Stanford

Ron Dror

Associate Professor of Computer Science and, by courtesy, of Molecular and Cellular Physiology and of Structural Biology

Curriculum Vitae available Online

CONTACT INFORMATION

- **Administrator**

  Carrie Petersen - Administrative Associate

  Email carriep1@stanford.edu

  Tel (650) 498-0615

Bio

BIO

Ron Dror is an Associate Professor of Computer Science and, by courtesy, Molecular and Cellular Physiology and Structural Biology at Stanford University, where he is also affiliated with the Institute for Computational and Mathematical Engineering, the Stanford Artificial Intelligence Lab, Bio-X, ChEM-H, and the Biophysics and Biomedical Informatics Programs. Dr. Dror's research at Stanford addresses a broad set of computational biology problems related to the spatial organization and dynamics of biomolecules and cells.

Before joining Stanford in March 2014, Dr. Dror served as second-in-command of D. E. Shaw Research, a hundred-person company, having joined in 2002 as its first hire. At DESRES, he focused on high-performance computing and biomolecular simulation—in particular, developing technology that accelerates molecular dynamics simulations by orders of magnitude, and applying these simulations to the study of protein function, protein folding, and protein-drug interactions (part of a project highlighted by Science as one of the top 10 scientific breakthroughs of 2010).

Dr. Dror earned a PhD in Electrical Engineering and Computer Science at MIT, an MPhil in Biological Sciences as a Churchill Scholar at the University of Cambridge, and both a BA in Mathematics and a BS in Electrical and Computer Engineering at Rice University, summa cum laude. As a student, he worked in genomics, vision, image analysis, and neuroscience. He has been awarded a Fulbright Scholarship and fellowships from the National Science Foundation, the Department of Defense, and the Whitaker Foundation, as well as a Gordon Bell Prize and several Best Paper awards.

ACADEMIC APPOINTMENTS

- Associate Professor, Computer Science
- Associate Professor (By courtesy), Molecular & Cellular Physiology
- Associate Professor (By courtesy), Structural Biology
- Member, Bio-X
- Faculty Fellow, Stanford ChEM-H
- Member, Wu Tsai Neurosciences Institute

HONORS AND AWARDS

- Gordon Bell Prize (Performance), ACM (2014)
- Best Paper Award, International Parallel and Distributed Processing Symposium (2013)
- Best Paper Award, ACM/IEEE Conference on Supercomputing (SC11) (2011)
- Breakthrough of the Year runner-up, Science Magazine (2010)
- Best Paper Award, ACM/IEEE Conference on Supercomputing (SC09) (2009)
- Gordon Bell Prize (Special Achievement), ACM (2009)
- Profiled in feature on “EECS Alums: Major Players and Thinkers", MIT Department of Electrical Engineering and Computer Science (2009)
- Best Paper Award, ACM/IEEE Conference on Supercomputing (SC06) (2006)

PROGRAM AFFILIATIONS

- Institute for Computational and Mathematical Engineering (ICME)

LINKS

- Dror Lab: http://drorlab.stanford.edu/

Teaching

COURSES

2018-19

- Seminar in Artificial Intelligence in Healthcare: CS 522 (Aut)

2017-18

- Computational Biology in Four Dimensions: BIOMEDIN 371, CME 371, CS 371 (Win)
- Computational Biology: Structure and Organization of Biomolecules and Cells: BIOE 279, BIOMEDIN 279, BIOPHYS 279, CME 279, CS 279 (Aut)
- Seminar in Artificial Intelligence in Healthcare: CS 522 (Aut)

2016-17

- Computational Biology in Four Dimensions: BIOMEDIN 371, BIOPHYS 371, CME 371, CS 371 (Win)
- Computational Biology: Structure and Organization of Biomolecules and Cells: BIOE 279, BIOMEDIN 279, BIOPHYS 279, CME 279, CS 279 (Aut)

2015-16

- Computational Biology in Four Dimensions: BIOMEDIN 371, BIOPHYS 371, CME 371, CS 371 (Win)
- Computational Biology: Structure and Organization of Biomolecules and Cells: BIOMEDIN 279, BIOPHYS 279, CME 279, CS 279 (Aut)

