

Electronic supplementary materials

Oxovanadium(IV/V) Lawsonsone-based complexes: Synthesis, characterization, DFT Studies, and multifunctional biological activities

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Contents

1. FTIR spectra

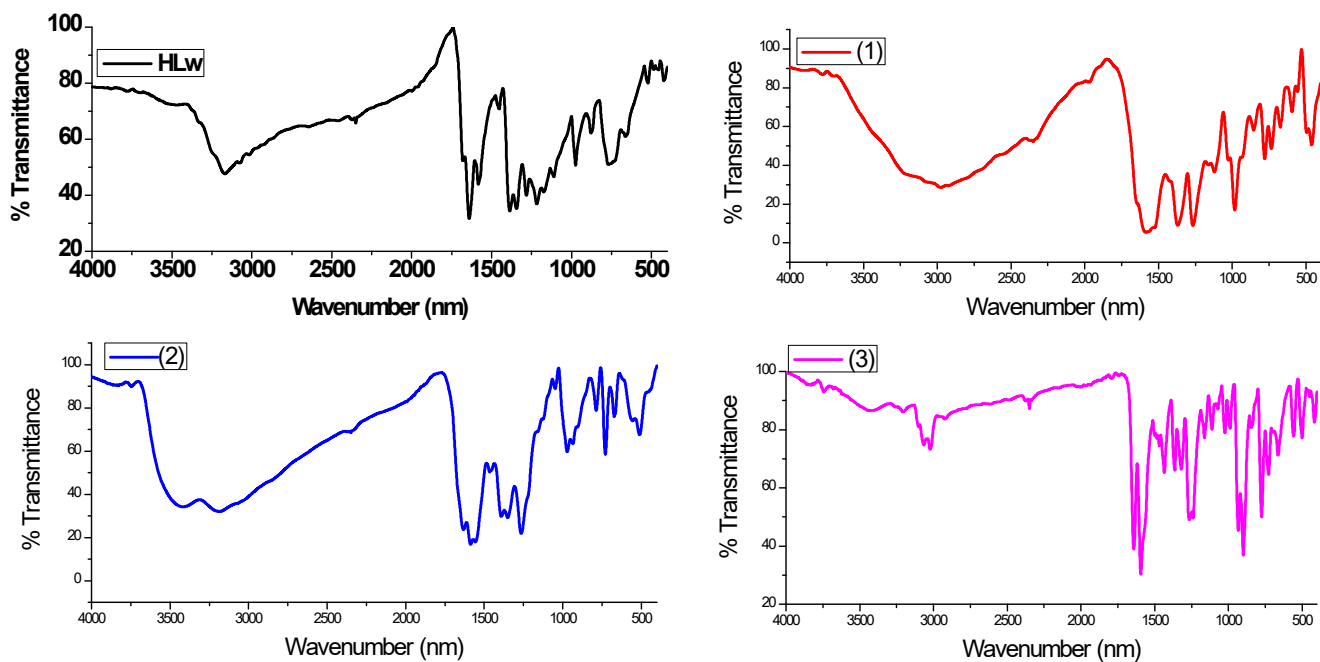


Fig. S1: FTIR spectra of the ligand (HLw) and its complexes (1 – 3)

