Supplementary material for the article:

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Supplementary Information

Half-sandwich ruthenium(II)-arene complexes: Synthesis, spectroscopic studies, biological properties and molecular modeling

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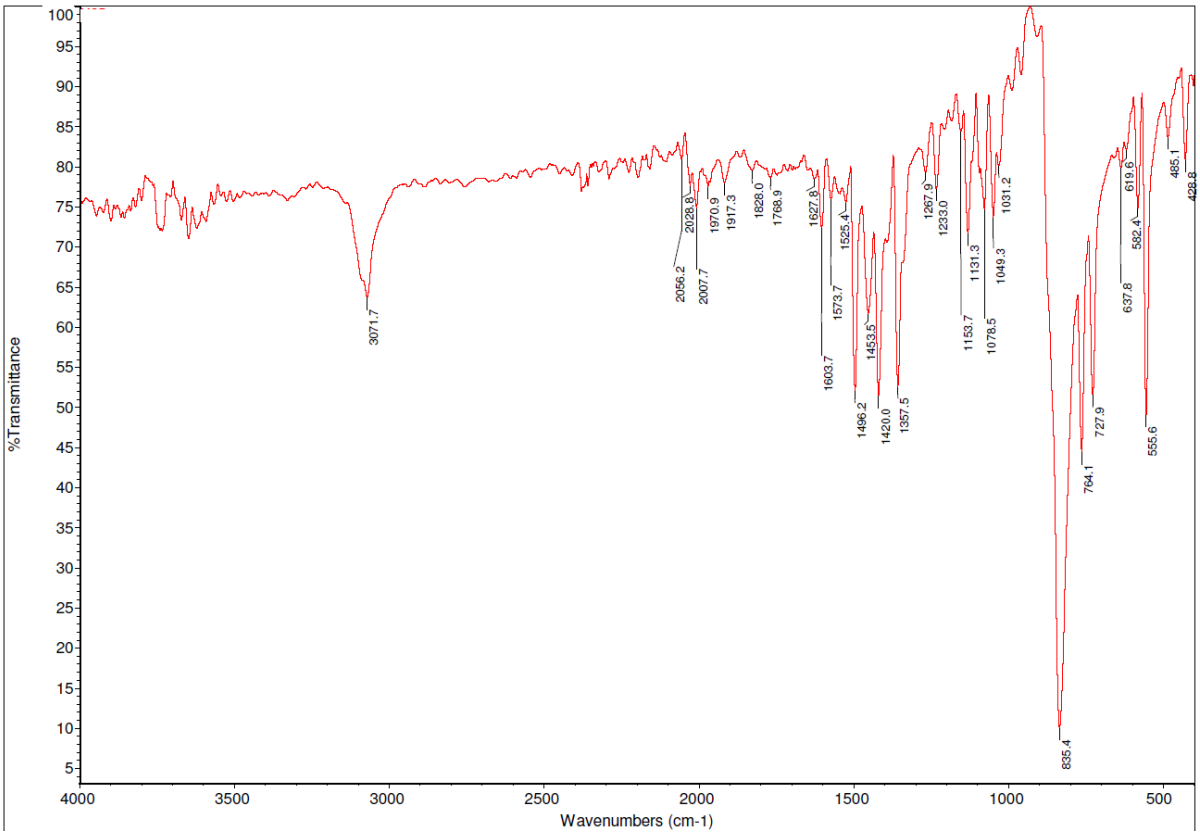


Figure S1. IR spectrum of complex **1**.

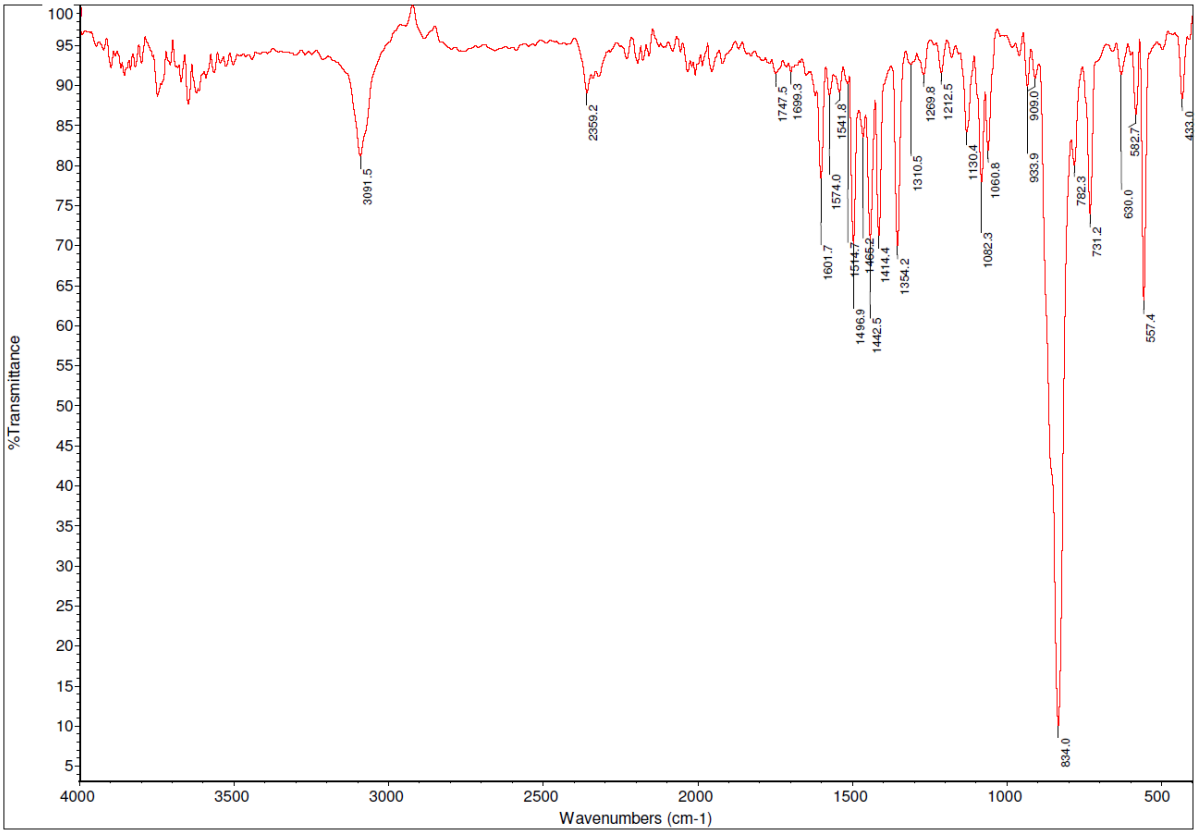


Figure S2. IR spectrum of complex **3**.

