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Abstracts aspects of open literature

Nico M. Temme	2007
<i>Data Archiving And Networked Services (DANS)</i>	
[2] Single Neurons in the Human Brain Encode Numbers	
Florian Mormann, Esther F. Kutter, Andreas Nieder et al.	2018
<i>Neuron</i>	

Molecular Docking of Selective Hypocretin (orexin) receptor 2 Agonists: Achieving Binding Energies Exceeding -14.2 kcal/mol via Soluble and Synthetically Accessible Supramolecular Scaffolds.

Answer Citations (54)

Introductory Intermediate Expert

Molecular Docking of Selective Orexin Receptor 2 Agonists.

- High-resolution cryo-EM structures of the active-state orexin receptor 2 (OX₂R) bound to both peptide and small-molecule agonists have revealed key interactions in the orthosteric binding pocket, enabling structure-based design of selective agonists [1](#).
- Small-molecule agonists bind deeply within the OX₂R orthosteric site, mimicking interactions of the endogenous peptide, which supports rational optimization of binding affinity and efficacy [1](#).
- While the provided sources do not report specific OX₂R agonists achieving binding energies below -14.2 kcal/mol, advanced molecular docking and free energy calculation methods—such as free energy perturbation (FEP) and alchemical simulations—are capable of predicting and optimizing such high-affinity interactions in GPCRs [2](#), [3](#).
- Supramolecular scaffolds with high solubility and synthetic accessibility, such as tripodal or foldamer-based systems, have demonstrated strong ligand-receptor binding through optimized hydrogen bonding, conformational preorganization, and intramolecular stabilization—factors that can significantly enhance binding affinity [4](#), [5](#), [1126/sciadv.1501240].

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