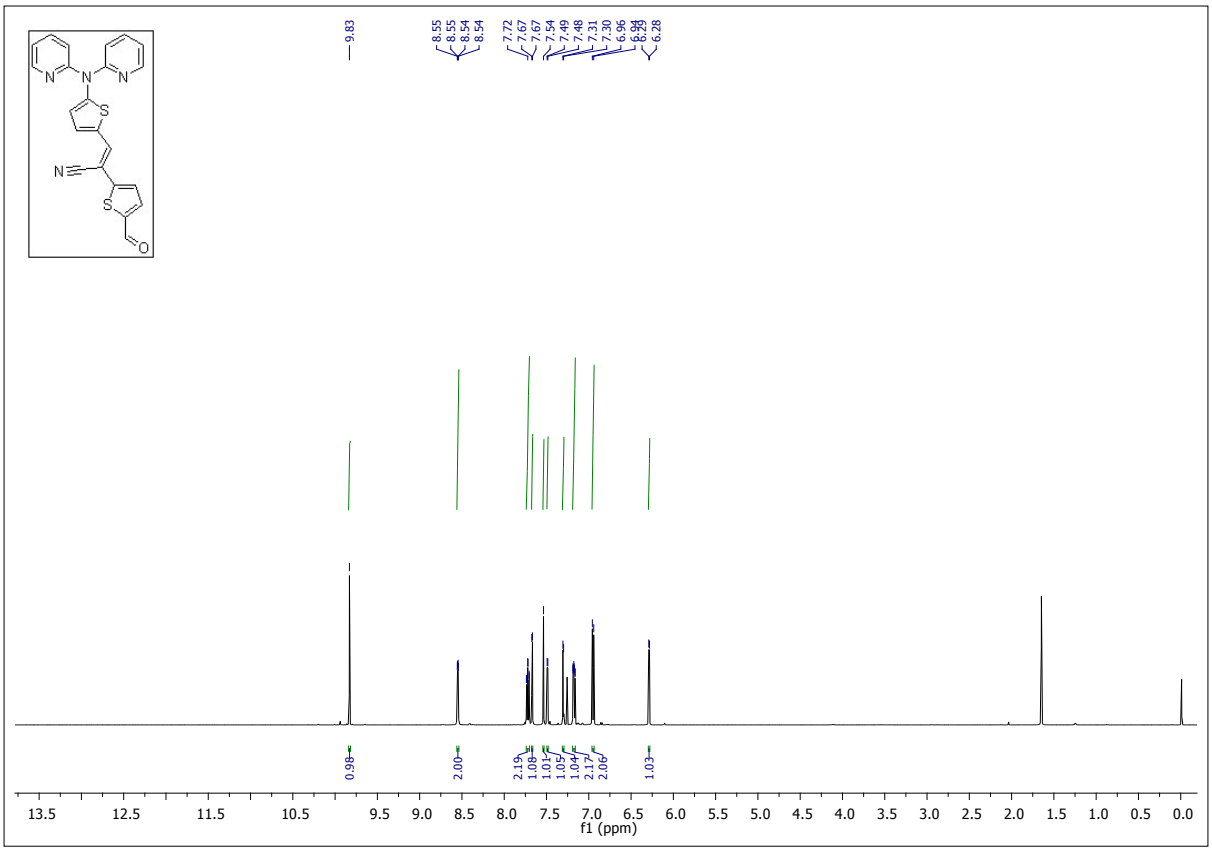

Figure S15: ^{1}H NMR spectrum of compound 4b

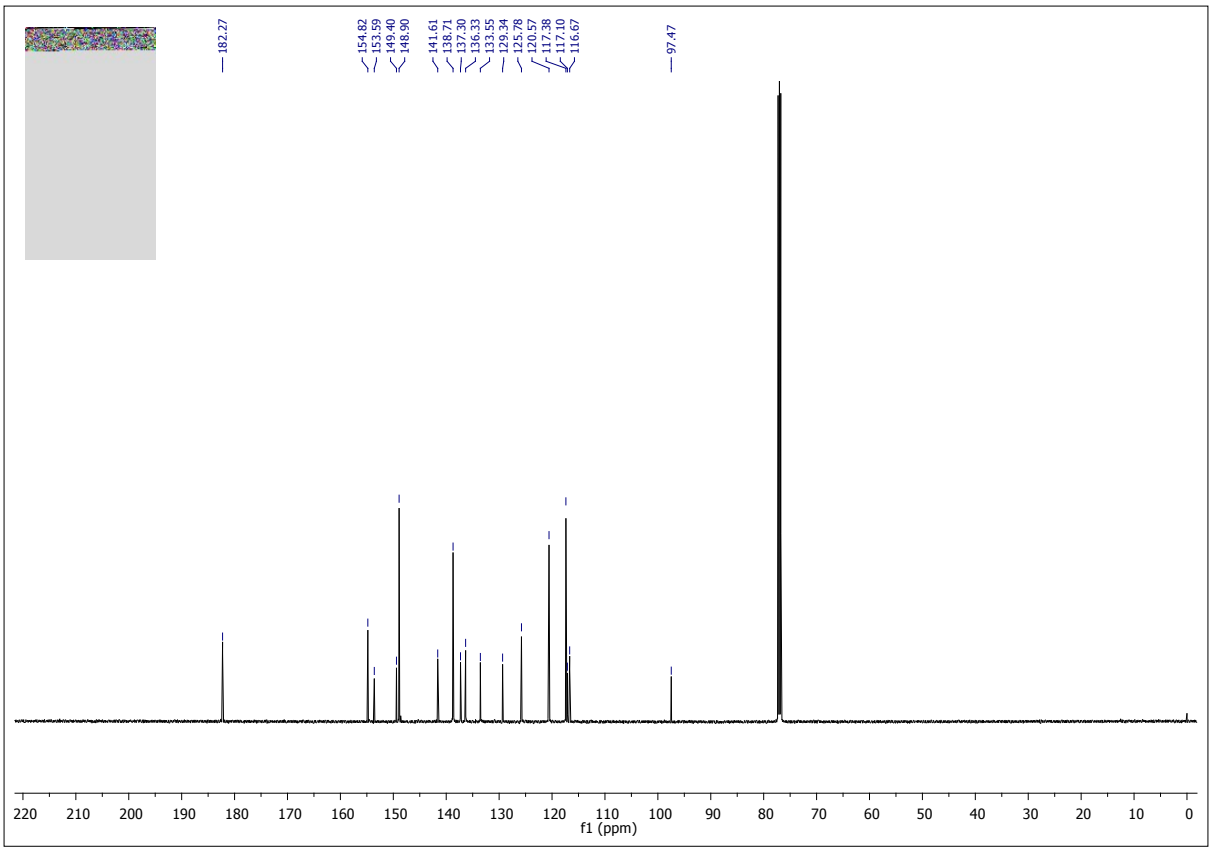

Figure S16: ^{13}C NMR spectrum of compound 4b

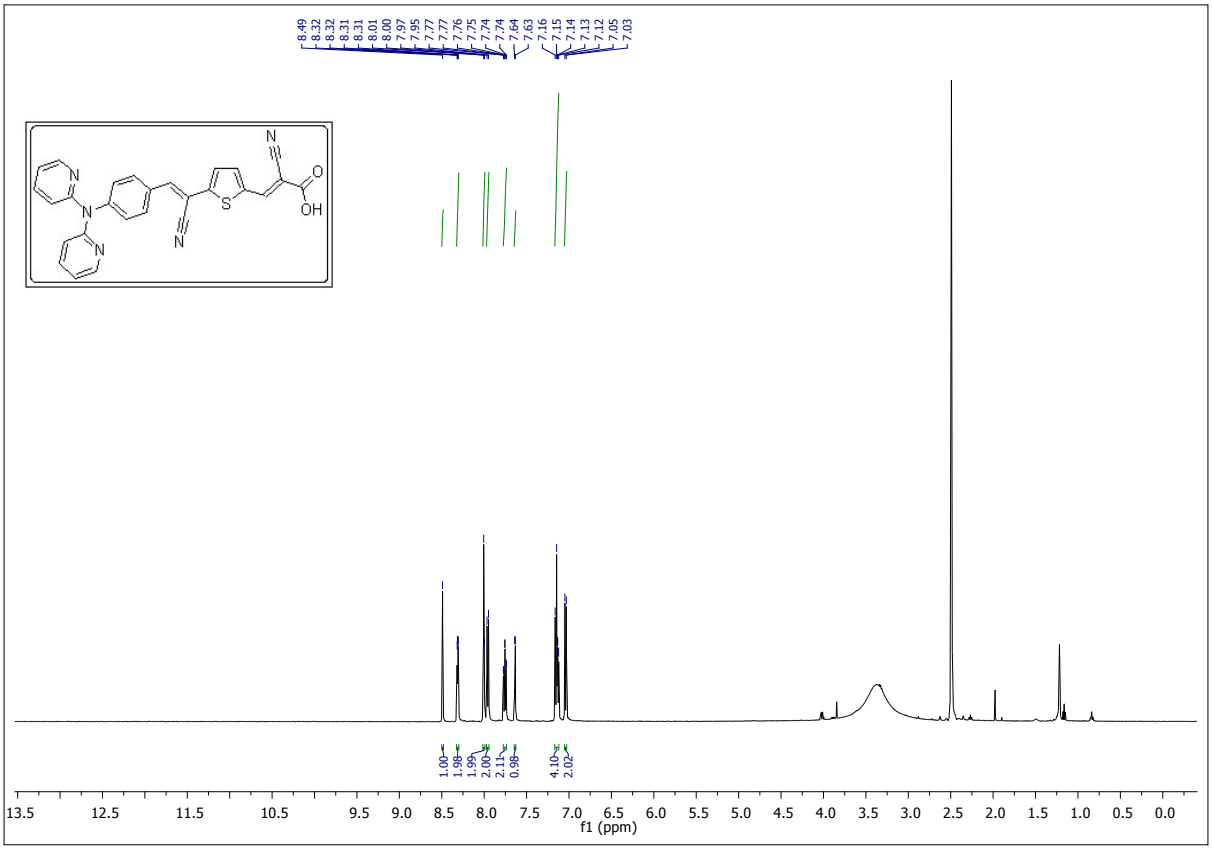

Figure S17: ^{1}H NMR spectrum of sensitizer DP1

