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ZBORNIK POVZETKOV
BOOK OF ABSTRACTS

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In silico and stability analyses of selected pesticides in use in Serbia

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Tebuconazole, pendimethalin, pyraclostrobin, propiconazole and famoxadone are pesticides approved as active substances in the formulations for the plants protection in the Republic of Serbia. Tebuconazole, propiconazole, pyraclostrobin, and famoxadone belong to fungicides, and pendimethalin is a herbicide [1].

The methanol solutions of tebuconazole, pendimethalin, propiconazole and famoxadone were kept tightly sealed in the fridge for 9 months, and the methanol solution of pyraclostrobin for 20 months. The solutions were then analysed using GC-MS [2]. *In silico* analyses consisted of optimization of the structures of selected pesticides by conformational search and their molecular docking against acetylcholine esterase (AChE) of *Mus musculus* and *Homo sapiens* under Schrodinger 2022-3. ADMET parameters of the compounds were calculated using QikProp v7.0 software running in normal mode (Schrödinger, Inc., New York, NY, USA).

GC-MS analysis showed that only the pyraclostrobin solution was degraded. Molecular docking showed that famoxadone was the strongest inhibitor of AChE in *M. musculus*, and propiconazole in *H. sapiens*. Two interactions are common for all investigated pesticides against AChE in *M. musculus*: His 381 and Phe 531. A different situation was observed in *H. sapiens*. They have no common contact with AChE, and in general less interactions with AChE were observed compared to *M. musculus*. The acute oral toxicities of pendimethalin, pyraclostrobin and famoxadone in mice/rats are > 4500 mg/kg [3], so their *in silico* inhibitory effects on AChE in *H. sapiens* were compared with those of approved Alzheimer's drugs (donepezil, rivastigmine and galantamine). Their Glide scores in kcal/mol (-4.72 for pendimethalin, -4.38 for pyraclostrobin and -4.80 for famoxadone) were better than those for donepezil (-3.90) and rivastigmine (-2.94). According to the calculated ADMET parameters, all selected pesticides are orally active.

Therefore, pendimethalin, pyraclostrobin and famoxadone can be considered for further studies in the treatment of Alzheimer's disease, and perhaps their less toxic modifications can be developed in the future, and more stable in case of the pyraclostrobin.

Keywords: pesticides, GC-MS, stability, Alzheimer's disease, molecular docking.

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