STANFORD ADVISEES

Doctoral Dissertation Reader (AC)

Tyler Shimko, Nathaniel Thomas

Postdoctoral Faculty Sponsor

Deniz Aydin, Carl-Mikael Suomivuori, Martin Voegele

Doctoral Dissertation Advisor (AC)

Robin Betz, Naomi Latorraca, Alex Powers

Doctoral Dissertation Co-Advisor (AC)

Mark Berger, Adrian Sanborn

Master's Program Advisor

Tushar Dhoot, Jason Li, Laura Miron, Blue Sheffer, Jonathan Tynan

Doctoral (Program)

Joe Paggi, Adrian Sanborn, Raphael Townshend, Alex Tseng

GRADUATE AND FELLOWSHIP PROGRAM AFFILIATIONS

- Biomedical Informatics (Phd Program)
- Biophysics (Phd Program)
- Molecular and Cellular Physiology (Phd Program)
- Neurosciences (Phd Program)
- Structural Biology (Phd Program)

Publications

PUBLICATIONS

- **Catalytic activation of beta-arrestin by GPCRs** *NATURE*
  Eichel, K., Jullie, D., Barsi-Rhyne, B., Latorraca, N. R., Masureel, M., Sibarita, J., Dror, R. O., von Zastrow, M.
  2018; 557 (7705): 381-+
- **Molecular mechanism of GPCR-mediated arrestin activation** *NATURE*
  Latorraca, N. R., Wang, J. K., Bauer, B., Townshend, R. L., Hollingsworth, S. A., Olivieri, J. E., Xu, H., Sommer, M. E., Dror, R. O.
  2018; 557 (7705): 452-+
- **Smoothened stimulation by membrane sterols drives Hedgehog pathway activity.** *Nature*
  Deshpande, I., Liang, J., Hedeen, D., Roberts, K. J., Zhang, Y., Ha, B., Latorraca, N. R., Faust, B., Dror, R. O., Beachy, P. A., Myers, B. R., Manglik, A.
  2019
- **Conformational transitions of a neurotensin receptor1-Gi1complex.** *Nature*
  Kato, H. E., Zhang, Y., Hu, H., Suomivuori, C., Kadji, F. M., Aoki, J., Krishna Kumar, K., Fonseca, R., Hilger, D., Huang, W., Latorraca, N. R., Inoue, A., Dror, et al
  2019
- **How Effectively Can Adaptive Sampling Methods Capture Spontaneous Ligand Binding?** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Betz, R. M., Dror, R. O.
  2019; 15 (3): 2053–63
- **Diverse GPCRs exhibit conserved water networks for stabilization and activation.** *Proceedings of the National Academy of Sciences of the United States of America*
  Venkatakrishnan, A. J., Ma, A. K., Fonseca, R., Latorraca, N. R., Kelly, B., Betz, R. M., Asawa, C., Kobilka, B. K., Dror, R. O.
  2019
- **Structure of a Signaling Cannabinoid Receptor 1-G Protein Complex** *CELL*
  Kumar, K., Shalev-Benami, M., Robertson, M. J., Hu, H., Banister, S. D., Hollingsworth, S. A., Latorraca, N. R., Kato, H. E., Hilger, D., Maeda, S., Weis, W. I., Farrens, D. L., Dror, et al
  2019; 176 (3): 448-+
- **Angiotensin Analogs with Divergent Bias Stabilize Distinct Receptor Conformations.** *Cell*
  Wingler, L. M., Elgeti, M., Hilger, D., Latorraca, N. R., Lerch, M. T., Staus, D. P., Dror, R. O., Kobilka, B. K., Hubbell, W. L., Lefkowitz, R. J.
  2019
- **Structure of a Signaling Cannabinoid Receptor 1-G Protein Complex.** *Cell*
  Krishna Kumar, K., Shalev-Benami, M., Robertson, M. J., Hu, H., Banister, S. D., Hollingsworth, S. A., Latorraca, N. R., Kato, H. E., Hilger, D., Maeda, S., Weis, W. I., Farrens, D. L., Dror, et al
  2018

