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A drug-like pyridine appended sulfonamide ligand and its platinum complex: Synthesis, characterization and biological applications

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Introduction and objectives: Pyridine derivatives are often used as drugs because of their characteristics such as basicity, stability, small molecular size, water solubility and hydrogen bond-forming ability. The objective of this study was to synthesize a pyridine appended sulfonamide ligand and its platinum complex and to identify their drug-like properties.

Methods: Novel ligand, N(SO_2pyridine)dpa (L1) and its corresponding platinum complex, Pt(N(SO_2pyridine)dpa)Cl_2 (C1) were synthesized and characterized by X-ray crystallography, ^{1}H NMR, FT-IR, UV-Vis and fluorescence spectroscopic methods. Biological target prediction was carried out using 'SwissTargetPrediction' and 'SwissADME' servers and 'PyRx 0.9.4' software was used for molecular docking.

Results: Structural data confirmed the formation of the compounds and the S-N bond length for L1 was 1.6331 Å, whereas for C1, it was 1.622 Å. According to ^{1}H NMR results, peaks of L1 were de-shielded upon binding with the metal and the singlet peak observed at 4.62 ppm for methylene protons appeared as two doublets at 5.28 ppm and 6.06 ppm in the spectrum of C1. L1 displayed high fluorescence intensity in the visible range; it was lowered in C1, possibly due to the quenching of fluorescence upon binding to the metal. *In silico* analysis of drug-likeness indicated that L1 complies with the Lipinski rule of five and L1 was predicted to bind with GABA-A receptor and cyclooxygenase-2 with calculated binding affinities of -6.0 kcal/mol and -7.0 kcal/mol, respectively.

Conclusions: Drug-likeness of the ligand indicated that these compounds can be further investigated as anxiolytic and anti-inflammatory drug leads.

Keywords: *Drug, Pyridine, Sulfonamide ligand, Platinum complex*