

Supporting information for :

Ruthenium Complex Dye with Designed Ligand Capable of Chelating Triiodide Anion for Dye-Sensitized Solar Cells

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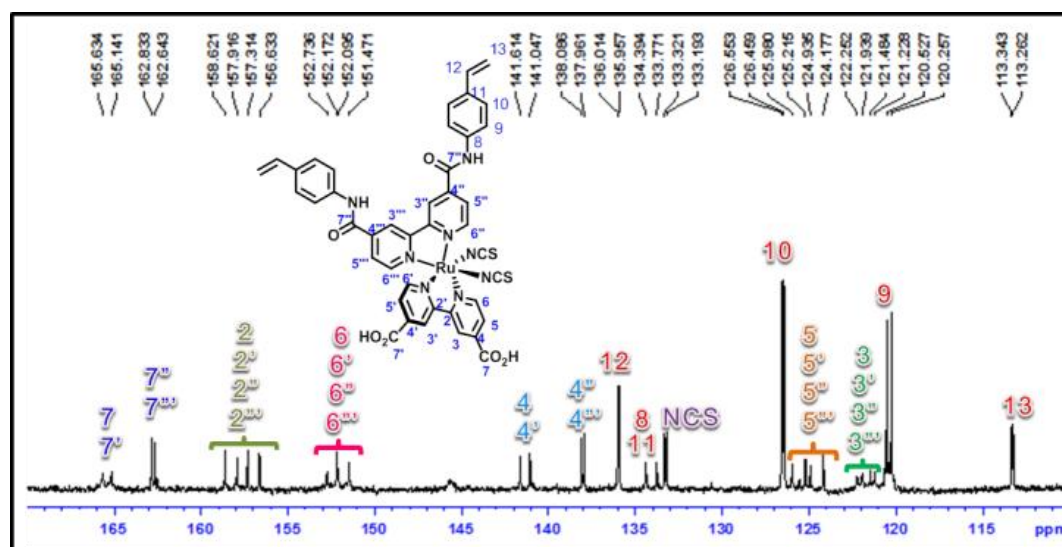


Fig. S1 ¹³C NMR spectrum of RuAS.

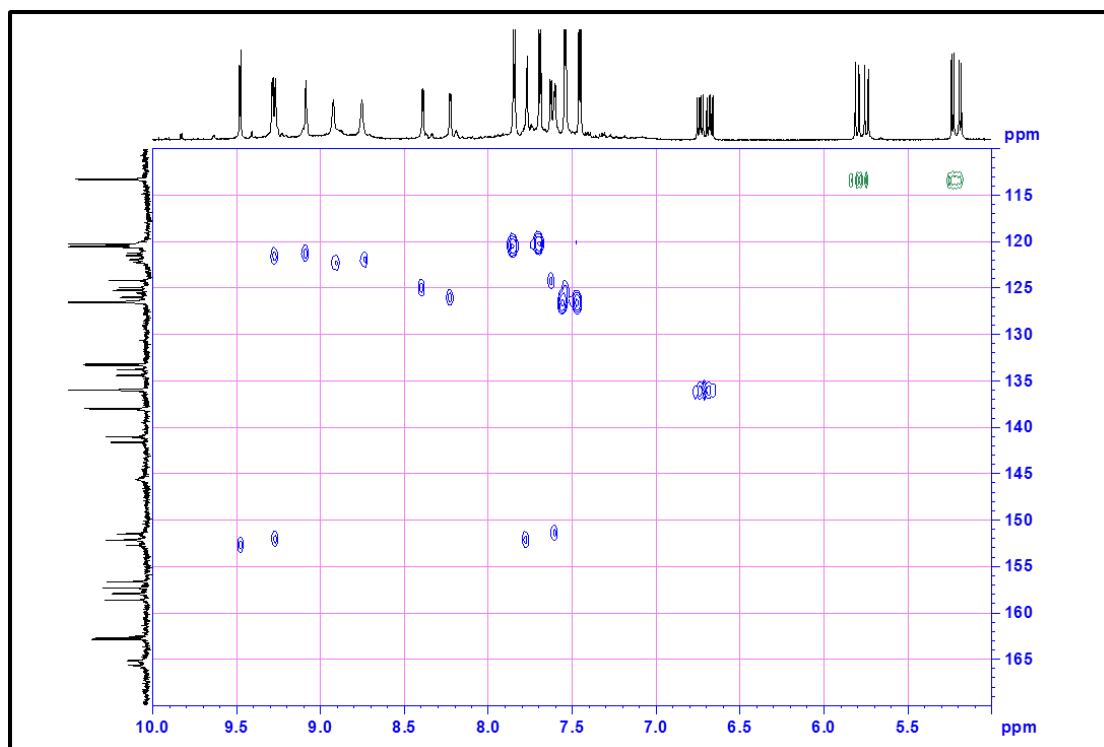


Fig. S2 HSQC spectrum of **RuAS**.

