Barry J Grant

List of Publications by Year in descending order

42 papers	4,533 citations	201385 27 h-index	243296 44 g-index
46 all docs	46 docs citations	46 times ranked	6124 citing authors

#	Article	IF	Citations
1	Bio3d: an R package for the comparative analysis of protein structures. Bioinformatics, 2006, 22, 2695-2696.	1.8	1,440
2	Drug hypersensitivity caused by alteration of the MHC-presented self-peptide repertoire. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 9959-9964.	3.3	354
3	Integrating protein structural dynamics and evolutionary analysis with Bio3D. BMC Bioinformatics, 2014, 15, 399.	1.2	292
4	Large conformational changes in proteins: signaling and other functions. Current Opinion in Structural Biology, 2010, 20, 142-147.	2.6	213
5	The <scp>Bio3D</scp> packages for structural bioinformatics. Protein Science, 2021, 30, 20-30.	3.1	200
6	Mapping the Nucleotide and Isoform-Dependent Structural and Dynamical Features of Ras Proteins. Structure, 2008, 16, 885-896.	1.6	191
7	Ras Conformational Switching: Simulating Nucleotide-Dependent Conformational Transitions with Accelerated Molecular Dynamics. PLoS Computational Biology, 2009, 5, e1000325.	1.5	157
8	Novel Allosteric Sites on Ras for Lead Generation. PLoS ONE, 2011, 6, e25711.	1.1	155
9	Targeted Molecular Dynamics Study of C-Loop Closure and Channel Gating in Nicotinic Receptors. PLoS Computational Biology, 2006, 2, e134.	1.5	113
10	Channel Opening Motion of Î±7 Nicotinic Acetylcholine Receptor as Suggested by Normal Mode Analysis. Journal of Molecular Biology, 2006, 355, 310-324.	2.0	104
11	Accessing a Hidden Conformation of the Maltose Binding Protein Using Accelerated Molecular Dynamics. PLoS Computational Biology, 2011, 7, e1002034.	1.5	102
12	Structural and Molecular Mechanisms of Cytokine-Mediated Endocrine Resistance in Human Breast Cancer Cells. Molecular Cell, 2017, 65, 1122-1135.e5.	4.5	99
13	Induced Fit or Conformational Selection? The Role of the Semi-closed State in the Maltose Binding Protein. Biochemistry, 2011, 50, 10530-10539.	1.2	88
14	A structural model for microtubule minus-end recognition and protection by CAMSAP proteins. Nature Structural and Molecular Biology, 2017, 24, 931-943.	3.6	86
15	Computational and biochemical characterization of two partially overlapping interfaces and multiple weak-affinity K-Ras dimers. Scientific Reports, 2017, 7, 40109.	1.6	85
16	The Distinct Conformational Dynamics of K-Ras and H-Ras A59G. PLoS Computational Biology, 2010, 6, e1000922.	1.5	79
17	Dynamic Coupling and Allosteric Networks in the Î± Subunit of Heterotrimeric G Proteins. Journal of Biological Chemistry, 2016, 291, 4742-4753.	1.6	66
18	Electrostatically Biased Binding of Kinesin to Microtubules. PLoS Biology, 2011, 9, e1001207.	2.6	64

#	Article	IF	Citations
19	Conformational Selection in G-Proteins: Lessons from Ras and Rho. Biophysical Journal, 2010, 99, L87-L89.	0.2	52
20	Kinesin-5 Allosteric Inhibitors Uncouple the Dynamics of Nucleotide, Microtubule, and Neck-Linker Binding Sites. Biophysical Journal, 2014, 107, 2204-2213.	0.2	52
21	Multivariate Analysis of Conserved Sequenceâ€“Structure Relationships in Kinesins: Coupling of the Active Site and a Tubulin-binding Sub-domain. Journal of Molecular Biology, 2007, 368, 1231-1248.	2.0	47
22	Mapping the Structural and Dynamical Features of Kinesin Motor Domains. PLoS Computational Biology, 2013, 9, e1003329.	1.5	39
23	Rapid Characterization of Allosteric Networks with Ensemble Normal Mode Analysis. Journal of Physical Chemistry B, 2016, 120, 8276-8288.	1.2	37
24	Online interactive analysis of protein structure ensembles with Bio3D-web. Bioinformatics, 2016, 32, 3510-3512.	1.8	37
25	Systems Structural Biology Analysis of Ligand Effects on ERÎ± Predicts Cellular Response to Environmental Estrogens and Anti-hormone Therapies. Cell Chemical Biology, 2017, 24, 35-45.	2.5	34
26	Neck linker docking is critical for Kinesin-1 force generation in cells but at a cost to motor speed and processivity. ELife, 2019, 8, .	2.8	31
27	Large-Scale Conformational Changes of Trypanosoma cruzi Proline Racemase Predicted by Accelerated Molecular Dynamics Simulation. PLoS Computational Biology, 2011, 7, e1002178.	1.5	30
28	LeuT Conformational Sampling Utilizing Accelerated Molecular Dynamics and Principal Component Analysis. Biophysical Journal, 2012, 103, L1-L3.	0.2	28
29	Calcium binding and allosteric signaling mechanisms for the sarcoplasmic reticulum Ca²⁺ ATPase. Protein Science, 2012, 21, 1429-1443.	3.1	28
30	Mapping the Processivity Determinants of the Kinesin-3 Motor Domain. Biophysical Journal, 2015, 109, 1537-1540.	0.2	28
31	Conformational Sampling and Nucleotide-Dependent Transitions of the GroEL Subunit Probed by Unbiased Molecular Dynamics Simulations. PLoS Computational Biology, 2011, 7, e1002004.	1.5	27
32	Altered chemomechanical coupling causes impaired motility of the kinesin-4 motors KIF27 and KIF7. Journal of Cell Biology, 2018, 217, 1319-1334.	2.3	25
33	Domain-Opening and Dynamic Coupling in the Î±-Subunit of Heterotrimeric G Proteins. Biophysical Journal, 2013, 105, L08-L10.	0.2	24
34	A posttranslational modification of the mitotic kinesin Eg5 that enhances its mechanochemical coupling and alters its mitotic function. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E1779-E1788.	3.3	24
35	Enrichment of Druggable Conformations from Apo Protein Structures Using Cosolvent-Accelerated Molecular Dynamics. Biology, 2015, 4, 344-366.	1.3	19
36	Comparative structural dynamic analysis of GTPases. PLoS Computational Biology, 2018, 14, e1006364.	1.5	18

#	Article	IF	Citations
37	Navigating the conformational landscape of G proteinâ€“coupled receptor kinases during allosteric activation. Journal of Biological Chemistry, 2017, 292, 16032-16043.	1.6	16
38	Identification of Potential Small Molecule Binding Pockets on Rho Family GTPases. PLoS ONE, 2012, 7, e40809.	1.1	15
39	Novel procedure for thermal equilibration in molecular dynamics simulation. Molecular Simulation, 2009, 35, 349-357.	0.9	9
40	Comparative Protein Structure Analysis with Bio3D-Web. Methods in Molecular Biology, 2020, 2112, 15-28.	0.4	7
41	sgTarget: a target selection resource for structural genomics. Nucleic Acids Research, 2006, 34, W225-W230.	6.5	6
42	Investigating Protein Sequence-structure-dynamics Relationships with Bio3D-web. Journal of Visualized Experiments, 2017, , .	0.2	2