polymers

MDPI

Supporting Information

Bis-Tridendate Ir(III) Polymer-Metallocomplexes: Hybrid, Main-Chain Polymer Phosphors for Orange – Red Light Emission

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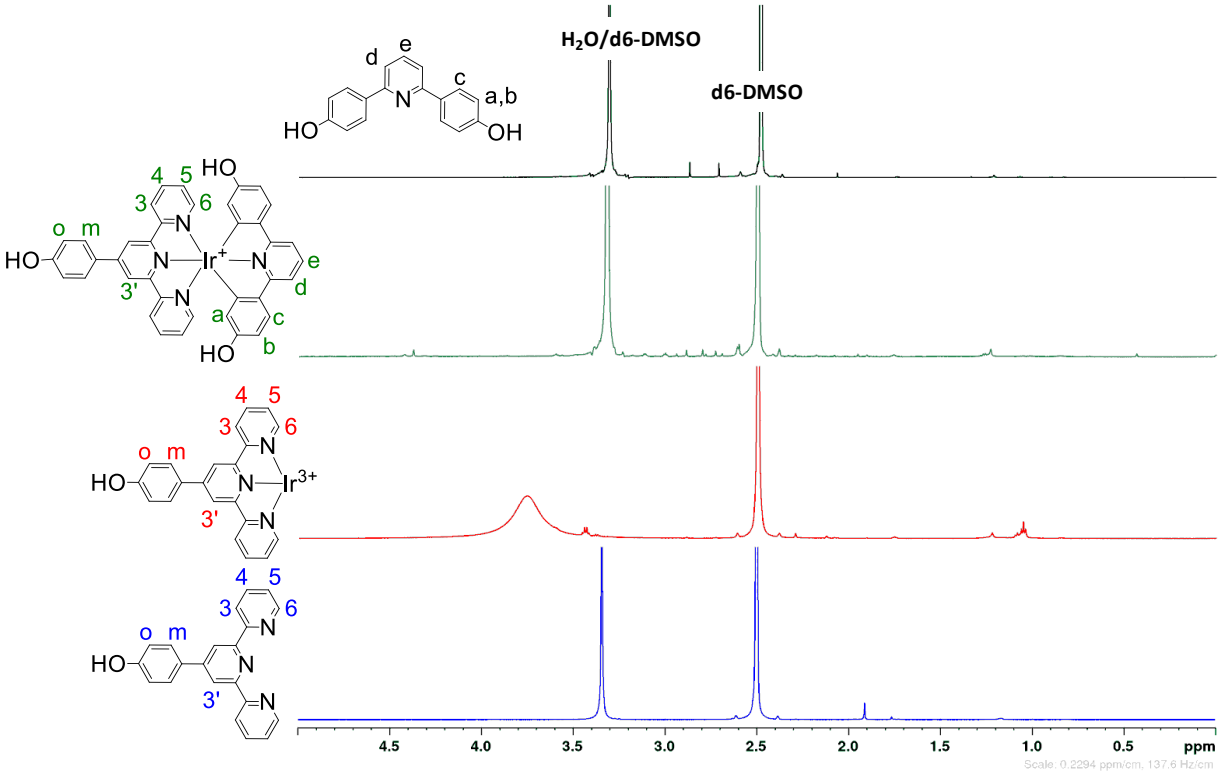

Figure S1. ^{1}H-NMR spectra area 5-0 ppm, of **HOtpy**, **HOtpy-IrCl$_3$**, **HOtpy-Ir-HOpy** and **HOpy** all in DMSO-d$_6$.