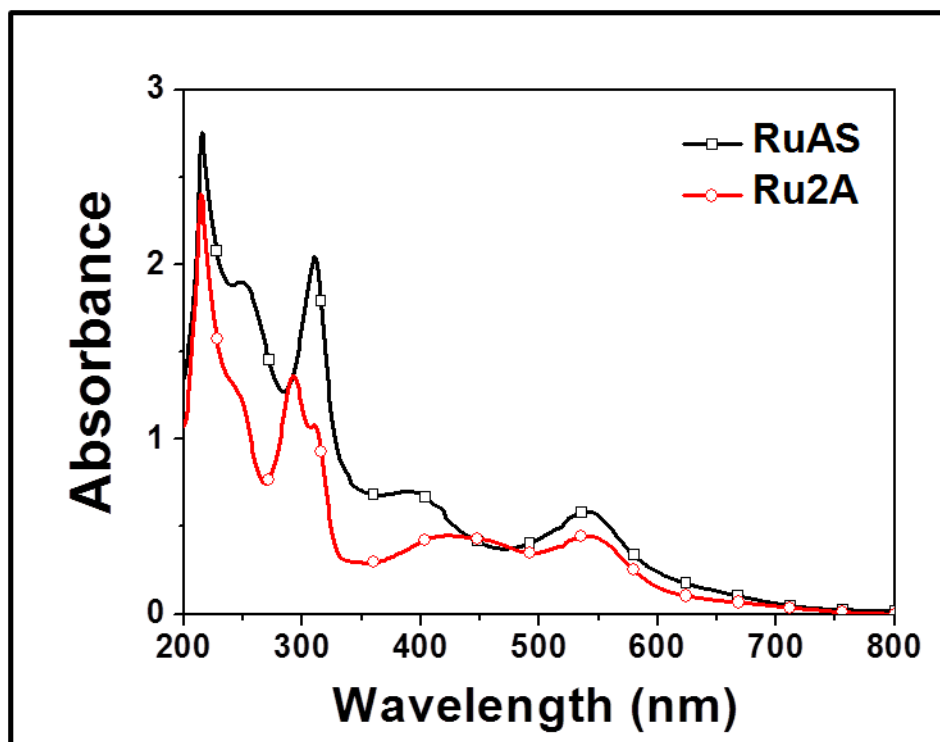


Fig. S3 UV-vis absorption spectra of **RuAS** and **Ru2A** in ACN/*t*-butanol (1:1 by volume) at a concentration of 50 μ M.

