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Synthesis and characterization of lipophilic triruthenium acetates bearing orthometallated phenanthrolines

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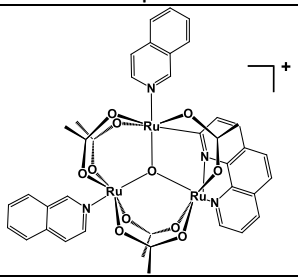
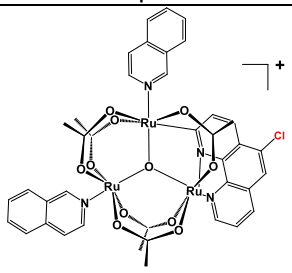
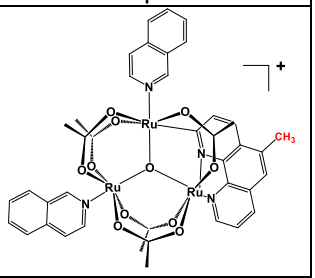
In the development of new drugs, lipophilicity is a feature of great interest, once this property can be related to the improvement of the interaction of the compound with biomolecules and its ability to cross cell membranes.[1] Regarding metal complexes, it is possible to modulate lipophilicity/hydrophilicity by the ligands in the coordination sphere, and lipophilic compounds can be achieved by the coordination of planar and hydrophobic structures, such as phenazines.[2] Furthermore, the inclusion of a metal-carbon bond is another way to enhance a lipophilic character in cyclometalated compounds.[3] Triruthenium acetates bearing hydrophobic ligands have shown promising anticancer and antitrypanosomal activities.[2] Therefore, we have synthesized two novel triruthenium acetates (**2** e **3**) aiming to improve the lipophilicity of such structures, by the inclusion of the extended ligand isoquinoline and the presence of orthometallated phenanthrolines. We have also investigated the impact of -Cl and -CH_3 on the lipophilicity of the complexes, using log P 1-octanol-water parameter. We have found positive values for log P, which indicates that all the complexes are lipophilic, although the presence of substituents seems to have no impact on the value. The chemical characterization of these complexes was done by spectroscopic methods (UV-Vis, IR, ^{1}H-NMR) and electrochemical experiments (cyclic and differential pulse voltammetry). Data for complex **2:** UV-Vis (λ (nm), log ε (L mol^{-1} cm^{-1})): 700, 3.87; 348, 4.17. FT-IR (ν(cm^{-1})): (ν_{as}(PF)), 1417 (ν_s(OCO)), 1540 (ν_{as}(OCO)). ^{1}H-NMR (CD_3CN) δacetates (ppm): 15.4, 7.34, 4.15, 0.00 and -1.22. Data for complex **3** is similar to **2**.

Table 1. Values of log P (1-octanol-water) at 37 ºC for three novel triruthenium acetates bearing orthometallated phenanthrolines.

	Complex **1**	Complex **2**	Complex **3**
			
log P at 37 ºC	0.73 ± 0.04	0.76 ± 0.04	0.77 ± 0.04

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References

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