PR-56

MODELING THE ANTITUBULIN ACTIVITY OF BENZIMIDAZOL-2-YL CARBAMATES: MINI-REVIEW

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Abstract. Computer modeling has become the commonly used method to explain biological activity of substances [1]. Despite the technical attractiveness of this approach, there are serious difficulties in creating a theoretical model that would correspond to the experimental data [2]. The purpose of this mini-review is to systematize scientific efforts to predict the binding site of benzimidazol-2-yl carbamate derivatives with β-tubulin. Interest in the generalization of these studies is due to the fact that while the crystal structure of the complex tubulin with methyl [5-(2-thienylcarbonyl)-1H-benzimidazol-2-yl] carbamate 1 was published only in 2015 (PDB id 5CA1, Figure 1), some details of the interaction of benzimidazol-2-yl carbamates with β-tubulin could be predicted before it. This mini-review summarizes the results of such works.

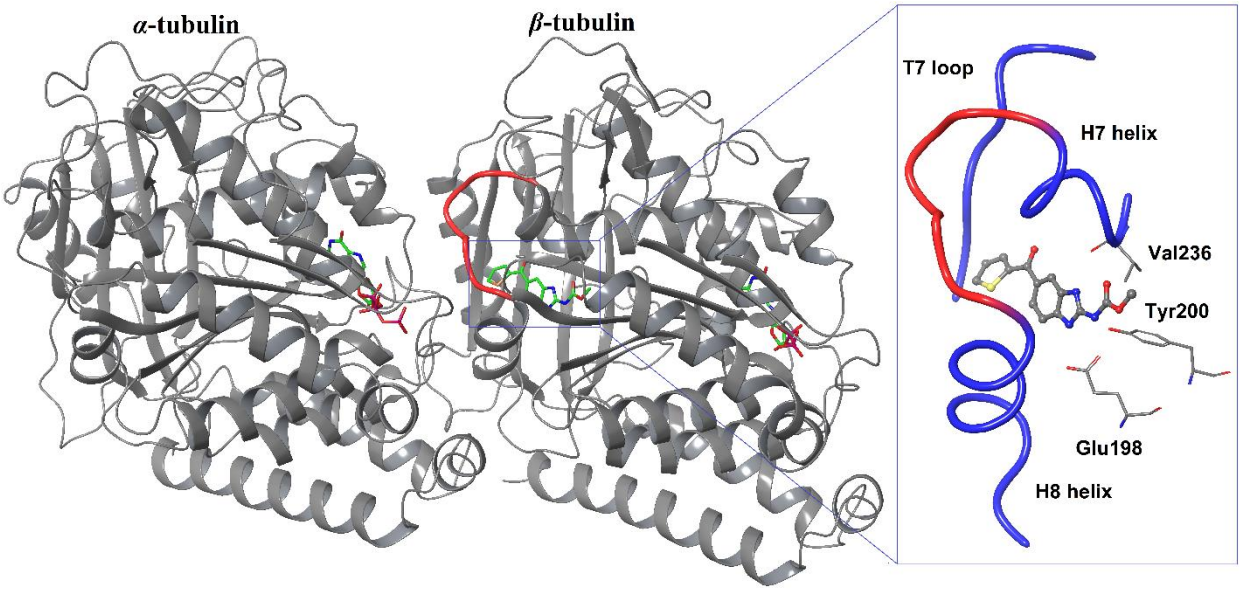

Figure 1. Nocodazole complex with tubulin (PDB id 5CA1).

References

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This research was supported by the Russian Foundation for Basic Research (grant No. 18-316-20018).