

Ron O. Dror

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PROFESSIONAL EXPERIENCE

Cheriton Family Professor, Stanford University 2014–present
Faculty member in the Departments of Computer Science and, by courtesy, Molecular and Cellular Physiology and Structural Biology. Affiliated with the Stanford Artificial Intelligence Lab, the Institute for Computational and Mathematical Engineering, Bio-X, ChEM-H, and the Biophysics and Biomedical Informatics Programs. Lead a research group that applies machine learning and physics-based simulation to structural biology in order to explain the workings of living systems and develop better medicines. Developed two new computational biology courses whose enrollment grew eight-fold over three years.

Senior Research Scientist and Special Advisor to the Chairman, D. E. Shaw Research 2002–2014
Second in command of a 110-person research group focused on accelerating simulations of biomolecules, whose work was highlighted by *Science* as one of the top ten scientific breakthroughs of 2010. Helped build the group after starting as the first hire, and managed interdisciplinary projects together with founder and chief scientist David E. Shaw. Oversaw the group's operations; managed substantial parts of the design process for Anton, a special-purpose molecular dynamics supercomputer, and Desmond, a fast molecular dynamics software package for standard computer clusters; and played a leadership role in various projects involving application of molecular dynamics simulations to proteins and ligands of biological and pharmaceutical interest.

Lead Artificial Intelligence Engineer, Arch Healthcare 2001–2002
Developed image-processing software to detect signs of cancer in mammograms.

EDUCATION

Massachusetts Institute of Technology 2002
Ph.D. in Electrical Engineering and Computer Science
Advisors: Alan Willsky and Edward Adelson
Research area: Machine learning and statistical inference for computer vision and genomics

University of Cambridge 1998
M.Phil. in Biological Sciences (Churchill Scholar)
Advisor: Simon Laughlin
Research area: Computational and experimental neuroscience (visual motion detection)

Rice University 1997
B.S. in Electrical Engineering and B.A. in Mathematics
Summa cum laude (1st in class)

AWARDS

Cheriton Family Professorship, Stanford University	2023
Best Paper Award, Conference on Neural Information Processing Systems (NeurIPS), Datasets & Benchmarks	2021
Intel Outstanding Researcher Award	2021
Ravi Faculty Scholar, Stanford University	2018
Gordon Bell Prize (Performance)	2014
Best Paper Award, International Parallel and Distributed Processing Symposium	2013
Best Paper Award, ACM/IEEE Conference on Supercomputing (SC11)	2011
Science Magazine Breakthrough of the Year runner-up (one of nine projects)	2010
Gordon Bell Prize (Special Achievement)	2009
Best Paper Award, ACM/IEEE Conference on Supercomputing (SC09)	2009
Profiled by MIT EECS Dept. in feature on “EECS Alums: Major Players and Thinkers”	2009
Best Paper Award, ACM/IEEE Conference on Supercomputing (SC06)	2006
Whitaker Foundation Fellowship in Biomedical Engineering	1999–2002
National Defense Science and Engineering Graduate Fellowship	1998–2001
Churchill Scholarship	1997–1998
National Science Foundation Graduate Fellowship	declined, 1998
Fulbright Scholarship	declined, 1997
MSTP Fellowship, Harvard-MIT M.D./Ph.D. Program	declined, 1997
Elected to Phi Beta Kappa, Sigma Xi, Tau Beta Pi, and Eta Kappa Nu	1996–2001
Graham Baker Studentship, highest scholastic standing in Rice University class	1996
William Marsh Rice Scholarship (full tuition)	1993–1997
Bronze Medalist, International Mathematical Olympiad (Istanbul, Turkey)	1993
National Merit Scholarship and National Science Scholarship	1992

PUBLICATION SUMMARY

I have published over 140 papers, including over 30 in *Nature*, *Science*, and *Cell*, generally considered the most selective scientific journals. My papers have been cited over 40,000 times, and my h-index is 85.

In the publication list below:

* indicates senior/corresponding authorship

† indicates papers based entirely on work done since arriving at Stanford

JOURNAL PAPERS

1. M. Xu, T. Neelands, A.S. Powers, Y. Liu, S.D. Miller, G. Pintilie, J. Du Bois, **R.O. Dror**, W. Chiu, M. Maduke. CryoEM structures of the human CLC-2 voltage gated chloride channel reveal a ball-and-chain gating mechanism. *eLife* (2024).†
2. N. Hoppe, S. Harrison, S.H. Hwang, Z. Chen, M. Karelina, I. Deshpande, C.M. Suomivuori, V.R. Palicharla, S.P. Berry, P. Tschaikner, D. Regele, D.F. Covey, E. Stefan, D.S. Marks, J.F. Reiter, **R.O. Dror**, A.S. Evers, S. Mukhopadhyay, A. Manglik. GPR161 structure uncovers the redundant role of sterol-regulated ciliary cAMP signaling in the Hedgehog pathway. *Nature Structural & Molecular Biology* (2024).†
3. A.S. Powers, H.H. Yu, P. Suriana, R.V. Koodli, T. Lu, J.M. Paggi, **R.O. Dror***. Geometric Deep Learning for Structure-Based Ligand Design. *ACS Central Science* (2023).†
4. M. Karelina, J.J. Noh, **R.O. Dror***. How accurately can one predict drug binding modes using AlphaFold models? *eLife* (2023).†
5. W.A. Burger, V. Pham, Z. Vuckovic, A.S. Powers, J.I. Mobbs, Y. Laloudakis, A. Glukhova, D. Wootten, A.B. Tobin, P.M. Sexton, S.M. Paul, C.C. Felder, R. Radostin, **R.O. Dror***, A. Christopoulos, C. Valant, and D.M. Thal. Xanomeline displays concomitant orthosteric and allosteric binding modes at the M4 mAChR. *Nature Communications*, 14(1): 5440 (2023).†
6. S. Tajima, Y.S. Kim, M. Fukuda, Y.J. Jo, P.Y. Wang, J.M. Paggi, M. Inoue, E.F.X. Byrne, K.E. Kishi, S. Nakamura, C. Ramakrishnan, S. Takaramoto, T. Nagata, M. Konno, M. Sugiura, K. Katayama, T.E. Matsui, K. Yamashita, S. Kim, H. Ikeda, J. Kim, H. Kandori, **R.O. Dror**, K. Inoue, K. Deisseroth, and H.E. Kato. Structural basis for ion selectivity in potassium-selective channelrhodopsins. *Cell* 186(20):4325-4344.e26 (2023).†
7. X. Xu, J. Shonberg, J. Kaindl, M.J. Clark, A. Stößel, L. Maul, D. Mayer, H. Hübner, K. Hirata, A.J. Venkatakrishnan, **R.O. Dror**, B.K. Kobilka, R.K. Sunahara, X. Liu and P. Gmeiner. Constrained catecholamines gain β2AR selectivity through allosteric effects on pocket dynamics. *Nature Communications* (2023).†
8. K.K. Kumar, M.J. Robertson, E. Thadhani, H. Wang, C.M. Suomivuori, A.S. Powers, L. Ji, S.P. Nikas, **R.O. Dror**, A. Inoue, A. Makriyannis, G. Skiniotis and B. Kobilka. Structural basis for activation of CB1 by an endocannabinoid analog. *Nature Communications* (2023).†
9. A.S. Powers, V. Pham, W.A. C. Burger, G. Thompson, Y. Laloudakis, P.M. Sexton, S.M. Paul, A. Christopoulos, D.M. Thal, C.C. Felder, C. Valant and **R.O. Dror***. Structural basis of efficacy-driven ligand selectivity at GPCRs. *Nature Chemical Biology* (2023).†
10. A.E. Daibani, J.M. Paggi, K. Kim, Y.D. Laloudakis, P. Popov, S.M. Bernhard, B.E. Krumm, R.H.J. Olsen, J. Diberto, F.I. Carroll, V. Katritch, B. Wünsch, **R.O. Dror*** and T. Che. Molecular mechanism of biased signaling at the kappa opioid receptor. *Nature Communications* (2023).†