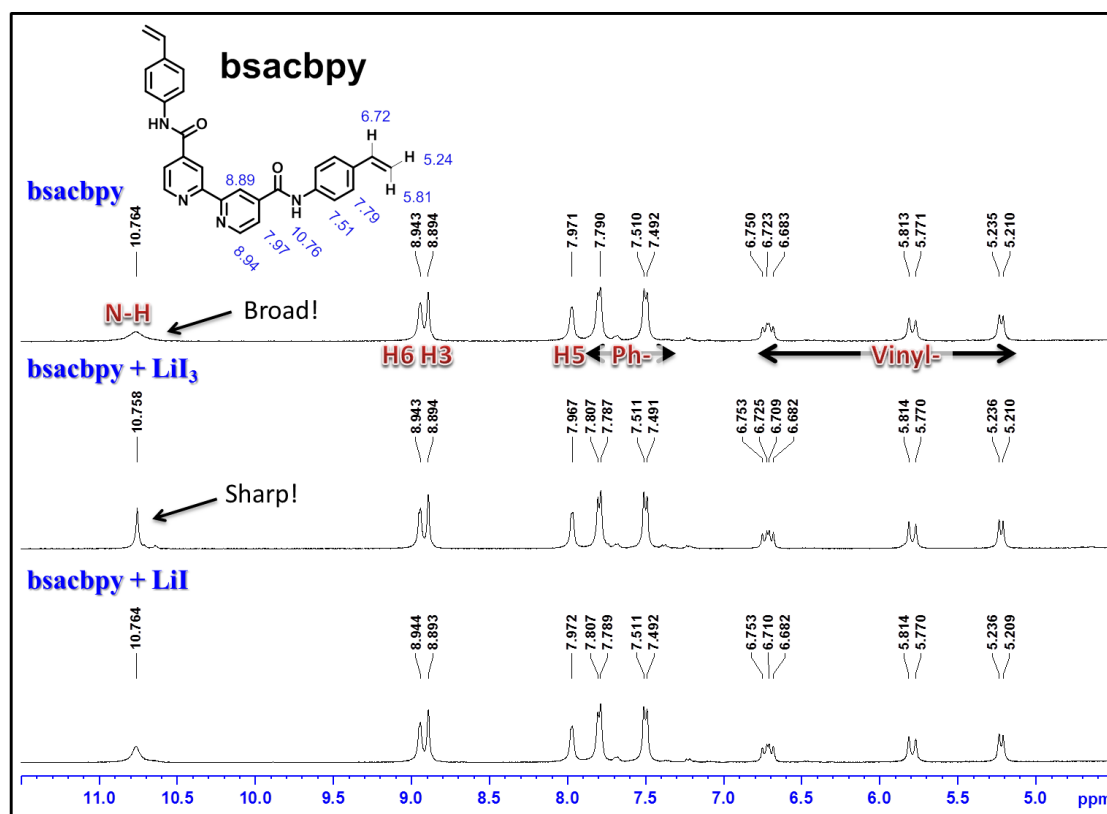


Fig. S4 ¹H NMR spectra of bsacbpy and its mixtures with equivalent concentration (0.01M) of LiI₃ and LiI, respectively. Note: The proton peak at 10.7 ppm contributed by the amide groups of bsacbpy became sharper after chelating I₃⁻, similar to the dimer of RuAS shown in Fig. 2.

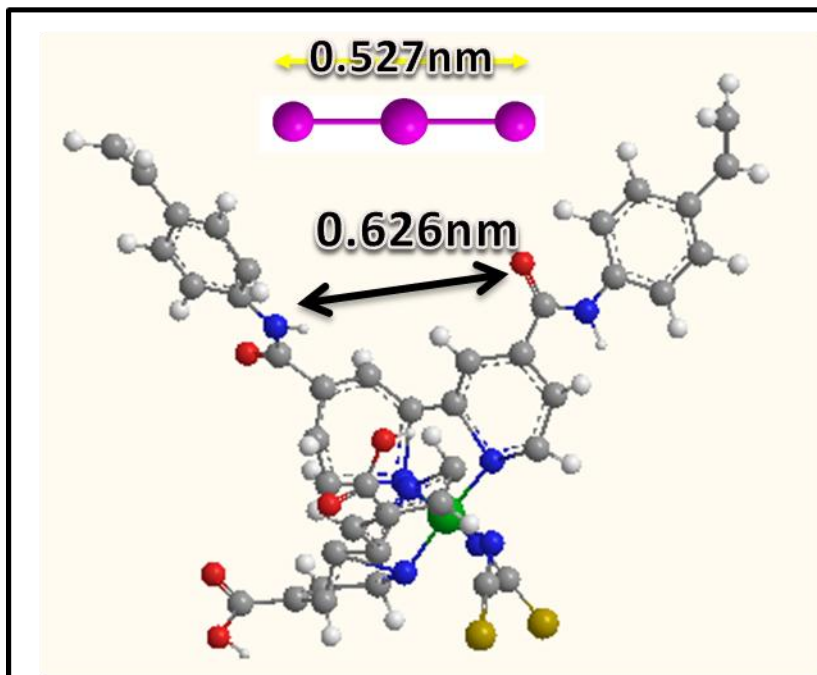


Fig. S5 Three dimensional configurations of **RuAS** and I_3^- molecules drawn by ChemBio3D. (The blue, green, grey, purple, red and white color is nitrogen, ruthenium, carbon, iodide, oxygen and hydrogen.)