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2. NMR spectra

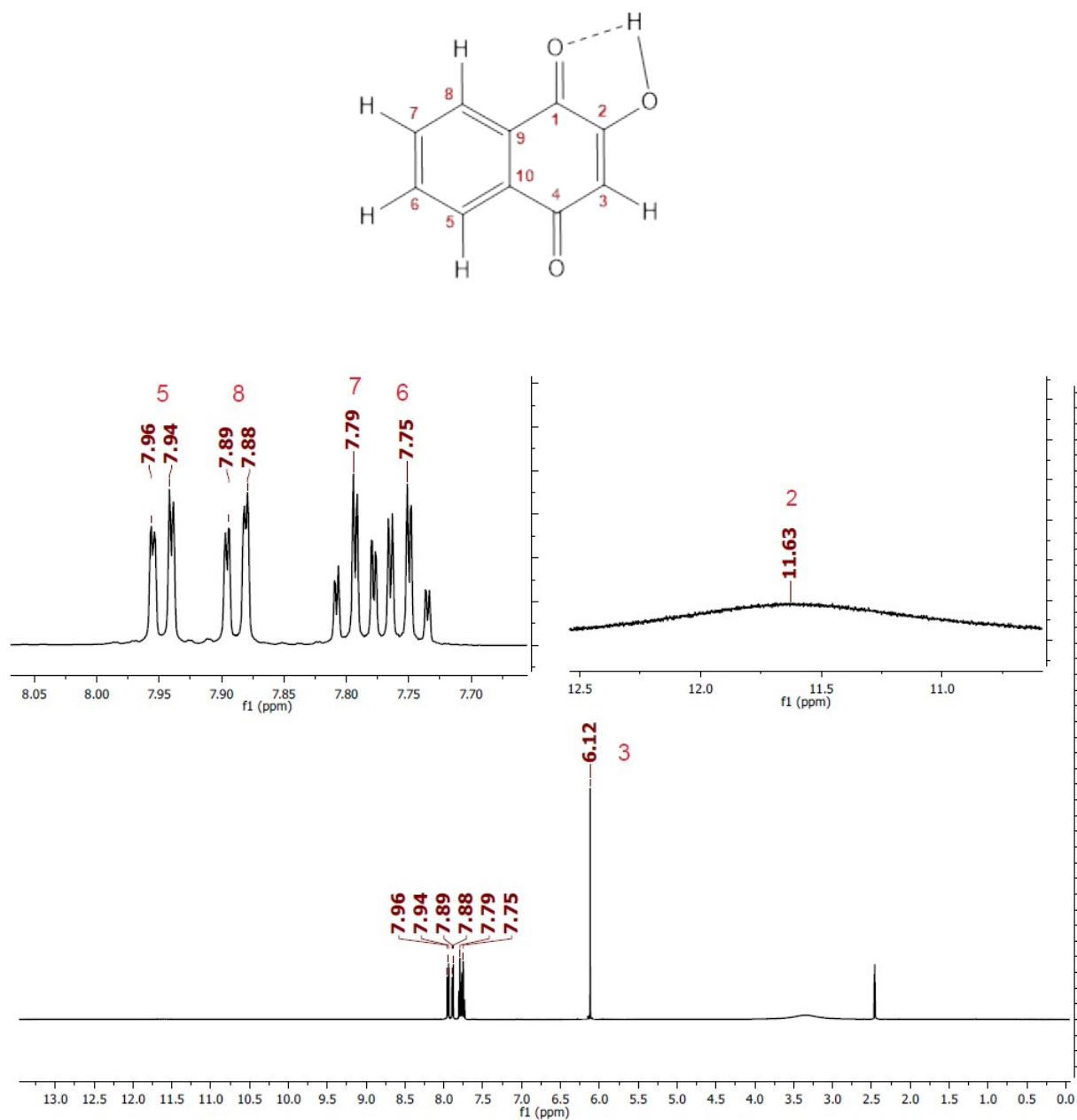


Fig. S2a: ^1H NMR spectrum of Lawsone (HLw) in DMSO-d_6 (400 MHz).

