Prof. Dr. Bojana Obradović

Editor-in-Chief

Dear Sir,

Please find enclosed the manuscript entitled "Spectroscopic and quantum chemical elucidation of newly synthesized 1-aryl-3-methyl-3-phenylpyrrolidine-2,5-diones as potentional anticonvulsant agents" by Jelena Petković Cvetković *et al.* to be submitted as an Original scientific paper to Hemijska industrija. All co-authors have seen and agree with the content of the manuscript and there is no financial interest to the report. We certify that the submission is not under review at any other publication.

Derivatives of succinimide (pyrrolidine-2,5-dione) are used as anticonvulsant drugs in the treatment of epilepsy for a long time. Additionally, these compounds have been recently recognized as promising materials for applications in optoelectronics and great effort is invested in their synthesis and characterization. In this manuscript, we present a spectroscopic and theoretical study of newly synthesized 1-aryl-3-methyl-3-phenylpyrrolidine-2,5-diones. The interpretation of effects of different substituents on the phenyl ring in the position 1 on the spectroscopic properties (UV, FT-IR, 1H and 13С NMR) is based on Hammett equation as well as on quantum-chemical calculations which have been performed by the DFT(B3LYP)/6-311G(d,p) method. It is demonstrated that substituents change the conjugation effect and further affect the pathways of intramolecular charge transfer (ICT). We have also analyzed the energy gaps between the HOMO and LUMO orbitals which is relevant not only for the ICT character, but also for the biological activity of compounds. Due to the potential biological activities of novel succinimide derivatives, an ADMET factor profiling and *in-silico* prediction by Pass program have been performed.

We hope that the editorial board and the reviewers will consider this study appealing enough to be a part of Hemijska industrija.

Sincerely yours,

Dr. Bojan Božić

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