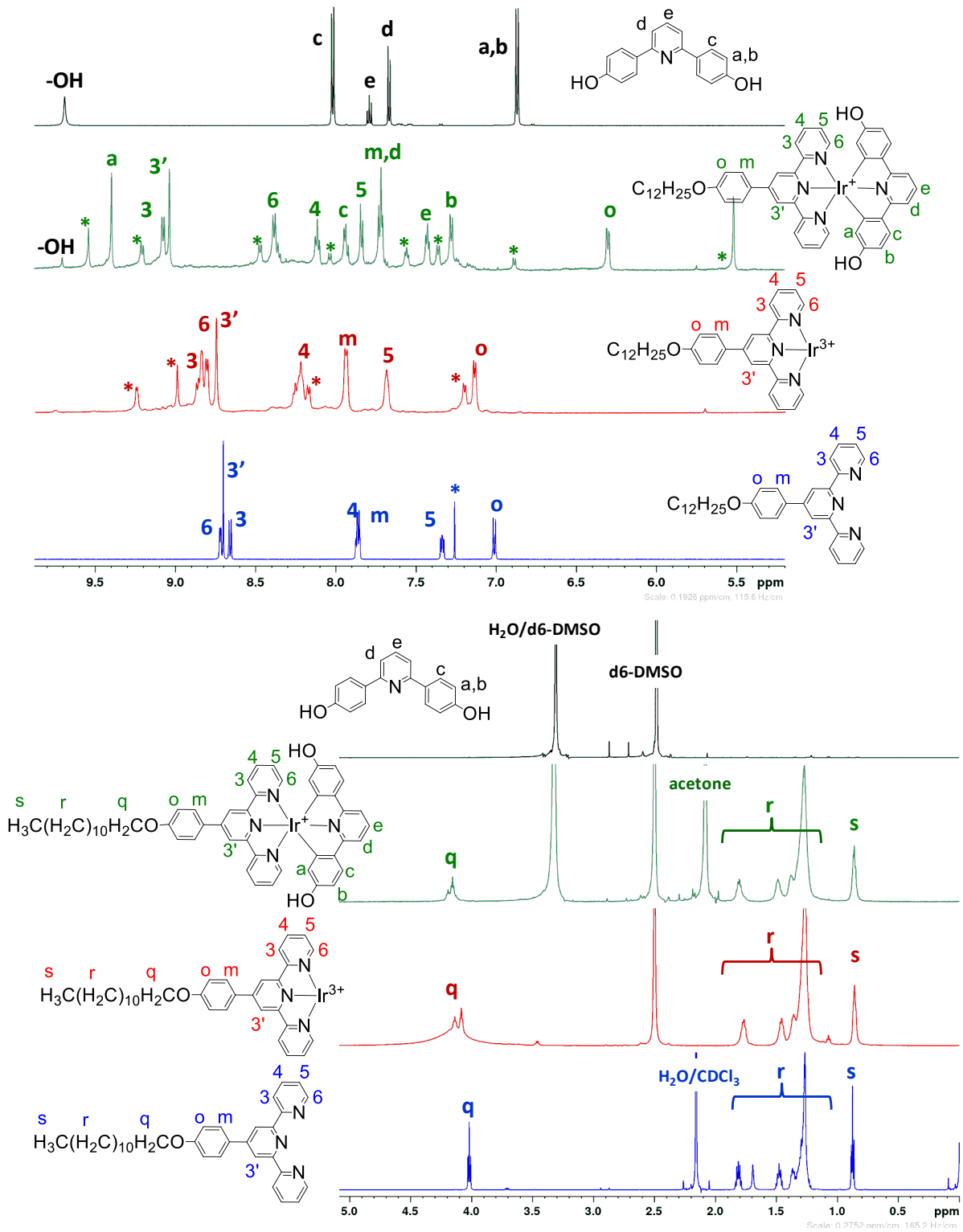

Figure S2. ^{1}H- NMR spectra of **C12Otpy** in $CDCl_3$, **C12Otpy-IrCl3** in DMSO-*d6* and **C12Otpy-Ir-HOpy** in DMSO-d_6. Peaks denoted with asterisks refer to alternative complexation modes or residual solvent traces.

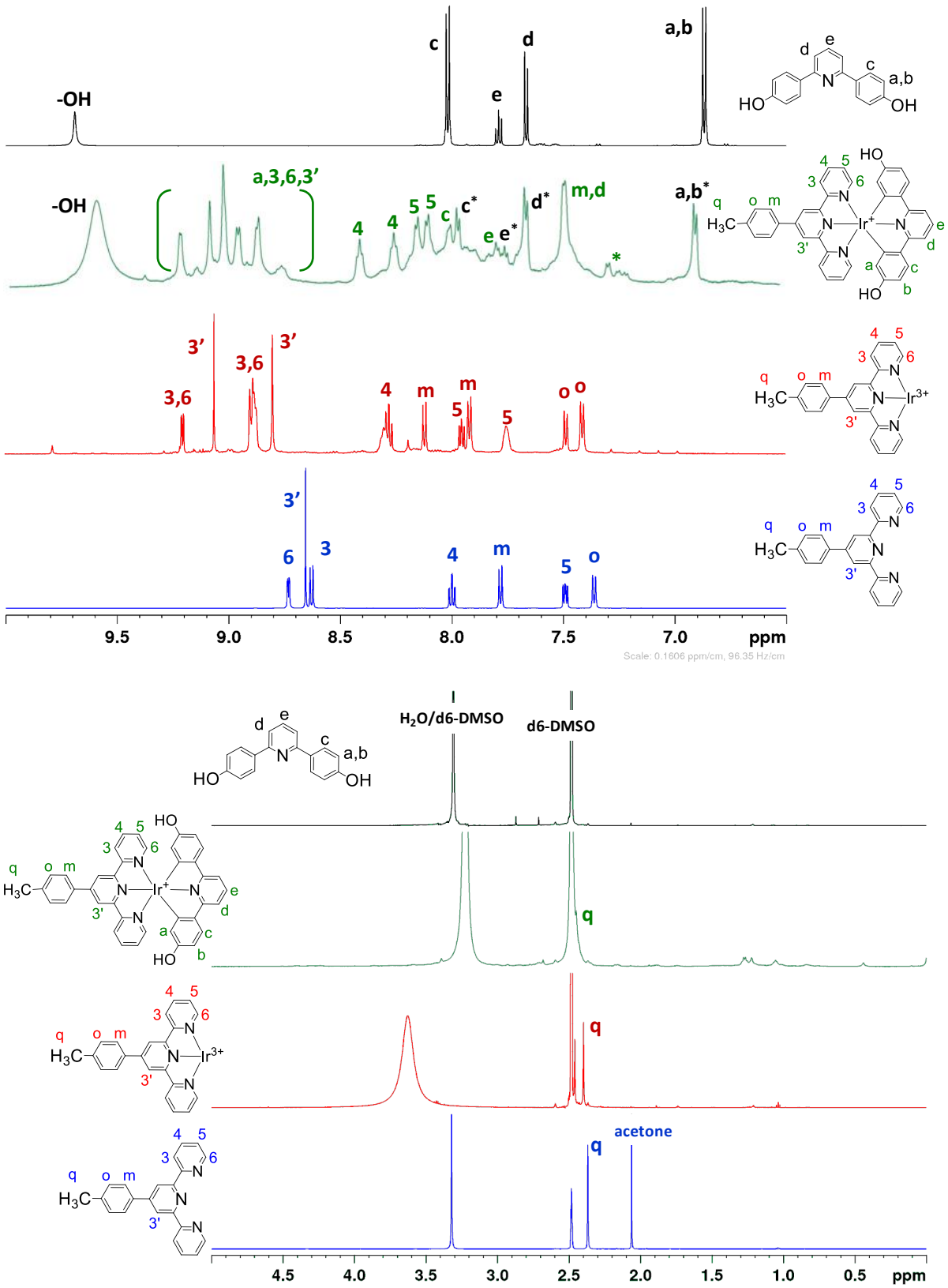

Figure S3. ^{1}H- NMR spectra of **CH$_3$tpy** in DMSO-*d6*, **CH$_3$tpy-IrCl$_3$** in DMSO-*d6* and **CH$_3$tpy-Ir-HOpy** in DMSO-*d$_6$*.

