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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(SO_2trimethylbenzene)dpa)Cl_2] (C1) and [Pt(N(SO_2chlorobenzene)dpa)Cl_2] (C2)}, derived from sulfonamide ligands; {N(SO_2trimethylbenzene) dpa (L1) and N(SO_2chlorobenzene)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 л-л*and n-л* 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

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The effect of the metal ion composition on the decarboxylation percentage of metal basic soap and level of unsaturation in producing green diesel

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The growing demand for fossil fuels has led to their depletion, causing higher fuel prices and threatening the sustainability of industrialized countries. Biodiesel is a renewable fuel produced through the trans-esterification of fatty acids, however, it has several technical issues such as lower energy density and less oxidation stability compared to petroleum diesel. Green diesel, an oxygen-free hydrocarbon-like fuel, produced through deoxygenation, solves the inefficiency issue of biodiesel. Deoxygenation techniques such as decarboxylation and decarbonylation are preferred to hydrodeoxygenation from an economic perspective. The decarboxylation of metal basic soap (MBS) is a promising method of deoxygenation for green diesel production, and the