

Supporting information

Development of Aldehyde Functionalized Iridium(III) Complexes Photosensitizers with Strong Visible-Light Absorption for Photocatalytic Hydrogen Generation from Water

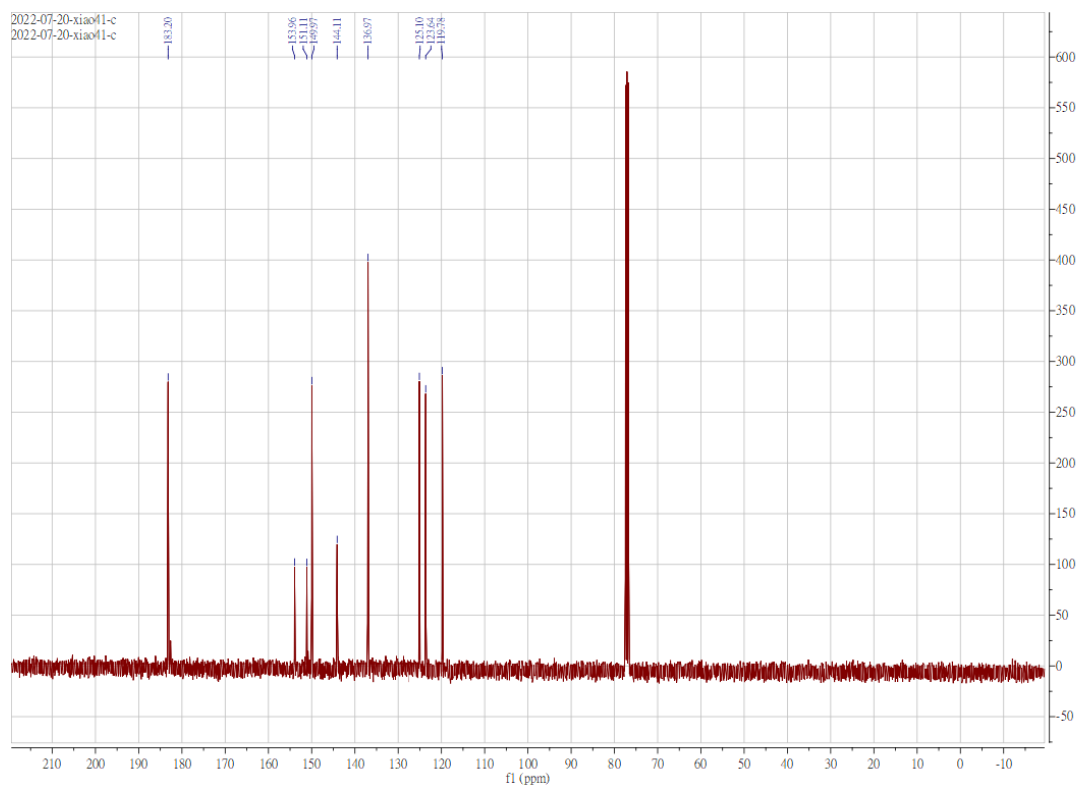
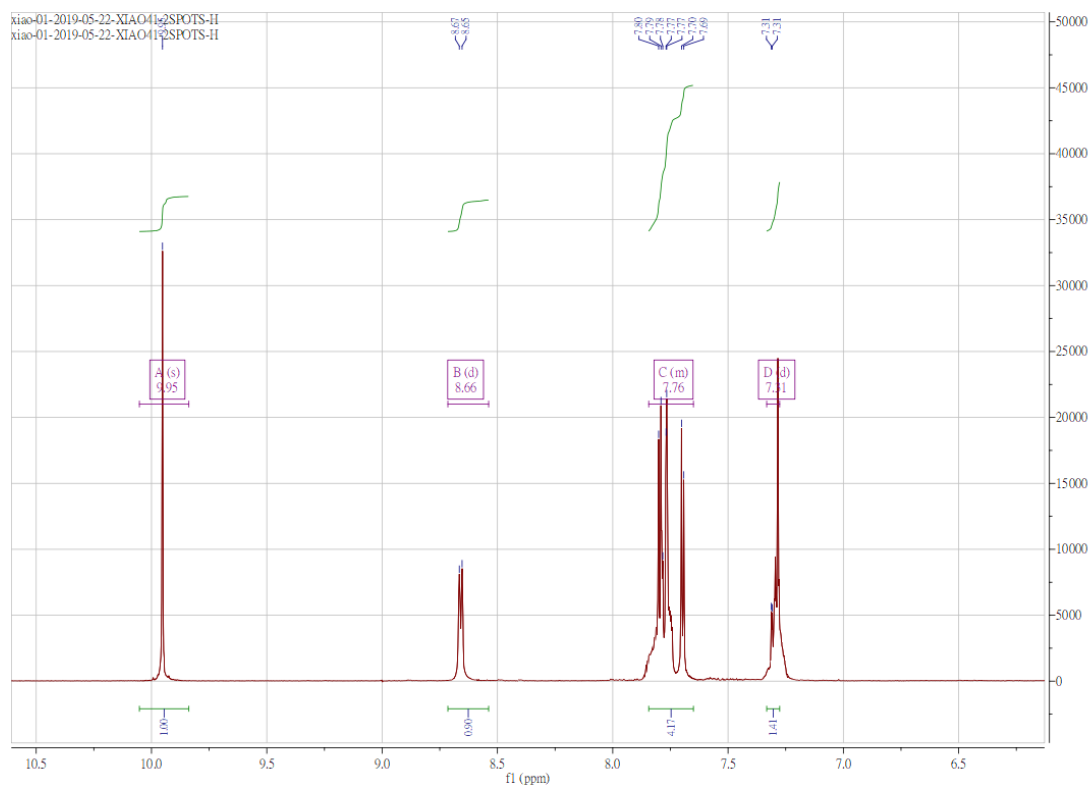
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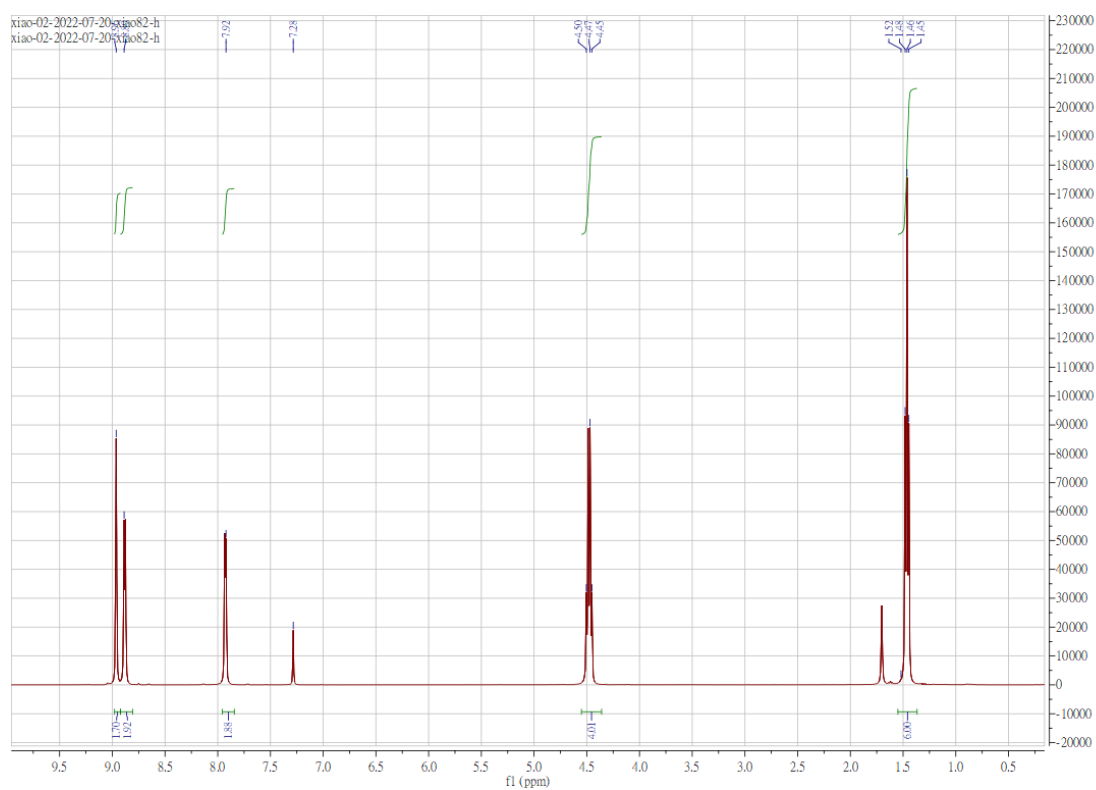