11. A.S. Powers, V. Pham, W.A. C. Burger, G. Thompson, Y. Laloudakis, P.M. Sexton, S.M. Paul, A. Christopoulos, D.M. Thal, C.C. Felder, C. Valant, and **R.O. Dror***. Structural basis of efficacy-driven ligand selectivity at GPCRs. *Nature Chemical Biology* **19**:805–814 (2023).†
12. S. Eismann, P. Suriana, B. Jing, R.J.L. Townshend, and **R.O. Dror***. Protein model quality assessment using rotation-equivariant transformations on point clouds. *Proteins* **91**:1089–1096 (2023).†
13. Q. Qu, W. Huang, D. Aydin, J.M. Paggi, A.B. Seven, H. Wang, S. Chakraborty, T. Che, J.F. DiBerto, M.J. Robertson, A. Inoue, C.-M. Suomivuori, B.L. Roth, S. Majumdar, **R.O. Dror***, B.K. Kobilka, and G. Skiniotis. Insights into distinct signaling profiles of the μOR activated by diverse agonists. *Nature Chemical Biology* (2022).†
14. B. Faust, C.B. Billesbølle, C.-M. Suomivuori, I. Singh, K. Zhang, N. Hoppe, A.F.M. Pinto, J.K. Diedrich, Y. Muftuoglu, M.W. Szkudlinski, A. Saghatelian, **R.O. Dror**, Y. Cheng, A. Manglik. Autoantibody mimicry of hormone action at the thyrotropin receptor. *Nature* **609**:846–853 (2022).†
15. C. Cao, X. Barros-Álvarez, S. Zhang, K. Kim, M.A. Dämgen, O. Panova, C.-M. Suomivuori, J.F. Fay, X. Zhong, B.E. Krumm, R.H. Gumpfer, A.B. Seven, M.J. Robertson, N.J. Krogan, R. Hüttenhain, D.E. Nichols, **R.O. Dror***, G. Skiniotis, B.L. Roth. Signaling snapshots of a serotonin receptor activated by the prototypical psychedelic LSD. *Neuron* **110**:P3154-3167.E7, (2022).†
16. K. Zhang, N. Horikoshi, S. Li, A.S. Powers, M.A. Hameedi, G.D. Pintilie, H.-D. Chae, Y.A. Khan, C.-M. Suomivuori, **R.O. Dror**, K.M. Sakamoto, W. Chiu, S. Wakatsuki. Cryo-EM, protein engineering, and simulation enable the development of peptide therapeutics against acute myeloid leukemia. *ACS Central Science* **8**:214–222 (2022).†
17. K.E. Kishi, Y.S. Kim, M. Fukuda, M. Inoue, T. Kusakizako, P.Y. Wang, C. Ramakrishnan, E.F. Byrne, E. Thadhani, J.M. Paggi, T.E. Matsui, K. Yamashita, T., M. Shibata, N. Nomura, S. Iwata, O. Nureki, **R.O. Dror**, K. Inoue, K. Deisseroth, and H.E. Kato. Structural basis for channel conduction in the pump-like channelrhodopsin ChRmine. *Cell* **185**: 672-689 (2022).†
18. N. Tsutsumi, S. Maeda, Q. Qu, M. Vögele, K.M. Jude, C.-M. Suomivuori, O. Panova, D. Waghray, H.E. Kato, A. Velasco, **R.O. Dror**, G. Skiniotis, B.K. Kobilka, and K.C. Garcia. Atypical structural snapshots of human cytomegalovirus GPCR interactions with host G proteins. *Science Advances* **8**:eabI5442 (2022).†
19. J.A. Harris, B. Faust, A.B. Gondin, M.A. Dämgen, C.-M. Suomivuori, N.A. Veldhuis, Y. Cheng, **R.O. Dror***, D.M. Thal, and A. Manglik. Selective G protein signaling driven by substance P–neurokinin receptor dynamics. *Nature Chemical Biology* **18**:109–115 (2022).†
20. L. Han, Q. Qu, D. Aydin, O. Panova, M.J. Robertson, Y. Xu, **R.O. Dror**, G. Skiniotis, and L. Feng. Structure and mechanism of the SGLT family of glucose transporters. *Nature* **601**:274–279 (2022).†
21. R.J.L. Townshend, S. Eismann, A.M. Watkins, R. Rangan, M. Karelina, R. Das, and **R.O. Dror***. Geometric deep learning of RNA structure. *Science* **373**:1047–1051 (2021). **Cover story**.†
22. J.M. Paggi, J.A. Belk, S.A. Hollingsworth, N. Villanueva, A.S. Powers, M.J. Clark, A.G. Chemparakthy, J.E. Tynan, T.K. Lau, R.K. Sunahara, and **R.O. Dror***. Leveraging non-structural data to predict structures and affinities of protein–ligand complexes. *Proceedings of the National Academy of Sciences of the United States of America*. **118**:e2112621118 (2021).†
23. C.A.P. Wood, J. Zhang, D. Aydin, Y. Xu, B.J. Andreone, U.H. Langen, **R.O. Dror**, C. Gu, L. Feng. Structure and mechanism of blood–brain-barrier lipid transporter MFSD2A. *Nature* **596**:444–448 (2021).†³

