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A highly efficient red electrophosphorescent iridium(III) complex containing phenyl quinazoline ligand in polymer light-emitting diodes

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PL quantum efficiency Φ:

The PL quantum efficiency of $(PQxD)_2Ir(pic)$ was measured in CH_2Cl_2 solution using Tris(2,2'-bipyridyl)ruthenium(II) ion ($Ru(bipy)_3^{2+}$) in aqueous solution as the reference (Φ_s = 0.042±0.002)[1]in the same apparatus. The PL quantum efficiency was calculated with the following equation[2-3]:

$$\Phi_x=\Phi_s \times (S_s/A_s)^{-1} \times (S_x/A_x) \times (n_s/n_x)^2$$

Where: Φ is PL quantum efficiency, the s subscript refers to the sample and x to the standard, A is absorbance at the excitation wavelength, S is the integrated emission area across the band and n is the refractive index of the solvent containing the sample.

The fluorescence emission spectra of the standard and sample were determined on the same apparatus under the same excitation intensity. Absorbance of sample and standard must be similar and small (e.g. below 0.05). The concentration of the standard solution and sample solution are almost limited, so n_s and n_x can be replaced by solvent. The refractive index of water and CH_2Cl_2 were known as 1.333 and 1.424 at room temperature, respectively. The PL quantum efficiency of $(PQxD)_2Ir(pic)$ in CH_2Cl_2 solution was determined to be 0.116.

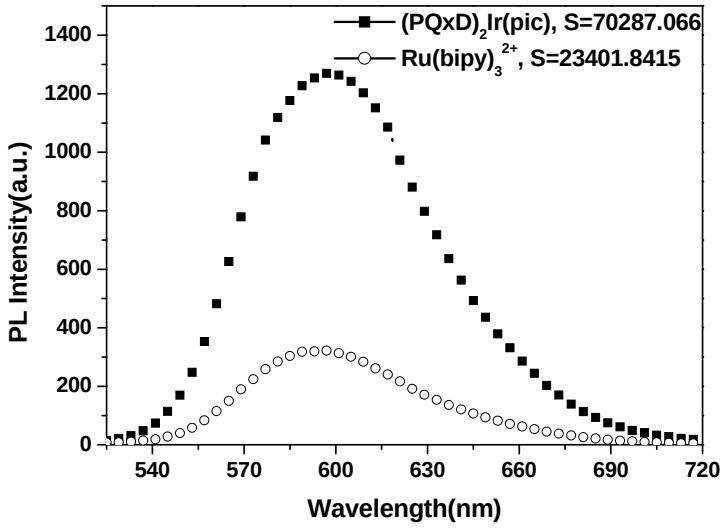

Figure S1. PL spectra of $(PQxD)_2Ir(pic)$ in CH_2Cl_2 solution and $Ru(bipy)_3^{2+}$ in aqueous solution at room temperature (λ_{em}=420nm).

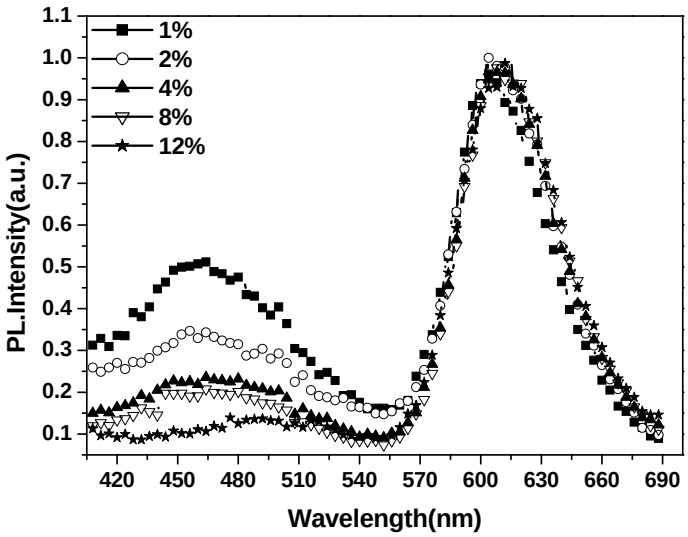

Figure S2. PL spectra of $(PQxD)_2Ir(pic)$/PVK-PBD films with different doping concentrations.