- **Publisher Correction: Structural insights into binding specificity, efficacy and bias of a beta2AR partial agonist.** *Nature chemical biology*
  Masureel, M., Zou, Y., Picard, L., van der Westhuizen, E., Mahoney, J. P., Rodrigues, J. P., Mildorf, T. J., Dror, R. O., Shaw, D. E., Bouvier, M., Pardon, E., Steyaert, J., Sunahara, et al
  2018
- **Structural insights into binding specificity, efficacy and bias of a beta2AR partial agonist.** *Nature chemical biology*
  Masureel, M., Zou, Y., Picard, L., van der Westhuizen, E., Mahoney, J. P., Rodrigues, J. P., Mildorf, T. J., Dror, R. O., Shaw, D. E., Bouvier, M., Pardon, E., Steyaert, J., Sunahara, et al
  2018; 14 (11): 1059–66
- **Entry from the Lipid Bilayer: A Possible Pathway for Inhibition of a Peptide G Protein-Coupled Receptor by a Lipophilic Small Molecule** *BIOCHEMISTRY*
  Bokoch, M. P., Jo, H., Valcourt, J. R., Srinivasan, Y., Pan, A. C., Capponi, S., Grabe, M., Dror, R. O., Shaw, D. E., DeGrado, W. F., Coughlin, S. R.
  2018; 57 (39): 5748–58
- **Structural basis for sigma(1) receptor ligand recognition** *NATURE STRUCTURAL & MOLECULAR BIOLOGY*
  Schmidt, H. R., Betz, R. M., Dror, R. O., Kruse, A. C.
  2018; 25 (10): 981-+
- **Molecular Dynamics Simulation for All.** *Neuron*
  Hollingsworth, S. A., Dror, R. O.
  2018; 99 (6): 1129–43
- **Structural mechanisms of selectivity and gating in anion channelrhodopsins.** *Nature*
  Kato, H. E., Kim, Y. S., Paggi, J. M., Evans, K. E., Allen, W. E., Richardson, C., Inoue, K., Ito, S., Ramakrishnan, C., Fenno, L. E., Yamashita, K., Hilger, D., Lee, et al
  2018
- **Crystal structure of the natural anion-conducting channelrhodopsin GtACR1.** *Nature*
  Kim, Y. S., Kato, H. E., Yamashita, K., Ito, S., Inoue, K., Ramakrishnan, C., Fenno, L. E., Evans, K. E., Paggi, J. M., Dror, R. O., Kandori, H., Kobilka, B. K., Deisseroth, et al
  2018
- **Structure of the μ-opioid receptor-Gi protein complex.** *Nature*
  Koehl, A., Hu, H., Maeda, S., Zhang, Y., Qu, Q., Paggi, J. M., Latorraca, N. R., Hilger, D., Dawson, R., Matile, H., Schertler, G. F., Granier, S., Weis, et al
  2018
- **One receptor, many partners: How do GPCRs stimulate diverse signaling proteins?**
  Dror, R.
  AMER CHEMICAL SOC.2018
- **Molecular simulation and machine learning for the design of finely tuned drugs**
  Dror, R.
  AMER CHEMICAL SOC.2018
- **G(i)- and G(s)-coupled GPCRs show different modes of G-protein binding** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Van Eps, N., Altenbach, C., Caro, L. N., Latorraca, N. R., Hollingsworth, S. A., Dror, R. O., Ernst, O. P., Hubbell, W. L.
  2018; 115 (10): 2383–88
- **Mechanism of Substrate Translocation in an Alternating Access Transporter**
  Latorraca, N. R., Fastman, N. M., Feng, L., Dror, R. O.
  CELL PRESS.2018: 207A
- **Structure-inspired design of beta-arrestin-biased ligands for aminergic GPCRs** *NATURE CHEMICAL BIOLOGY*
  McCorvy, J. D., Butler, K. V., Kelly, B., Rechsteiner, K., Karpiak, J., Betz, R. M., Kormos, B. L., Shoichet, B. K., Dror, R. O., Jin, J., Roth, B. L.
  2018; 14 (2): 126-+
- **Structure-inspired design of #-arrestin-biased ligands for aminergic GPCRs** *Nature Chemical Biology*
  McCorvy, J. D., Butler, K. V., Kelly, B., Rechsteiner, K., Karpiak, J., Betz, R. M., Kormos, B. L., Shoichet, B. K., Dror, R. O., Jin, J., Roth, B. L.

