Molecular docking study of a novel series of pyrazolines as potential inhibitors of phosphodiesterase type 5 (PDE5)

Istraživanje nove serije pirazolina kao potencijalnih inhibitora fosfodiesteraze tipa 5 (PDE5) metodom molekularnog uklapanja

Vesna Rastija¹, Maja Molnar², Harshad Brahmbhatt²

¹ Faculty of Agrobiotechnical Sciences Osijek, Josip Juraj Strossmayer University of Osijek, Vladimira Preloga 1, HR-31000 Osijek, Croatia, vrastija@pfos.hr
² Faculty of Food Technology Osijek, Josip Juraj Strossmayer University of Osijek, Franje Kuhaca 20, 31000 Osijek, Croatia, maja.molnar@ptfos.hr; brahmbhatthurshad@hotmail.com

Phosphodiesterase type 5 (PDE5) is a cyclic guanosine monophosphate (cGMP)-specific enzyme and mostly expressed in smooth muscle tissue of corpus cavernosum, heart, lung, platelets, prostate, urethra, bladder, liver, brain, and stomach. Inhibitors of PDE5, prevent the hydrolysis of cGMP and become effective treatment to diseases associated with low cGMP level, such as pulmonary arterial hypertension. [1] It has been well-documented that pyrazole-containing compounds diverse chemotherapeutic potentials, such as antileukemic and antiproliferative agents. Beside, halogenated organic compounds has been widely use as many drug candidates. [2] Recently, we have synthesized a novel series of halogenated pyrazolines. Molecular docking study was performed to explain in silico the binding interaction with the PDE5 (PDB: 4oew). Molecular docking has confirmed that compound 5-(2,6-dimethoxyphenyl)-3-(4-fluorophenyl)-4,5-dihydro-1H-pyrazole-1-carbaldehyde has lowest total energy binding (-105,69 kcal/mol). The binding interactions of the most active compound have shown strong hydrogen bonding and van der Waals interactions with the target protein.

![Molecular structure of derivate of pyrazoline as the most promising inhibitor of phosphodiesterase type 5.](image)

Figure 1. Molecular structure of derivate of pyrazoline as the most promising inhibitor of phosphodiesterase type 5.

References