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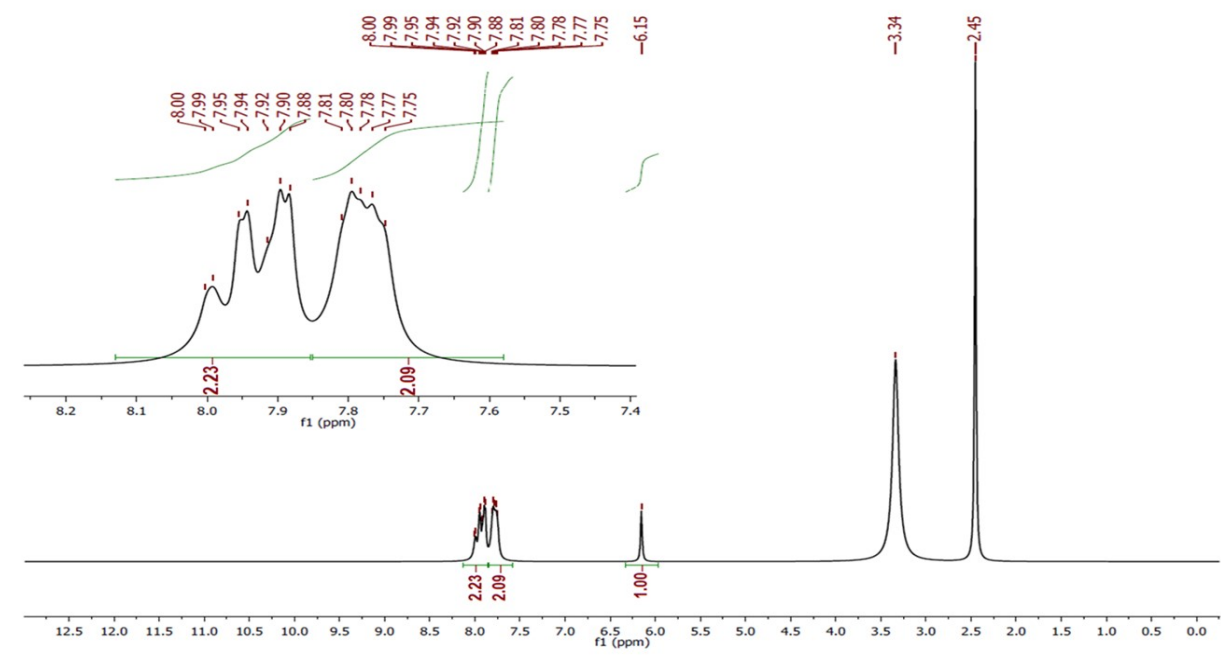


Fig. S2b: ^1H NMR spectrum of Complex (2) in DMSO-d_6 (400 MHz).