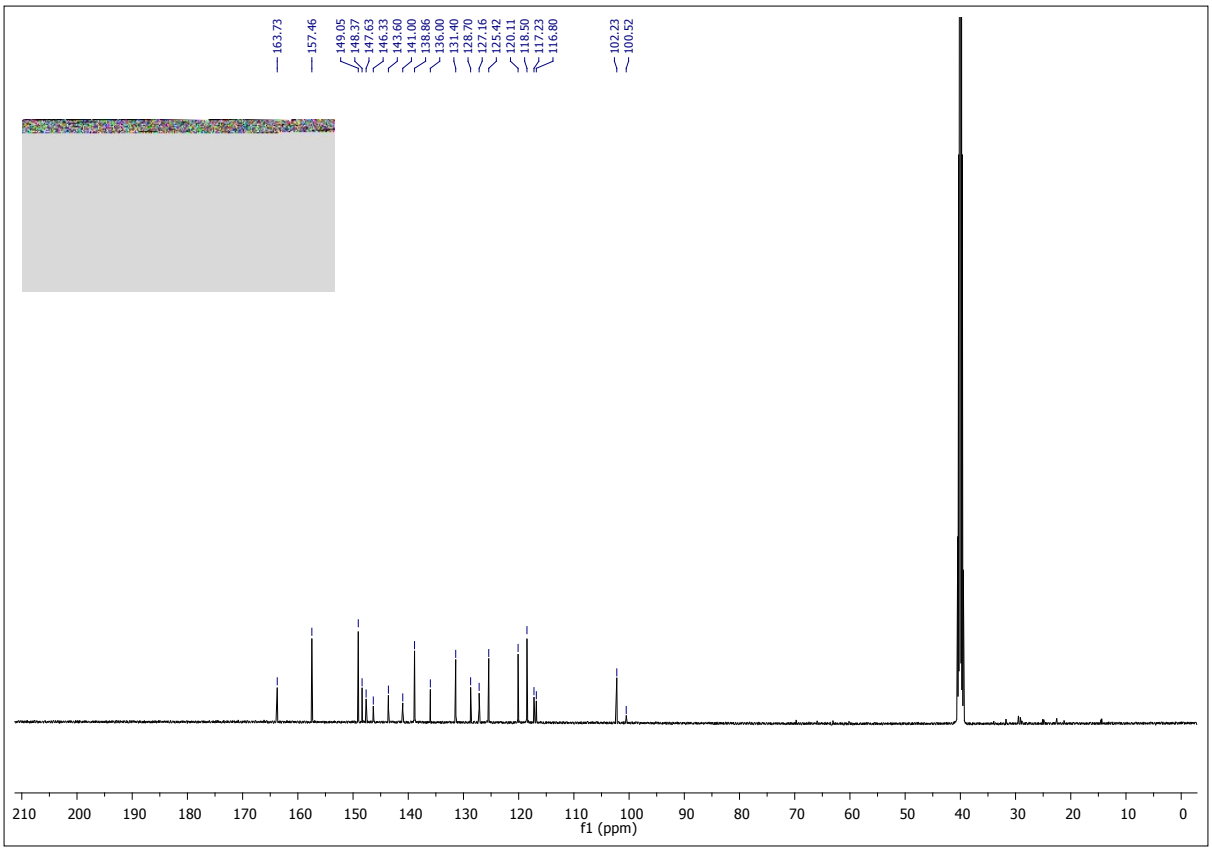

Figure S18: ^{13}C NMR spectrum of sensitizer DP1

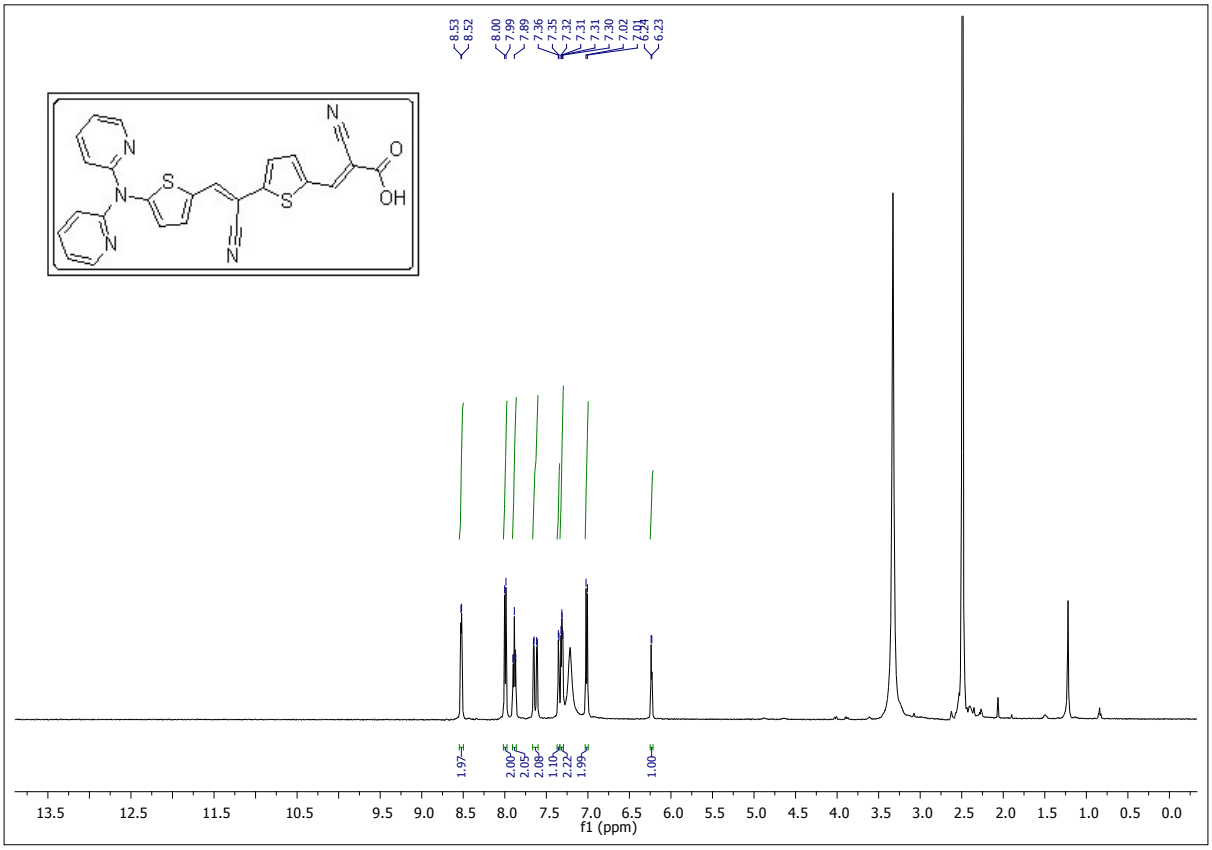

Figure S19: ^{1}H NMR spectrum of sensitizer DP2

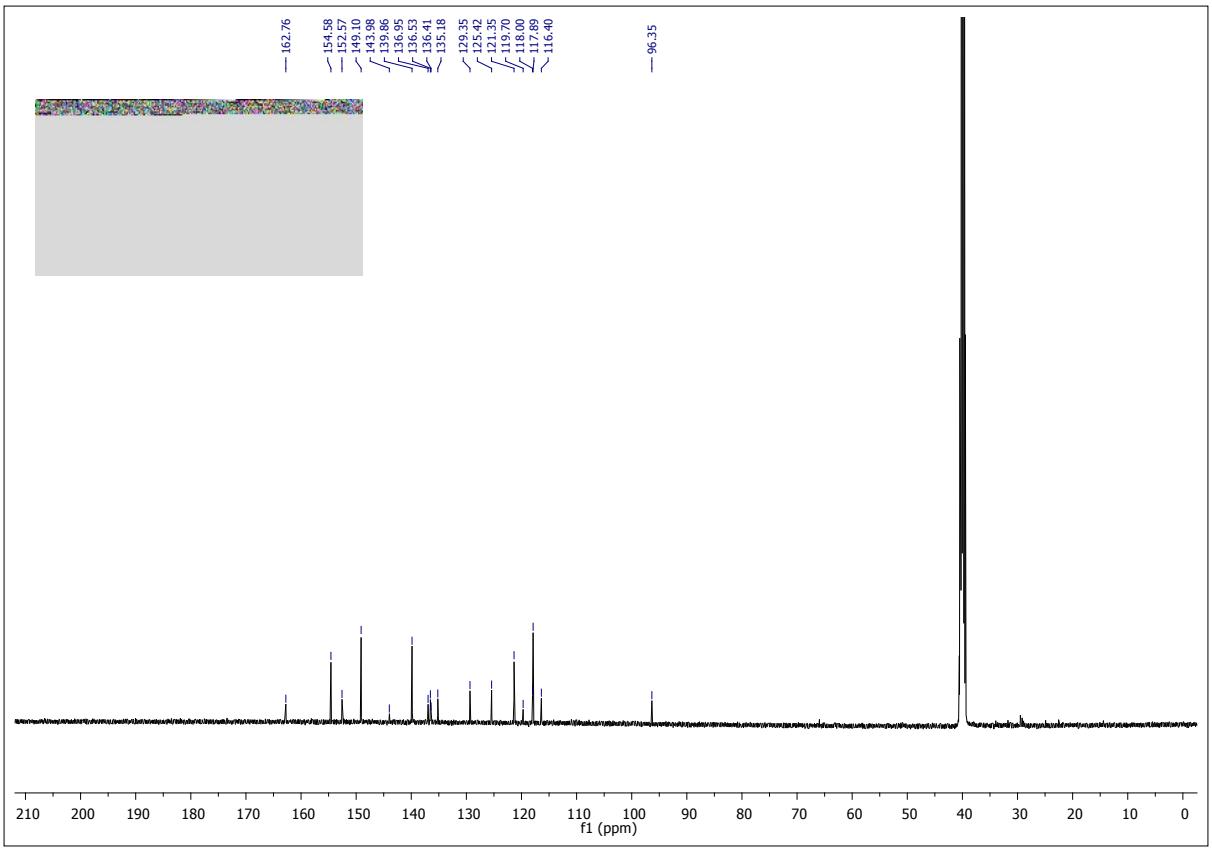

Figure S20: ^{13}C NMR spectrum of sensitizer DP2