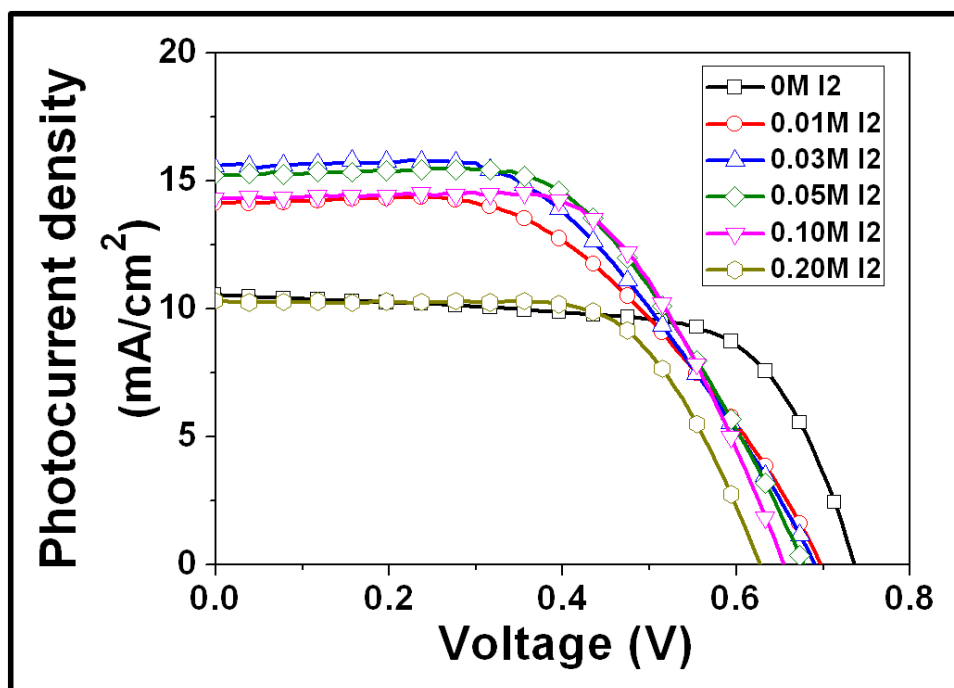
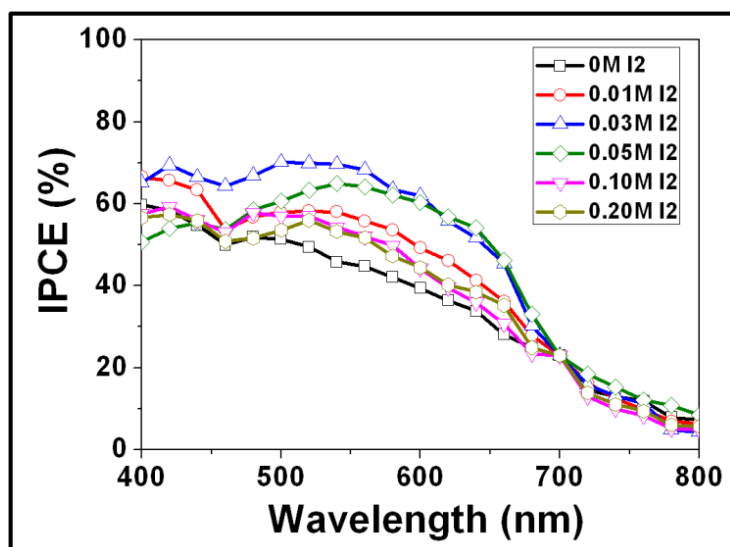


Fig. S6 Photocurrent-voltage plots of DSSC based on **Ru2A** with various I₂ concentrations of liquid electrolyte under AM 1.5 full sunlight.

(a)



(b)

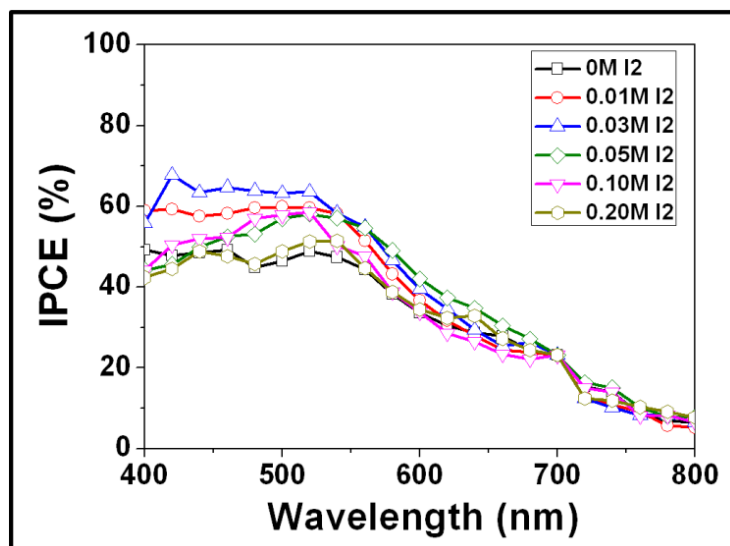


Fig. S7 IPCE spectra of the DSSCs with (a) RuAS and (b) Ru2A containing various I₂ concentrations in the liquid electrolyte.

Table S1 Photovoltaic properties of DSSC with Ru2A containing various I₂ concentrations in the liquid electrolyte under 100 mWcm⁻² illumination.

[I₂] (M)	PCE (%)	Jsc (mAcm⁻²)	Voc (V)	ff
0	5.19	10.54	0.738	0.67
0.01	4.92	13.62	0.703	0.51
0.03	5.53	15.59	0.692	0.51
0.05	5.90	15.20	0.680	0.57
0.10	5.90	14.30	0.659	0.63
0.20	4.37	10.30	0.639	0.66