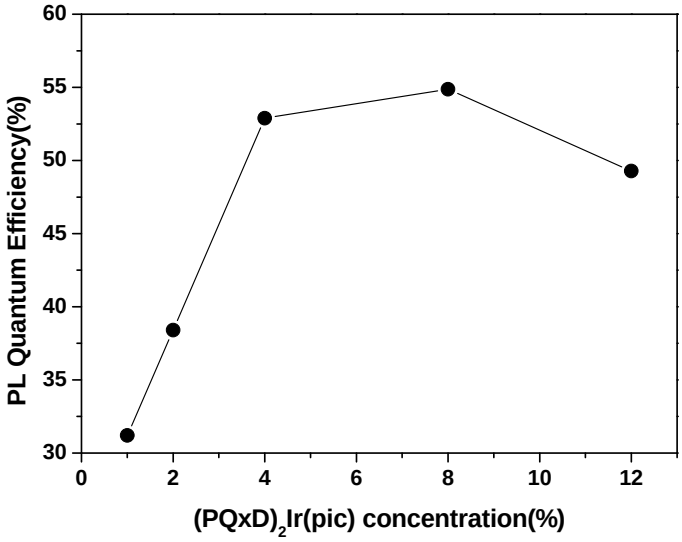

Figure S3. PL quantum efficiency of $(PQxD)_2Ir(pic)$/PVK-PBD films with different doping concentrations.