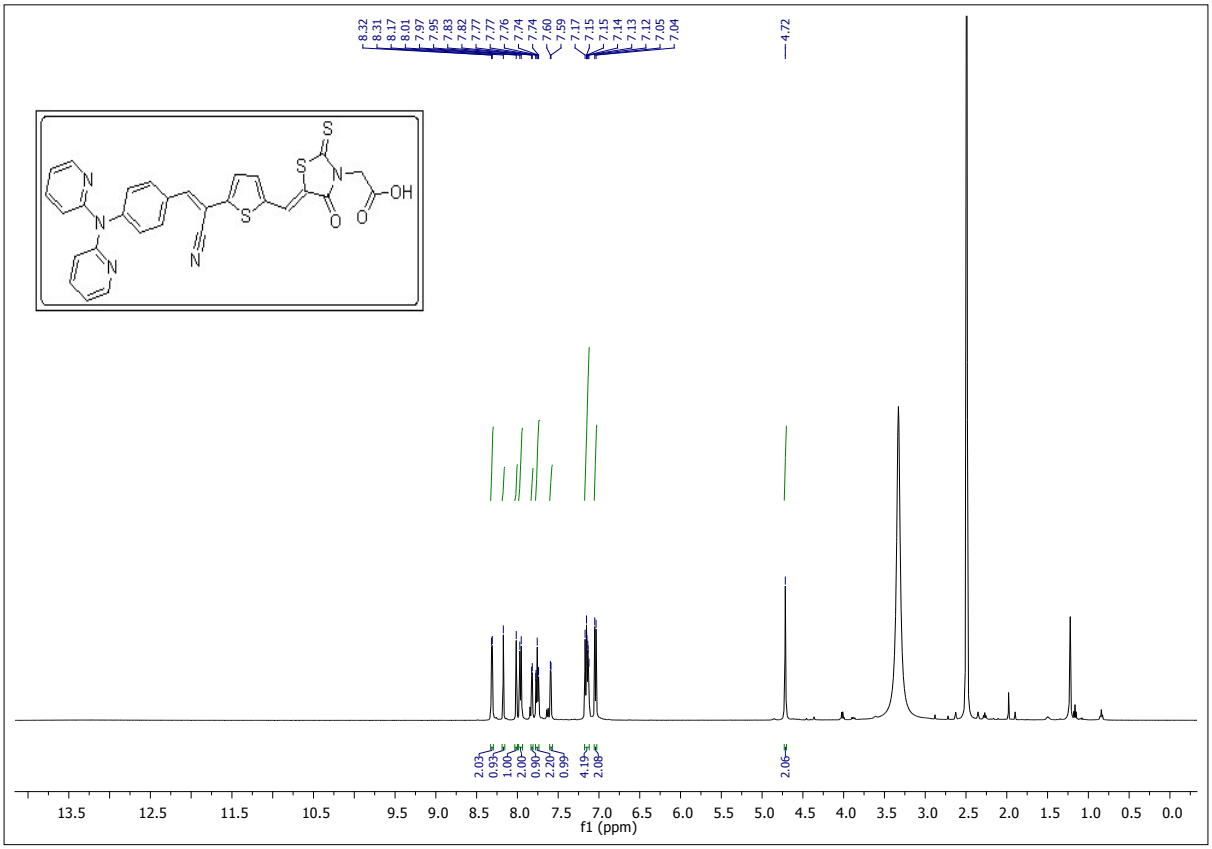

Figure S21: ^{1}H NMR spectrum of sensitizer DP3

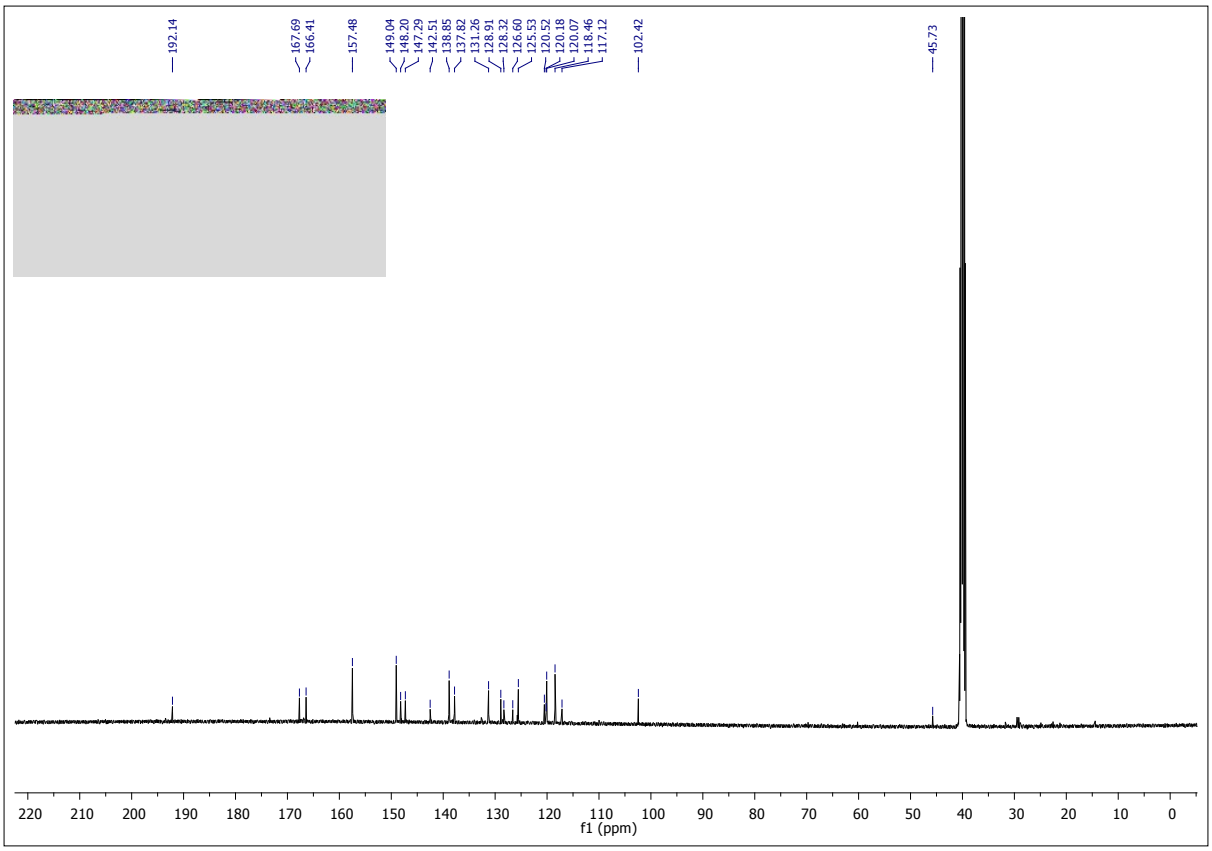

Figure S22: ^{13}C NMR spectrum of sensitizer DP3

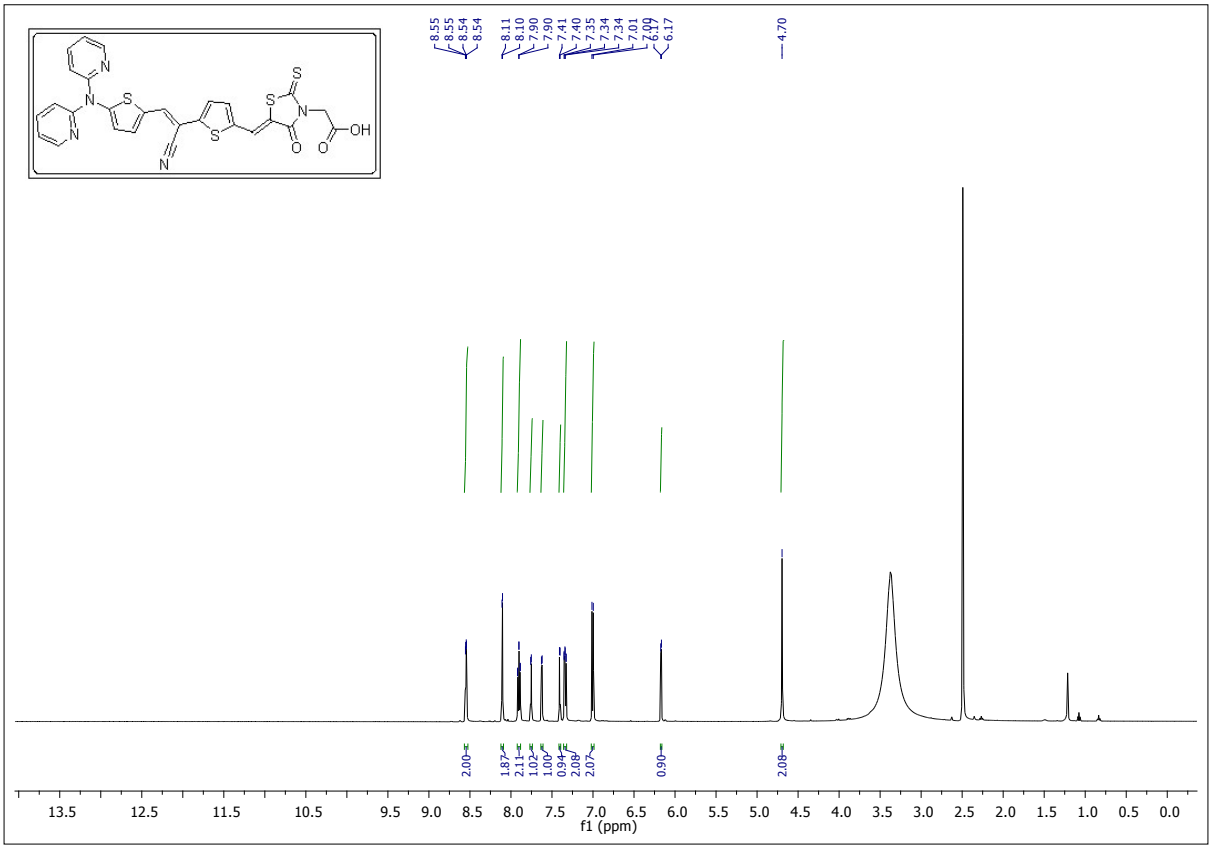