Figure S5. ¹H NMR spectrum of diethyl [2,2'-bipyridine]-4,4'-dicarboxylate in CDCl₃

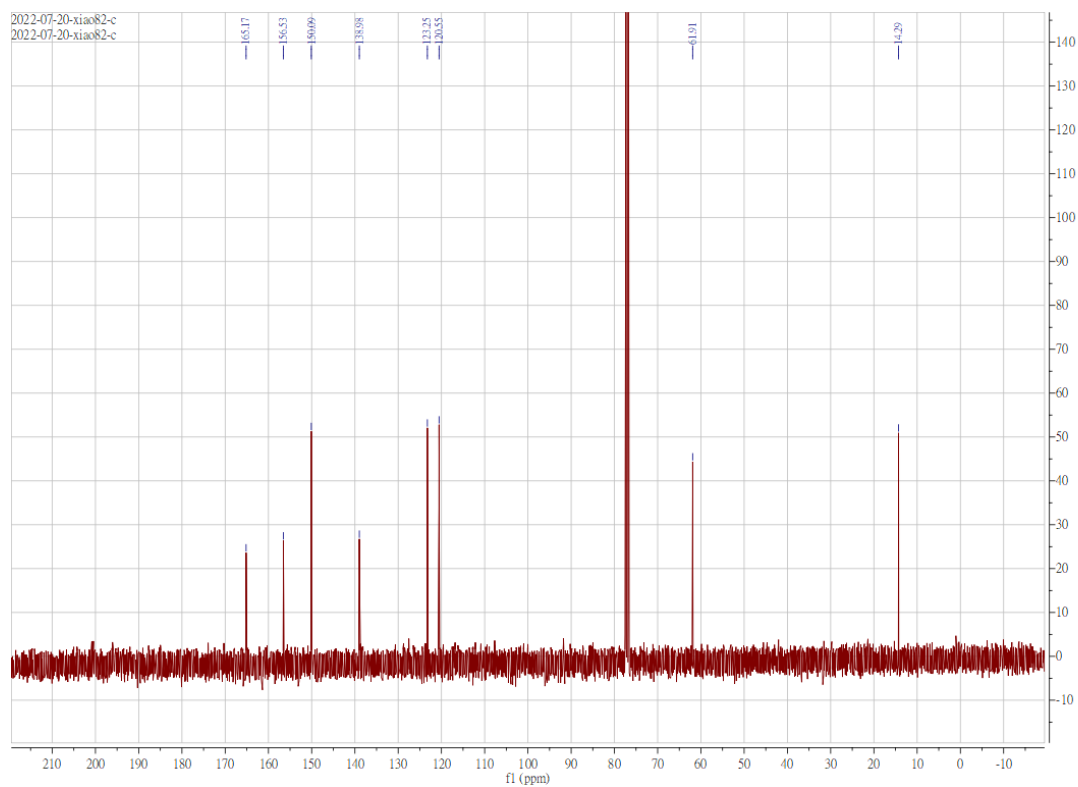


Figure S6. ¹³C NMR spectrum of diethyl [2,2'-bipyridine]-4,4'-dicarboxylate in CDCl₃

