Biological evaluation of tris-heteroleptic ruthenium complexes with DNA and BSA, docking studies analysis

S. Balou, M. Apostolopoulou, J. Stetou, C.A. Mitsopoulou

Inorganic Chemistry Laboratory, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou 15771, Greece

Presenting Author: sbalou@chem.uoa.gr

The coordination chemistry of ruthenium complexes with polypyridyl ligands is one of the most extensively studied area for potential anticancer drugs due to their catalytic reactions, photochemistry and redox properties [1-3]. As it has been proven, the interactions of these complexes with biomolecules such as CT-DNA and serum transport proteins are of great importance [4]. There is a plethora of ruthenium complexes with bidentate chelating ligands such as 2,2'-bipyridine (bpy) or 1,10-phenanthroline (phen) which exhibit intriguing interactions with biomolecules and show significant anticancer activity. Furthermore, the ligand 2-(2-pyridyl)-quinoxaline (pq) shows medicinal interest because of its antibacterial and anticancer activity [5,6].

For all the aforementioned reasons, two tris-chelated ruthenium polypyridyl complexes were synthesized in our laboratory. The interactions of these metal compounds with biomolecules delve into their possible anticancer properties. Both complexes $[Ru(pq)(bpy)_2](PF_6)_2$ and $[Ru(bpy)(phen)(pq)](PF_6)_2$, were studied for their binding affinity to bovine serum albumin (BSA) by UV-Visible absorption and emission spectroscopy. Finally, in an effort to evaluate their biological activity, DNA and BSA docking studies were performed.

References

- 1. M. Frezza et al., Curr. Pharm. Des., vol. 16, no. 16, pp. 1813–1825, Jun. 2010.
- A. K. Sahu, D. K. Dash, K. Mishra, S. P. Mishra, R. Yadav, and P. Kashyap, M. S. Seehra and A. D. Bristow, Eds. InTech, 2018.
- 3. M. Ganeshpandian, M. Palaniandavar, A. Muruganantham, S. K. Ghosh, A. Riyasdeen, and M. A. Akbarsha, Appl. Organomet. Chem., vol. 32, no. 3, p. e4154, Mar. 2018.
- 4. V. Brabec and J. Kasparkova, Coord. Chem. Rev., vol. 376, pp. 75–94, Dec. 2018.
- R. L. Williams, H. N. Toft, B. Winkel, and K. J. Brewer, Inorg. Chem., vol. 42, no. 14, pp. 4394–4400, Jul. 2003.
- 6. C. A. Mitsopoulou and C. Dagas, Bioinorg. Chem. Appl., vol. 2010, 2010,