Figure S23: ^{1}H NMR spectrum of sensitizer DP4

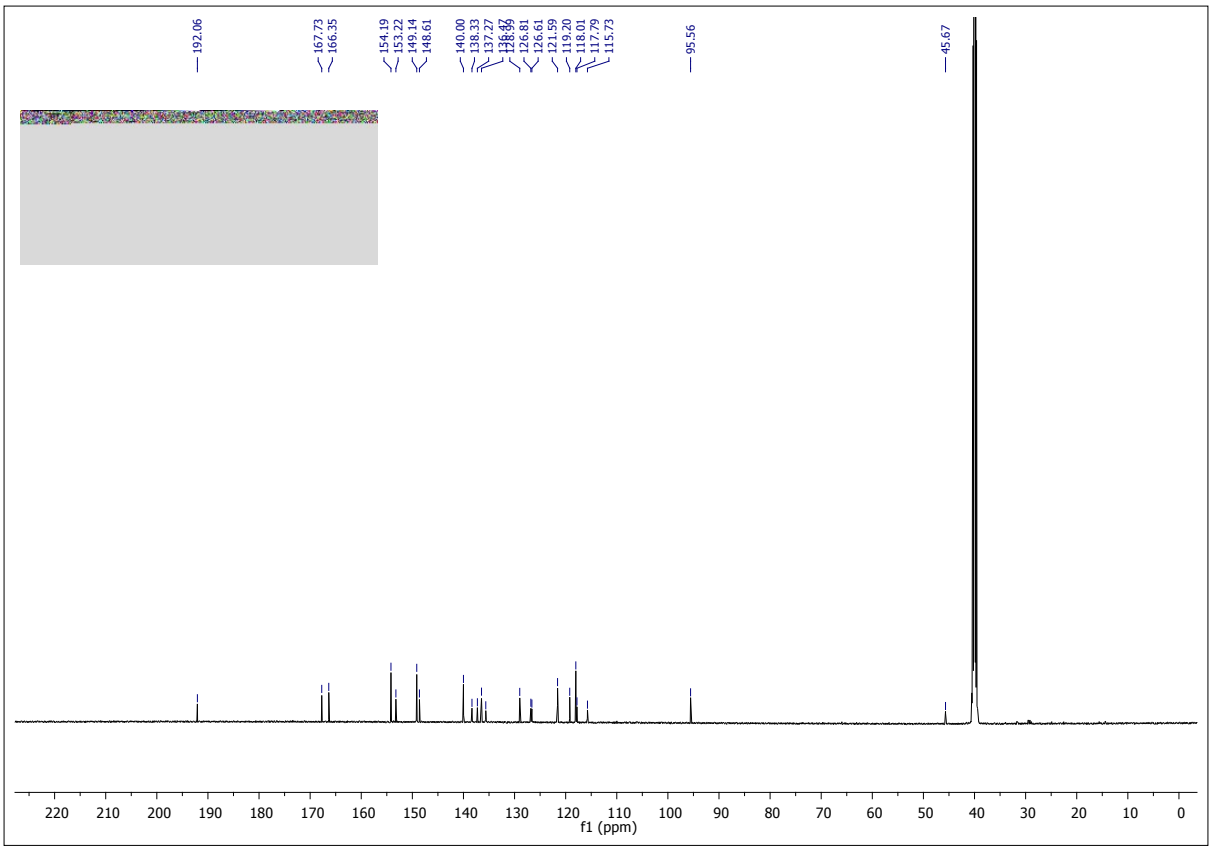

Figure S24: ^{13}C NMR spectrum of sensitizer DP4

Table S1. Electrochemical characterization of DP sensitizers by DFT calculations.

Sensitizer	HOMO (eV)	LUMO (eV)	LUMO+1 (eV)	HL-gap	HL+1-gap