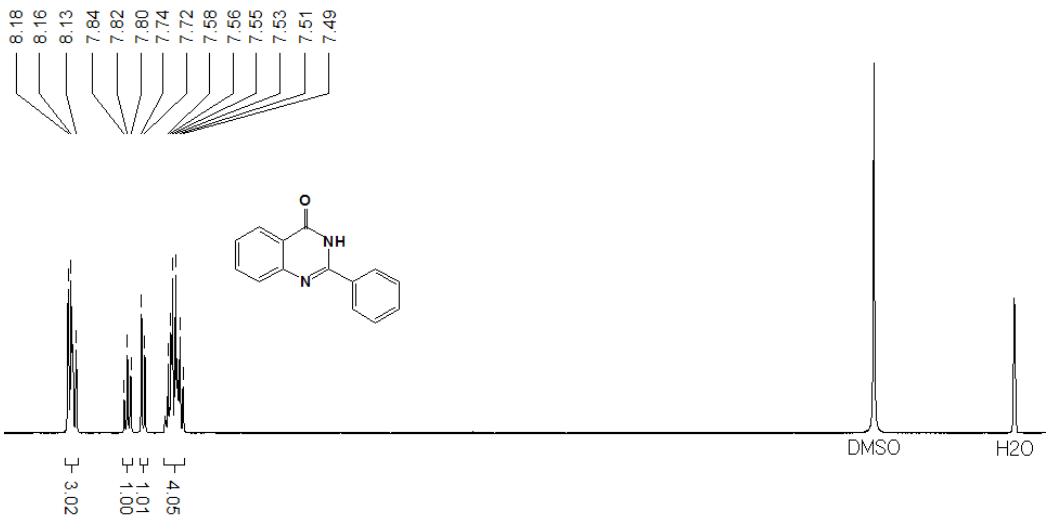

Figure S4. ^{1}H NMR of **2-phenylquinazolin-4(3H)-one (1)** in DMSO-d_6

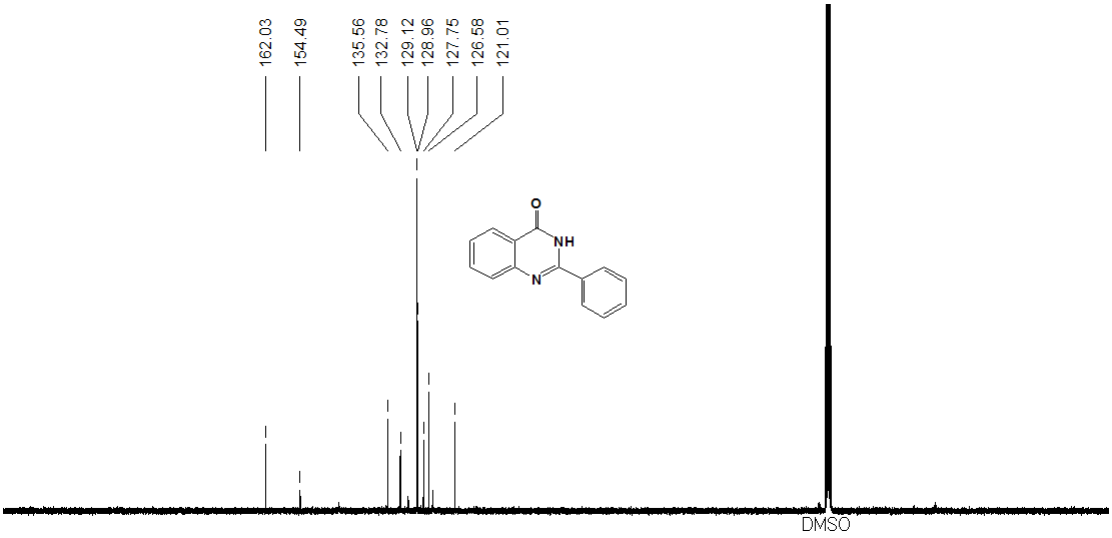

Figure S5. ^{13}C NMR of **2-phenylquinazolin-4(3H)-one (1)** in DMSO-d_6