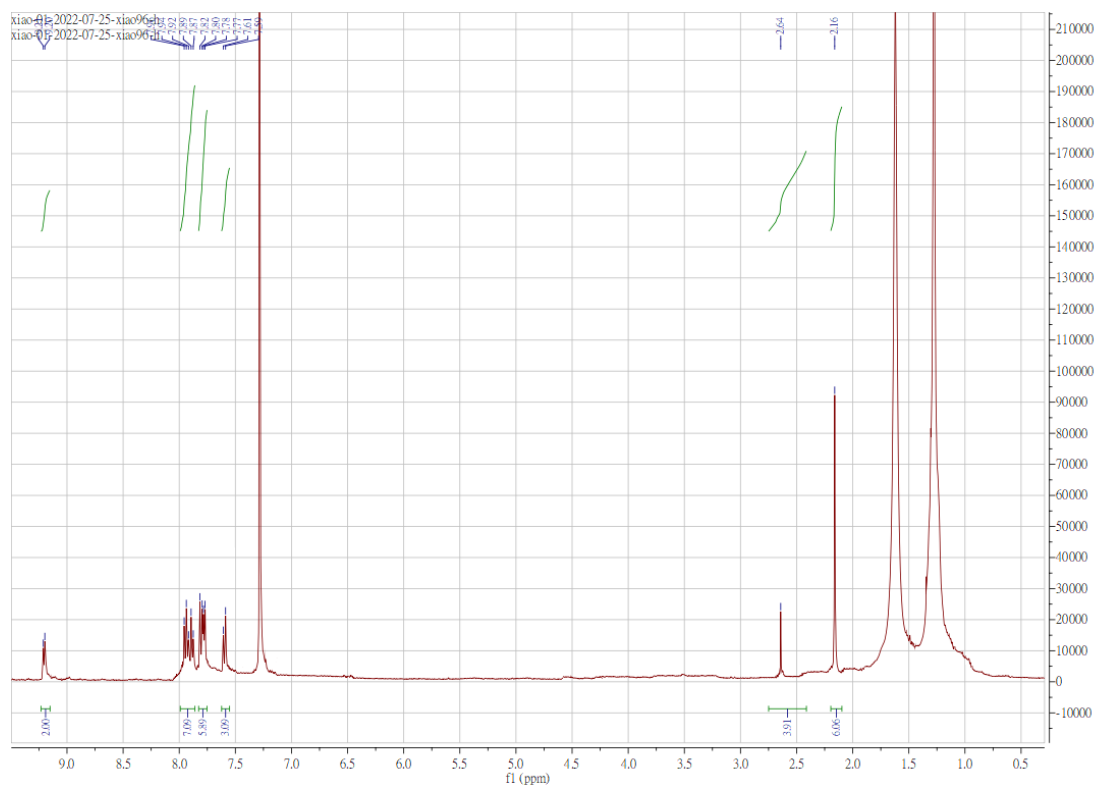


Figure S7. ^1H NMR spectrum of Ir1 in CDCl_3

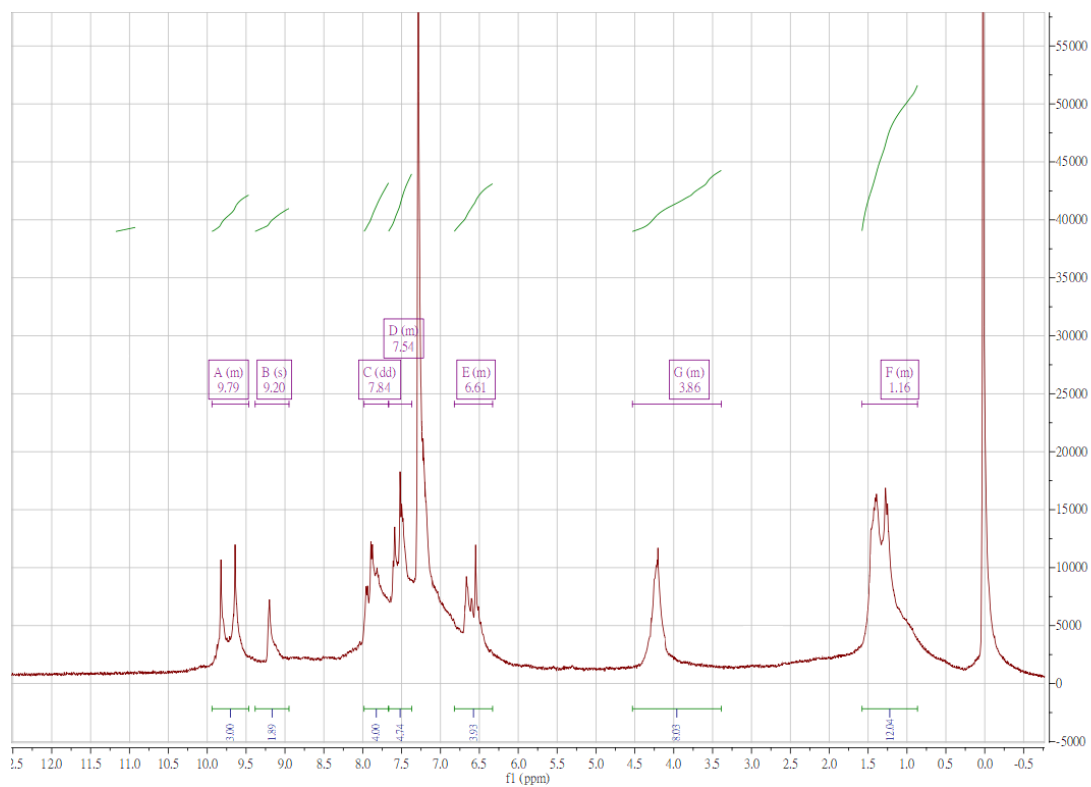


Figure S8. ^1H NMR spectrum of Ir2 in CDCl_3

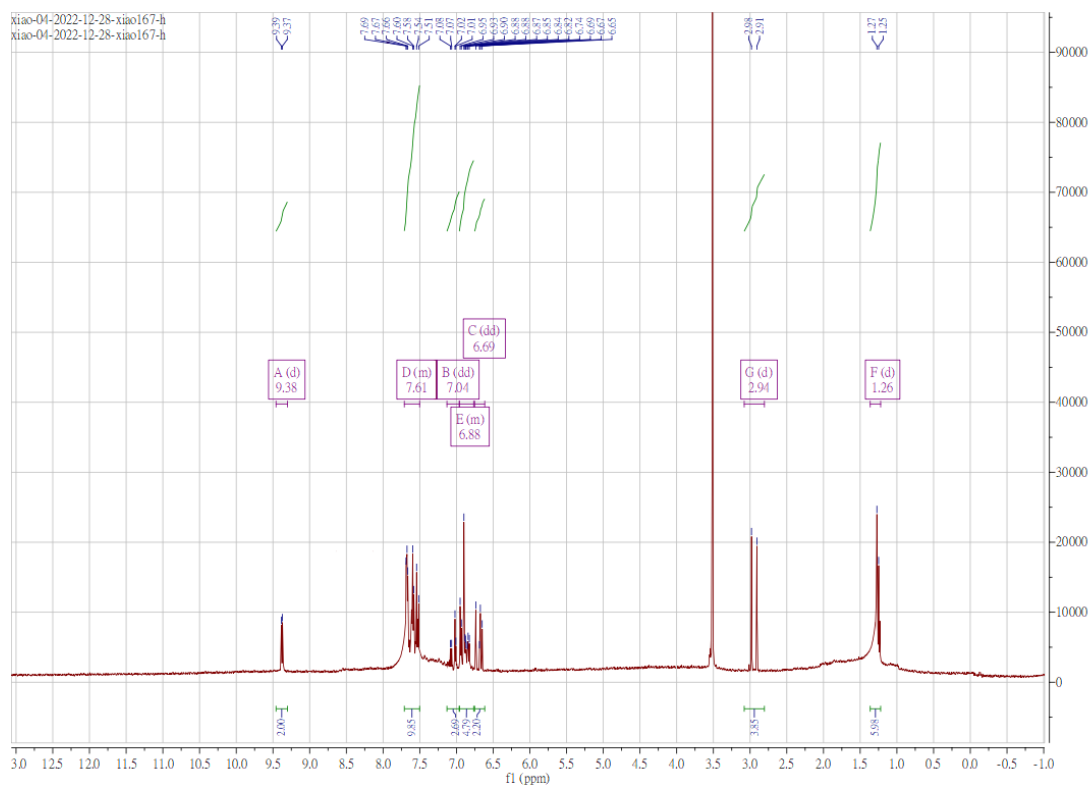


Figure S9. ^1H NMR spectrum of Ir3 in CDCl_3

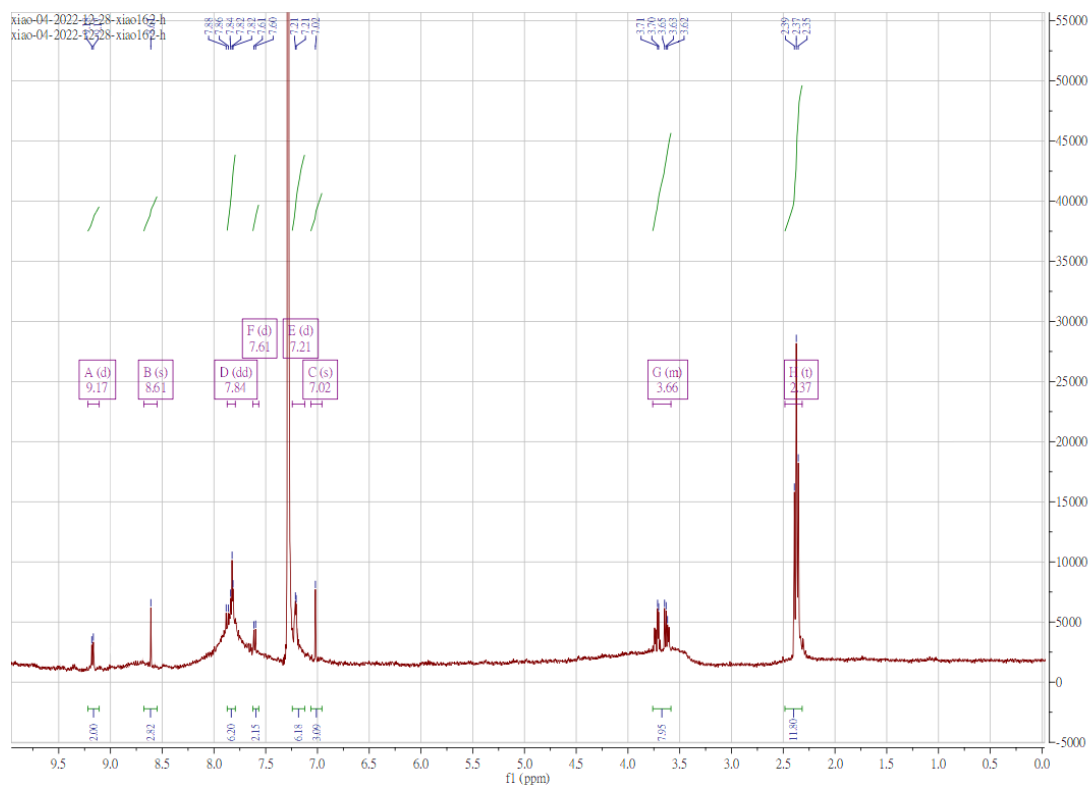