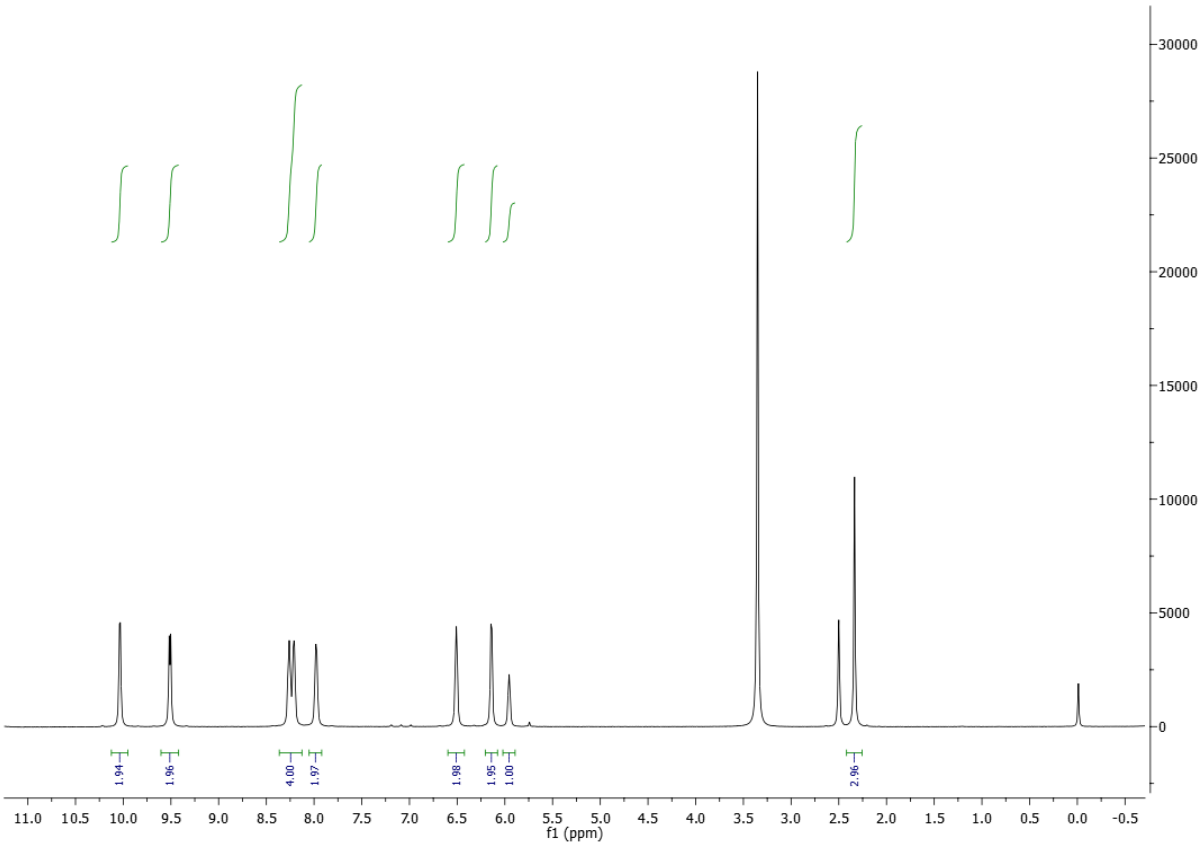


Figure S3. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of complex **1**.

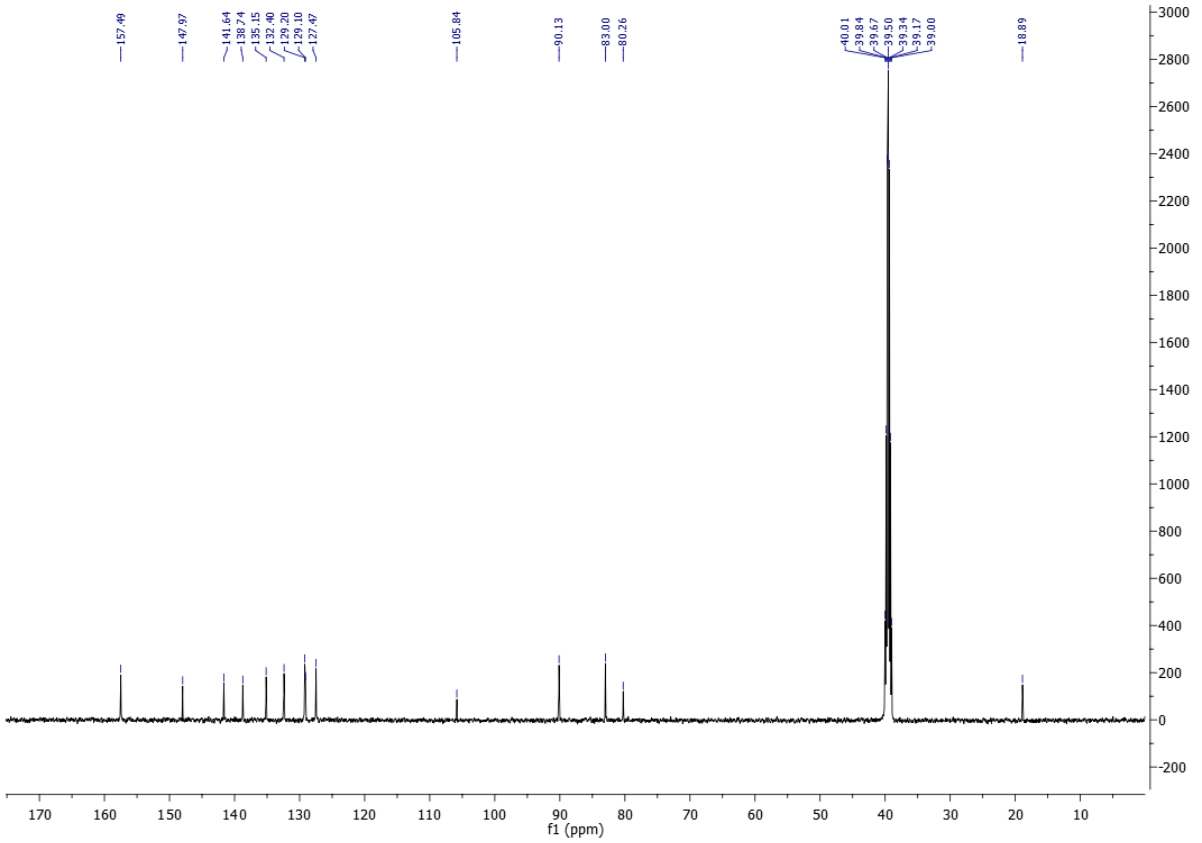


Figure S4. ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of complex **1**.