DP1	-5.498	-3.0626	-1.958	2.435	3.539
DP2	-5.297	-2.9211	-1.866	2.372	3.426
DP3	-5.425	-3.058	-2.096	2.367	3.328
DP4	-5.211	-2.945	-2.053	2.266	3.158

Table S2 Electronic transition data obtained by TD-B3LYP/6-311++G(d,p) level for each molecule in the DMF solution.

Sensitizers	States	λ_{max} (nm)	f	LHE	Excited energy (eV)	Transition character
DP1	S_1	573	1.323	0.9525	2.16	H → L (99.56%)
	S_2	412	0.503	0.6859	3.01	H-1 → L (84.53%), H → L+1 (15.13%)
	S_3	383	0.073	0.1547	3.24	H-1 → L (14.66%), H → L+1 (80.46%).
DP2	S_1	594	1.644	0.9773	2.08	H → L (99.34%)
	S_2	452	0.441	0.6377	2.74	H-1 → L (91.32%), H → L (8.06%)
	S_3	431	0.001	0.0023	2.87	H-2 → L (89.48%), H-2 → L+1 (7.54%), H-2 → L+2 (2.79%).
DP3	S_1	575	1.658	0.9780	2.15	H → L (99.97%)
	S_2	406	0.156	0.3017	3.05	H-1 → L (26.79%), H → L+1 (71.62%)
	S_3	366	0.016	0.0362	3.38	H-1 → L (71.49%), H → L+1 (24.72%).
DP4	S_1	610	1.808	0.9844	2.03	H → L (99.79%)
	S_2	441	0.312	0.5124	2.81	H-1 → L (28.27%), H → L+1 (70.47%)
	S_3	422	0.001	0.0023	2.93	H-2 → L (87.51%), H-2 → L+1 (9.31%).