24. B. Kelly, S.A. Hollingsworth, D.C. Blakemore, R.M. Owen, R.I. Storer, N.A. Swain, D. Aydin, R. Torella, J.S. Warmus, and **R.O. Dror***. Delineating the ligand–receptor interactions that lead to biased signaling at the μ -opioid receptor. *Journal of Chemical Informatics and Modeling* **61**:3696–3707 (2021).†
25. A.L. Sanborn, B.T. Yeh, J.T. Feigerle, C.V. Hao, R.J.L. Townshend, E.L. Aiden, **R.O. Dror**, and R.D. Kornberg. Simple biochemical features underlie transcriptional activation domain diversity and dynamic, fuzzy binding to Mediator. *eLife* **10**:e68068 (2021).†
26. M. Jagota, R.J.L. Townshend, L. Kang, D.A. Bushnell, **R.O. Dror**, R.D. Kornberg, and M. Azubel. Gold nanoparticles and tilt pairs to assess protein flexibility by cryo-electron microscopy. *Ultramicroscopy* **227**:1133026 (2021).†
27. K.E. Komolov, S.M. Sulon, A. Bhardwaj, S.C. van Keulen, N.M. Duc, D.K. Laurinavichyute, H.J. Lou, B.E.T. Ka, Y. Chung, **R.O. Dror**, and J.L. Benovic. Structure of a GRK5-calmodulin complex reveals molecular mechanism of GRK activation and substrate targeting. *Molecular Cell* **81**:323–339 (2021).†
28. C.-M. Suomivuori, N.R. Latorraca, L.M. Wingler, S. Eismann, M.C. King, A.L.W. Kleinhenz, M.A. Skiba, D.P. Staus, A.C. Kruse, R.J. Lefkowitz, and **R.O. Dror***. Molecular mechanism of biased signaling in a prototypical G protein-coupled receptor. *Science* **367**:881–887 (2020).†
29. N.R. Latorraca, M. Masureel, S.A. Hollingsworth, F.M. Heydenreich, C.-M. Suomivuori, C. Brinton, R.J.L. Townshend, M. Bouvier, B.K. Kobilka, and **R.O. Dror***. How GPCR phosphorylation patterns orchestrate arrestin-mediated signaling. *Cell* **183**:1813–1825 (2020).†
30. L.M. Wingler, M.A. Skiba, C. McMahon, D.P. Staus, A.W. Kleinhenz, C.-M. Suomivuori, N.R. Latorraca, **R.O. Dror**, R.J. Lefkowitz, and A.C. Kruse. Angiotensin and biased analogs induce structurally distinct active conformations within a GPCR. *Science* **367**:888–892 (2020).†
31. S. Eismann, R.J.L. Townshend, N. Thomas, M. Jagota, B. Jing, and **R.O. Dror***. Hierarchical, rotation-equivariant neural networks to select structural models of protein complexes. *Proteins* **89**:493–501 (2020).†
32. C.B. Billesbølle, C.M. Azumaya, R.C. Kretsch, A.S. Powers, S. Gonen, S. Schneider, T. Arvedson, **R.O. Dror**, Y. Cheng, and A. Manglik. Structure of hepcidin-bound ferroportin reveals iron homeostatic mechanisms. *Nature* **586**:80–811 (2020).†
33. E.M. Jones, N.B. Lubock, A.J. Venkatakrishnan, J. Wang, A.M. Tseng, J.M. Paggi, N.R. Latorraca, D. Cancilla, M. Satyadi, J.E. Davis, M.M. Babu, **R.O. Dror***, and S. Kosuri. Structural and Functional Characterization of G Protein-Coupled Receptors with Deep Mutational Scanning. *eLife* **9**:e54895 (2020).†
34. T.A. Chew, B.J. Orlando, J. Zhang, N.R. Latorraca, A. Wang, S.A. Hollingsworth, D.H. Chen, **R.O. Dror**, M. Liao and L. Feng. Structure and mechanism of the cation–chloride cotransporter NKCC1. *Nature* **572**:488–492 (2019).†
35. S.A. Hollingsworth, B. Kelly, C. Valant, J.A. Michaelis, O. Mastromihalis, G. Thompson, A.J. Venkatakrishnan, S. Hertig, P.J. Scammells, P.M. Sexton, C.C. Felder, A. Christopoulos and **R.O. Dror***. Cryptic pocket formation underlies allosteric modulator selectivity at muscarinic GPCRs. *Nature Communications* **10**:3289 (2019).†
36. H.E. Kato, Y. Zhang, H. Hu, C.M. Suomivuori, F.M.N. Kadji, J. Aoki, K.K. Kumar, R. Fonseca, D. Hilger, W. Huang, N. R. Latorraca, A. Inoue, **R.O. Dror**, B.K. Kobilka and G. Skiniotis. Conformational transitions of a neuropeptidergic receptor 1–Gi1 complex. *Nature* **572**:80–85 (2019).†

37. I. Deshpande, J. Liang, D. Hedeen, K.J. Roberts, Y. Zhang, B. Ha, N.R. Latorraca, B. Faust, **R.O. Dror**, P.A. Beachy, B.R. Myers and A. Manglik. Smoothened stimulation by membrane sterols drives Hedgehog pathway activity. *Nature* **571**:284–288 (2019).†
38. A.J. Venkatakrishnan, A. Ma, R. Fonseca, N.R. Latorraca, B. Kelly, R.M. Betz, C. Asawa, B.K. Kobilka, and **R.O. Dror***. Diverse GPCRs exhibit conserved water networks for stabilization and activation. *Proceedings of the National Academy of Sciences of the United States of America* **116**:3288–3292 (2019).†
39. L.M. Wingler, E. Matthias, D. Hilger, N.R. Latorraca, M.T. Lerch, D.P. Staus, **R.O. Dror***, B.K. Kobilka, W.L. Hubbell, and R.J. Lefkowitz. Angiotensin analogs with divergent bias stabilize distinct receptor conformations. *Cell* **176**:468–478 (2019).†
40. R. Betz and **R.O. Dror***. How effectively can adaptive sampling methods capture spontaneous ligand binding? *Journal of Chemical Theory and Computation* **15**:2053–2063 (2019).†
41. K.K. Kumar, M. Shalev-Benami, M.J. Robertson, H. Hu, S.D. Banister, S.A. Hollingsworth, N.R. Latorraca, H.E. Kato, D. Hilger, S. Maeda, W.I. Weis, D.L. Farrens, **R.O. Dror**, S.V. Malhotra, B.K. Kobilka, and G. Skiniotis. Structure of a signaling cannabinoid receptor 1-G protein complex. *Cell* **176**:448–458 (2019).†
42. S.A. Hollingsworth and **R.O. Dror***. Molecular dynamics simulation for all. *Neuron* **99**:1129–1143 (2018).†
43. H.E. Kato, Y.S. Kim, J.M. Paggi, K.E. Evans, W.E. Allen, C. Richardson, K. Inoue, S. Ito, C. Ramakrishnan, Lief E. Fenno, K. Yamashita, D. Hilger, S.Y. Lee, A. Berndt, K. Shen, H. Kandori, **R.O. Dror**, B.K. Kobilka, and K. Deisseroth. Structural mechanisms of selectivity and gating in anion channelrhodopsins. *Nature* **561**:349–354 (2018).†
44. Y.S. Kim, H.E. Kato, K. Yamashita, S. Ito, K. Inoue, C. Ramakrishnan, L.E. Fenno, K.E. Evans, J.M. Paggi, **R.O. Dror**, H. Kandori, B.K. Kobilka, and K. Deisseroth. Crystal structure of a natural anion-conducting channelrhodopsin GtACR1. *Nature* **561**:343–348 (2018).†
45. H.R. Schmidt, R.M. Betz, **R.O. Dror**, and A.C. Kruse. Structural basis for sigma-1 receptor ligand recognition. *Nature Structural & Molecular Biology* **25**:981–987 (2018).†
46. N.R. Latorraca, J.K. Wang, B. Bauer, R.J.L. Townshend, S.A. Hollingsworth, J.E. Olivieri, H.E. Xu, M.E. Sommer, and **R.O. Dror***. Molecular mechanism of GPCR-mediated arrestin activation. *Nature* **557**:452–456 (2018).†
47. K. Eichel, D. Jullié, B. Barsi-Rhyne, N.R. Latorraca, M. Masureel, J. Sibarita, **R.O. Dror**, and M. von Zastrow. Catalytic activation of β-arrestin by GPCRs. *Nature* **557**:381–386 (2018).†
48. A. Koehl, H. Hu, S. Maeda, Y. Zhang, Q. Qu, J.M. Paggi, N.R. Latorraca, D. Hilger, R. Dawson, H. Matile, G.F.X. Schertler, S. Granier, W.I. Weis, **R.O. Dror**, A. Manglik, G. Skiniotis, B.K. Kobilka. Structure of the μ opioid receptor-Gi protein complex. *Nature* **558**:547–552 (2018).†
49. N. van Eps, C. Altenbach, L.N. Caro, N.R. Latorraca, S.A. Hollingsworth, **R.O. Dror**, O.P. Ernst and W.L. Hubbell. Gi- and Gs-coupled GPCRs show different modes of G-protein binding. *Proceedings of the National Academy of Sciences of the United States of America* **115**:2383–2388 (2018).†
50. J.D. McCorry, K.V. Butler, B. Kelly, K. Rechsteiner, J. Karpia, R.M. Betz, B.L. Kormos, B.K. Shoichet, **R.O. Dror***, J. Jin, B.L. Roth. Structure-inspired design of β-arrestin-biased ligands for aminergic GPCRs. *Nature Chemical Biology* **14**:126–134 (2018).†
51. M. Masureel, Y. Zou, L. Picard, E. Westhuizen, J.P. Mahoney, J.P.G.L. Rodrigues, T.J. Mildorf, **R.O. Dror**, D.E. Shaw, M. Bouvier, E. Pardon, J. Steyaert, R.K. Sunahara, W.I. Weis, C. Zhang, and B.K. Kobilka. Structural insights into binding specificity, efficacy and bias of a β2AR partial agonist. *Nature Chemical Biology* **14**:1059–1066 (2018).

