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| **CoMFA STUDY AS AN EFFICIENT APPROACH FOR THE DESIGN OF BIOLOGICALLY ACTIVE BIS-1,2,4-TRIAZOLES** |
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| **SLIVKA Mikhailo1,2, MOYZESH Olexander1, GRYGORKA Hanna1, KOROL Nataliya1,** **FIZER Maksym3, MARIYCHUK Ruslan2** |
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| *1Uzhhorod National University, Uzhhorod, Ukraine, mikhailo.slivka@uzhnu.edu.ua, +380999408740**2University of Presov, Presov, Slovak Republic, ruslan.mariychuk@unipo.sk**3Institute of Chemistry Slovak Academy of Sciences, Bratislava, Slovak Republic, mmfizer@gmail.com* |
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| *Computational approaches became an efficient and a suitable technique for the design of significant compounds with valuable properties, prediction of interaction particularities and could calculate lot of other important values. CoMFA (Comparative molecular field analysis) study is an advance that develops and compars the steric and* [*electrostatic interaction*](https://www.sciencedirect.com/topics/chemistry/electrostatic-interaction) *fields in the 3D space around set of aligned congeneric molecules and correlating this comparison with variation in their biological activity.**Using the example of the series of prenyl-alkylated bis-1,2,4-triazole derivatives, the theoretical investigations included CoMFA studies for the target compounds were carried out. For this purpose, an online tool https://www.3d-qsar.com was used. The r2 for steric model field was 0.665, for the electrostatic – 0.363. The q2**are -0.425 and -0.572 corresponding. The common values of r2 and q2**for both model fields are 0.697 and -0.646. Obtained statistical results for both steric and electrostatic model fields and based on these data, we got predicted activities and built the corresponding correlation curve with the existing experimental results. The generated electrostatic contour maps demonstrated that electronegative substituents are proper in the region of triazole ring or terminal methyl group of prenyl substituent and electropositive substituents are satisfied in the field of double bond of prenyl group, aromatic substituents and C6 in the cases of alkyl groups in the 4th position of triazole ring. The generated steric contour maps demonstrated that bulky substituents are proper in the region of triazole rings and prenyl groups and are not satisfied to be added into the substituents in the 4th position.**Thus, as the result of current study, we determine the best directions for functionalization of novel series of bis-1,2,4-triazoles, which would increase the biological activities of target compounds.* |
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| ***Keywords****: Synthetic Design, CoMFA, bis-Triazoles, Eco-friendly Approaches* |
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| ***Biography*** |  |  |
| D:\ElCycl\foto_Slivka.jpg | *Mikhailo Slivka was born in Uzhhorod, Ukraine in 1974. He graduated with honors from Uzhhorod National University in 1996 and obtained his Ph.D. in organic chemistry at Institute of Organic Chemistry in Kyiv (Ukraine), in 2001. His Dr.Sc. thesis was devoted to electrophilic cyclization reaction of 1,2,4-triazoles. At present, he is Professor and research group leader at Uzhhorod National University (Uzhhorod, Ukraine). His scientific interests include synthesis of functional and condensed heterocycles via intramolecular electrophilic cyclization via green approaches, investigations of the reactivity of fused heterocycles and their application.* |