Indole conjugates – synthesis, structural analysis and evaluation of biological activity

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The aim of my doctoral thesis was to synthesize indole conjugates and their complexes, as well as to analyze the structure and evaluate the biological activity of the obtained compounds.

Using gramine, I synthesized over thirty new indole-azole conjugates in which the azole is attached to the indole through a methylene linker. Based on their structure, they can be divided into three groups: 1) indole-imidazole, 2) indole-thioketone, and 3) indole-pyrazole. The conjugates of the first group were used as ligands in the complexation reaction with zinc chloride.

All new derivatives were characterized by mass spectrometry, FT-IR, and NMR spectroscopy and for most of them the crystal structures were determined.

In collaboration with the Faculty of Biology of Adam Mickiewicz University, I investigated the compounds' hemolytic and antioxidant properties. Molecular docking allowed us to determine the affinity of selected derivatives to enzymes involved in oxidative stress.

In addition, studies in collaboration with the University of Life Sciences in Poznań determined the compounds' antibacterial and antifungal properties. Also, the druglikeness of all conjugates and complexes were tested using *in silico* methods.

A comprehensive analysis of the biological activity of the obtained derivatives established the relationship between the compound's chemical structure and its biological properties.