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Ph.D. Student in Biophysics, admitted Autumn 2014

Publications

PUBLICATIONS

- **A Quantitative and Predictive Model for RNA Binding by Human Pumilio Proteins** *MOLECULAR CELL*
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- **Blind tests of RNA-protein binding affinity prediction** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Kappel, K., Jarmoskaite, I., Vaidyanathan, P. P., Greenleaf, W. J., Herschlag, D., Das, R.
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- **De novo computational RNA modeling into cryo-EM maps of large ribonucleoprotein complexes.** *Nature methods*
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2018
- **Sampling Native-like Structures of RNA-Protein Complexes through Rosetta Folding and Docking.** *Structure (London, England : 1993)*
Kappel, K., Das, R.
2018
- **Architecture of an HIV-1 reverse transcriptase initiation complex.** *Nature*
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- **The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design.** *Journal of chemical theory and computation*
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- **RNA-Puzzles Round III: 3D RNA structure prediction of five riboswitches and one ribozyme.** *RNA (New York, N.Y.)*
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2017
- **Blind tests of RNA nearest-neighbor energy prediction** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Chou, F., Kladwang, W., Kappel, K., Das, R.
2016; 113 (30): 8430-8435
- **Accelerated molecular dynamics simulations of ligand binding to a muscarinic G-protein-coupled receptor.** *Quarterly reviews of biophysics*
Kappel, K., Miao, Y., McCammon, J. A.
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- **The binding mechanism, multiple binding modes, and allosteric regulation of Staphylococcus aureus Sortase A probed by molecular dynamics simulations.** *Protein science : a publication of the Protein Society*

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