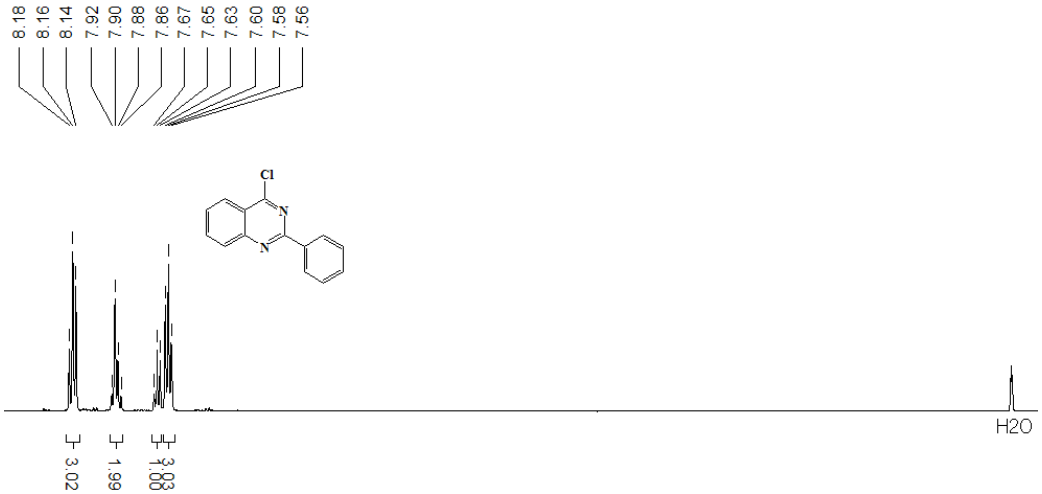

Figure S6. ^{1}H NMR of **4-chloro-2-phenylquinazoline(2)** in $CDCl_3$

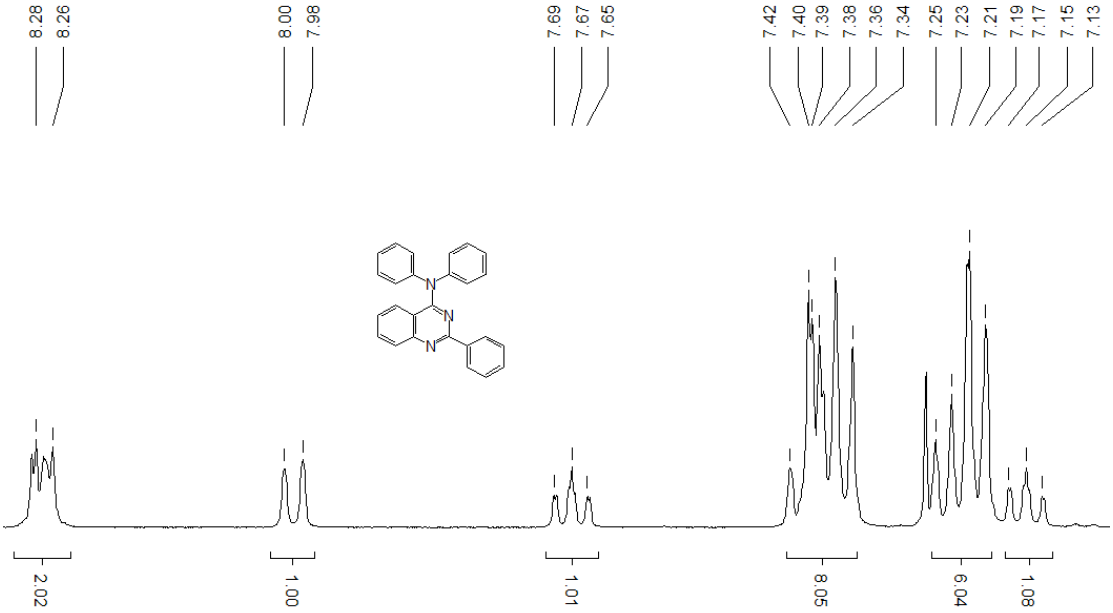

Figure S7. ^{1}H NMR of **N,N,2-triphenylquinazolin-4-amine (HPQxD)** in $CDCl_3$