2018: 126-134

- **D-4 dopamine receptor high-resolution structures enable the discovery of selective agonists** *SCIENCE*
  Wang, S., Wacker, D., Levit, A., Che, T., Betz, R. M., McCorvy, J. D., Venkatakrishnan, A. J., Huang, X., Dror, R. O., Shoichet, B. K., Roth, B. L.
  2017; 358 (6361): 381-+

- **Mechanism of substrate translocation in an alternating access transporter**
  Dror, R.
  AMER CHEMICAL SOC.2017

- **Revealing the structural basis for GPCR signaling through atomic-level simulation**
  Dror, R.
  AMER CHEMICAL SOC.2017

- **Structural and Functional Analysis of a beta(2)-Adrenergic Receptor Complex with GRK5** *CELL*
  Komolov, K. E., Du, Y., Nguyen Minh Duc, N. M., Betz, R. M., Rodrigues, J. P., Leib, R. D., Patra, D., Skiniotis, G., Adams, C. M., Dror, R. O., Chung, K. Y., Kobilka, B. K., Benovic, et al
  2017; 169 (3): 407-?

- **Mechanism of Substrate Translocation in an Alternating Access Transporter** *CELL*
  Latorraca, N. R., Fastman, N. M., Venkatakrishnan, A. J., Frommer, W. B., Dror, R. O., Feng, L.
  2017; 169 (1): 96-?

- **Crystal Structure of an LSD-Bound Human Serotonin Receptor.** *Cell*
  Wacker, D., Wang, S., McCorvy, J. D., Betz, R. M., Venkatakrishnan, A. J., Levit, A., Lansu, K., Schools, Z. L., Che, T., Nichols, D. E., Shoichet, B. K., Dror, R. O., Roth, et al
  2017; 168 (3): 377-389 e12

- **GPCR Dynamics: Structures in Motion** *CHEMICAL REVIEWS*
  Latorraca, N. R., Venkatakrishnan, A. J., Dror, R. O.
  2017; 117 (1): 139-155

- **Mechanism of intracellular allosteric #2AR antagonist revealed by X-ray crystal structure.** *Nature*
  Liu, X., Ahn, S., Kahsai, A. W., Meng, K. C., Latorraca, N. R., Pani, B., Venkatakrishnan, A. J., Masoudi, A., Weis, W. I., Dror, R. O., Chen, X., Lefkowitz, R. J., Kobilka, et al
  2017; 548 (7668): 480–84

- **Identification of Phosphorylation Codes for Arrestin Recruitment by G Protein-Coupled Receptors.** *Cell*
  Zhou, X. E., He, Y., de Waal, P. W., Gao, X., Kang, Y., Van Eps, N., Yin, Y., Pal, K., Goswami, D., White, T. A., Barty, A., Latorraca, N. R., Chapman, et al
  2017; 170 (3): 457–69.e13

- **Mechanism of intracellular allosteric #2AR antagonist revealed by X-ray crystal structure** *Nature*
  Liu, X., Ahn, S., Kahsai, A. W., Meng, K. C., Latorraca, N. R., Pani, B., Venkatakrishnan, A., Masoudi, A., Weis, W. I., Dror, R. O., Chen, X., Lefkowitz, R. J., Kobilka, et al
  2017: 480-484

- **D4 dopamine receptor high-resolution structures enable the discovery of selective agonists** *Science*
  Wang, S., Wacker, D., Levit, A., Che, T., Betz, R. M., McCorvy, J. D., Venkatakrishnan, A., Huang, X. P., Dror, R. O., Shoichet, B. K., Roth, B. L.
  2017: 381-386