52. M.P. Bokoch, H. Jo, J.R. Valcourt, Y. Srinivasan, A.C. Pan, S. Capponi, M. Grabe, **R.O. Dror**, D.E. Shaw, W.F. DeGrado, and S.R. Coughlin. Entry from the lipid bilayer: a possible pathway for inhibition of a peptide G protein-coupled receptor by a lipophilic small molecule. *Biochemistry* **57**:5748–5758 (2018).
53. S. Wang, D. Wacker, A. Levit, T. Che, R.M. Betz, J.D. McCory, A.J. Venkatakrishnan, X.-P. Huang, **R.O. Dror**, B.K. Shoichet, and B.L. Roth. D4 dopamine receptor high-resolution structures enable the discovery of selective agonists. *Science* **358**: 381–386 (2017).†
54. X. Liu, S. Ahn, A.W. Kahsai, K.C. Meng, N.R. Latorraca, B. Pani, A.J. Venkatakrishnan, A. Masoudi, W.I. Weis, **R.O. Dror**, X. Chen, R.J. Lefkowitz, and B.K. Kobilka. Mechanism of intracellular allosteric β_2 AR antagonist revealed by X-ray crystal structure. *Nature* **548**: 480–484 (2017).†
55. X.E. Zhou, Y. He, P.W. de Waal, X. Gao, Y. Kang, N. Van Eps, Y. Yin, K. Pal, D. Goswami, T.A. White, A. Barty, N.R. Latorraca, H.N. Chapman, W.L. Hubbell, **R.O. Dror**, R.C. Stevens, V. Cherezov, V.V. Gurevich, P.R. Griffin, O.P. Ernst, K. Melcher, and H.E. Xu. Identification of phosphorylation codes for arrestin recruitment by G protein-coupled receptors. *Cell* **170**: 457–469 (2017).†
56. N.R. Latorraca, N.M. Fastman, A.J. Venkatakrishnan, W.B. Frommer, **R.O. Dror***, and L. Feng. Mechanism of substrate translocation in an alternating access transporter. *Cell* **169**: 96-107 (2017).†
57. D. Wacker, S. Wang, J.D. McCory, R.M. Betz, A.J. Venkatakrishnan, A. Levit, K. Lansu, Z. Schools, T. Che, D.E. Nichols, B.K. Shoichet, **R.O. Dror***, and B.L. Roth. Crystal structure of an LSD-bound human serotonin receptor. *Cell* **168**: 377-389 (2017). **Cover story.**†
58. K.E. Komolov, Y. Du, N.M. Duc, R.M. Betz, J.P.G.L.M. Rodrigues, R.D. Leib, D. Patra, G. Skiniotis, C.M. Adams, **R.O. Dror**, K.Y. Chung, B.K. Kobilka, and J.L. Benovic. Structural and functional analysis of a β 2-adrenergic receptor complex with GRK5. *Cell* **169**: 407-421 (2017).†
59. N.R. Latorraca, A.J. Venkatakrishnan, and **R.O. Dror***. GPCR dynamics: structures in motion. *Chemical Reviews* **117**: 139–155 (2017).†
60. Crystal structure of a full-length human tetraspanin reveals a cholesterol-binding pocket. B. Zimmerman, B. Kelly, T. Seegar, B.J. McMillan, **R.O. Dror**, A.C. Kruse, and S. Blacklow. *Cell* **167**: 1041–1051 (2016).†
61. S. Hertig, N.R. Latorraca, and **R.O. Dror***. Revealing atomic-level mechanisms of protein allostery with molecular dynamics simulations. *PLOS Computational Biology*. **12**: e1004746 (2016).†
62. D. Guo, A.C. Pan, **R.O. Dror**, T. Mocking, R. Liu, L. Heitman, D.E. Shaw, and A.P. IJzerman. Molecular basis of ligand dissociation from the adenosine A_{2A} receptor. *Molecular Pharmacology* **89**: 485–491 (2016).
63. W. Huang, A. Manglik, A.J. Venkatakrishnan, T. Laeremans, E.N. Feinberg, A.L. Sanborn, H. Kato, K.E. Livingston, T.S. Thorsen, R. Kling, S. Granier, P. Gmeiner, S.M. Husbands, J.R. Traynor, W.I. Weis, J. Steyaert, **R.O. Dror**, and B.K. Kobilka. Structural insights into μ -opioid receptor activation. *Nature* **524**: 315–321 (2015).†
64. **R.O. Dror***, T.J. Mildorf, D. Hilger, A. Manglik, D.W. Borhani, D.H. Arlow, A. Philippse, N. Villanueva, Z. Yang, M. Lerch, W.L. Hubbell, B.K. Kobilka, R.K. Sunahara, and D.E. Shaw. Structural basis for nucleotide exchange in heterotrimeric G proteins. *Science* **348**: 1361–1365 (2015).
65. J.S. Burg, J.R. Ingram, A.J. Venkatakrishnan, K.M. Jude, A. Dukkipati, E.N. Feinberg, A. Angelini, D. Waghray, **R.O. Dror**, H.L. Ploegh, and K.C. Garcia. Structural basis for chemokine recognition and activation of a viral G protein-coupled receptor. *Science* **347**: 1113–1117 (2015).†

66. Z. Fan, R.O. Dror*, T.J. Mildorf, S. Piana, and D.E. Shaw. 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* **112**: 7454–7459 (2015).
67. A. Ranganathan, R.O. Dror, J. Carlsson. Insights into the role of Asp^{792.50} in β_2 adrenergic receptor activation from molecular dynamics simulations. *Biochemistry* **53**: 7283–7296 (2014).†
68. R.O. Dror*, H.F. Green, C. Valant, D.W. Borhani, J.R. Valcourt, A.C. Pan, D.H. Arlow, M. Canals, J.R. Lane, R. Rahmani, J.B. Baell, P.M. Sexton, A. Christopoulos, and D.E. Shaw. Structural basis for modulation of a GPCR by allosteric drugs. *Nature* **503**: 295–299 (2013).
69. R. Nygaard, Y. Zou, R.O. Dror, T.J. Mildorf, D.H. Arlow, A. Manglik, A.C. Pan, C.W. Liu, J.J. Fung, M.P. Bokoch, F.S. Thian, T.S. Kobilka, D.E. Shaw, L. Mueller, R.S. Prosser, and B.K. Kobilka. The dynamic process of β_2 -adrenergic receptor activation. *Cell* **152**: 532–542 (2013).
70. A. Arkhipov, Y. Shan, E.T. Kim, R.O. Dror, and D.E. Shaw. Her2 activation mechanism reflects evolutionary preservation of asymmetric ectodomain dimers in the human EGFR family. *eLife* **2**: e00708 (2013).
71. A.C. Pan, D.W. Borhani, R.O. Dror, and D.E. Shaw. Molecular determinants of drug-receptor binding kinetics. *Drug Discovery Today* **18**: 667–673 (2013).
72. R.A. Lippert, C. Predescu, D.J. Ierardi, K.M. Mackenzie, M.P. Eastwood, R.O. Dror, and D.E. Shaw. Accurate and efficient integration for molecular dynamics simulations at constant temperature and pressure. *Journal of Chemical Physics* **139**: 164106 (2013).
73. T.H. Kim, K.Y. Chung, A. Manglik, A.L. Hansen, R.O. Dror, T.J. Mildorf, D.E. Shaw, B.K. Kobilka, and R.S. Prosser. The role of ligands on the equilibria between functional states of a G protein-coupled receptor. *Journal of the American Chemical Society* **135**: 9465–9474 (2013).
74. R.O. Dror*, R.M. Dirks, J.P. Grossman, H. Xu, and D.E. Shaw. Biomolecular simulation: A computational microscope for molecular biology. *Annual Review of Biophysics* **41**: 429–452 (2012).
75. C. Zhang, Y. Srinivasan, D.H. Arlow, J.J. Fung, D. Palmer, Y. Zheng, H.F. Green, A. Pandey, R.O. Dror, D.E. Shaw, W.I. Weis, S.R. Coughlin, and B.K. Kobilka. High-resolution crystal structure of human protease-activated receptor 1. *Nature* **492**: 387–392 (2012).
76. M.Ø. Jensen, V. Jogini, D.W. Borhani, A.E. Lefler, R.O. Dror, and D.E. Shaw. Mechanism of voltage gating in K⁺ channels. *Science* **336**: 229–233 (2012).
77. Y. Shan, M.P. Eastwood, X. Zhang, E.T. Kim, A. Arkhipov, R.O. Dror, J. Jumper, J. Kuriyan, and D.E. Shaw. Oncogenic mutations counteract intrinsic disorder in the EGFR kinase and promote receptor dimerization. *Cell* **149**: 860–870 (2012).
78. A.C. Kruse, J. Hu, A.C. Pan, D.H. Arlow, D.M. Rosenbaum, E. Rosemond, H.F. Green, T. Liu, P.S. Chae, R.O. Dror, D.E. Shaw, W.I. Weis, J. Wess, and B.K. Kobilka. Structure and dynamics of the M₃ muscarinic acetylcholine receptor. *Nature* **482**: 552–556 (2012).
79. A. Raval, S. Piana, M.P. Eastwood, R.O. Dror, and D.E. Shaw. Refinement of protein structure homology models via long, all-atom molecular dynamics simulations. *Proteins: Structure, Function, and Bioinformatics* **80**: 2071–2079 (2012).
80. C. Predescu, R.A. Lippert, M.P. Eastwood, D.J. Ierardi, H. Xu, M.Ø. Jensen, K.J. Bowers, J. Gullingsrud, C.A. Rendleman, R.O. Dror, and D.E. Shaw. Computationally efficient molecular dynamics integrators with improved sampling accuracy. *Molecular Physics* **110**: 967–983 (2012).