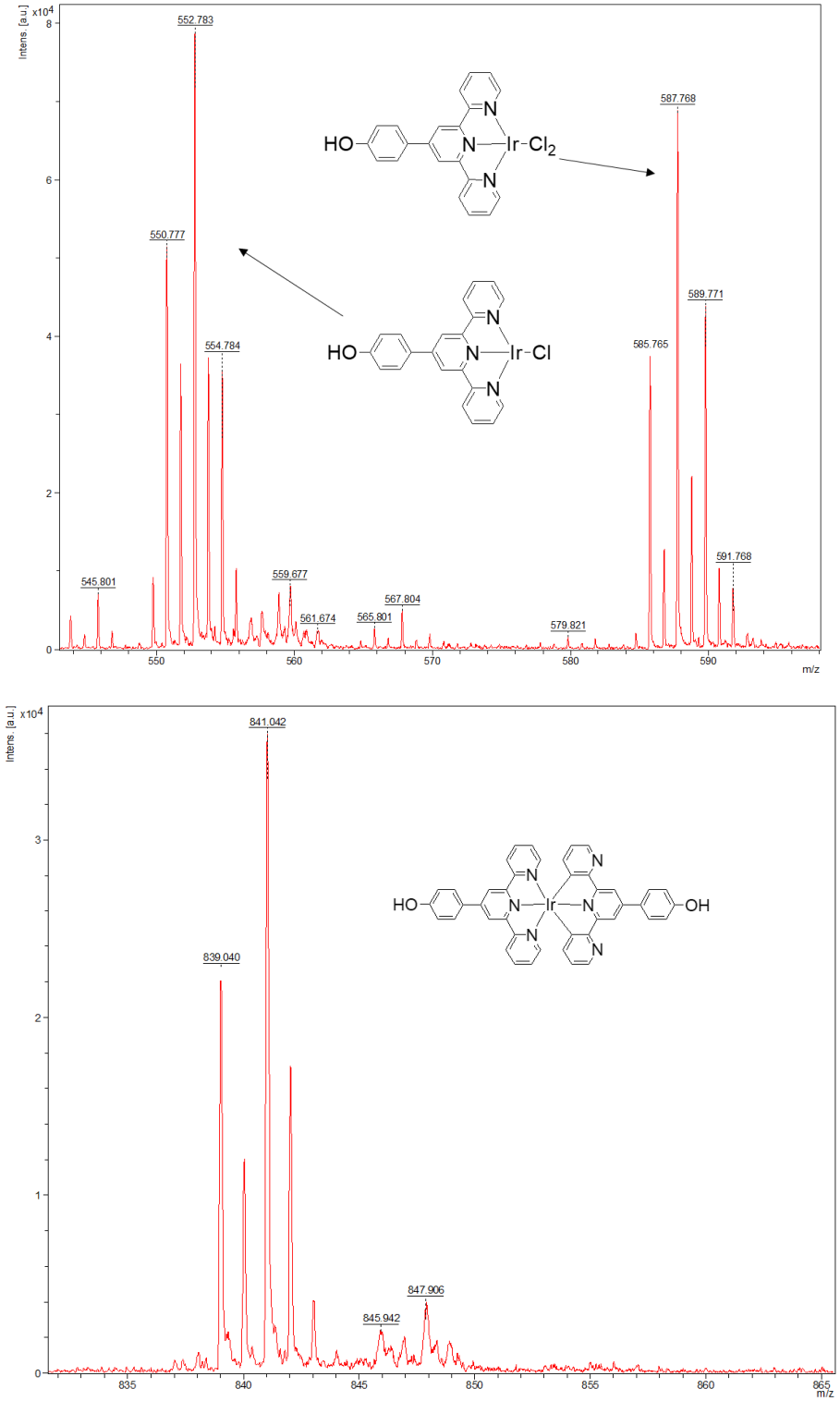

Figure S4. LDI – TOF/MS spectra of **HOtpy-IrCl3.**

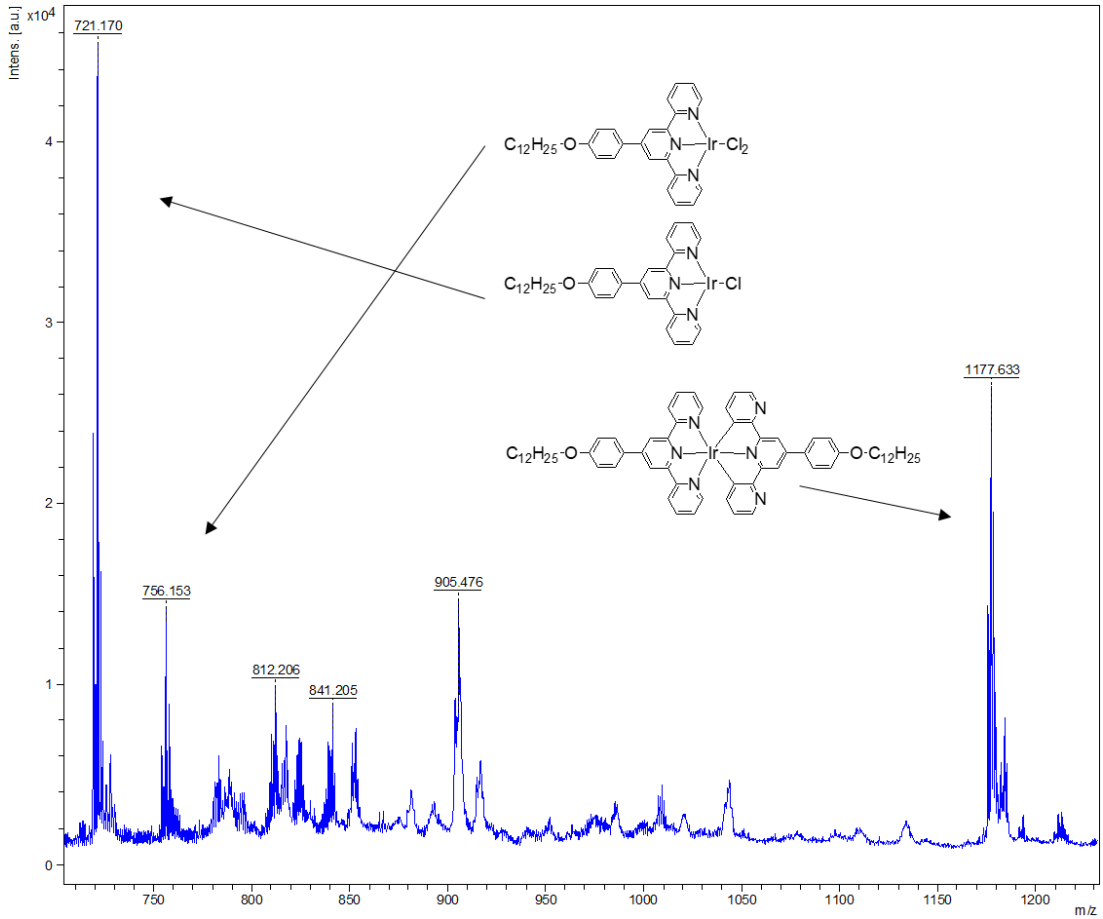

Figure S5. LDI – TOF/MS spectra of **C_{12}Otpy-$IrCl_3$**

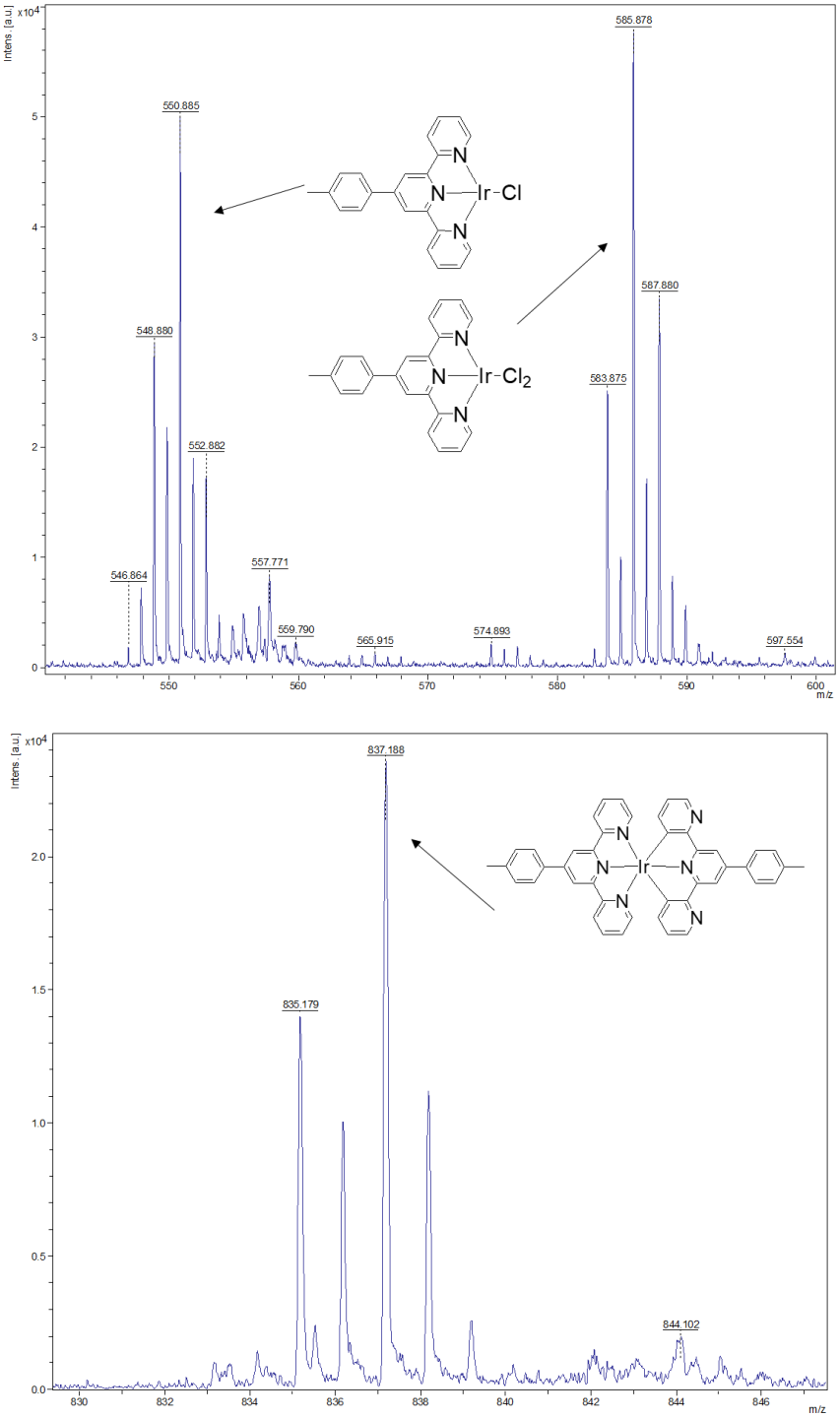

Figure S6. LDI – TOF/MS spectra of **CH_3tpy-$IrCl_3$**