- **Structural and functional analysis of a #2-adrenergic receptor complex with GRK5** *Cell*
  Komolov, K. E., Du, Y., Duc, N. M., Betz, R. M., Rodrigues, J. M., Leib, R. D., Patra, D., Skiniotis, G., Adams, C. M., Dror, R. O., Chung, K. Y., Kobilka, B. K., Benovic, et al
  2017: 407-421

- **Identification of phosphorylation codes for arrestin recruitment by G protein-coupled receptors** *Cell*
  Zhou, X. E., He, Y., de Waal, P. W., Gao, X., Kang, Y., Van Eps, N., Yin, Y., Pal, K., Goswami, D., White, T. A., Barty, A., Latorraca, N. R., Chapman, et al
  2017: 457-469

- **Crystal Structure of a Full-Length Human Tetraspanin Reveals a Cholesterol-Binding Pocket** *CELL*
  Zimmerman, B., Kelly, B., McMillan, B. J., Seegar, T. C., Dror, R. O., Kruse, A. C., Blacklow, S. C.

2016; 167 (4): 1041-?

- **Revealing Atomic-Level Mechanisms of Protein Allostery with Molecular Dynamics Simulations** *PLOS COMPUTATIONAL BIOLOGY*
  Hertig, S., Latorraca, N. R., Dror, R. O.
  2016; 12 (6)
- **Molecular Basis of Ligand Dissociation from the Adenosine A(2A) Receptor** *MOLECULAR PHARMACOLOGY*
  Guo, D., Pan, A. C., Dror, R. O., Mocking, T., Liu, R., Heitman, L. H., Shaw, D. E., IJzerman, A. P.
  2016; 89 (5): 485-491
- **Structural insights into mu-opioid receptor activation** *NATURE*
  Huang, W., Manglik, A., Venkatakrishnan, A. J., Laeremans, T., Feinberg, E. N., Sanborn, A. L., Kato, H. E., Livingston, K. E., Thorsen, T. S., Kling, R. C., Granier, S., Gmeiner, P., Husbands, et al
  2015; 524 (7565): 315-?
- **Structural basis for nucleotide exchange in heterotrimeric G proteins** *SCIENCE*
  Dror, R. O., Mildorf, T. J., Hilger, D., Manglik, A., Borhani, D. W., Arlow, D. H., Philippsen, A., Villanueva, N., Yang, Z., Lerch, M. T., Hubbell, W. L., Kobilka, B. K., Sunahara, et al
  2015; 348 (6241): 1361-1365
- **Identifying localized changes in large systems: Change-point detection for biomolecular simulations** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Fan, Z., Dror, R. O., Mildorf, T. J., Piana, S., Shaw, D. E.
  2015; 112 (24): 7454-7459
- **Structural basis for chemokine recognition and activation of a viral G protein-coupled receptor** *SCIENCE*
  Burg, J. S., Ingram, J. R., Venkatakrishnan, A. J., Jude, K. M., Dukkipati, A., Feinberg, E. N., Angelini, A., Waghray, D., Dror, R. O., Ploegh, H. L., Garcia, K. C.
  2015; 347 (6226): 1113-1117
- **Insights into the Role of Asp79(2.50) in beta(2) Adrenergic Receptor Activation from Molecular Dynamics Simulations** *BIOCHEMISTRY*
  Ranganathan, A., Dror, R. O., Carlsson, J.
  2014; 53 (46): 7283-7296
- **Anton 2: Raising the bar for performance and programmability in a special-purpose molecular dynamics supercomputer** *SC14: INTERNATIONAL CONFERENCE FOR HIGH PERFORMANCE COMPUTING, NETWORKING, STORAGE AND ANALYSIS*
  Shaw, D. E., Grossman, J. P., Bank, J. A., Batson, B., Butts, J. A., Chao, J. C., Deneroff, M. M., Dror, R. O., Even, A., Fenton, C. H., Forte, A., Gagliardo, J., Gill, et al
  2014: 41-53
- **The role of ligands on the equilibria between functional States of a g protein-coupled receptor.** *Journal of the American Chemical Society*
  Kim, T. H., Chung, K. Y., Manglik, A., Hansen, A. L., Dror, R. O., Mildorf, T. J., Shaw, D. E., Kobilka, B. K., Prosser, R. S.
  2013; 135 (25): 9465-9474
- **Hardware Support for Fine-Grained Event-Driven Computation in Anton 2** *ACM SIGPLAN NOTICES*
  Grossman, J. P., Kuskin, J. S., Bank, J. A., Theobald, M., Dror, R. O., Ierardi, D. J., Larson, R. H., Ben Schafer, U., Towles, B., Young, C., Shaw, D. E.
  2013; 48 (4): 549-560
- **The Dynamic Process of beta(2)-Adrenergic Receptor Activation** *CELL*
  Nygaard, R., Zou, Y., Dror, R. O., Mildorf, T. J., Arlow, D. H., Manglik, A., Pan, A. C., Liu, C. W., Fung, J. J., Bokoch, M. P., Thian, F. S., Kobilka, T. S., Shaw, et al
  2013; 152 (3): 532-542
- **The dynamic process of #2-adrenergic receptor activation** *Cell*
  Nygaard, R., Zou, Y., Dror, R. O., Mildorf, T. J., Arlow, D. H., Manglik, A., Pan, A. C., Liu, C. W., Fung, J. J., Bokoch, M. P., Thian, F. S., Kobilka, T. S., Shaw, et al
  2013: 532-542
- **Extending the generality of molecular dynamics simulations on a special-purpose machine** *IEEE 27TH INTERNATIONAL PARALLEL AND DISTRIBUTED PROCESSING SYMPOSIUM (IPDPS 2013)*
  Scarpazza, D. P., Ierardi, D. J., Lerer, A. K., Mackenzie, K. M., Pan, A. C., Bank, J. A., Chow, E., Dror, R. O., Grossman, J. P., Killebrew, D., Moraes, M. A., Predescu, C., Salmon, et al