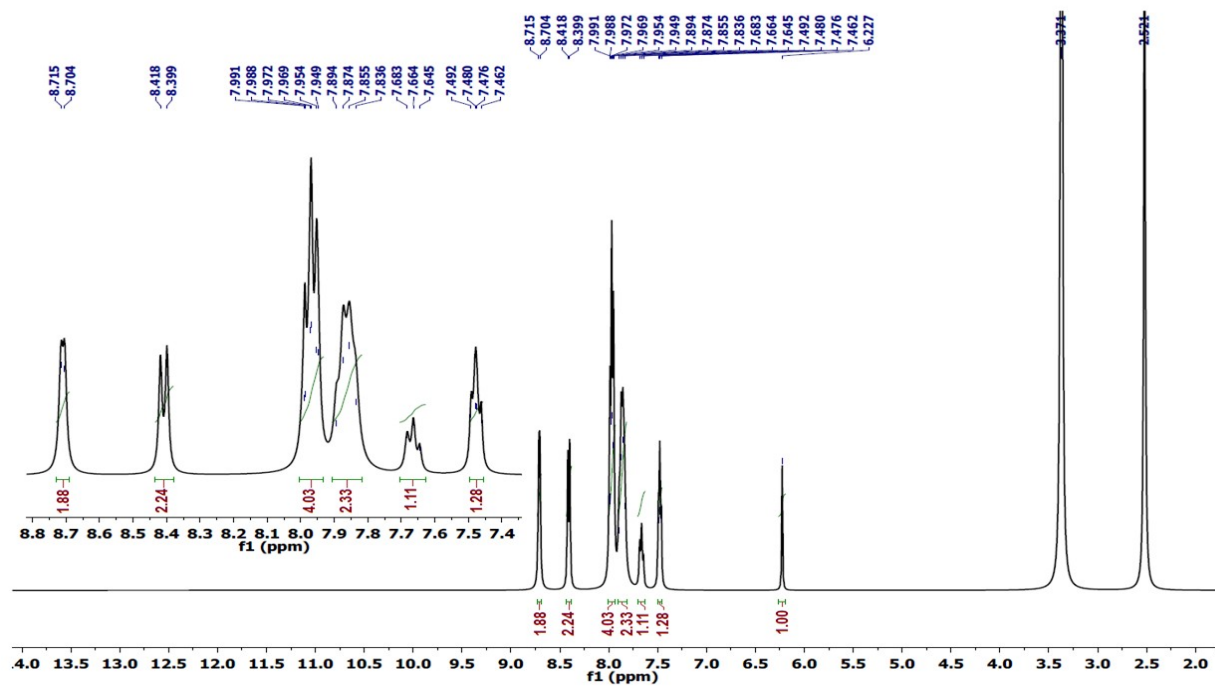
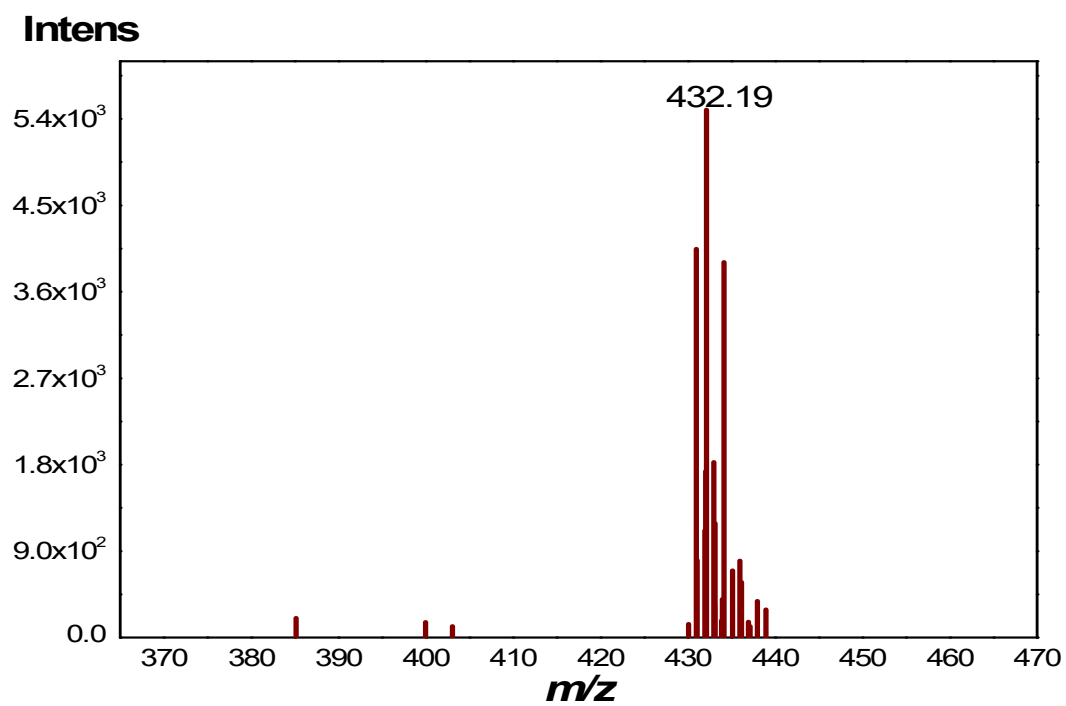


Fig. S2C: ^1H NMR spectrum of Complex (3) in DMSO-d_6 (400 MHz).

