



*Electronic Processes in Organic and  
Inorganic Materials  
(ICEPOM-12)*

**June 1 - 5, 2020  
Kamianets-Podilskyi, Ukraine**

*With support of*  
**Taras Shevchenko National University of Kyiv  
Institute of Physics, NASU  
Kamianets-Podilskyi National Ivan Ohienko University**



**ICEPOM-12**  
**Conference abstracts**

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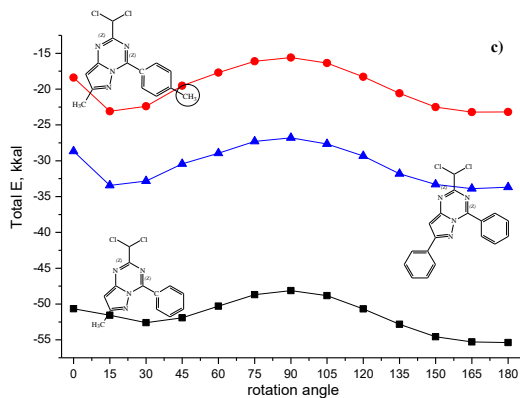
## ENERGY OF THE ROTATION BARRIERS PHENYL SUBSTITUENTS IN PYRAZOLO[1,5-*a*][1,3,5]TRIAZINES AS A FACTOR THE STABILIZATION OF [PHARMACOPHORE-BIOMOLECULE] COMPLEX

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The heterocyclic compounds with branched conjugated systems can generate the enough complementary structure with the many biopolymers, what is considered as an important condition for increasing of selectivity to potential targets. It was found that pyrazolo[1,5-*a*][1,3,5]triazines exhibit higher anticancer activity, by inhibiting cancer cell enzymes [1]. Then it could be assumed that the branched  $\pi$ -electronic system of the phenyl cycle should effectively participate in the mechanism of interaction of the pharmacophore with certain protein molecules.



In the interaction of pyrazolo[1,5-*a*][1,3,5]triazines with biomolecules, torsion angles of phenyl substituents play an important role for the formation and stabilization of the complex. The performed calculations give the barriers of the phenyl substituents in different positions varied appreciably. Firstly, it can be seen that the rotation barriers for phenyl introduced into the 5- and 6-membered ring of the heterocyclic

“platform” are significantly different ( $\approx 6$  kcal/mol). It should be noted that both barriers noticeably decrease with the simultaneous introduction of two phenyl substituents ( $\approx 3$  kcal/mol), i.e., the expansion of the entire conjugated system causes a decrease in the rotation barriers of phenyl cycles. A decrease in the barrier occurs even when a weak donor methyl substituent is introduced into the *p*-position of the phenyl residue.

It can be assumed that a decrease in the rotation barriers of phenyl substituents will lead to a decrease in the activation energy of the interaction of pharmacophore substances with biologically active molecules (proteins, nucleic acids). Thus, the [Pharmacophore-Biomolecule] complex will form more easily and have higher stability.

[1] Sun L., Bera, H., & Chui, W. K. *Eur. J. of Med. Chem.*, **2013**, 65, 1–11.

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