Figure S10. ^1H NMR spectrum of Ir4 in CDCl_3



Figure S11. MS result of L1



Figure S12. MS result of L2

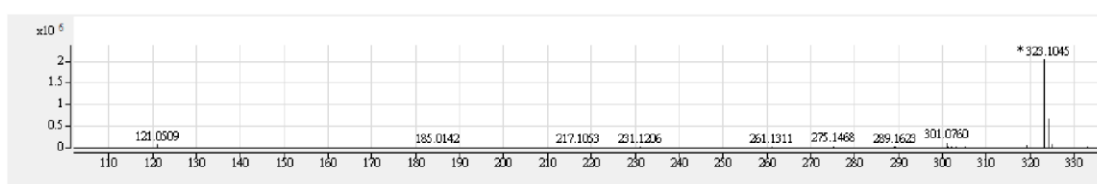


Figure S13. MS result of diethyl [2,2'-bipyridine]-4,4'-dicarboxylate



Figure S13. MS result of Ir1

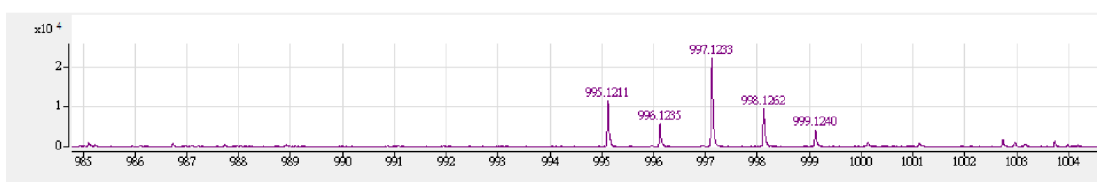


Figure S14. MS result of Ir2

