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Molecular design of a new class of inhibitors for ion channel of influenza protein

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Motivation: A design of novel anti-influenza drugs is a task of great importance due to a capability of influenza viruses to infect fast a large human population by occasional cross of inter-species barriers and to rapid mutate.
Methods: Transport of H^+ ion through ion channel of protein M2 of cell membrane can be blocked by drug molecule bound inside of ion channel. A new class of molecular blockers is suggested. Binding mode and binding energies are calculated for a set of novel molecular structures constructed on the base of diazobicyclooctane.
Results: A set of molecular structures as a derivatives of leading compound is suggested. Binding modes and energies of binding are calculated by method of hierarchical blind docking [1]. A molecular structure of an optimal molecular blocker is suggested.
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References

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