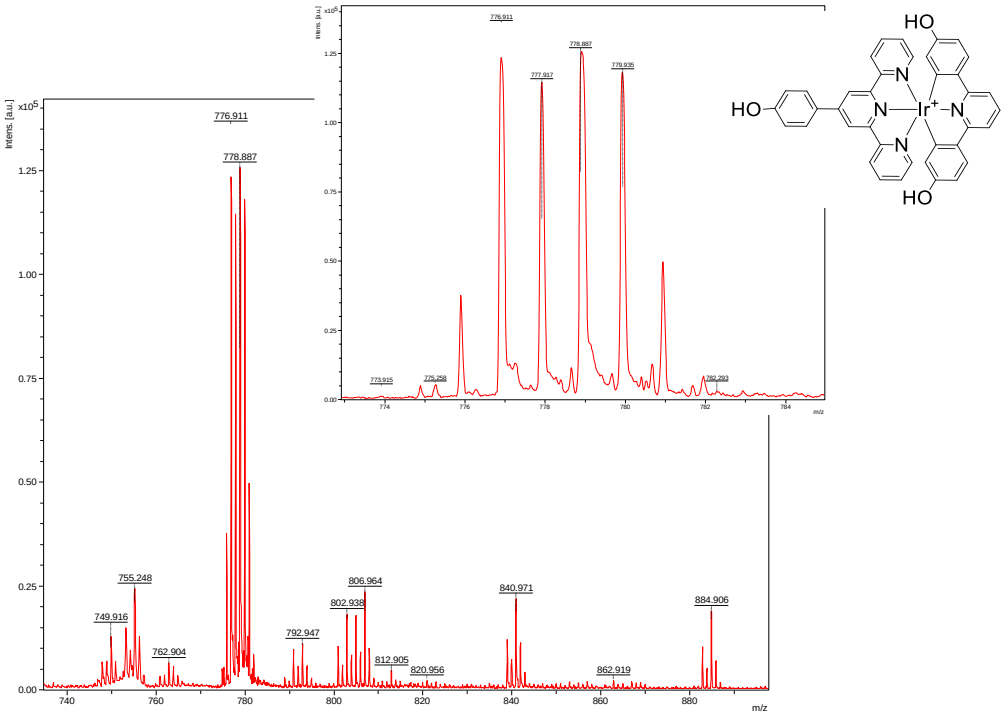

Figure S7. LDI – TOF/MS spectra of **HOtpy-Ir-HOpy**

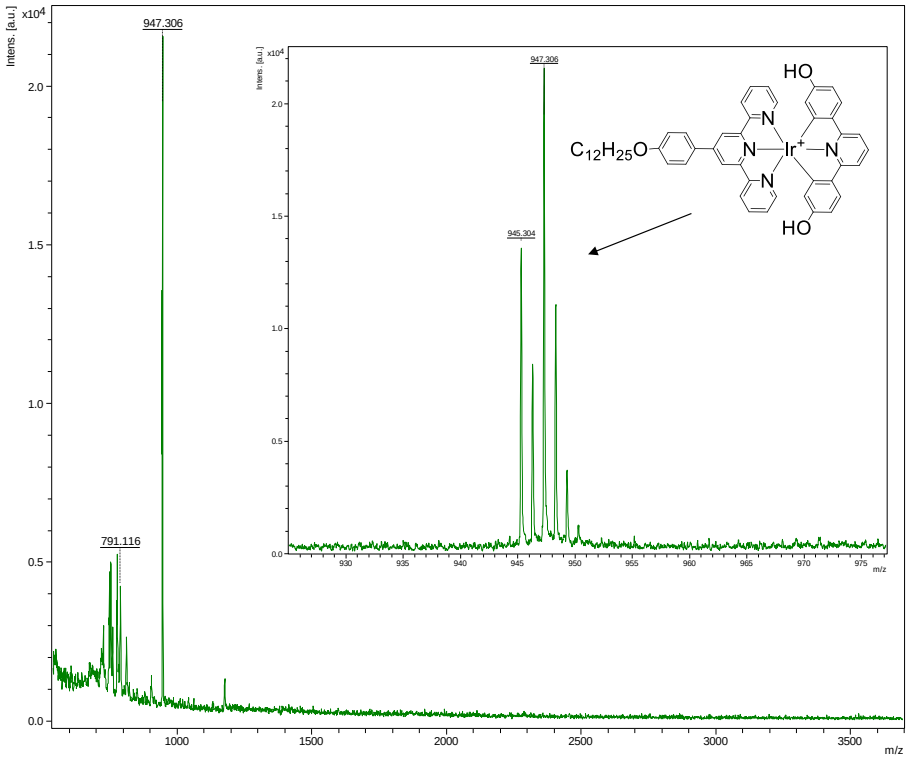

Figure S8. LDI-TOF MS spectra of **C_{12}Otpy-Ir-HOpy.**

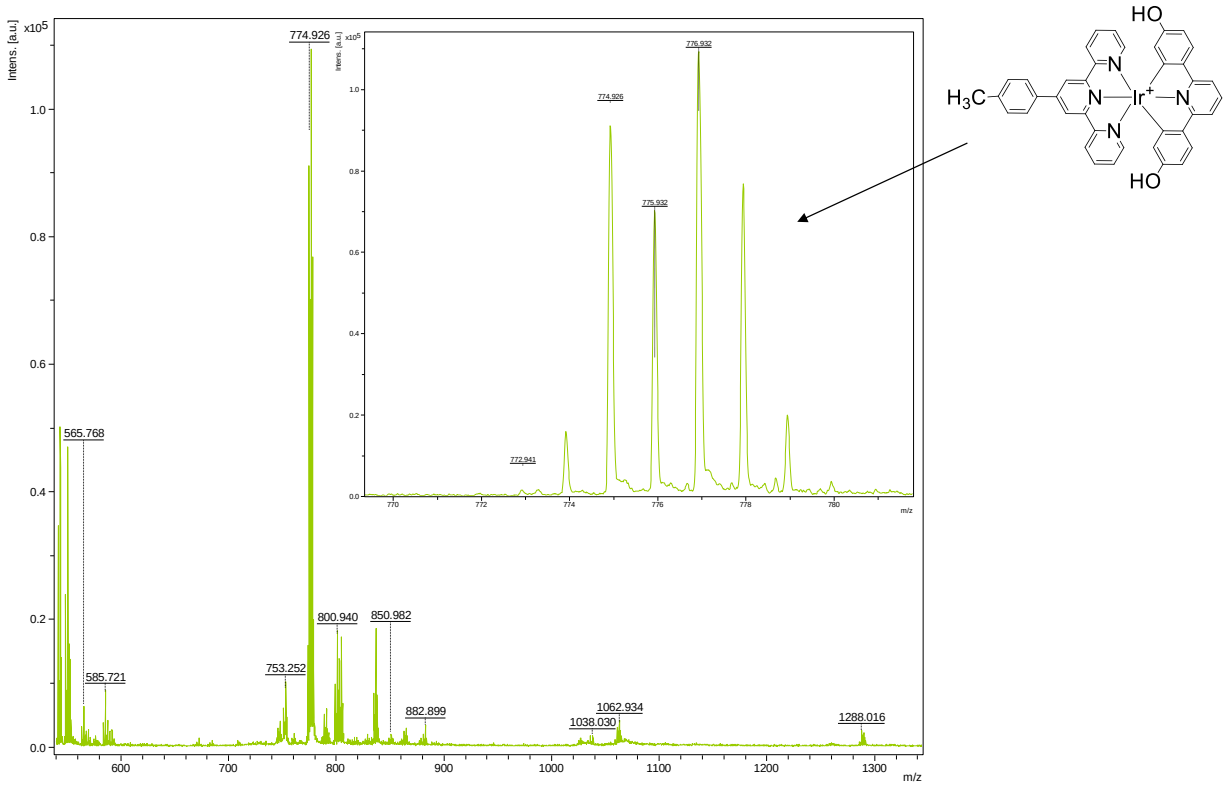

Figure S9. LDI – TOF/MS spectra of **CH3tpy-Ir-HOpy**