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3. ESI-MS spectra



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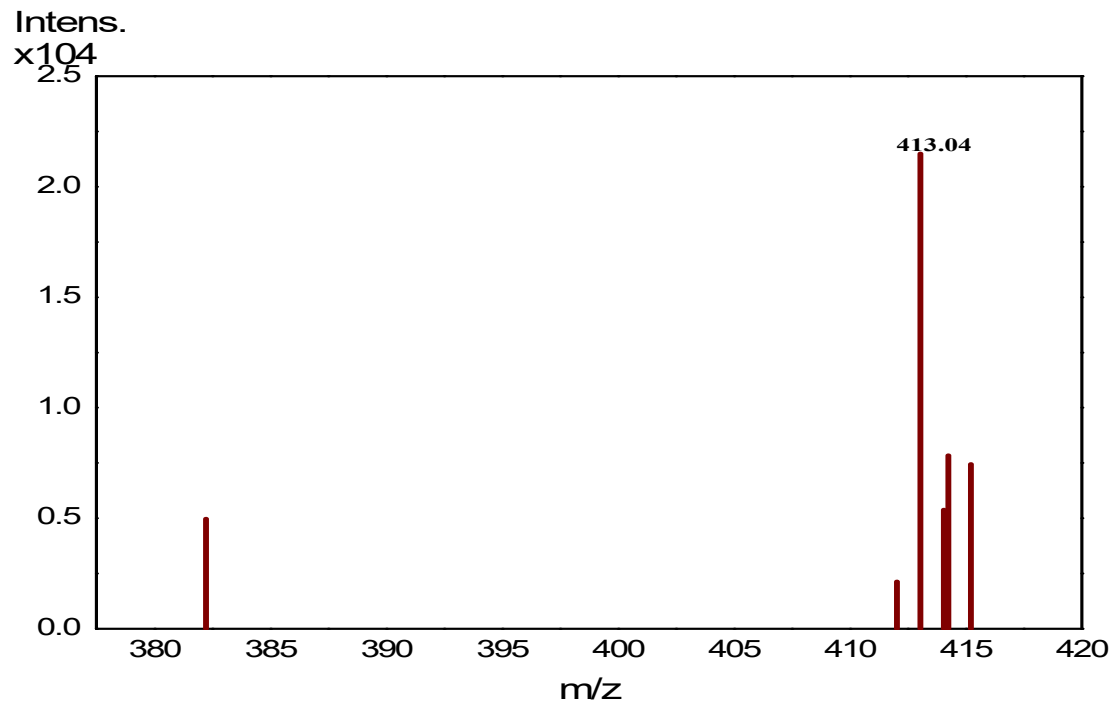