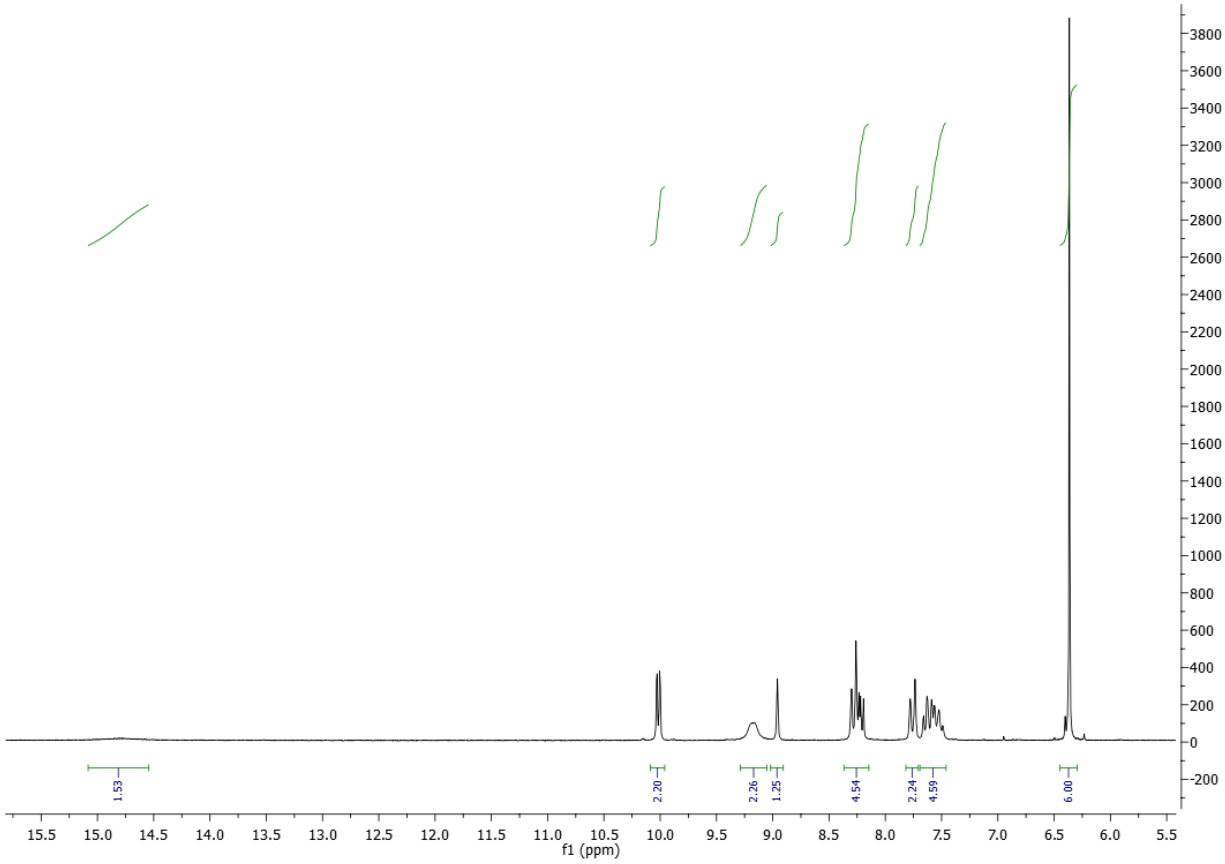


Figure S5. ^{1}H NMR (200 MHz, DMSO-d_6) spectrum of complex **3**.

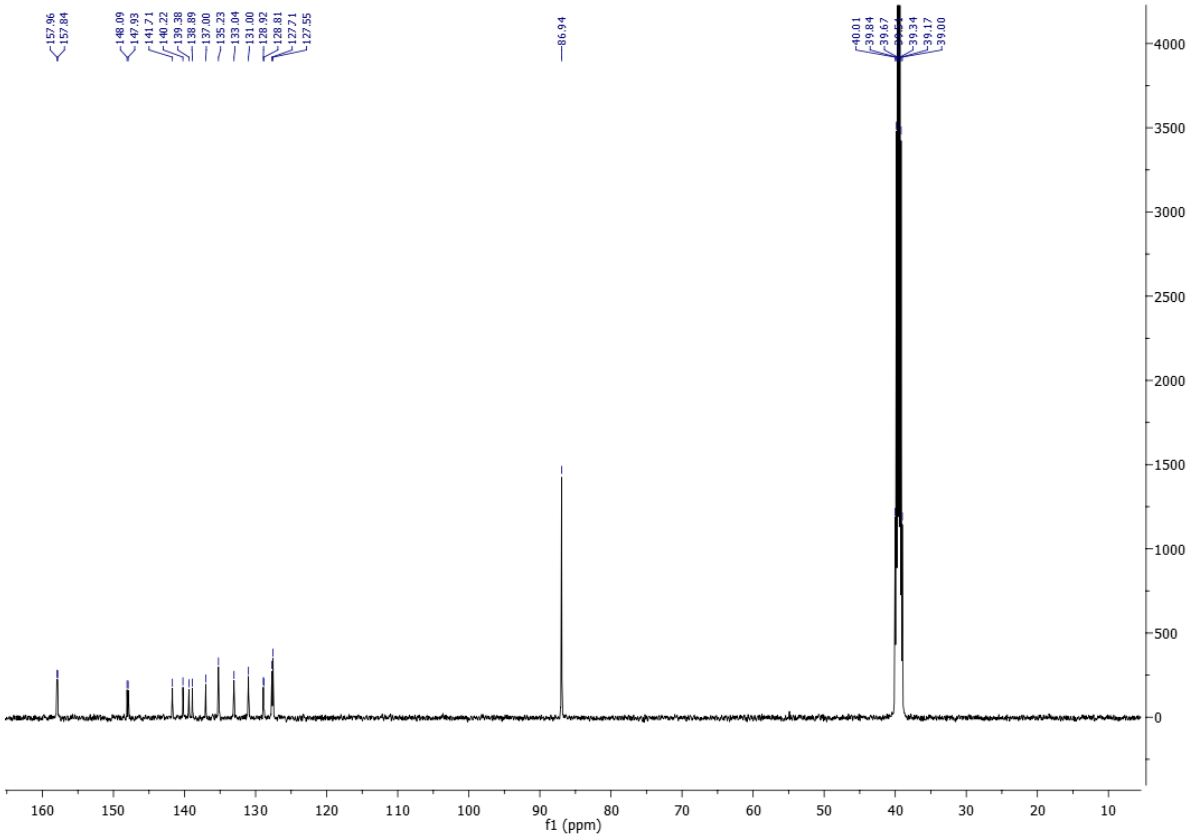


Figure S6. ^{13}C NMR (50 MHz, DMSO-d_6) spectrum of complex **3**.