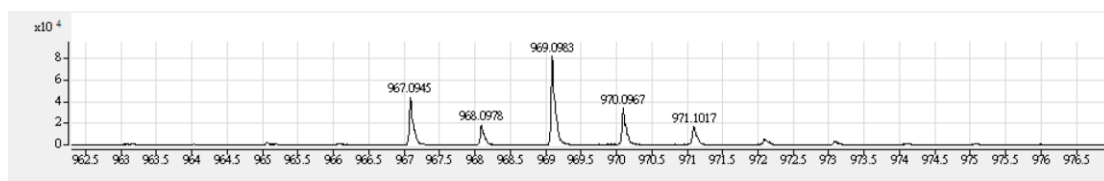


Figure S15. MS result of Ir₃



Figure S16. MS result of Ir₄

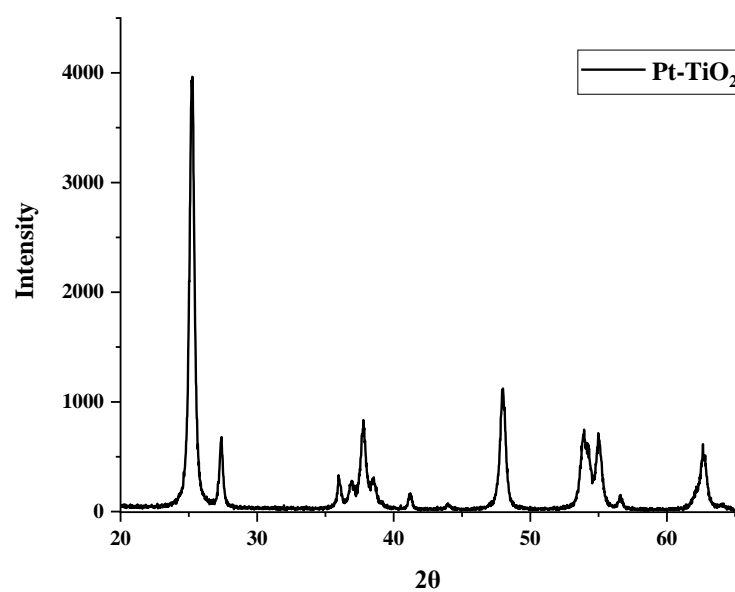


Figure S17. XRD patterns of Pt-TiO₂

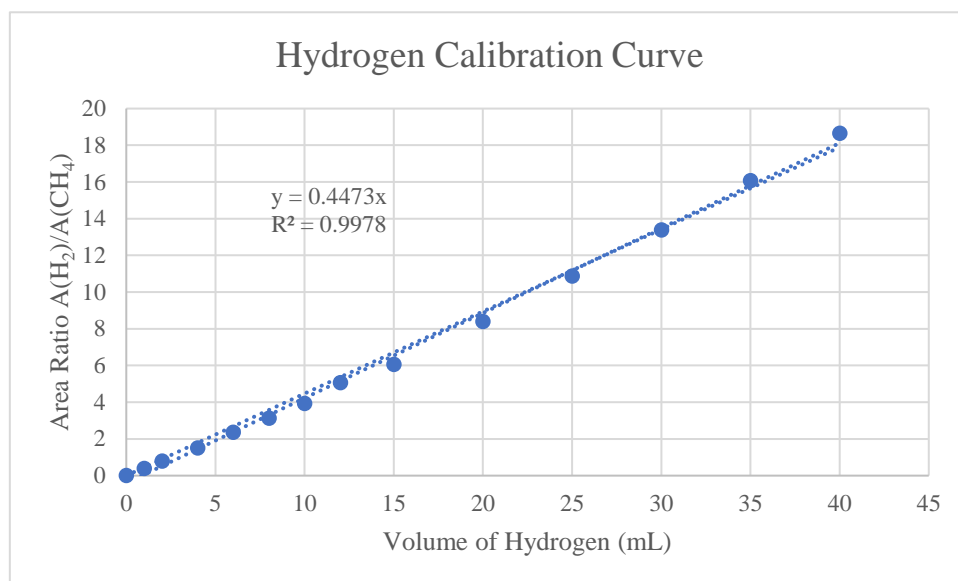


Figure S18. Calibration plot of the signal ratio (H_2/CH_4) vs. amount of H_2 obtained from GC analysis.

