BOOK OF ABSTRACTS

COST Training School

COST action CA21101 COSY

Multiscale modeling of the properties of compounds: From isolated molecules to 3D materials relevant for industrial and astrophysical applications

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Self-discriminating assembly and biorecognition of a spirohydantoin derived from α-tetralone

Anita M. Lazić,[1] Ivana S. Đorđević,[2] Lidija D. Radovanović,[3] Dragan M. Popović,[2] Jelena R. Rogan,[3] Nemanja P. Trišović,[3] Goran V. Janjić [2]

[1]Innovation Center, Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, [2]Department of Chemistry, University of Belgrade – Institute of Chemistry, Technology and Metallurgy – National Institute of the Republic of Serbia, Belgrade, Serbia, [3]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

The hierarchical development of the crystal structure of racemic 3-(4-methoxybenzyl)-6,7-benzo-1,3-diazaspiro[4.5]decane-2,4-dione was analyzed through cooperativity of various homo and heterochiral dimeric motifs associated with the presence of different intermolecular interactions, namely strong N–H···O and weaker C–H···O, C–H···π and PILOs.[1] Although a bigger number of the contacts in the environment of the tetralin unit results from its larger contact surface, the 4-methoxybenzyl unit provides a greater contribution to the overall stabilization. In addition, the investigated compound is identified as a potential inhibitor of kinase enzymes and AG protein-coupled receptors, with a slightly higher affinity for the later enzyme. An analysis of the nature of the amino acid residues around the tetralin and 4-methoxy benzyl units revealed that interactions with nonpolar groups are the most prevalent and even more numerous than interactions with other amino acid residues (polar, positive and negative).

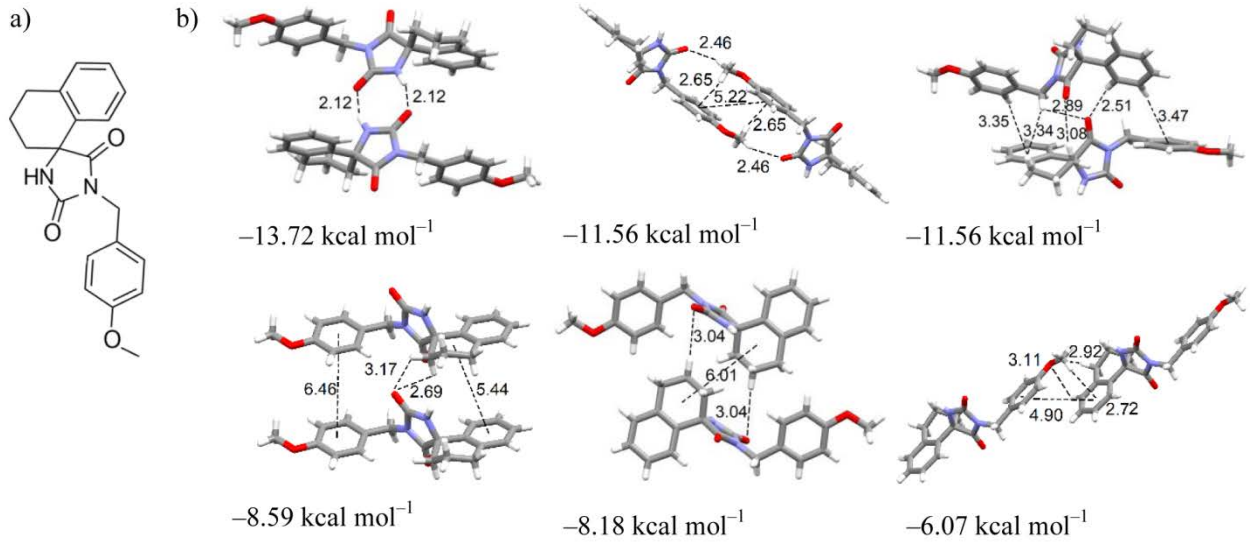

Fig 1. a) Chemical structure of 3-(4-methoxybenzyl)-6,7-benzo-1,3-diazaspiro[4.5]decan-2,4-dione and b) Dimer motifs observed in the crystal structure with their interaction energies.

References:

1. A. M. Lazić, I. S. Đorđević, L. D. Radovanović, D. M. Popović, J. R. Rogan, G. V. Janjić, N. P. Trišović, *ChemPlusChem* (2020), **85**(6), 1220.