81. S. Piana, K. Lindorff-Larsen, R.M. Dirks, J.K. Salmon, **R.O. Dror**, and D.E. Shaw. Evaluating the effects of cutoffs and treatment of long-range electrostatics in protein folding simulations. *PLoS ONE* **7**: e39918 (2012).
82. Lindorff-Larsen, P. Maragakis, S. Piana, M.P. Eastwood, **R.O. Dror**, and D.E. Shaw. Systematic validation of protein force fields against experimental data. *PLoS ONE* **7**: e32131 (2012).
83. **R.O. Dror***, D.H. Arlow, P. Maragakis, T.J. Mildorf, A.C. Pan, H. Xu, D.W. Borhani, and D.E. Shaw. Activation mechanism of the β_2 -adrenergic receptor. *Proceedings of the National Academy of Sciences of the United States of America*. **108**: 18684–18689 (2011).
84. K. Lindorff-Larsen, S. Piana, **R.O. Dror**, and D.E. Shaw. How fast-folding proteins fold. *Science*, **334**: 517–520 (2011).
85. **R.O. Dror***, A.C. Pan, D.H. Arlow, D.W. Borhani, P. Maragakis, Y. Shan, H. Xu, and D.E. Shaw. Pathway and mechanism of drug binding to G protein-coupled receptors. *Proceedings of the National Academy of Sciences of the United States of America*, **108**: 13118–13123 (2011).
86. Y. Shan, E.T. Kim, M.P. Eastwood, **R.O. Dror**, M.A. Seeliger, and D.E. Shaw. How does a drug molecule find its target binding site? *Journal of the American Chemical Society*, **133**: 9181–9183 (2011).
87. **R.O. Dror***, J.P. Grossman, K.M. Mackenzie, B. Towles, E. Chow, J.K. Salmon, C. Young, J.A. Bank, B. Batson, M.M. Deneroff, J.S. Kuskin, R.H. Larson, M.A. Moraes, and D.E. Shaw. Overcoming communication latency barriers in massively parallel scientific computation. *IEEE Micro*, **31**: 8–19 (2011).
88. D.M. Rosenbaum, C. Zhang, J.A. Lyons, R. Holl, D. Aragao, D.H. Arlow, S.G.F. Rasmussen, H.-J. Choi, B.T. DeVree, R.K. Sunahara, P.S. Chae, S.H. Gellman, **R.O. Dror**, D.E. Shaw, W.I. Weis, M. Caffrey, P. Gmeiner, and B.K. Kobilka. Structure and function of an irreversible agonist- β_2 adrenoceptor complex. *Nature* **469**: 236–240 (2011).
89. D.E. Shaw, P. Maragakis, K. Lindorff-Larsen, S. Piana, **R.O. Dror**, M.P. Eastwood, J.A. Bank, J.M. Jumper, J.K. Salmon, Y. Shan, and W. Wriggers. Atomic-level characterization of the structural dynamics of proteins. *Science*, **330**: 341–346 (2010).
90. **R.O. Dror**, M. \emptyset . Jensen, D.W. Borhani, and D.E. Shaw. Exploring atomic resolution physiology on a femtosecond to millisecond timescale using molecular dynamics simulations. *Journal of General Physiology*, **135**: 555–562 (2010).
91. M.P. Eastwood, K.A. Stafford, R.A. Lippert, M. \emptyset . Jensen, P. Maragakis, C. Predescu, **R.O. Dror**, and D.E. Shaw. Equipartition and the calculation of temperature in biomolecular simulations. *Journal of Chemical Theory and Computation*, **6**: 2045–2058 (2010).
92. M. \emptyset . Jensen, D.W. Borhani, K. Lindorff-Larsen, P. Maragakis, V. Jogini, M.P. Eastwood, **R.O. Dror**, and D.E. Shaw. Principles of conduction and hydrophobic gating in K $^{+}$ channels. *Proceedings of the National Academy of Sciences of the United States of America*, **107**: 5833–5838 (2010).
93. K. Lindorff-Larsen, S. Piana, K. Palmo, P. Maragakis, J.L. Klepeis, **R.O. Dror**, and D.E. Shaw. Improved side-chain torsion potentials for the Amber ff99SB protein force field. *Proteins: Structure, Function, and Bioinformatics*, **78**: 1950–1958 (2010).
94. K.J. Bowers, R.A. Lippert, **R.O. Dror**, and D.E. Shaw. Improved twiddle access for fast Fourier transforms. *IEEE Transactions on Signal Processing*, **58**: 1122–1130 (2010).
95. D.K. Shenfeld, H. Xu, M.P. Eastwood, **R.O. Dror**, and D.E. Shaw. Minimizing thermodynamic length to select intermediate states for free-energy calculations and replica-exchange simulations. *Physical Review E*, **80**: 046705-1–046705-4 (2009).