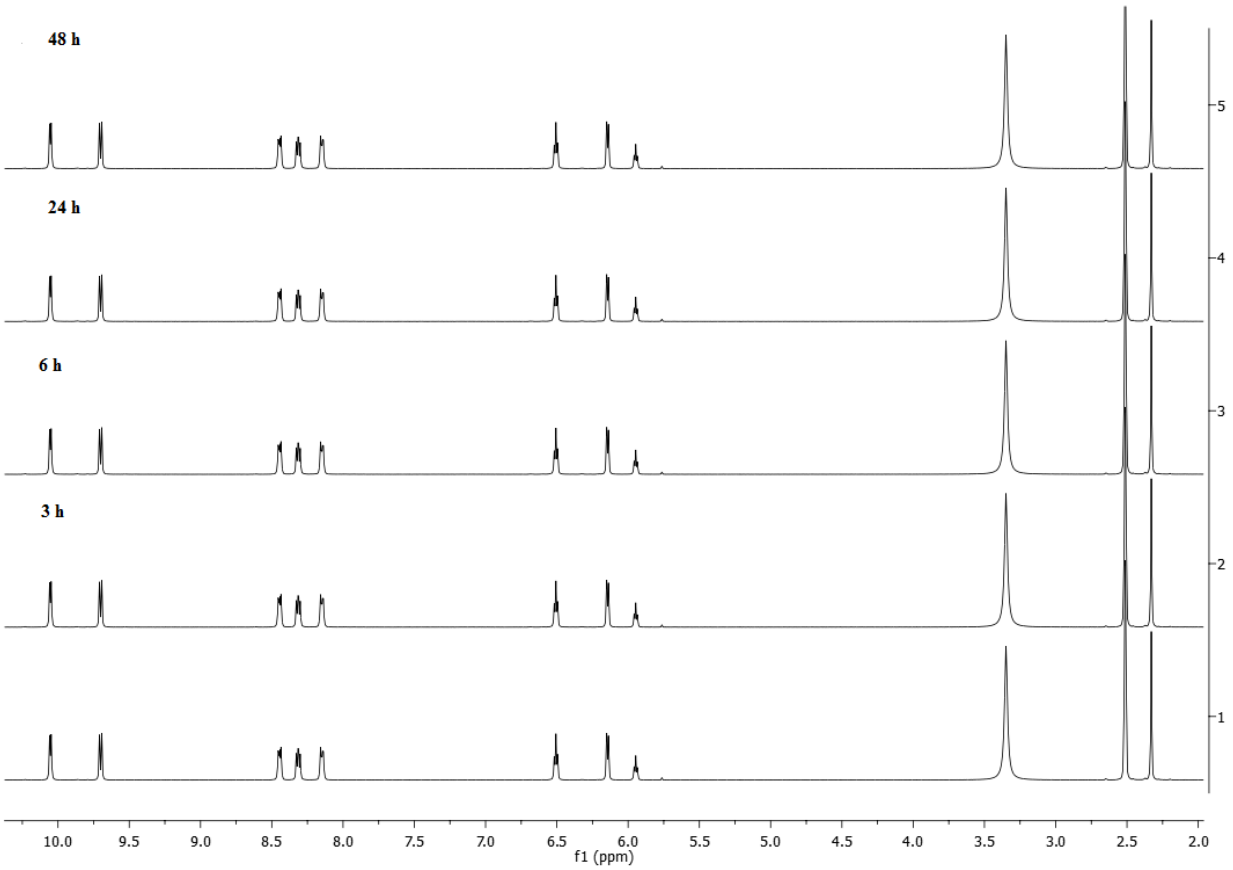


Figure S7. ^{1}H NMR (500 MHz, DMSO-d_6) spectra of complex **1** during 48 h.

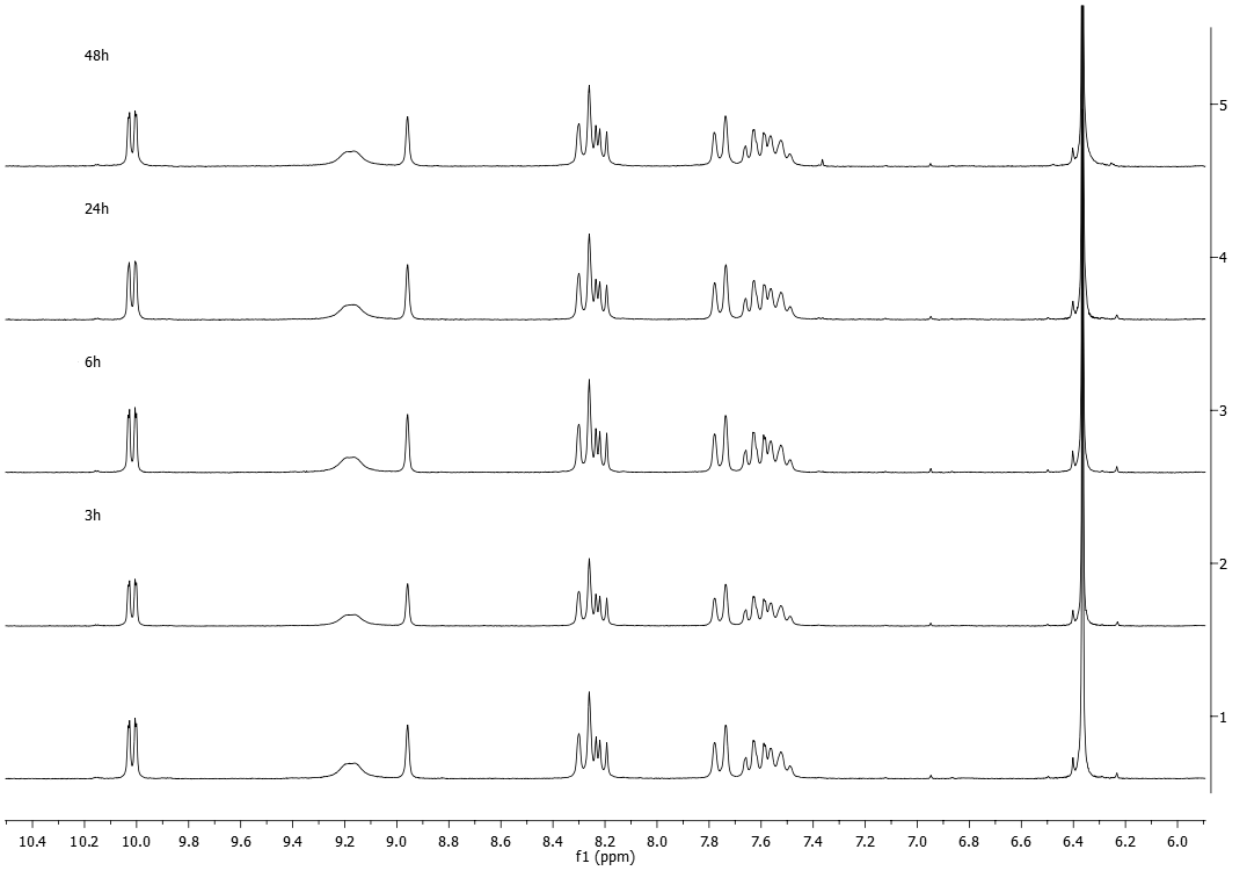


Figure S8. ^{1}H NMR (500 MHz, DMSO-d_6) spectra of complex **3** during 48 h.