Fig.S3a. ESI-MS spectrum of **complex (1)**

Fig.S3b. ESI-MS spectrum of **complex (2)**

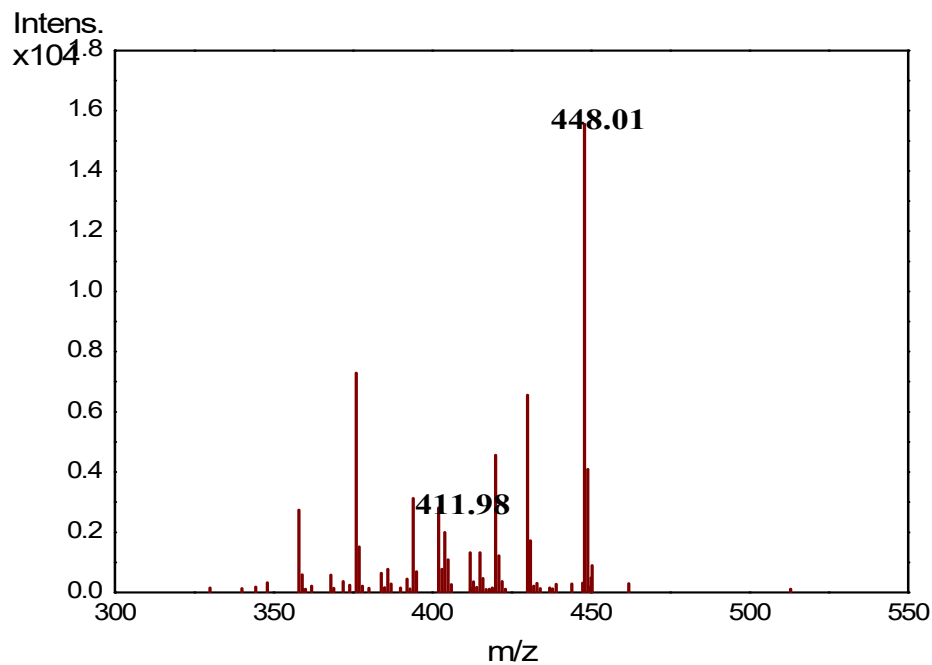


Fig.S3
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4. TGA diagrams :

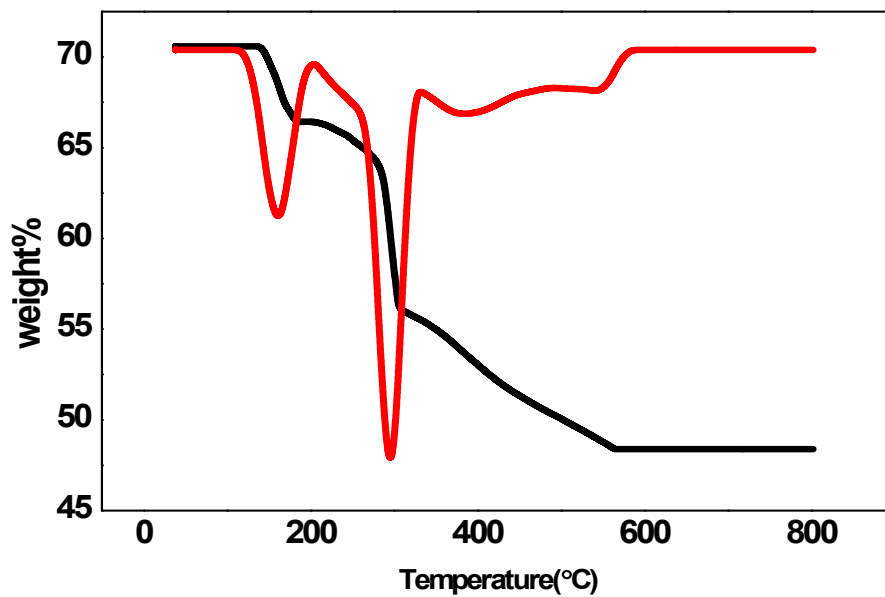


Fig. S4a:TGA of [VO(Lw)₂(H₂O)].H₂O (1)

