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Palladium(II) Complex Bearing Diphosphines Moiety: Synthesis, Characterization and Biological Activity

Abdul Afiq Nazmi Abdul Aziz[a], Khairil Anuar Jantan[ab*]

Structured Abstract

Background: Palladium complexes have garnered interest due to their unique chemical properties and potential biomedical applications, including antimicrobial activity. PdI_2(dppf) ([1,1′-*Bis*-(diphenylphosphino)ferrocene]diiodopalldium(II)]) represents a promising candidate, showcasing versatile coordination chemistry and stability. This study focuses on synthesizing and characterizing PdI_2(dppf) and evaluating its antimicrobial potential. The study also using *In Silico* studies to predict the therapeutic potential of PdI_2(dppf).

Methods: PdI_2(dppf) was synthesized by reacting $(Ph_4P)_2[Pd_2I_6]$ with dppf in acetone under ambient conditions. Characterization included Fourier Transform Infrared (FTIR), UV-Visible Analysis, ^{1}H and ^{31}P Nuclear Magnetic Resonance (NMR), CHNS/O Analysis and Thermogravymetric Analysis (TGA). The antimicrobial properties were assessed using the Kirby-Bauer disk diffusion method on Mueller-Hinton agar (MHA), targeting Gram-positive and Gram-negative bacterial strains. *In Silico* studies using SwissADME and ProTox-III computational methods to predict the compound's drug-likeness and toxicity profile.

Results: PdI_2(dppf) was obtained as an red precipitate with high purity and stability. FTIR spectra confirmed the coordination of dppf with palladium through significant peaks at 1480–1430 cm^{-1} (C=C stretches) and 1200–900 cm^{-1} (P–C bonds). UV-Vis spectroscopy revealed absorbance at 330 nm, indicative of metal-ligand charge transfer. NMR spectra provided detailed insights into the chemical environment of the complex. The antimicrobial assay demonstrated PdI_2(dppf)'s moderate activity against tested bacterial strains, with an inhibition zone of 6-13 mm at 4 different concentrations which are 1mL, 2mL, 3mL and 4mL. PdI_2(dppf) categorized as toxicity class 4 and have a possibility for drug development.

Conclusion: PdI_2(dppf) was successfully synthesized and characterized, confirming its structural and electronic properties. Preliminary antimicrobial tests highlight its potential as a therapeutic agent, warranting further studies on its biological applications and toxicity profile. Toxicity and pharmacokinetics profile of [PdI_2(dppf)] complexes succesfully done.

Keywords: PdI_2(dppf), palladium complex, 1,1′-Bis(diphenylphosphino)ferrocene, antimicrobial activity

*Correspondence: khairil0323@uitm.edu.my

[a] School of Chemistry & Environment, Faculty of Applied Sciences, Universiti Teknologi MARA, Shah Alam, Malaysia

[b] Multifunctional Nanoporous Material Research Group (MULNA), Universiti Teknologi MARA, Shah Alam, Malaysia