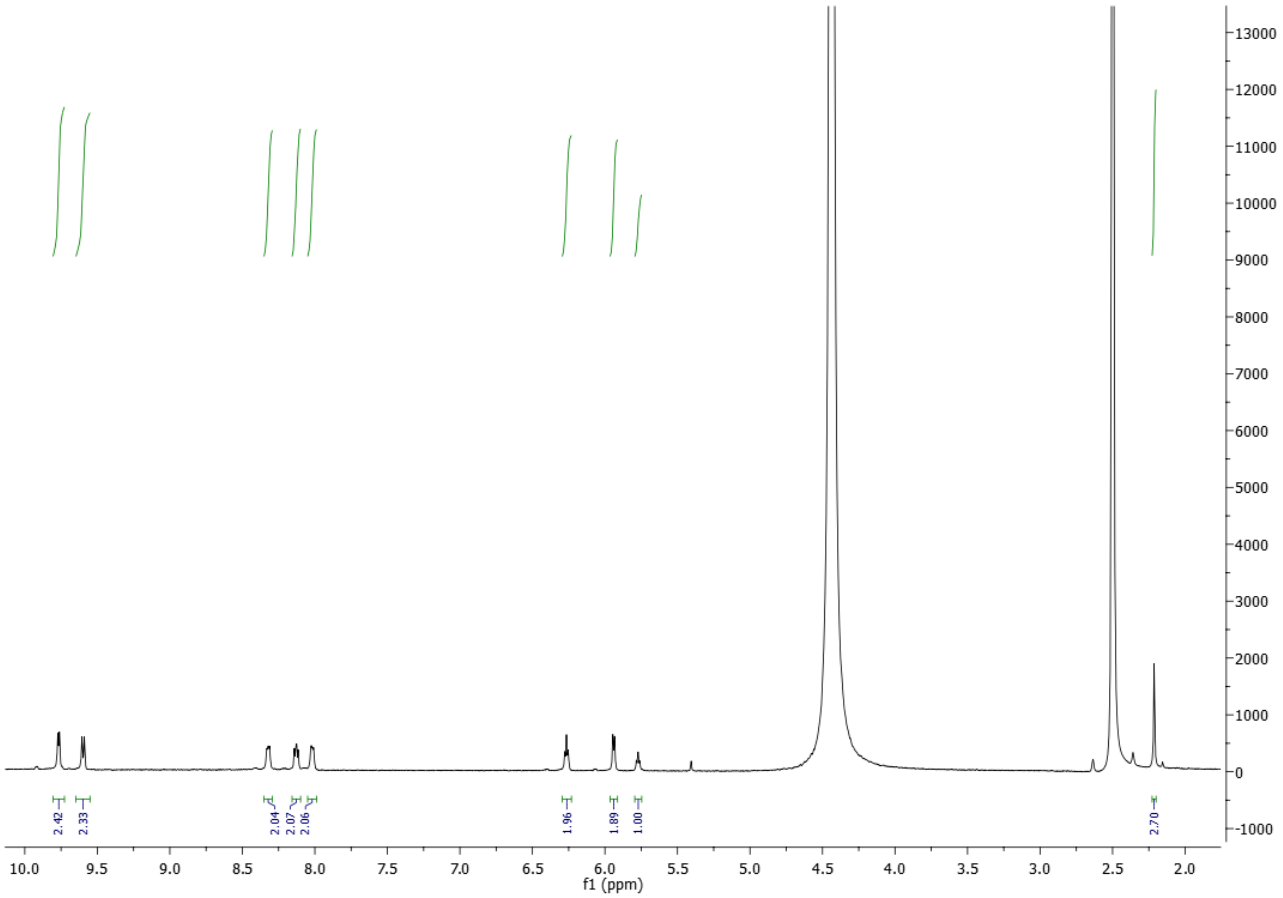


Figure S9. ^{1}H NMR (500 MHz, DMSO-d_6/D_2O) spectra of complex **1**.

