



Synthesis and characterization of trimethylbenzene and chlorobenzene derivatized platinum complexes towards biological applications

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Synthesis of metal-based complexes as potential therapeutic agents for diseases like cancer, arthritis is a recent topic of interest. With the intention of identifying novel drug leads with potential biological applications, novel platinum complexes; {[Pt(N(SO₂trimethylbenzene)dpa)Cl₂] (C1) and [Pt(N(SO₂chlorobenzene)dpa)Cl₂] (C2)}, derived from sulfonamide ligands; {N(SO₂trimethylbenzene) dpa (L1) and N(SO₂chlorobenzene)dpa (L2)} were synthesized. These compounds were characterized by 1H NMR, X-ray crystallography, 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. Structural data confirm the formation of the compounds and the S-N bond length for L1 was 1.6273 Å whereas for the C1 it was 1.6461 Å. In 1H NMR data, the peaks of L1 were de-shielded upon binding with the metal and the singlet peak observed at 4.53 ppm for methylene protons appeared as two

doublets (5.08 ppm, 6.09 ppm) in the spectrum of C1. Similarly, in L2, a singlet peak observed at 4.56 ppm for methylene protons appeared as two doublets (5.23 ppm, 6.02 ppm) in the spectrum of C2. L1 shows high energy absorption bands at 205 nm and 227 - 295 nm due to intraligand π-π* and n-π* transitions whereas C1 displays absorption bands at 205 nm, 229 nm and 275 nm. L2 shows high energy absorption bands at 204 nm, 237 nm and 254 nm and C2 shows absorption bands at 204 nm and 275 nm. Both L1 and L2 display high fluorescence intensities in the visible range which have lowered in corresponding platinum complexes. *In silico* analysis of drug-likeness indicates that ligands comply with the Lipinski rule of five and they are predicted to bind with Cyclooxygenase-2 and L1 is predicted to bind with a calculated binding affinity of -6.9 kcal/mol showing their potential to be used as anti-inflammatory drug leads.

Keywords:

Anti-inflammatory, chlorobenzene, platinum, trimethylbenzene