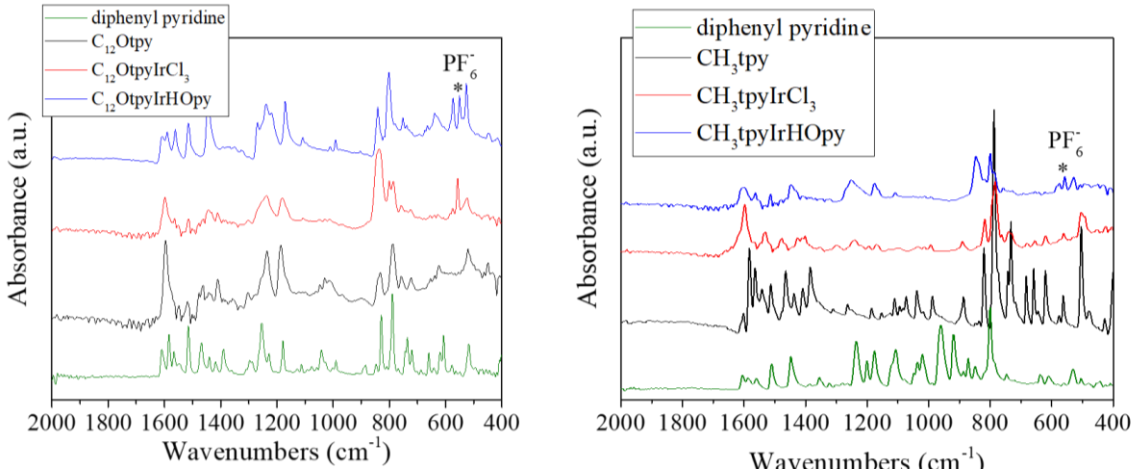

Figure S10. ATR spectra of the **monomeric Ir(III) complexes** based on the **C12Otpy** and **CH3tpy** ligands.

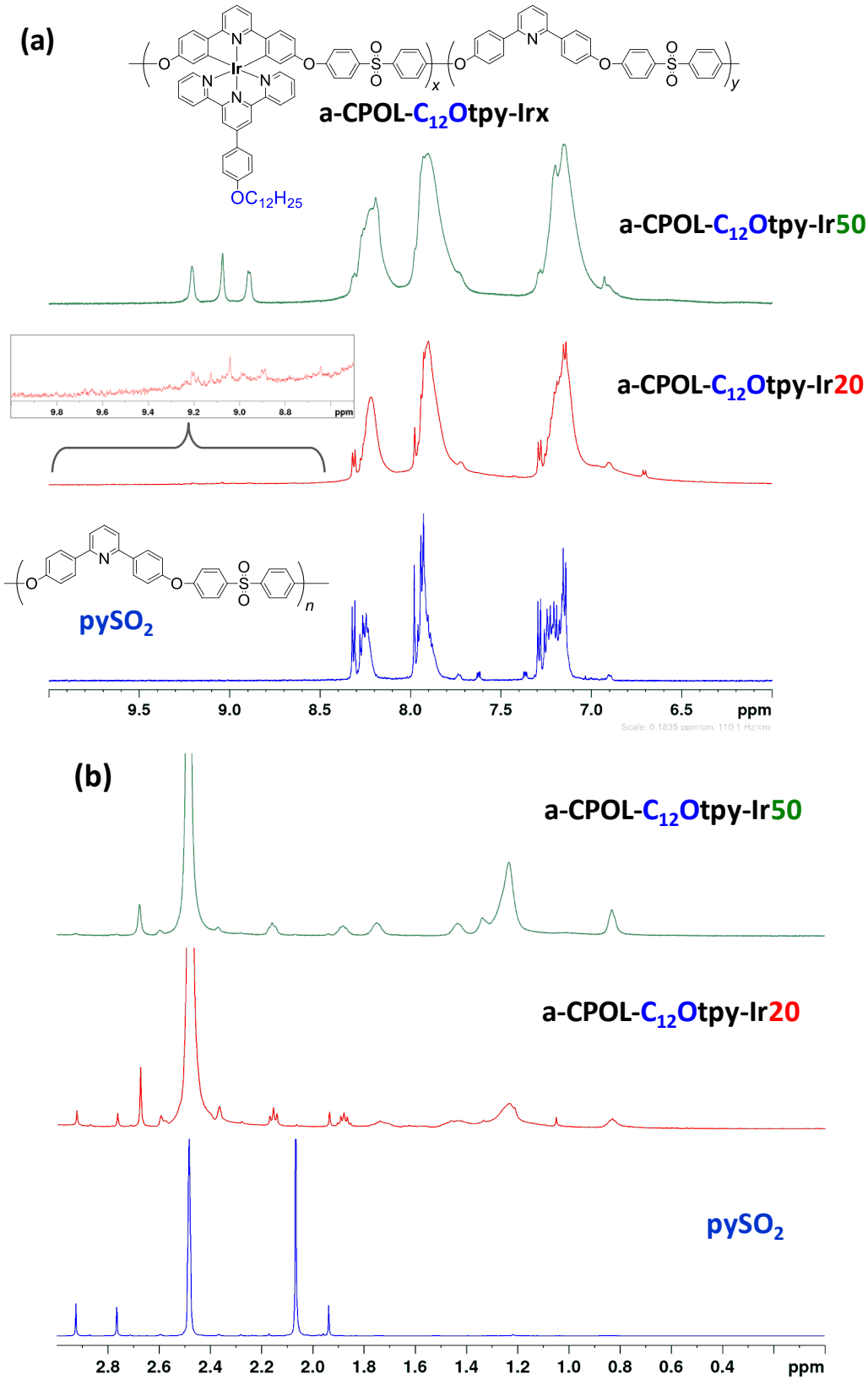

Figure S11. ^{1}H-NMR spectra of **a-CPOL-C$_{12}$Otpy-Irx** (where x=20% red and x=50% green) prepared by the "post polymerization" complexation method, and of the uncomplexated homopolymer ligand **pySO$_2$** in DMSO-d_6. **(a)** shows the region of 10-6 ppm and **(b)** the region 3-0 ppm. The inset in **(a)** shows a magnification of the 10ppm – 8.5ppm area of the **a-CPOL-C$_{12}$Otpy-Ir20** spectrum.