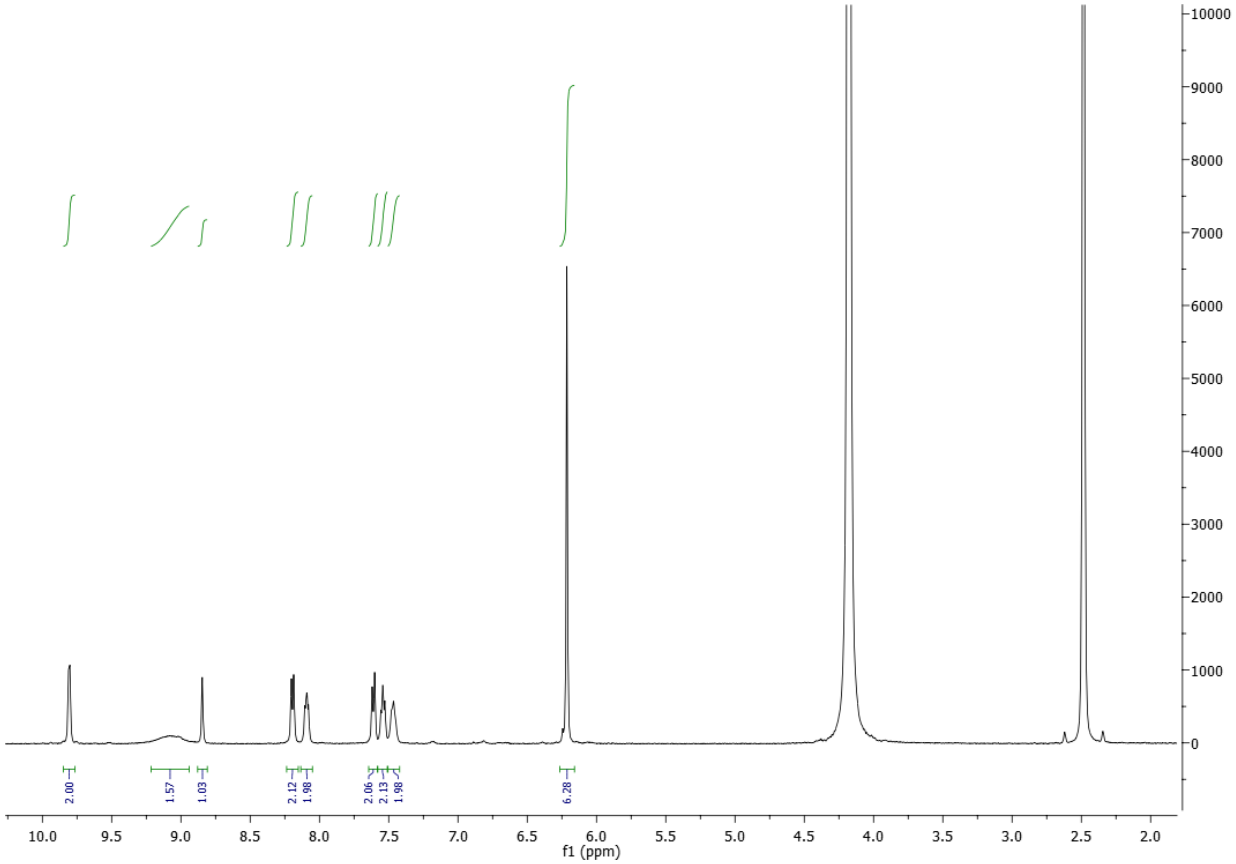


Figure S10. ^{1}H NMR (500 MHz, DMSO-d_6/D_2O) spectra of complex **3**.

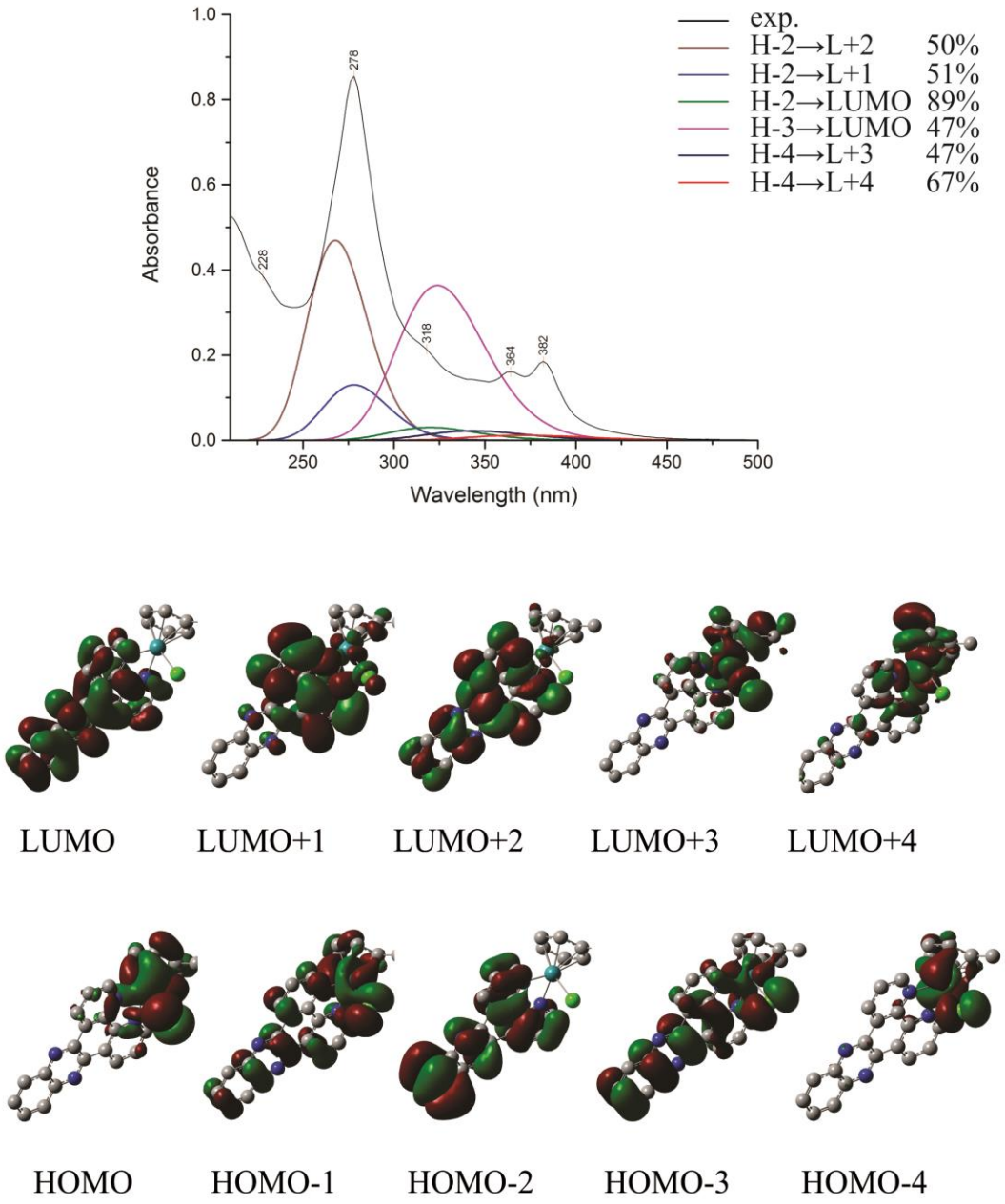


Figure S11. Experimental UV-Vis spectra, calculated the electronic transitions and molecular orbitals of complex **1**. The black line with marked numbers represent experimental UV-Vis curve; Colored curves represent calculated transitions where H-2, H-3, H-4 correspond to HOMO-2, HOMO-3, HOMO-4 while L+1, L+2, L+3, L+4 stand for LUMO+1, LUMO+2, LUMO+3, LUMO+4.