2013: 933-945

- **Structural basis for modulation of a GPCR by allosteric drugs** *Nature*
  Dror, R. O., Green, H. F., Valant, C., Borhani, D. W., Valcourt, J. R., Pan, A. C., Arlow, D. H., Canals, M., Lane, J. R., Rahmani, R., Baell, J. B., Sexton, P. M., Christopoulos, et al
  2013: 295-299

- **High-resolution crystal structure of human protease-activated receptor 1** *NATURE*
  Zhang, C., Srinivasan, Y., Arlow, D. H., Fung, J. J., Palmer, D., Zheng, Y., Green, H. F., Pandey, A., Dror, R. O., Shaw, D. E., Weis, W. I., Coughlin, S. R., Kobilka, et al
  2012; 492 (7429): 387-?

- **Refinement of protein structure homology models via long, all-atom molecular dynamics simulations** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
  Raval, A., Piana, S., Eastwood, M. P., Dror, R. O., Shaw, D. E.
  2012; 80 (8): 2071-2079

- **Evaluating the Effects of Cutoffs and Treatment of Long-range Electrostatics in Protein Folding Simulations** *PLOS ONE*
  Piana, S., Lindorff-Larsen, K., Dirks, R. M., Salmon, J. K., Dror, R. O., Shaw, D. E.
  2012; 7 (6)

- **Oncogenic Mutations Counteract Intrinsic Disorder in the EGFR Kinase and Promote Receptor Dimerization** *CELL*
  Shan, Y., Eastwood, M. P., Zhang, X., Kim, E. T., Arkhipov, A., Dror, R. O., Jumper, J., Kuriyan, J., Shaw, D. E.
  2012; 149 (4): 860-870

- **Structure and dynamics of the M3 muscarinic acetylcholine receptor** *NATURE*
  Kruse, A. C., Hu, J., Pan, A. C., Arlow, D. H., Rosenbaum, D. M., Rosemond, E., Green, H. F., Liu, T., Chae, P. S., Dror, R. O., Shaw, D. E., Weis, W. I., Wess, et al
  2012; 482 (7386): 552-556

