

Supplementary Materials: Half-Sandwich Ru(II) Halogenido, Valproato and 4-Phenylbutyrato Complexes Containing 2,2'-Dipyridylamine: Synthesis, Characterization, Solution Chemistry and In Vitro Cytotoxicity

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Table S1. Parameters of selected non-covalent contacts (Å, °) detected in the crystal structure of [Ru(η^6 -*p*-cym)(dpa)I]PF₆ (3).

Contact	<i>d</i> (D–H) (Å)	<i>d</i> (H...A) (Å)	<i>d</i> (D–H...A) (Å)	$\angle$ (D–H...A) (°)
N2–H2A...F4 ⁱ	0.85(2)	2.40(3)	3.096(3)	140(3)
N2–H2A...F6 ⁱ	0.85(2)	2.14(3)	2.953(3)	161(3)
C3–H3A...F6 ⁱ	0.95	2.60	3.351(3)	136.3(2)
C4–H4A...F1 ⁱⁱ	0.95	2.53	3.210(4)	128.7(2)
C4–H4A...F5 ⁱⁱ	0.95	2.61	3.557(4)	173.8(2)
C15–H15A...F3 ⁱⁱⁱ	0.95	2.47	3.069(4)	121.1(2)
C16–H16A...F3 ⁱⁱⁱ	0.95	2.48	3.068(3)	120.44(14)

Symmetry codes: (i) $x - 1, y, z$; (ii) $1 - x, -y, 1 - z$; (iii) $2 - x, 1 - y, 1 - z$.

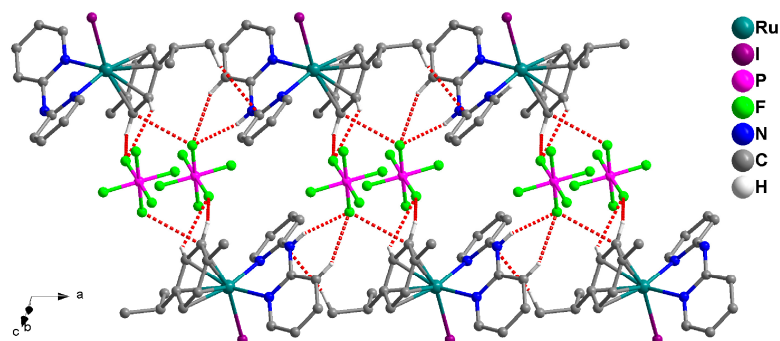


Figure S1. Part of the crystal structure of [Ru(η^6 -*p*-cym)(dpa)I]PF₆ (3) with non-covalent contacts depicted by red dashed lines. The hydrogen atoms not involved into the non-covalent contacts have been omitted for clarity.

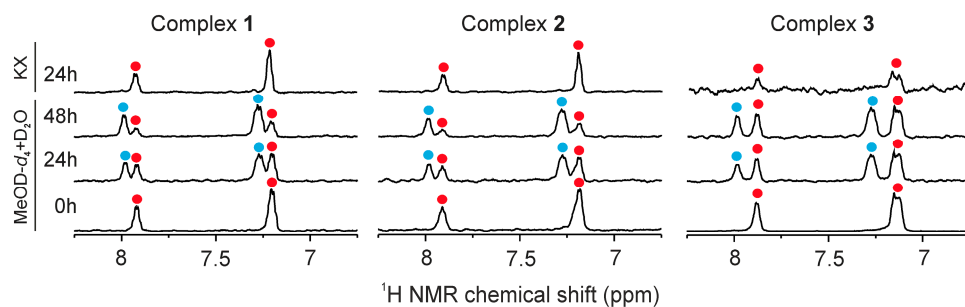


Figure S2. ¹H-NMR spectra acquired on 10% MeOD-*d*₄/90% D₂O solutions for the halogenido complexes 1–3 in different time points (0 h, 24 h and 48 h) and after the addition of the appropriate potassium halogenide (KX = KCl (for 1), KBr (for 2) or KI (for 3)). The signals of the initial complex are labelled by the red spheres, while the signals of hydrolysates are labelled by the blue ones.