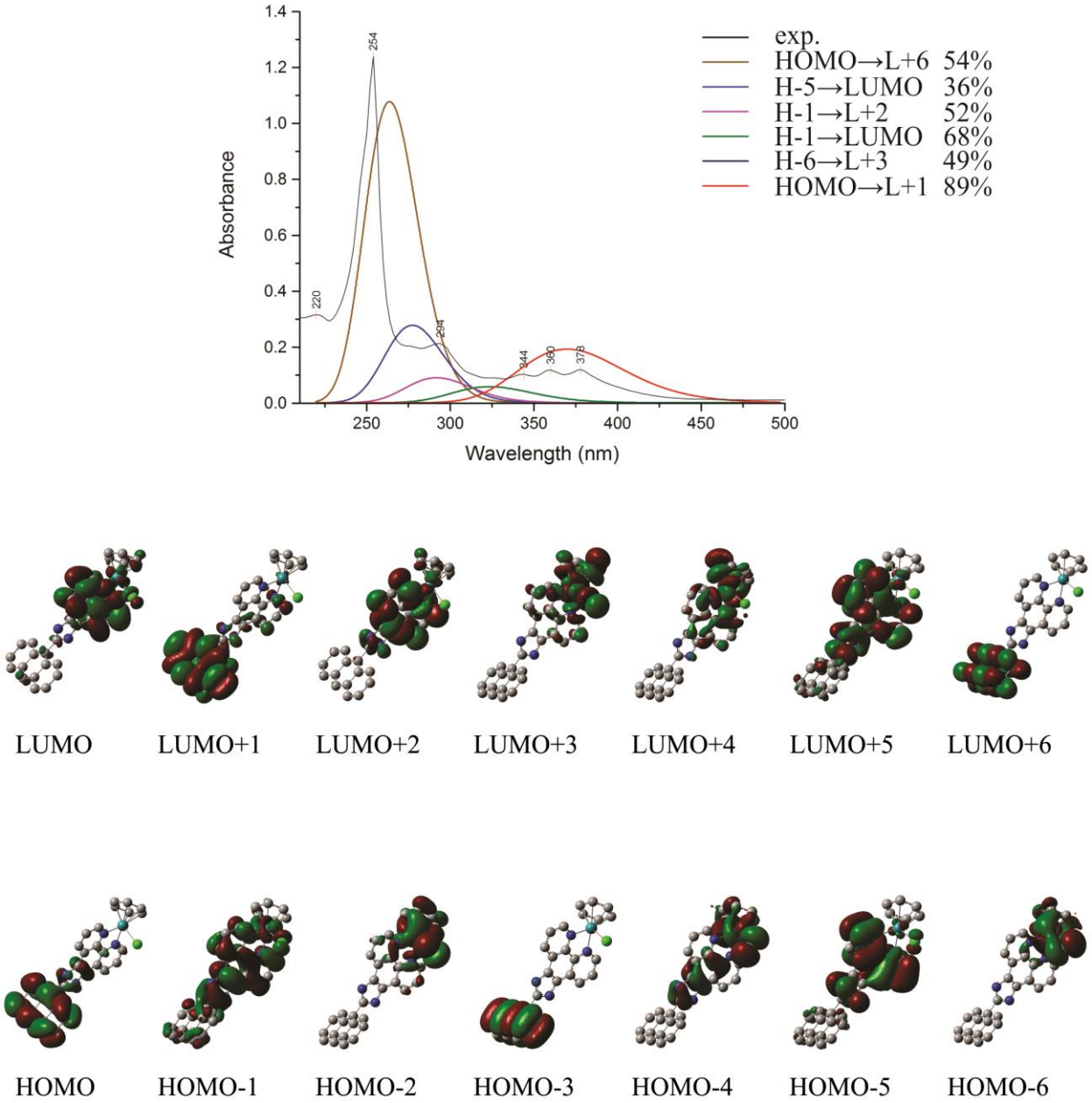
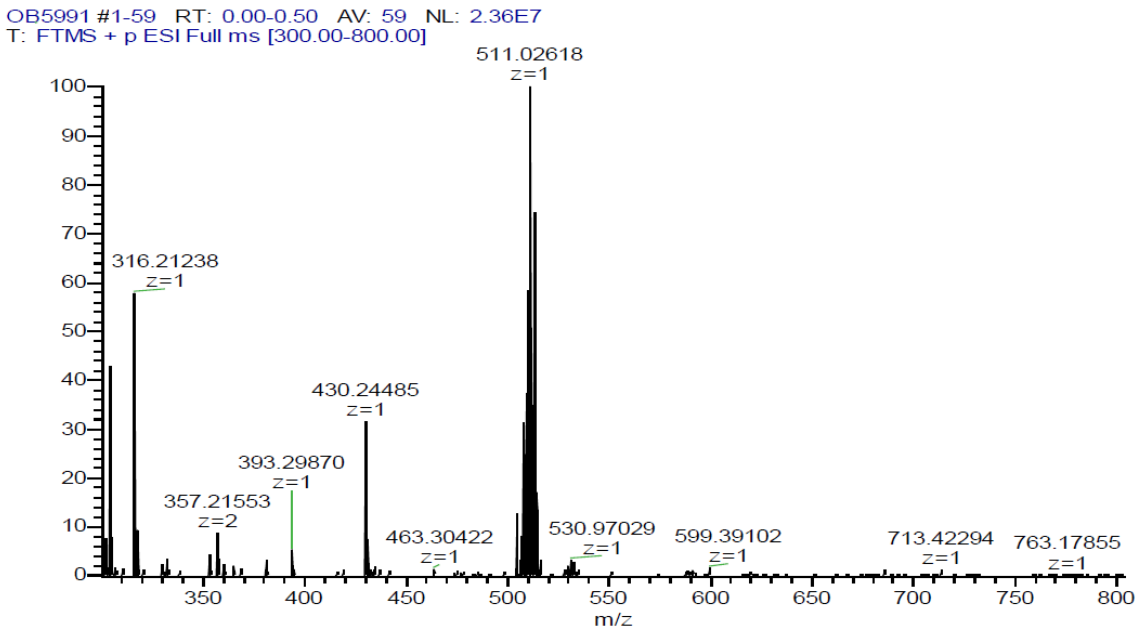
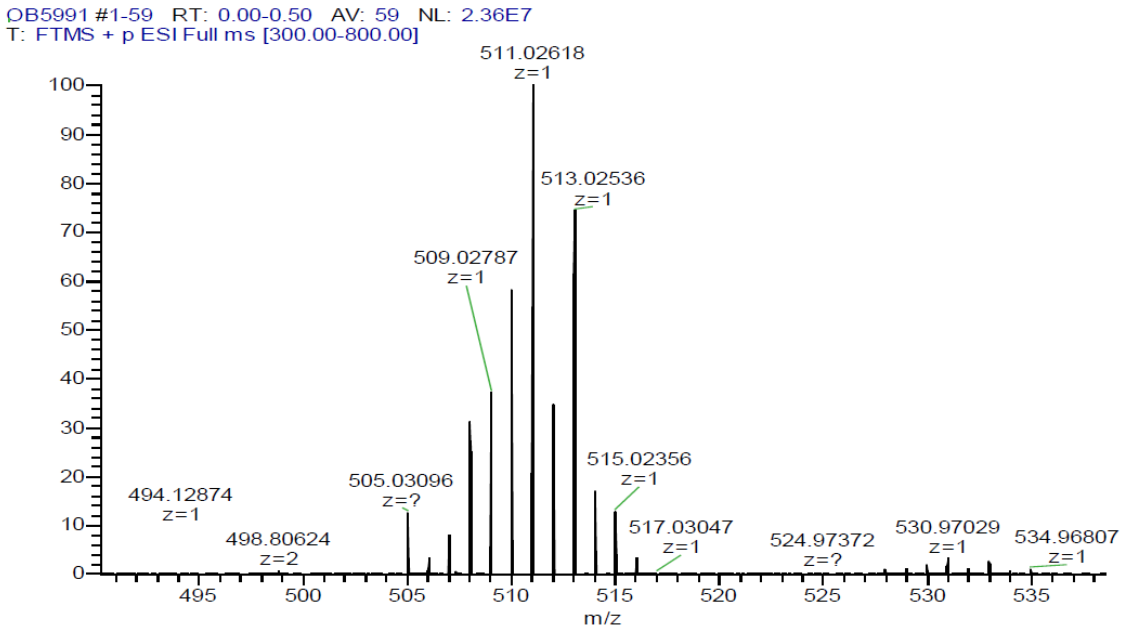