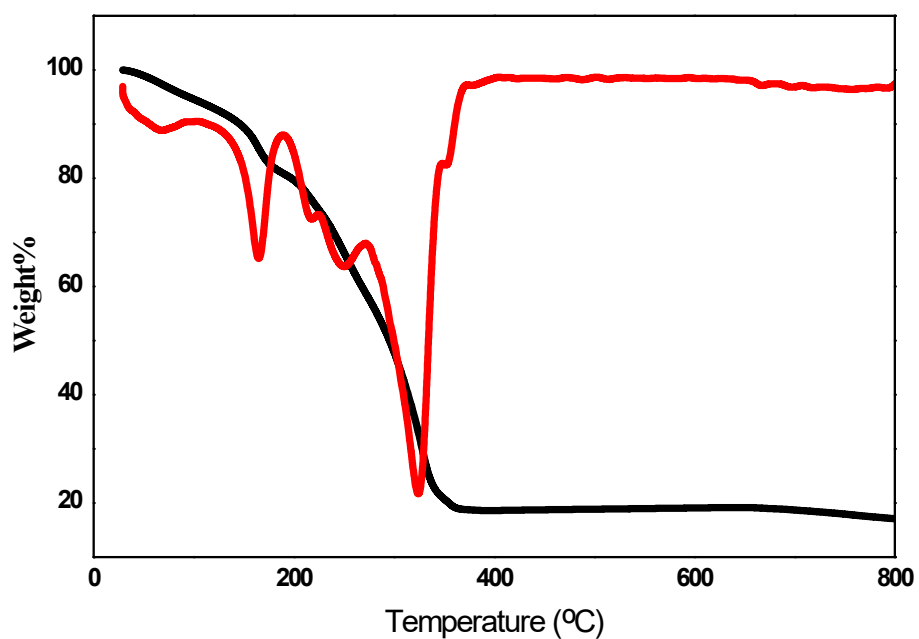


Fig. S4b:TGA of [VO(Lw)₂Cl].H₂O (2)

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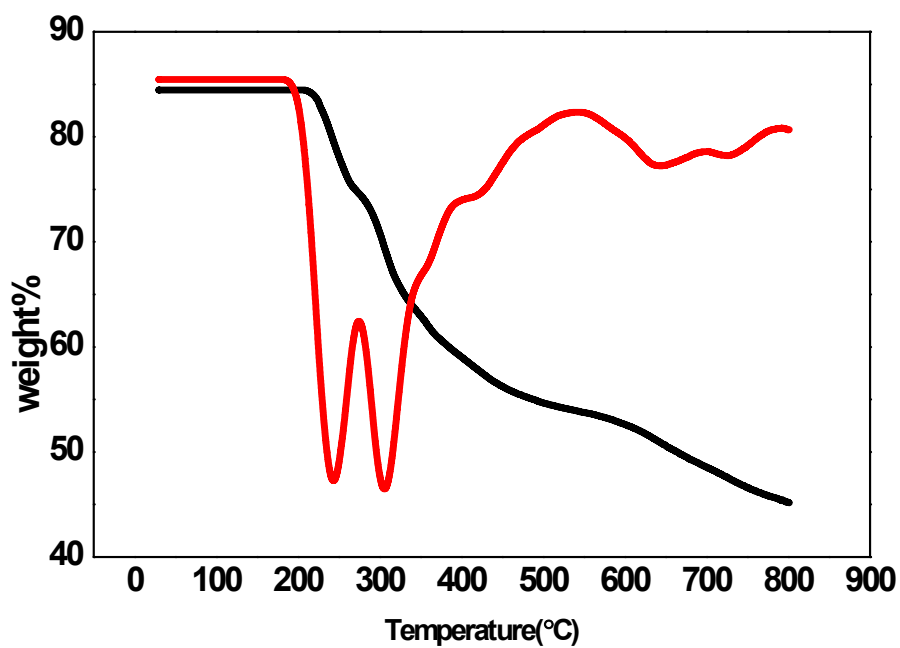
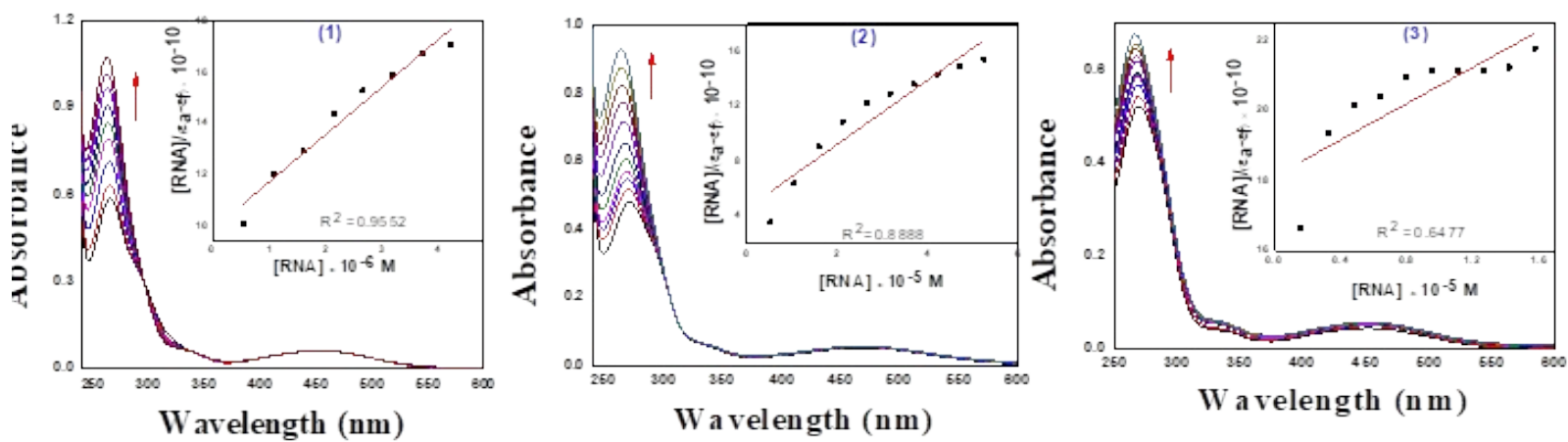