- **Systematic Validation of Protein Force Fields against Experimental Data** *PLOS ONE*
  Lindorff-Larsen, K., Maragakis, P., Piana, S., Eastwood, M. P., Dror, R. O., Shaw, D. E.
  2012; 7 (2)

- **Biomolecular Simulation: A Computational Microscope for Molecular Biology** *ANNUAL REVIEW OF BIOPHYSICS, VOL 41*
  Dror, R. O., Dirks, R. M., Grossman, J. P., Xu, H., Shaw, D. E.
  2012; 41: 429-452

- **Computationally efficient molecular dynamics integrators with improved sampling accuracy** *MOLECULAR PHYSICS*
  Predescu, C., Lippert, R. A., Eastwood, M. P., Ierardi, D., Xu, H., Jensen, M. O., Bowers, K. J., Gullingsrud, J., Rendleman, C. A., Dror, R. O., Shaw, D. E.
  2012; 110 (9-10): 967-983

- **Mechanism of voltage gating in K+ channels** *Science*
  Jensen, M. O., Jogini, V., Borhani, D. W., Lefler, A. E., Dror, R. O., Shaw, D. E.
  2012: 229-233

- **How Fast-Folding Proteins Fold** *SCIENCE*
  Lindorff-Larsen, K., Piana, S., Dror, R. O., Shaw, D. E.
  2011; 334 (6055): 517-520

- **Pathway and mechanism of drug binding to G-protein-coupled receptors** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
  Dror, R. O., Pan, A. C., Arlow, D. H., Borhani, D. W., Maragakis, P., Shan, Y., Xu, H., Shaw, D. E.
  2011; 108 (32): 13118-13123

- **How Does a Drug Molecule Find Its Target Binding Site?** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Shan, Y., Kim, E. T., Eastwood, M. P., Dror, R. O., Seeliger, M. A., Shaw, D. E.
  2011; 133 (24): 9181-9183

- **OVERCOMING COMMUNICATION LATENCY BARRIERS IN MASSIVELY PARALLEL SCIENTIFIC COMPUTATION** *IEEE MICRO*

Dror, R. O., Grossman, J. P., Mackenzie, K. M., Towles, B., Chow, E., Salmon, J. K., Young, C., Bank, J. A., Batson, B., Deneroff, M. M., Kuskin, J. S., Larson, R. H., Moraes, et al

2011; 31 (3): 8-19

- **Structure and function of an irreversible agonist-beta(2) adrenoceptor complex** *NATURE*

  Rosenbaum, D. M., Zhang, C., Lyons, J. A., Holl, R., Aragao, D., Arlow, D. H., Rasmussen, S. G., Choi, H., DeVree, B. T., Sunahara, R. K., Chae, P. S., Gellman, S. H., Dror, et al

  2011; 469 (7329): 236-240

- **Activation mechanism of the #2-adrenergic receptor** *Proceedings of the National Academy of Sciences of the United States of America*

  Dror, R. O., Arlow, D. H., Maragakis, P., Mildorf, T. J., Pan, A. C., Xu, H., Borhani, D. W., Shaw, D. E.

  2011: 18684-18689

- **Radix-8 Digit-by-Rounding: Achieving High-Performance Reciprocals, Square Roots, and Reciprocal Square Roots** *2011 20TH IEEE SYMPOSIUM ON COMPUTER ARITHMETIC (ARITH-20)*

  Butts, J. A., Tang, P. T., Dror, R. O., Shaw, D. E.

  2011: 149-158

- **Structure and function of an irreversible agonist–#2 adrenoceptor complex** *Nature*

  Rosenbaum, D. M., Zhang, C., Lyons, J. A., Holl, R., Aragao, D., Arlow, D. H., Rasmussen, S. F., Choi, H. J., DeVree, B. T., Sunahara, R. K., Chae, P. S., Gellman, S. H., Dror, et al

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