Figure S12. Experimental UV-Vis spectra, calculated the electronic transitions and molecular orbitals of complex **3**. The black line with marked numbers represent experimental UV-Vis curve; Colored curves represent calculated transitions where H-1, H-5, H-6 correspond to HOMO-1, HOMO-5, HOMO-6 while L+1, L+2, L+3, L+6 stand for LUMO+1, LUMO+2, LUMO+3, LUMO+6.

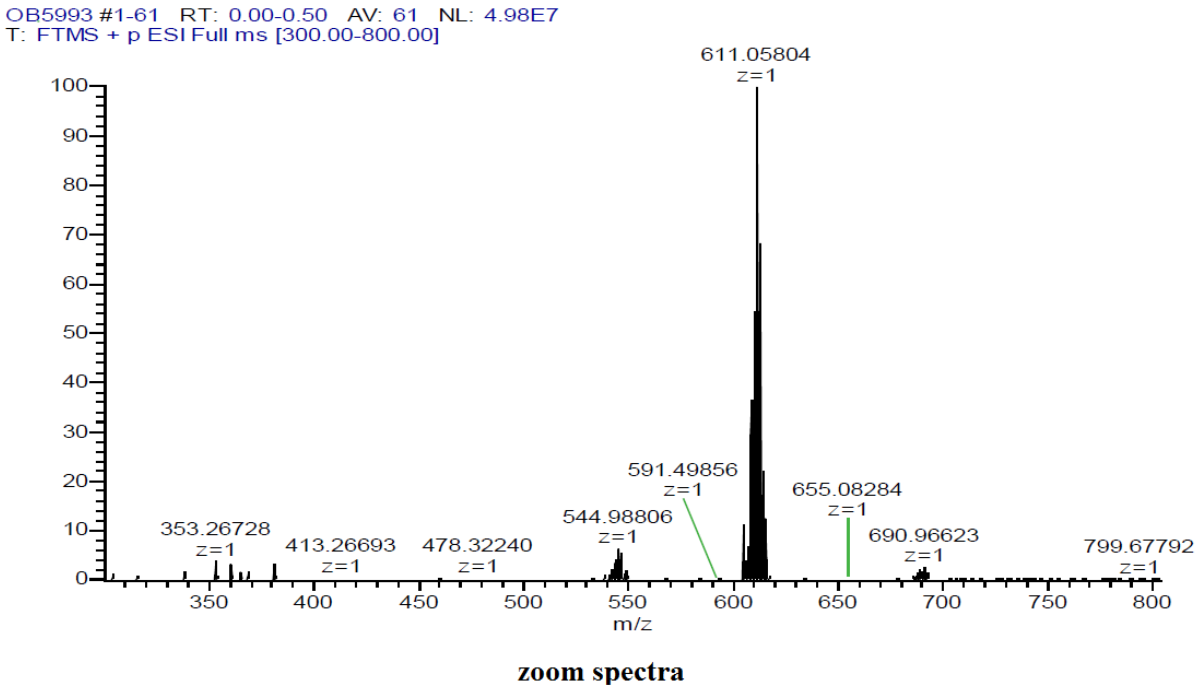


zoom spectra

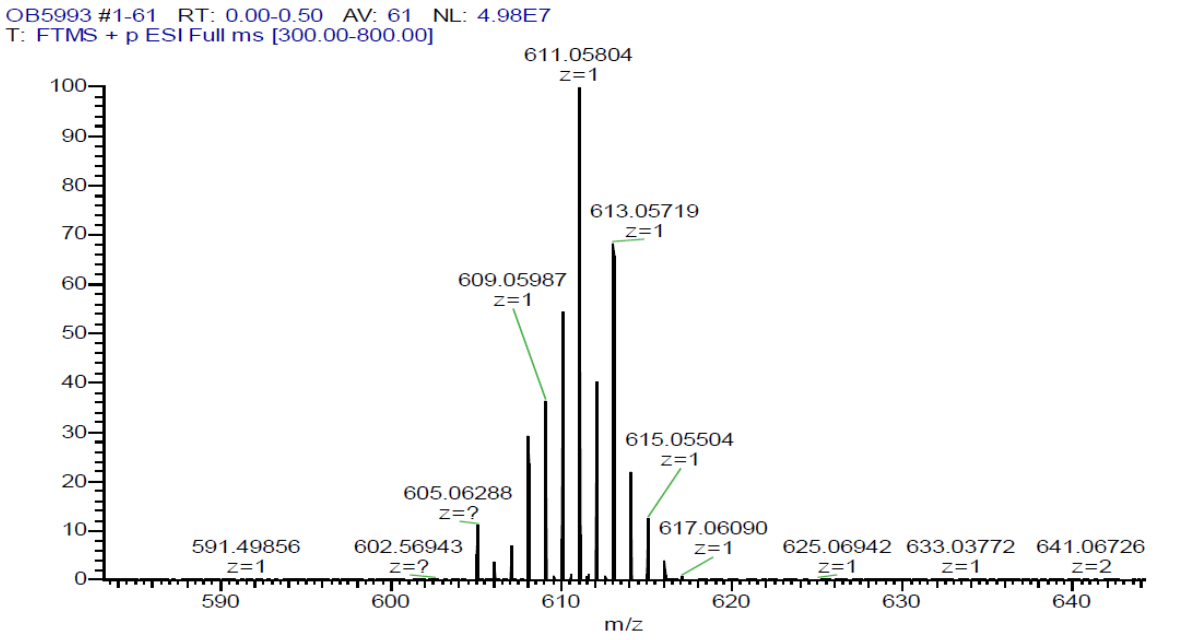


Exact mass	Observed mass	Error (ppm)
511.02635	511.08618	0.33

Figure S13. Mass spectra of complex **1**.



zoom spectra



Exact mass	Observed mass	Error (ppm)
611.05765	611.05804	0.64

Figure S14. Mass spectra of complex **3**.