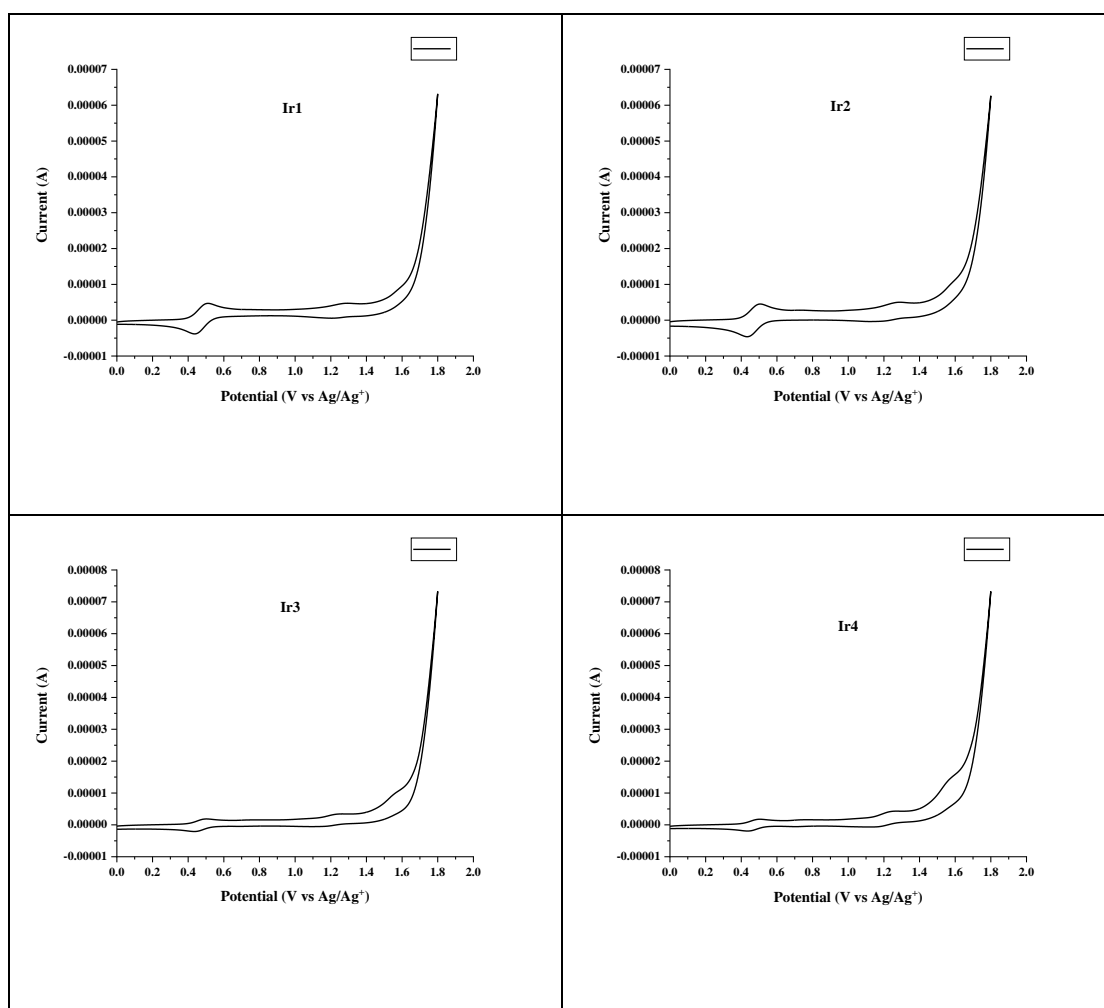


Figure S19. Cyclic voltammograms of Ir1–Ir4.

