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New Cyclopalladated Complexes Containing 2,5-Dimethyl-1,3,4-Thiadiazole: Synthesis, Characterization and Antineoplastic Activity

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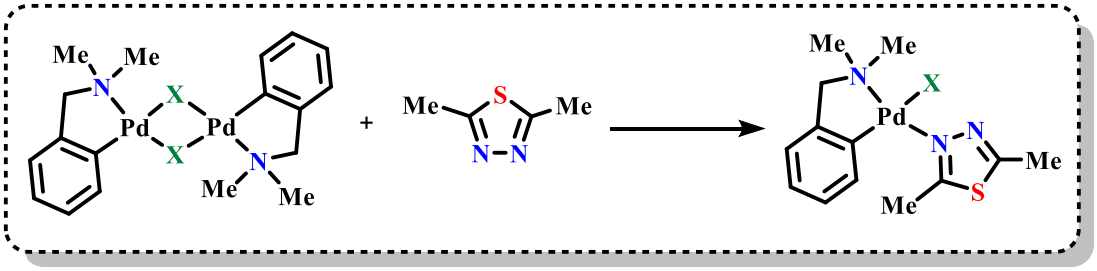
Palladium complexes have received significant attention in research focused on the synthesis of coordination compounds with potential biological applications. The palladium(II) ion, known for its tetracoordinated nature, adopts a square planar structure. This geometric and electronic configuration is similar to that of platinum(II) compounds, which are already recognized for their biological applications, especially in antineoplastic treatments. Cyclopalladated compounds have greater stability in biological systems compared to other palladium(II) complexes, demonstrating greater efficacy even at low concentrations.[1] The activity of a compound depends not only on the nature of the metal ion, but also on the ligands present. Thiadiazoles are organic compounds characterized by a heterocyclic structure containing one sulphur and two nitrogen atoms. They can have different isomers, with the 1,3,4-thiadiazole configuration being the most frequently reported for its biological activities.[2] Given these facts, our research aimed to synthesize and structurally characterize new palladium(II) cyclopalladated complexes containing *N,N*-dimethylbenzylamine (dmba), 2,5-dimethyl-1,3,4-thiadiazole (dtz) and a halogen (X = Cl, Br, I) as ligands. The compounds were synthesized from the cleavage of $[Pd(dmba)(\mu\text{-}X)]_2$ by the thiadiazole compound. They were characterized using thermogravimetric analysis (TG), infrared spectroscopy (FTIR), Nuclear Magnetic Resonance spectroscopy (NMR) and single crystal X-ray diffraction. The compounds synthesized proved to be effective in reducing the cell viability of HepG2 and MCF-7 and are potential antineoplastic agents.



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References

1. Czarnomysy, R.; Radomska, D.; Bielawski, K.; Szewczyk, O. K.; Roszczenk, P.; *Int. J. Mol. Sci.*, **2021**, *22*, 8271.
2. Anthwal, T.; Paliwal, S.; Nain, S.; *Chemistry* **2022**, *4*, 1654.