Fig. S4c:TGA of $[\text{VO}_2(\text{Lw})(\text{bpy})]$ (3)



5. RNA absorption study

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Fig.S5: Electronic spectral changes of the complexes (1–3) (50 μM) before and after the addition of (b) tRNA (0 – 100 μM), in Tris–HCl buffer (pH 7.2)) (inset: Plot of $[\text{RNA}]$ vs. $[\text{RNA}] / (\epsilon_a - \epsilon_f)$)).

6. DNA emission Study

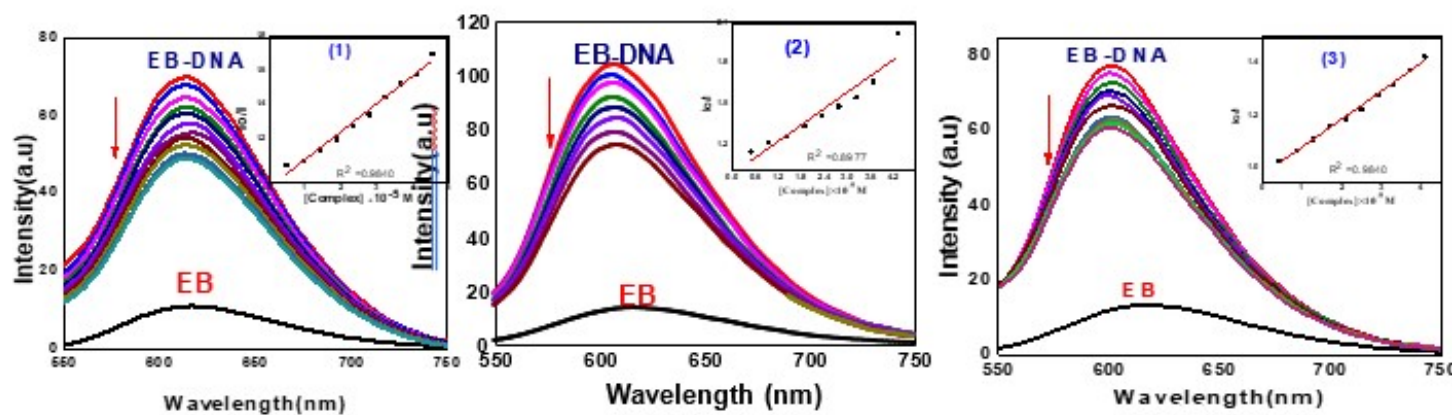


Fig.S6: Fluorescence spectra of EB –DNA complex in the presence of different concentrations of the complexes (1-3), (Inset: plots of I_0/I vs. $[\text{complex}]$).