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	The <scp>Bio3D</scp> packages for structural bioinformatics. Protein Science, 2021, 30, 20-30.	3.1	200
2	Comparative Protein Structure Analysis with Bio3D-Web. Methods in Molecular Biology, 2020, 2112, 15-28.	0.4	7
3	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
4	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
5	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
6	Comparative structural dynamic analysis of GTPases. PLoS Computational Biology, 2018, 14, e1006364.	1.5	18
7	Computational and biochemical characterization of two partially overlapping interfaces and multiple weak-affinity K-Ras dimers. Scientific Reports, 2017, 7, 40109.	1.6	85
8	Structural and Molecular Mechanisms of Cytokine-Mediated Endocrine Resistance in Human Breast Cancer Cells. Molecular Cell, 2017, 65, 1122-1135.e5.	4.5	99
9	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
10	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
11	Investigating Protein Sequence-structure-dynamics Relationships with Bio3D-web. Journal of Visualized Experiments, 2017, , .	0.2	2
12	Navigating the conformational landscape of G proteinâ€“coupled receptor kinases during allosteric activation. Journal of Biological Chemistry, 2017, 292, 16032-16043.	1.6	16
13	Rapid Characterization of Allosteric Networks with Ensemble Normal Mode Analysis. Journal of Physical Chemistry B, 2016, 120, 8276-8288.	1.2	37
14	Online interactive analysis of protein structure ensembles with Bio3D-web. Bioinformatics, 2016, 32, 3510-3512.	1.8	37
15	Dynamic Coupling and Allosteric Networks in the Î± Subunit of Heterotrimeric G Proteins. Journal of Biological Chemistry, 2016, 291, 4742-4753.	1.6	66
16	Enrichment of Druggable Conformations from Apo Protein Structures Using Cosolvent-Accelerated Molecular Dynamics. Biology, 2015, 4, 344-366.	1.3	19
17	Mapping the Processivity Determinants of the Kinesin-3 Motor Domain. Biophysical Journal, 2015, 109, 1537-1540.	0.2	28
18	Integrating protein structural dynamics and evolutionary analysis with Bio3D. BMC Bioinformatics, 2014, 15, 399.	1.2	292

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19	Kinesin-5 Allosteric Inhibitors Uncouple the Dynamics of Nucleotide, Microtubule, and Neck-Linker Binding Sites. Biophysical Journal, 2014, 107, 2204-2213.	0.2	52
20	Domain-Opening and Dynamic Coupling in the Î±-Subunit of Heterotrimeric G Proteins. Biophysical Journal, 2013, 105, L08-L10.	0.2	24
21	Mapping the Structural and Dynamical Features of Kinesin Motor Domains. PLoS Computational Biology, 2013, 9, e1003329.	1.5	39
22	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
23	LeuT Conformational Sampling Utilizing Accelerated Molecular Dynamics and Principal Component Analysis. Biophysical Journal, 2012, 103, L1-L3.	0.2	28
24	Calcium binding and allosteric signaling mechanisms for the sarcoplasmic reticulum Ca²⁺ ATPase. Protein Science, 2012, 21, 1429-1443.	3.1	28
25	Identification of Potential Small Molecule Binding Pockets on Rho Family GTPases. PLoS ONE, 2012, 7, e40809.	1.1	15
26	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
27	Electrostatically Biased Binding of Kinesin to Microtubules. PLoS Biology, 2011, 9, e1001207.	2.6	64
28	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
29	Large-Scale Conformational Changes of Trypanosoma cruzi Proline Racemase Predicted by Accelerated Molecular Dynamics Simulation. PLoS Computational Biology, 2011, 7, e1002178.	1.5	30
30	Accessing a Hidden Conformation of the Maltose Binding Protein Using Accelerated Molecular Dynamics. PLoS Computational Biology, 2011, 7, e1002034.	1.5	102
31	Novel Allosteric Sites on Ras for Lead Generation. PLoS ONE, 2011, 6, e25711.	1.1	155
32	Large conformational changes in proteins: signaling and other functions. Current Opinion in Structural Biology, 2010, 20, 142-147.	2.6	213
33	The Distinct Conformational Dynamics of K-Ras and H-Ras A59G. PLoS Computational Biology, 2010, 6, e1000922.	1.5	79
34	Conformational Selection in G-Proteins: Lessons from Ras and Rho. Biophysical Journal, 2010, 99, L87-L89.	0.2	52
35	Novel procedure for thermal equilibration in molecular dynamics simulation. Molecular Simulation, 2009, 35, 349-357.	0.9	9
36	Ras Conformational Switching: Simulating Nucleotide-Dependent Conformational Transitions with Accelerated Molecular Dynamics. PLoS Computational Biology, 2009, 5, e1000325.	1.5	157

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37	Mapping the Nucleotide and Isoform-Dependent Structural and Dynamical Features of Ras Proteins. Structure, 2008, 16, 885-896.	1.6	191
38	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
39	sgTarget: a target selection resource for structural genomics. Nucleic Acids Research, 2006, 34, W225-W230.	6.5	6
40	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
41	Bio3d: an R package for the comparative analysis of protein structures. Bioinformatics, 2006, 22, 2695-2696.	1.8	1,440
42	Targeted Molecular Dynamics Study of C-Loop Closure and Channel Gating in Nicotinic Receptors. PLoS Computational Biology, 2006, 2, e134.	1.5	113