96. W. Wriggers, K.A. Stafford, Y. Shan, S. Piana, P. Maragakis, K. Lindorff-Larsen, P.J. Miller, M.P. Eastwood, **R.O. Dror**, and D.E. Shaw. Automated event detection and activity monitoring in long molecular dynamics simulations. *Journal of Chemical Theory and Computation*, **5**: 2595–2605, (2009).
97. **R.O. Dror**, D.H. Arlow, D.W. Borhani, M.Ø. Jensen, S. Piana, and D.E. Shaw. Identification of two distinct inactive conformations of the β_2 -adrenergic receptor reconciles structural and biochemical observations. *Proceedings of the National Academy of Sciences of the United States of America*, **106**: 4689–4694 (2009).
98. Y. Shan, M.A. Seeliger, M.P. Eastwood, F. Frank, H. Xu, M.Ø. Jensen, **R.O. Dror**, J. Kuriyan, and D.E. Shaw. A conserved protonation-dependent switch controls drug binding in the Abl kinase. *Proceedings of the National Academy of Sciences of the United States of America*, **106**: 139–144 (2009).
99. J.L. Klepeis, K. Lindorff-Larsen, **R.O. Dror**, and D.E. Shaw. Long-timescale molecular dynamics simulations of protein structure and function. *Current Opinion in Structural Biology*, **19**: 1–18 (2009).
100. M.Ø. Jensen, **R.O. Dror**, H. Xu, D.W. Borhani, I.T. Arkin, M.P. Eastwood, and D.E. Shaw. Dynamic control of slow water transport by aquaporin O: implications for hydration and junction stability in the eye lens. *Proceedings of the National Academy of Sciences of the United States of America*, **105**: 14430–14435 (2008).
101. D.E. Shaw, M.M. Deneroff, **R.O. Dror**, J.S. Kuskin, R.H. Larson, J.K. Salmon, C. Young, B. Batson, K.J. Bowers, J.C. Chao, M.P. Eastwood, J. Gagliardo, J.P. Grossman, C.R. Ho, D.J. Ierardi, I. Kolossváry, J.L. Klepeis, T. Layman, C. McLeavey, M.A. Moraes, R. Mueller, E.C. Priest, Y. Shan, J. Spengler, M. Theobald, B. Towles, and S.C. Wang. Anton, a special-purpose machine for molecular dynamics simulation. *Communications of the ACM*, **51**: 91–97 (2008).
102. P. Maragakis, K. Lindorff-Larsen, M.P. Eastwood, **R.O. Dror**, J.L. Klepeis, I.T. Arkin, M.Ø. Jensen, H. Xu, N. Trbovic, R.A. Friesner, A.G. Palmer, and D.E. Shaw. Microsecond molecular dynamics simulation shows effect of slow loop dynamics on backbone amide order parameters of proteins. *Journal of Physical Chemistry B*, **112**: 6155–6158 (2008).
103. I.T. Arkin, H. Xu, M.Ø. Jensen, E. Arbely, E.R. Bennett, K.J. Bowers, E. Chow, **R.O. Dror**, M.P. Eastwood, R. Flitman-Tene, B.A. Gregersen, J.L. Klepeis, I. Kolossváry, Y. Shan, and D.E. Shaw. Mechanism of Na^+/H^+ antiporting. *Science* **317**: 799–803 (2007).
104. R.A. Lippert, K.J. Bowers, **R.O. Dror**, M.P. Eastwood, B.A. Gregersen, J.L. Klepeis, I. Kolossváry, and D.E. Shaw. A common, avoidable source of error in molecular dynamics integrators. *Journal of Chemical Physics* **126**: 046101 (2007).
105. K.J. Bowers, **R.O. Dror**, and D.E. Shaw. Zonal methods for the parallel execution of range-limited N-body simulations. *Journal of Computational Physics* **221**: 303–329 (2007).
106. K.J. Bowers, **R.O. Dror**, and D.E. Shaw. The midpoint method for parallelization of particle simulations. *Journal of Chemical Physics* **124**: 184109 (2006).
107. Y. Shan, J.L. Klepeis, M.P. Eastwood, **R.O. Dror**, and D.E. Shaw. Gaussian split Ewald: A fast Ewald mesh method for molecular simulation. *Journal of Chemical Physics* **122**: 054101 (2005).
108. **R.O. Dror***, A.S. Willsky, and E.H. Adelson. Statistical characterization of real-world illumination. *Journal of Vision* **4**: 821–837 (2004).

109. R.O. Dror*, J.G. Murnick, N.J. Rinaldi, V.D. Marinescu, R.M. Rifkin, and R.A. Young. Bayesian estimation of transcript levels using a general model of array measurement noise. *Journal of Computational Biology* **10**: 433–452 (2003).
110. R.W. Fleming, R.O. Dror, and E.H. Adelson. Real-world illumination and the perception of surface reflectance properties. *Journal of Vision* **3**: 347–368 (2003).
111. R.O. Dror, D.C. O’Carroll, and S.B. Laughlin. Accuracy of velocity estimation by Reichardt correlators. *Journal of the Optical Society of America A* **18**: 241–252 (2001).
112. R.O. Dror, C.C. Canavier, R.J. Butera, J.W. Clark, and J.H. Byrne. A mathematical criterion based on phase response curves for stability in a ring of coupled oscillators. *Biological Cybernetics* **80**: 11–23 (1999).
113. C.C. Canavier, R.J. Butera, R.O. Dror, D.A. Baxter, J.W. Clark, and J.H. Byrne. Phase response characteristics of model neurons determine which patterns are expressed in a ring circuit model of gait generation. *Biological Cybernetics* **77**: 367–380 (1997).
114. R.O. Dror, S. Ganguli, and R.S. Strichartz. A search for best constants in the Hardy-Littlewood maximal theorem. *Journal of Fourier Analysis and Applications* **2**: 473–86 (1996).

REFEREED CONFERENCE PAPERS

115. M. Xu, A.S. Powers, R.O. Dror, S. Ermon, J. Leskovec. Geometric Latent Diffusion Models for 3D Molecular Generation. *Proceedings of International Conference on Machine Learning (ICML)* (2023).
116. P. Suriana, J.M. Paggi, and R.O. Dror. FlexVDW: A machine learning approach to account for protein flexibility in ligand docking. *Proceedings of the Workshop on Machine Learning for Drug Design at the International Conference on Learning Representations (ICLR)* (2023).
117. D.D. Liu, L. Melo, A. Costa, M. Vögele, R.J.L. Townshend, R.O. Dror*. Euclidean Transformers for Macromolecular Structures: Lessons Learned. *Proceedings of the Workshop on Computational Biology at the International Conference on Machine Learning (ICML)* (2022).
118. A.S. Powers, H. Yu, P. Suriana, and R.O. Dror*. Fragment-based ligand generation guided by geometric deep learning on protein-ligand structure. *Proceedings of the Workshop on Machine Learning for Drug Design at the International Conference on Learning Representations (ICLR)* (2022).
119. R.J.L. Townshend, M. Vögele, P. Suriana, A. Derry, A.S. Powers, Y. Laloudakis, S. Balachandar, B. Jing, B.M. Anderson, S. Eismann, R. Kondor, R.B. Altman, and R.O. Dror*. ATOM3D: tasks on molecules in three dimensions. *Advances in Neural Information Processing Systems 34* (NeurIPS 2021). **Best Paper Award** (Datasets & Benchmarks).†
120. B. Jing, S. Eismann, P. Suriana, R.J.L. Townshend, and R.O. Dror*. Learning from protein structure with Geometric Vector Perceptrons. *Proceedings of the International Conference on Learning Representations (ICLR 2021)*.†
121. R.J.L. Townshend, R. Bedi, P. Suriana, and R.O. Dror*. End-to-end learning on 3D protein structure for interface prediction. *Advances in Neural Information Processing Systems 32* (NeurIPS 2019).†