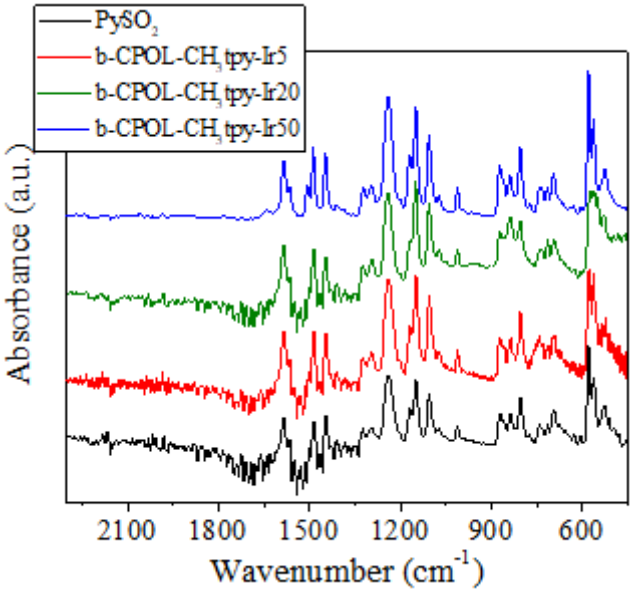

Figure S12. ATR spectra of the polymeric Ir(III) complexes **b-CPOL-CH3tpy-Irx.**

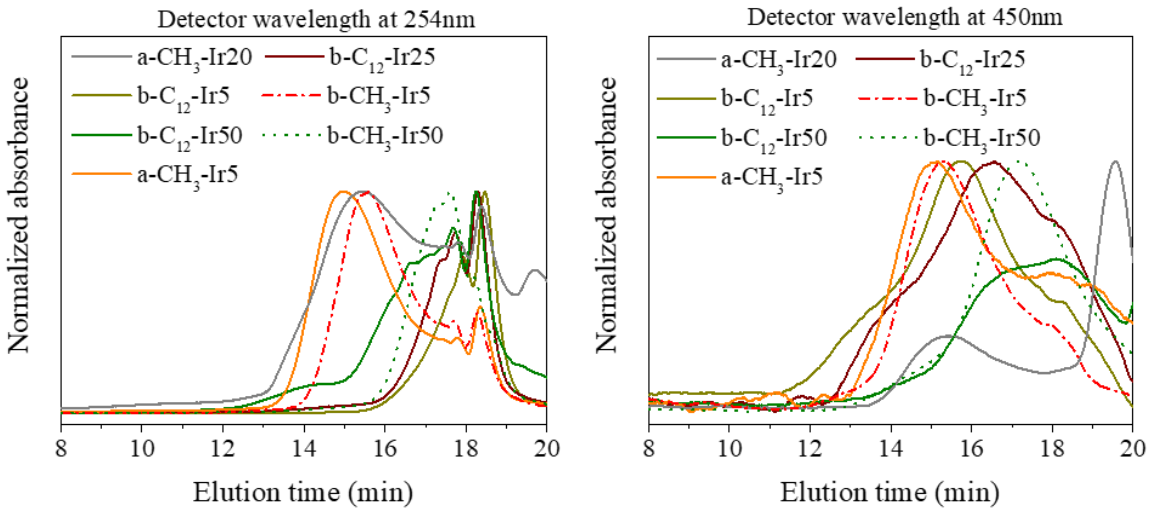

Figure S13. GPC trace of **a-CPOL-Rtpy-Irx** (indicated as **a-R-Irx**) and **b-CPOL-Rtpy-Irx** (indicated as **b-R-Irx**) with the detector set at 254nm (left) and at 450nm (right).

