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ADD-ONS TO MOLECULAR MODELING METHODS: IMPROVEMENT IN ACTIVITY PREDICTION

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The basic task of molecular modeling consists of several parts:[1]

• Development and application of molecular modeling methods as the first stage of directed synthesis, allowing (a) to predict the structures of products of directed synthesis, (b) to establish reaction mechanisms and (c) to determine key electronic and spatial effects that control the synthesis process and determine the activity of individual molecules, and active classes of compounds and complexes.

• practical validation of predictive modeling methods by obtaining substances with properties specified during modeling.

Methods and practical results of research:

1. FEP (Free Energy Perturbation):

• Syk kinase inhibitors. A set of new Syk kinase inhibitors (non-Hodgkin lymphoma and rheumatoid arthritis) in the submicromolar concentration range was modeled and synthesized;[2]

• selective inhibitor of ABL tyrosine kinases PF-114. PF-114 inhibits T315I and other mutant forms of the BCR/ABL protein (resistant forms of chronic myeloid leukemia).[3]

2. Searching for active sites for a specific ligand on the entire protein surface[4] allows one to determine both the implicit active site of the protein and previously undetected secondary activity. An inhibitor of the main protease COVID-19 has been identified[5] as a secondary activity of a known drug.

3. QM-cluster methodology (quantum chemical methods): a method for calculating the affinity of bioisosteres has been developed.[6]

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