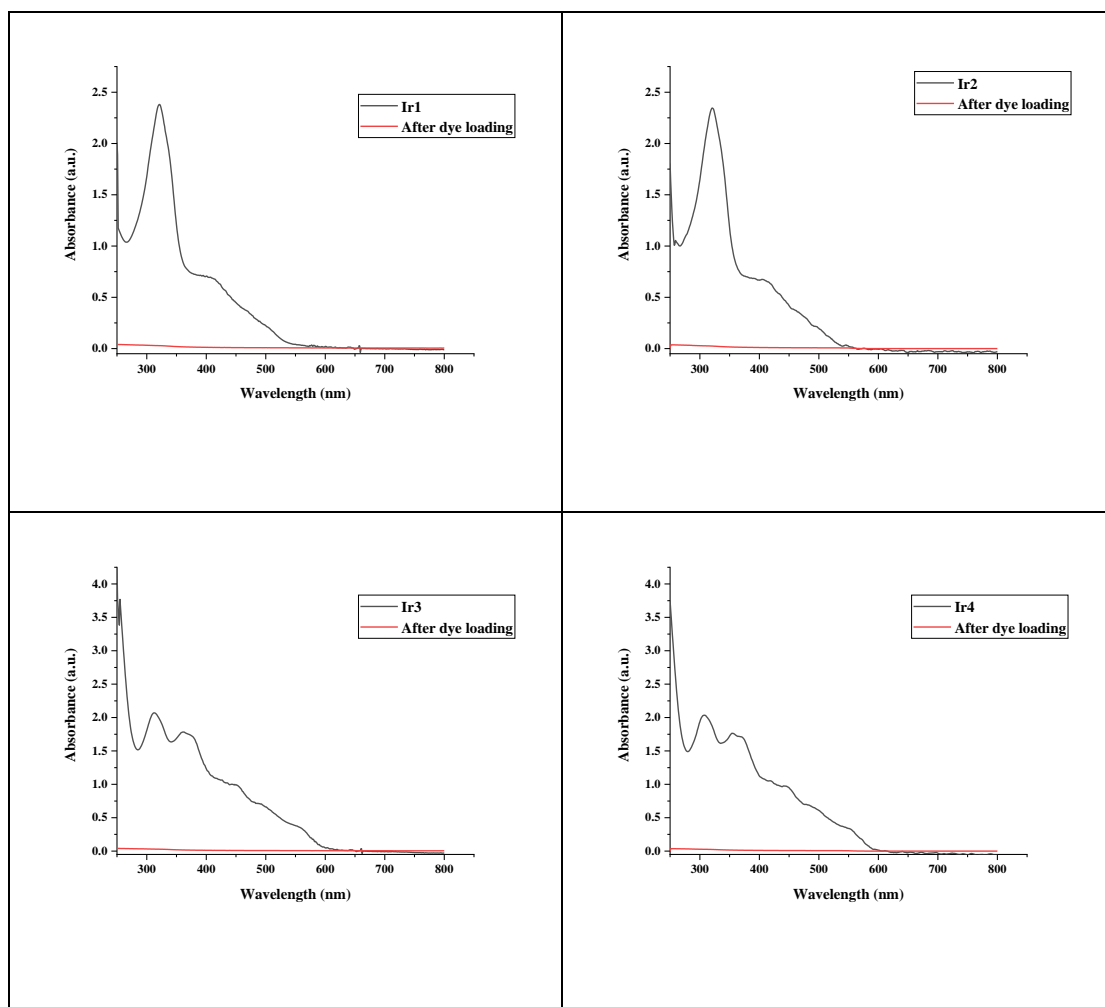


Figure S20. UV/Vis absorption spectra of **Ir1** to **Ir4** before and after dye loading in CH_2Cl_2 solution at 293 K

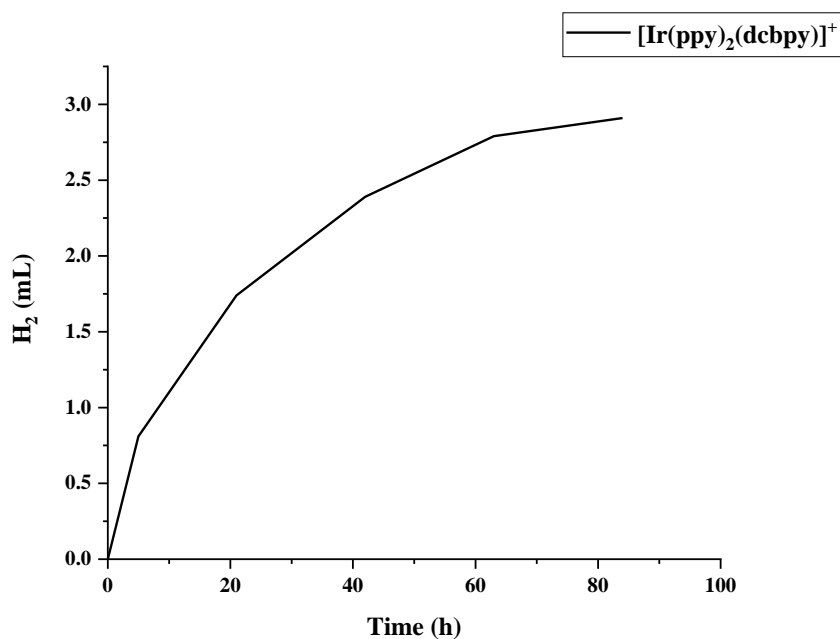


Figure S21. Photocatalytic H₂ generation curves of **[Ir(ppy)₂(dcbpy)]⁺** under blue LED irradiation (50 mW).

Table S1. Photocatalytic H₂ generation data with **[Ir(ppy)₂(dcbpy)]⁺** under blue light irradiation.

Dye	Time /h	H ₂ /mL	TON ^[a]	TOF ^[b] /h ⁻¹	TOF _i ^[c] /h ⁻¹	Activity _i ^[d] /μmol g ⁻¹ h ⁻¹	AQY _i % ^[e]
[Ir(ppy)₂(dcbpy)]⁺	84	2.91	1900	22.6	105.8	66122	0.42

[a] Turnover number (TON) of H₂ was calculated as twice of the number of moles of H₂ produced over the number of moles of PS attached to platinized TiO₂. [b] Turnover frequency (TOF) was calculated per hour. [c] Initial turnover frequency (TOF_i) in the first 5 h. [d] Initial photocatalytic activity (Activity_i) is defined as the number of micromoles of H₂ evolved per gram of platinum loaded per hour. [e] Initial apparent quantum yield percentage (AQY_i).

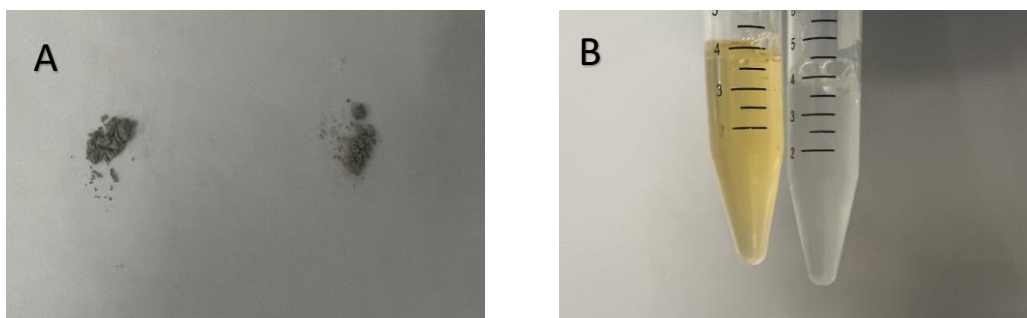


Figure S22. (A) TiO₂ composite material with **Ir4** before (left) and after (right) irradiation. (B) AA aqueous solution before (right) and after (left) irradiation.