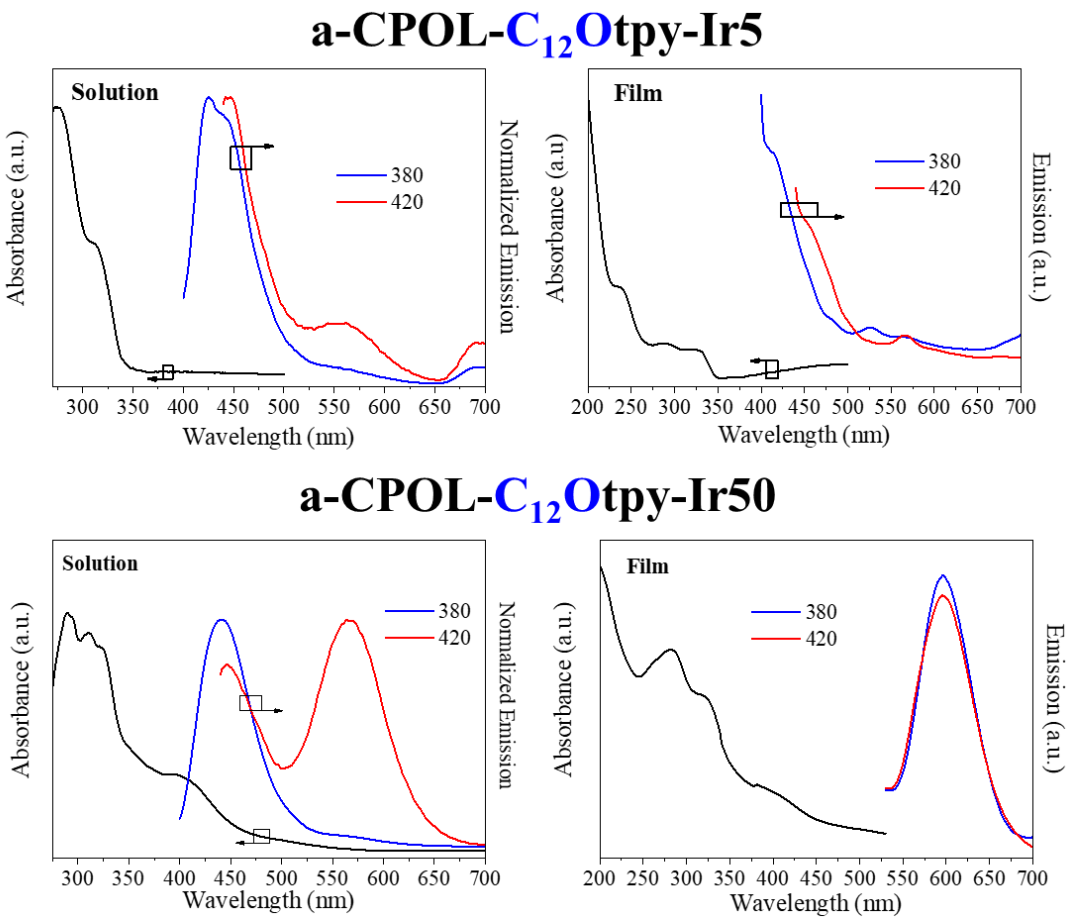

Figure S14. Absorption (black) and emission (color) spectra of the polymeric complexes **a-CPOL-C12Otpy-Irx** where **x=5, 50** recorded in 1,1′,2,2′-TCE solution (left) and thin film (right)

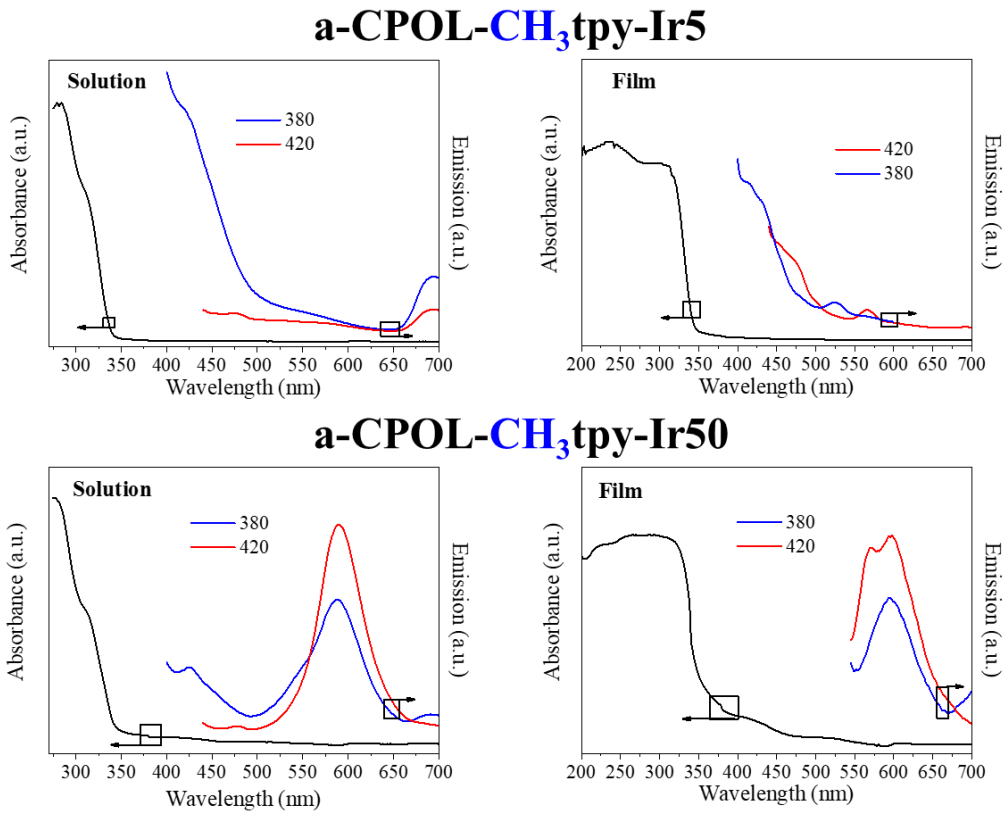

Figure S15. Absorption (black) and emission (colored) spectra of the polymeric complexes **a-CPOL-CH3tpy-Irx** where **x=5, 50** recorded in 1,1′,2,2′-TCE solution (left) and thin film (right)

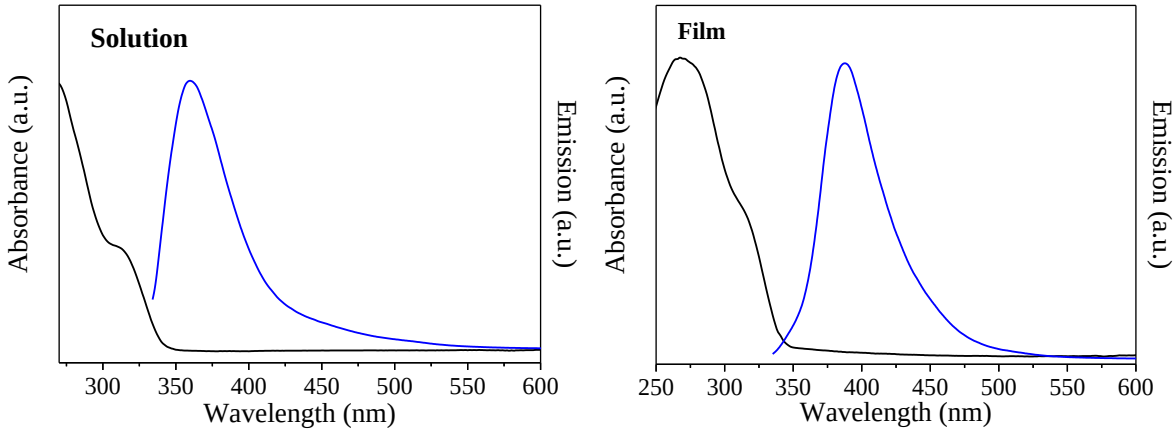

Figure S16. Absorption and emission spectra of **pySO2** in (a) solution using DMA and in (b) thin film form