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Synthesis and spectroscopic characterization of novel sulfonamide-based picolylamine ligands and their platinum(II) complexes towards potential biological applications

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The design and development of platinum(II) complexes remain a focal point in coordination chemistry due to their diverse applications in medicinal inorganic chemistry. Sulfonamide derivatives, in particular, offer versatile coordination environments and biological relevance. Herein, we report the successful synthesis of three new sulfonamide derivatized ligands with a 2-picolylamine moiety: N(SO_2-1-naphthalene)-2-picolylamine (L1), N(SO_2-2-naphthalene)-2-picolylamine (L2), and N(SO_2Me_2Nnap)-2-picolylamine (L3). These ligands were subsequently utilized to synthesize a series of three novel platinum(II) complexes: *cis*-[PtCl2(N(SO2-1-naphthalene)-2-picolylamine)] complex (C1), *cis*-[PtCl2(N(SO2-2-naphthalene)-2-picolylamine)] complex (C2), and *cis*-[PtCl2(N(SO2Me2Nnap)-2-picolylamine)] complex (C3). The structural properties of both the free ligands and the resulting metal complexes were comprehensively elucidated using spectroscopic techniques. X-ray crystallographic data revealed the crystal system of L3 ligand to be monoclinic, and the space group is P21/n. Fourier Transform Infrared (FTIR) spectroscopy confirmed the coordination of the ligands to the platinum center, specifically highlighting shifts in the S-N stretching frequencies which appear at lower wavenumbers compared to that of the corresponding free ligands. ^{1}H NMR spectral data provided detailed insights into the proton environments, showing characteristic downfield shifts upon complexation with the Pt(II) metal center. Furthermore, UV–Visible spectrophotometric measurements of all three Pt(II) complexes show a hypsochromic shift compared to the corresponding free ligands in the absorption spectra in methanol. These results collectively confirm the successful bidentate coordination of the picolylamine-sulfonamide scaffold to the platinum(II) center in a cis configuration. *In silico* Swiss target predictions suggest that human cyclooxygenase-2 as a potential target for L1, L2 and L3 ligands. This study may offer a pathway for further investigation into their potential biological applications such as anticancer and anti-inflammatory properties.

Keywords:

platinum complexes; 2-picolylamine; sulfonamide; anti-cancer; cyclooxygenase-2

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