122. D.E. Shaw, J.P. Grossman, J.A. Bank, B. Batson, J.A. Butts, J.C. Chao, M.M. Deneroff, R.O. Dror, A. Even, C.H. Fenton, A. Forte, J. Gagliardo, G. Gill, B. Greskamp, C.R. Ho, D.J. Ierardi, L. Iserovich, J.S. Kuskin, R.H. Larson, T. Layman, L.-S. Lee, A.K. Lerer, C. Li, D. Killebrew, K.M. Mackenzie, Shark Y.-H. Mok, M.A. Moraes, R. Mueller, L.J. Nociolo, J.L. Peticolas, T. Quan, D. Ramot, J.K. Salmon, D.P. Scarpazza, U.B. Schafer, N. Siddique, C.W. Snyder, J. Spengler, P.T.P. Tang, M. Theobald, H. Toma, B. Towles, B. Vitale, S.C. Wang, and C. Young. Anton 2: raising the bar for performance and programmability in a special-purpose molecular dynamics supercomputer. *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC14)*. Piscataway, NJ: IEEE. 41–53 (2014). **Gordon Bell Prize**.
123. D.P. Scarpazza, D.J. Ierardi, A.K. Lerer, K. M. Mackenzie, A.C. Pan, J.A. Bank, E. Chow, R.O. Dror, J.P. Grossman, D. Killebrew, M.A. Moraes, C. Predescu, J.K. Salmon, and D.E. Shaw. Extending the generality of molecular dynamics simulations on a special-purpose machine. *Proceedings of the 27th IEEE International Parallel and Distributed Processing Symposium (IPDPS)*. Boston, MA: IEEE Computer Society. 933–945 (2013). **Best Paper Award (Applications Track)**.
124. J.P. Grossman, J.S. Kuskin, J.A. Bank, M. Theobald, R.O. Dror, D.J. Ierardi, R.H. Larson, U.B. Schafer, B. Towles, C. Young, and D.E. Shaw. Hardware support for fine-grained event-driven computation in Anton 2. *Proceedings of the Eighteenth International Conference on Architectural Support for Programming Languages and Operating Systems (ASPLOS)*. New York, NY: ACM. 549–560 (2013).
125. J.K. Salmon, M.A. Moraes, R.O. Dror, and D.E. Shaw. Parallel random numbers: as easy as 1, 2, 3. *Proceedings of the Conference for High Performance Computing, Networking, Storage and Analysis (SC11)*. New York, NY: IEEE (2011). **Best Paper Award**.
126. J.A. Butts, P.T.P. Tang, R.O. Dror, and D.E. Shaw. Radix-8 digit-by-rounding: achieving high-performance reciprocals, square roots, and reciprocal square roots. *Proceedings of the 20th IEEE Symposium on Computer Arithmetic (ARITH20)*. Washington, DC: IEEE Computer Society (2011).
127. P.T.P. Tang, J.A. Butts, R.O. Dror, and D.E. Shaw. Tight certification techniques for digit-by-rounding algorithms with application to a new $1/\sqrt{x}$ design. *Proceedings of the 20th IEEE Symposium on Computer Arithmetic (ARITH20)*. Washington, DC: IEEE Computer Society (2011).
128. R.O. Dror, J.P. Grossman, K.M. Mackenzie, B. Towles, E. Chow, J.K. Salmon, C. Young, J.A. Bank, B. Batson, M.M. Deneroff, J.S. Kuskin, R.H. Larson, M.A. Moraes, and D.E. Shaw. Exploiting 162-nanosecond end-to-end communication latency on Anton. *Proceedings of the Conference for High Performance Computing, Networking, Storage and Analysis (SC10)*. New York, NY: IEEE (2010). **Best Paper Award Finalist**.
129. T. Tu, C.A. Rendleman, P. Miller, F. Sacerdoti, R.O. Dror, and D.E. Shaw. Accelerating parallel analysis of scientific simulation data via Zazen. *Proceedings of the USENIX Conference on File and Storage Technologies (FAST)*. Berkeley, CA: USENIX Association (2010).
130. D.E. Shaw, R.O. Dror, J.K. Salmon, J.P. Grossman, K.M. Mackenzie, J.A. Bank, C. Young, M.M. Deneroff, B. Batson, K.J. Bowers, E. Chow, M.P. Eastwood, D.J. Ierardi, J.L. Klepeis, J.S. Kuskin, R.H. Larson, K. Lindorff-Larsen, P. Maragakis, M.A. Moraes, S. Piana, Y. Shan, and B. Towles. Millisecond-scale molecular dynamics simulation on Anton. *Proceedings of the Conference for High Performance Computing, Networking, Storage and Analysis (SC09)*. New York, NY: ACM (2009). **Gordon Bell Prize; Best Paper Award**.

131. C. Young, J.A. Bank, **R.O. Dror**, J.P. Grossman, J.K. Salmon, and D. E. Shaw. A $32 \times 32 \times 32$, spatially distributed 3D FFT in five microseconds on Anton. *Proceedings of the Conference for High Performance Computing, Networking, Storage and Analysis (SC09)*. New York, NY: ACM (2009).
132. **R.O. Dror**, M.Ø. Jensen, and D.E. Shaw. Elucidating membrane protein function through long-timescale molecular dynamics simulation. *Proceedings of the IEEE Engineering in Medicine and Biology Society (EMBC)*. New York, NY: IEEE (2009).
133. C.R. Ho, M. Theobald, B. Batson, J.P. Grossman, S.C. Wang, J. Gagliardo, M.M. Deneroff, **R.O. Dror**, and D.E. Shaw. Post-silicon debug using formal verification waypoints. *Proceedings of the Design and Verification Conference and Exhibition (DVCon)*, San Jose (2009).
134. T. Tu, C.A. Rendleman, D.W. Borhani, **R.O. Dror**, J. Gullingsrud, M.Ø. Jensen, J.L. Klepeis, P. Maragakis, P. Miller, K.A. Stafford, and D.E. Shaw. A scalable parallel framework for analyzing terascale molecular dynamics trajectories. *Proceedings of the ACM/IEEE Conference on Supercomputing (SC08)*. New York, NY: IEEE (2008). **Best Paper Award Finalist**.
135. J.P. Grossman, C. Young, J.A. Bank, K. Mackenzie, D.J. Ierardi, J.K. Salmon, **R.O. Dror**, and D.E. Shaw. Simulation and embedded software development for Anton, a parallel machine with heterogenous multicore ASICs. *Proceedings of the 6th IEEE/ACM/IFIP International Conference on Hardware/Software Codesign and System Synthesis (CODES/ISSS)*. New York, NY: ACM (2008).
136. J.P. Grossman, J.K. Salmon, C.R. Ho, D.J. Ierardi, B. Towles, B. Batson, J. Spengler, S.C. Wang, R. Mueller, M. Theobald, C. Young, J. Gagliardo, M.M. Deneroff, **R.O. Dror**, and D.E. Shaw. Hierarchical simulation-based verification of Anton, a special-purpose parallel machine. *Proceedings of the 26th IEEE International Conference on Computer Design (ICCD)*. New York, NY: IEEE (2008).
137. C.R. Ho, M. Theobald, M.M. Deneroff, **R.O. Dror**, J. Gagliardo, and D.E. Shaw. Early formal verification of conditional coverage points to identify intrinsically hard-to-verify logic. *Proceedings of the 45th Design Automation Conference (DAC)*, Anaheim (2008).
138. R.H. Larson, J.K. Salmon, **R.O. Dror**, M.M. Deneroff, R.C. Young, J.P. Grossman, Y. Shan, J.L. Klepeis, and D.E. Shaw. High-throughput pairwise point interactions in Anton, a specialized machine for molecular dynamics simulation. *Proceedings of the 14th International Symposium on High-Performance Computer Architecture (HPCA)*. New York, NY: IEEE (2008).
139. J.S. Kuskin, R.C. Young, J.P. Grossman, B. Batson, M.M. Deneroff, **R.O. Dror**, and D.E. Shaw. Incorporating flexibility in Anton, a specialized machine for molecular dynamics simulation. *Proceedings of the 14th International Symposium on High-Performance Computer Architecture (HPCA)*. New York, NY: IEEE (2008).
140. D.E. Shaw, M.M. Deneroff, **R.O. Dror**, J.S. Kuskin, R.H. Larson, J.K. Salmon, C. Young, B. Batson, K.J. Bowers, J.C. Chao, M.P. Eastwood, J. Gagliardo, J.P. Grossman, C.R. Ho, D.J. Ierardi, I. Kolossváry, J.L. Klepeis, T. Layman, C. McLeavey, M.A. Moraes, R. Mueller, E.C. Priest, Y. Shan, J. Spengler, M. Theobald, B. Towles, and S.C. Wang. Anton: A special-purpose machine for molecular dynamics simulation. *Proceedings of the 34rd Annual International Symposium on Computer Architecture (ISCA)*. New York, NY: ACM (2007).
141. K.J. Bowers, E. Chow, H. Xu, **R.O. Dror**, M.P. Eastwood, B.A. Gregersen, J.L. Klepeis, I. Kolossváry, M.A. Moraes, F.D. Sacerdoti, J.K. Salmon, Y. Shan, and D.E. Shaw. Scalable algorithms for molecular dynamics simulations on commodity clusters. *Proceedings of the ACM/IEEE Conference on Supercomputing (SC06)*. New York, NY: IEEE (2006). **Best Paper Award**.

