

## Accepted Manuscript

Title: Structural insight into the glucokinase-ligands interactions. Molecular docking study

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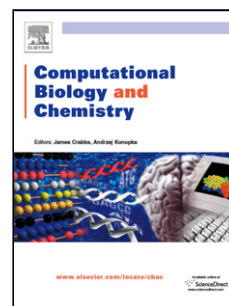
PII: S1476-9271(16)30264-X  
DOI: <http://dx.doi.org/doi:10.1016/j.compbiolchem.2016.08.001>  
Reference: CBAC 6571

To appear in: *Computational Biology and Chemistry*

Received date: 27-5-2016  
Revised date: 27-7-2016  
Accepted date: 7-8-2016

Please cite this article as: Ermakova, Elena, Structural insight into the glucokinase-ligands interactions. Molecular docking study. *Computational Biology and Chemistry* <http://dx.doi.org/10.1016/j.compbiolchem.2016.08.001>

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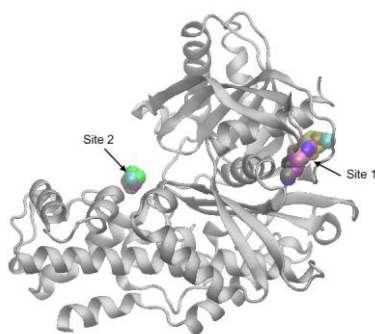
**Structural insight into the glucokinase-ligands interactions. Molecular docking study.**

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**Graphical abstract****HIGHLIGHTS:**

- Docking simulation was performed to study interaction of glucokinase with ligands
- AutoDock and Vina programs accurately reproduce the experimental ligand poses
- Correlation between free energy of binding and bioactivity of activators is discussed

**Abstract**

Glucokinase (GK) plays a key role in the regulation of hepatic glucose metabolism. Inactivation of GK is associated with diabetes, and an increase of its activity is linked to hypoglycemia.

Possibility to regulate the GK activity using small chemical compounds as allosteric activators

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