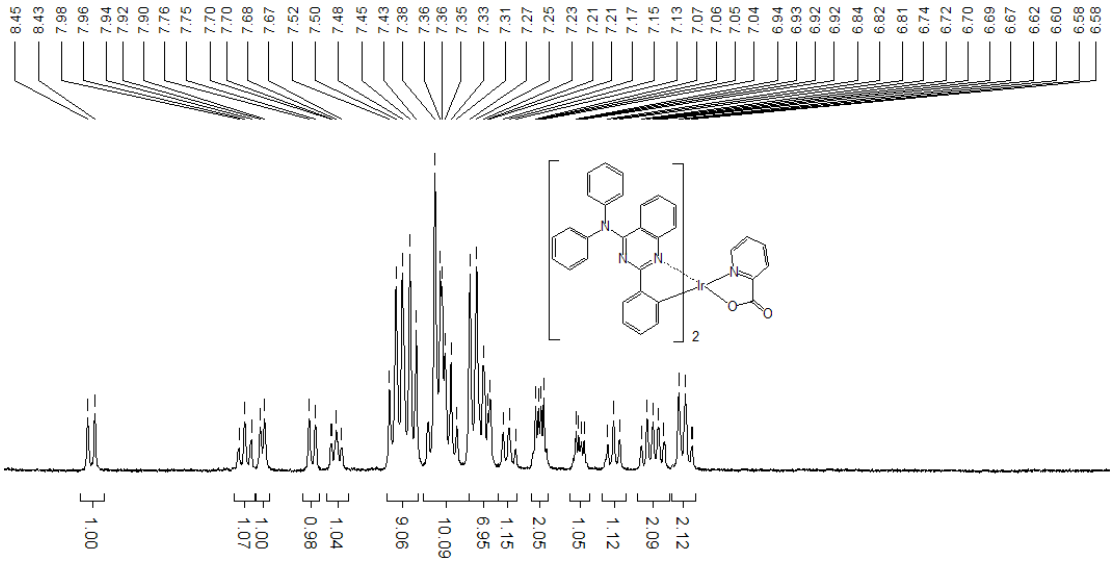

Figure S8. ^{1}H NMR of **$(PQxD)_2Ir(pic)$** in $CDCl_3$

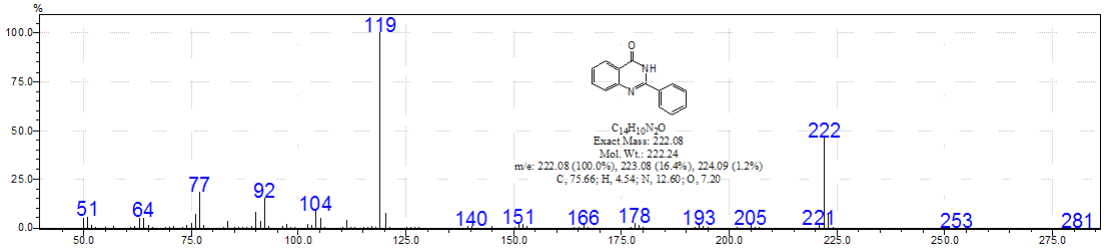

Figure S9. GC-MS of **2-phenylquinazolin-4(3H)-one (1)**

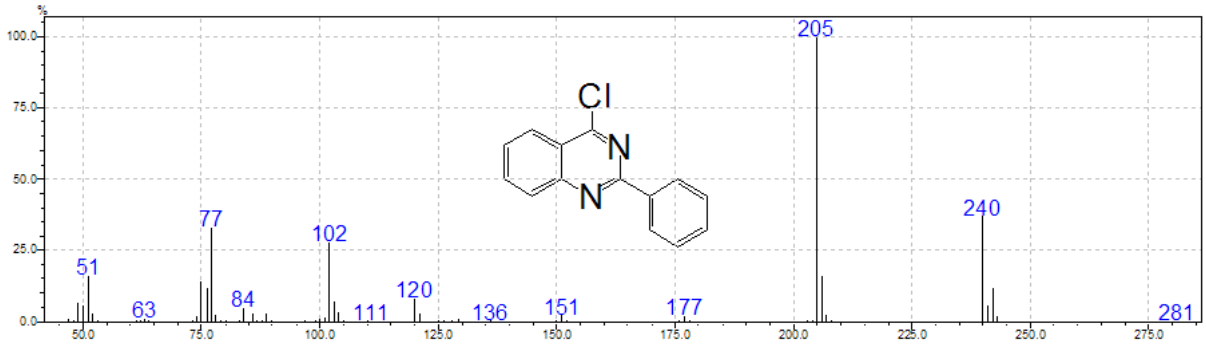

Figure S10. GC-MS of **4-chloro-2-phenylquinazoline(2)**

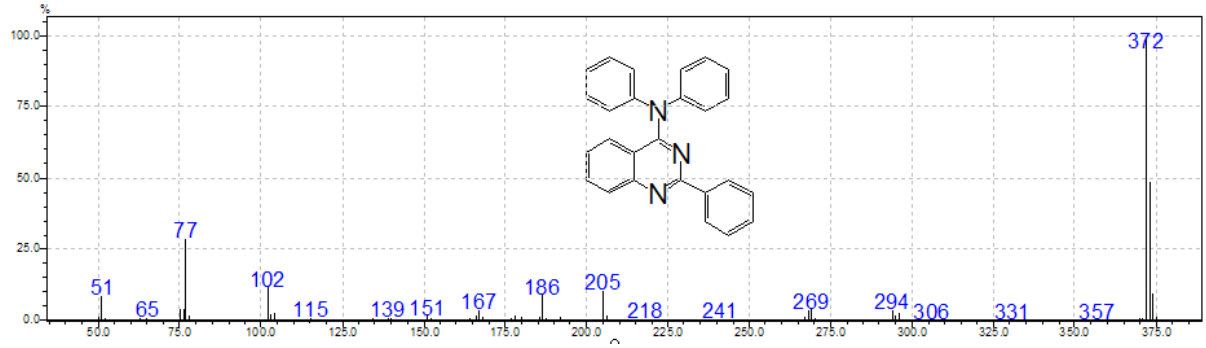

Figure S11. GC-MS of **N,N,2-triphenylquinazolin-4-amine (HPQxD)**

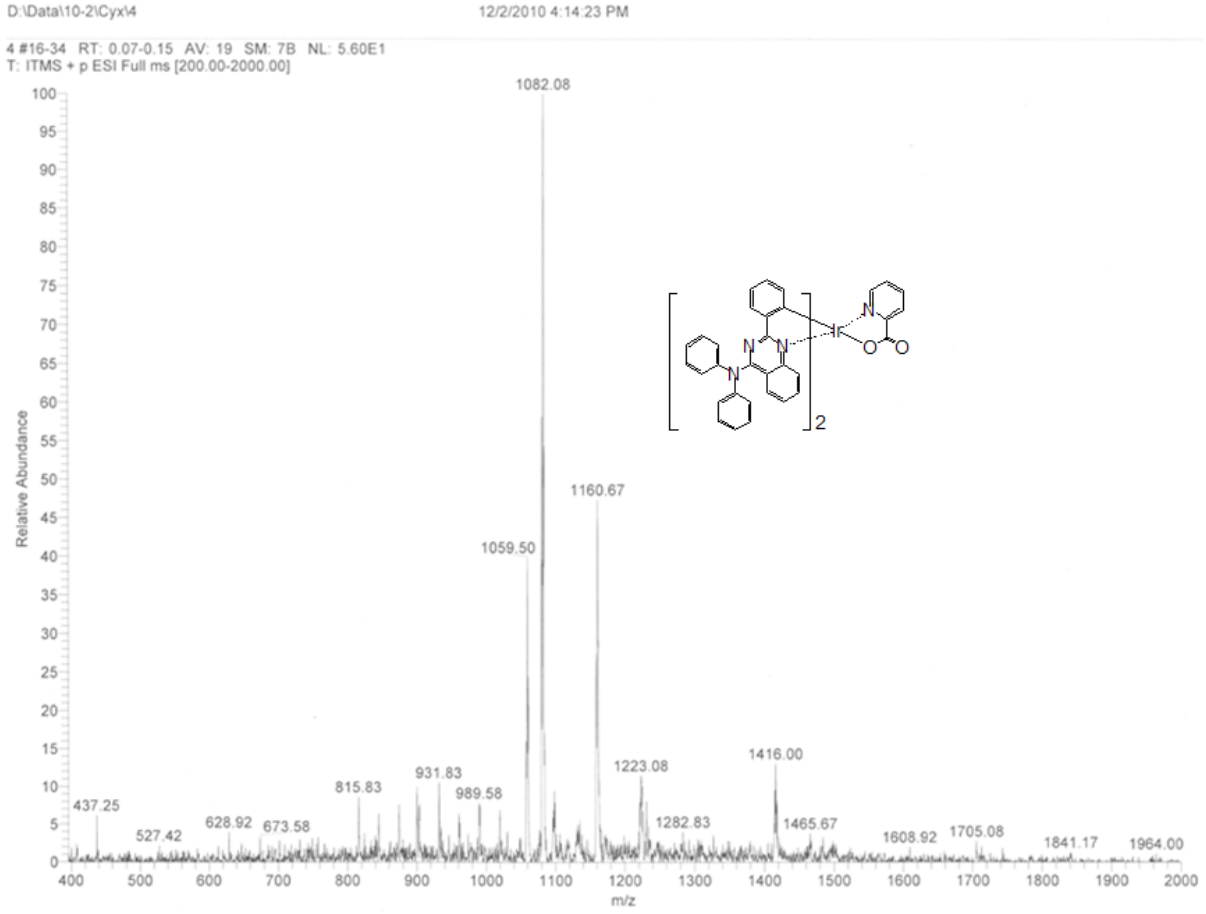

Figure S12. ESI-MS of **$(PQxD)_2Ir(pic)$**

References:

1. J. Van Houten and R. J. Watts, *Journal of the American Chemical Society*, 1976, **98**, 4853-4858.
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3. J. Huang, *Synthesis, Characterization and Electroluminescent Properties of Solution-Processable Small Red Light-emitting Molecular Materials*, Guang Zhou, South China University of Technology, **2011.06.09**, 34-35.