142. K.J. Bowers, **R.O. Dror**, and D.E. Shaw. Overview of neutral territory methods for the parallel evaluation of pairwise particle interactions. *Proceedings of the Scientific Discovery through Advanced Computing (SciDAC)*, San Francisco, June 2005. *Journal of Physics: Conference Series* 16:300–304 (2005).
143. **R.O. Dror***, J.G. Murnick, N.J. Rinaldi, V.D. Marinescu, R.M. Rifkin, and R.A. Young. A Bayesian approach to transcript estimation from gene array data: The BEAM technique. *Proceedings of the Sixth Annual International Conference on Research in Computational Molecular Biology (RECOMB)*, Washington, DC (2002).
144. **R.O. Dror**, T.K. Leung, E.H. Adelson, and A.S. Willsky. Statistics of real-world illumination. *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, Hawaii (2001).
145. **R.O. Dror**, E.H. Adelson, and A.S. Willsky. Recognition of surface reflectance properties from a single image under unknown real-world illumination. *Proceedings of the Workshop on Identifying Objects Across Variations in Lighting at the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, Hawaii (2001).
146. R.W. Fleming, **R.O. Dror**, and E.H. Adelson. How do humans determine reflectance properties under unknown illumination? *Proceedings of the Workshop on Identifying Objects Across Variations in Lighting at the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, Hawaii (2001).
147. **R.O. Dror**, E.H. Adelson, and A.S. Willsky. Surface reflectance estimation and natural illumination statistics. *Proceedings of the Second International Workshop on Statistical and Computational Theories of Vision at the IEEE International Conference on Computer Vision (ICCV)*, Vancouver (2001).
148. **R.O. Dror**, E.H. Adelson, and A.S. Willsky. Estimating surface reflectance properties from images under unknown illumination. *Proceedings of SPIE 4299: Human Vision and Electronic Imaging VI (HVEI)*, San Jose (2001).
149. **R.O. Dror**, D.C. O’Carroll, and S.B. Laughlin. The role of natural image statistics in biological motion estimation. *IEEE International Workshop on Biologically Motivated Computer Vision (BMVC)*, Seoul (2000). *Lecture Notes in Computer Science* 1811: 492–501 (2000).

BOOK CHAPTERS

150. E. Chow, J.L. Klepeis, C.A. Rendleman, **R.O. Dror**, and D.E. Shaw. New technologies for molecular dynamics simulations. In *Comprehensive Biophysics*, E.H. Egelman, ed., Amsterdam: Elsevier. 9:86–104 (2012).
151. **R.O. Dror***, C. Young, and D.E. Shaw. Anton: A special-purpose molecular simulation machine. In *Encyclopedia of Parallel Computing*, D. Padua, ed., New York, NY: Springer (2011).
152. **R.O. Dror***, A.C. Pan, D.H. Arlow, and D.E. Shaw. Probing the conformational dynamics of GPCRs with molecular dynamics simulation. In *G Protein-Coupled Receptors: From Structure to Function*. J. Giraldo and J.-P. Pin, eds., London: Royal Society of Chemistry, 384–400 (2011).

THESES

153. **R.O. Dror**. Surface reflectance recognition and real-world illumination statistics. Ph.D. thesis, Massachusetts Institute of Technology (2002).
154. **R.O. Dror**. Accuracy of visual velocity estimation by Reichardt correlators. M.Phil. thesis, University of Cambridge (1998).

TEACHING

Summary

I created two completely new computational biology courses, CS 279 and CS 371, after arriving at Stanford in 2014. The former has grown from 17 to 180 students, and the latter has grown from 5 to 45 students. I also coordinated two for-credit seminar series in computational biomedicine, which have attracted thousands of students. Comments on recent student evaluations include:

“Best class I've taken at Stanford so far. Ron is an incredible lecturer that makes the most complex topics seem simple.”

“One of the best teachers I've had at Stanford in all four years as an undergrad ... one of the best courses I've taken at Stanford.”

Computer Science (CS) 279: Computational Biology: Structure and Organization of Biomolecules and Cells

Cross-listed in Computational and Mathematical Engineering, Bioengineering, Biophysics, and Biomedical Informatics

Stanford, 2014, 2015, 2016, 2017, 2019, 2020, 2021, 2022, 2023

<http://cs279.stanford.edu>

Computational techniques for investigating and designing the three-dimensional structure and dynamics of biomolecules and cells. These computational methods play an increasingly important role in drug discovery, medicine, bioengineering, and molecular biology. Course topics include protein structure prediction, protein design, drug screening, molecular simulation, cellular-level simulation, image analysis for microscopy, and methods for solving structures from crystallography and electron microscopy data.

Computer Science (CS) 371: Computational Biology in Four Dimensions

Cross-listed in Computational and Mathematical Engineering, Biophysics, and Biomedical Informatics
Stanford, 2014, 2016, 2017, 2018

<http://cs371.stanford.edu>

Cutting-edge research on computational techniques for investigating and designing the three-dimensional structure and dynamics of biomolecules, cells, and everything in between. These techniques, which draw on approaches ranging from physics-based simulation to machine learning, play an increasingly important role in drug discovery, medicine, bioengineering, and molecular biology. Course is devoted primarily to reading, presentation, discussion, and critique of papers describing important recent research developments.

Computer Science (CS) 229: Machine Learning

Stanford, 2018

<http://cs229.stanford.edu>

Topics: statistical pattern recognition, linear and non-linear regression, non-parametric methods, exponential family, GLMs, support vector machines, kernel methods, model/feature selection, learning theory, VC dimension, clustering, density estimation, EM, dimensionality reduction, ICA, PCA, reinforcement learning and adaptive control, Markov decision processes, approximate dynamic programming, and policy search. Prerequisites: linear algebra, and basic probability and statistics.

Computer Science (CS) 522: Seminar on Artificial Intelligence in Healthcare

Stanford, 2017, 2018, 2019, 2020, 2021, 2023

Artificial intelligence is poised to make radical changes in healthcare, transforming areas such as diagnosis, genomics, surgical robotics, and drug discovery. In the coming years, artificial intelligence has the potential to lower healthcare costs, identify more effective treatments, and facilitate prevention and early detection of diseases. This class features prominent researchers, physicians,

entrepreneurs, and venture capitalists, all sharing their thoughts on the future of healthcare. Each year, I run this course in collaboration with a different set of student organizers.

Computer Science (CS) 109: Introduction to Probability for Computer Scientists

Stanford, 2015

Topics include: counting and combinatorics, random variables, conditional probability, independence, distributions, expectation, point estimation, and limit theorems. Applications of probability in computer science including machine learning and the use of probability in the analysis of algorithms.

Computational and Mathematical Engineering (CME) 500: Seminar on Computation and Mathematics in Biology

Stanford, 2014

This course serves as the main seminar series of the Institute for Computational and Mathematical Engineering. My version featured experts on a variety of topics in computational and mathematical biology.