Literature

Reviews

CRISPR–Cas9 Structures and Mechanisms

Simulations

Cas9-catalyzed DNA Cleavage Generates Staggered Ends: Evidence from Molecular Dynamics Simulations

Probing the structural dynamics of the CRISPR-Cas9 RNA-guided DNA-cleavage system by coarse-grained modeling

Striking Plasticity of CRISPR-Cas9 and Key Role of Non-target DNA, as Revealed by Molecular Simulations

CRISPR-Cas9 conformational activation as elucidated from enhanced molecular simulations

Experiments with structural & mechanistic focus.

DNA interrogation by the CRISPR RNA-guided endonuclease Cas9

Massively Parallel Biophysical Analysis of CRISPR-Cas Complexes on Next Generation Sequencing Chips

Cas9 domain fluctuations by FRET

Structures and mechanisms by Cryo-EM Cell 2017

Biophysical models of specificity.

DNA targeting specificity of RNA-guided Cas9 nucleases (https://crispr.bme.gatech.edu/): Contains experimental data about the specificity. They also have a server based on the data.

A Biophysical Model of CRISPR/Cas9 Activity for Rational Design of Genome Editing and Gene Regulation: This is a simple biophysical model used to predict the specificity of the sgRNA based on the sequence. They split the process in 3 steps and add the free energy change of each process to calculate a binding energy.

High-fidelity CRISPR–Cas9 nucleases with no detectable genome-wide off-target effects : Mutations on residues that bind to the phosphate backbone of the DNA can improve the specificity.

Cleavage

https://www.nature.com/articles/srep37584.pdf

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3110985/

QM:MM Simulations

Gamess+Tinker http://cfm.ehu.es/ricardo/master/intranet_ESCMAN/WinGAMESS/manuals/simomm.pdf (advantages: free, disadvantages: might not run well)

Gaussian+Gromacs http://www.gromacs.org/Downloads/Installation_Instructions/compiling_QMMM (advantages: will work well, Scuseria will likely help; disadvantages: will likely be limited to Rice U comp. resources.)

Mechanistic Insight into Catalytic Activity of BBA-Metallonucleases (This model system, *Vibrio vulnificus*, is thought to have the same cleavage mechanism as the HNH domain.)

Catalytic Mechanisms of Restriction and Homing Endonucleases (A general overview of both one- and two-metal reactions, not specifically theory-oriented.)

The Nucleophile in Ribozyme Catalysis (Not directly related, but an analogous cleavage reaction. The SI also has lots of detailed information on their QM /MM simulations.)

RNA coarse grain models:

http://pubs.acs.org/doi/abs/10.1021/jp104926t

http://rnajournal.cshlp.org/content/14/6/1164.long

Layman news:

https://www.wired.com/2017/06/crispr-mutations

https://hms.harvard.edu/news/bringing-crispr-focus