Carol Beth Post

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Ubiquitin Câ€Terminal Hydrolase L1: Biochemical and Cellular Characterization of a Covalent Cyanopyrrolidineâ€Based Inhibitor. ChemBioChem, 2020, 21, 712-722.	2.6	32
2	Substrate binding to Src: A new perspective on tyrosine kinase substrate recognition from NMR and molecular dynamics. Protein Science, 2020, 29, 350-359.	7.6	9
3	All-atom adaptively biased path optimization of Src kinase conformational inactivation: Switched electrostatic network in the concerted motion of $\hat{I}\pm C$ helix and the activation loop. Journal of Chemical Physics, 2020, 153, 175101.	3.0	7
4	Application of a Substrate-Mediated Selection with c-Src Tyrosine Kinase to a DNA-Encoded Chemical Library. Molecules, 2019, 24, 2764.	3.8	14
5	NmrLineGuru: Standalone and User-Friendly GUIs for Fast 1D NMR Lineshape Simulation and Analysis of Multi-State Equilibrium Binding Models. Scientific Reports, 2019, 9, 16023.	3.3	7
6	Protein Conformational Transitions from All-Atom Adaptively Biased Path Optimization. Journal of Chemical Theory and Computation, 2018, 14, 5372-5382.	5.3	6
7	Entropic allostery dominates the phosphorylationâ€dependent regulation of Syk tyrosine kinase release from immunoreceptor tyrosineâ€based activation motifs. Protein Science, 2018, 27, 1780-1796.	7.6	11
8	A minimization principle for transition paths of maximum flux for collective variables. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	1
9	A simple method for NMR t1 noise suppression. Journal of Magnetic Resonance, 2017, 276, 43-50.	2.1	18
10	Editorial overview: Theory & computation. Current Opinion in Structural Biology, 2017, 43, iv-vi.	5.7	1
11	Evaluating the dynamics and electrostatic interactions of folded proteins in implicit solvents. Protein Science, 2016, 25, 204-218.	7.6	7
12	Insights into the allosteric regulation of Syk association with receptor ITAM, a multi-state equilibrium. Physical Chemistry Chemical Physics, 2016, 18, 5807-5818.	2.8	14
13	Effects of impaired membrane interactions on α-synuclein aggregation and neurotoxicity. Neurobiology of Disease, 2015, 79, 150-163.	4.4	73
14	Shake, rattle, and roll: Impact of the dynamics of flavivirus particles on their interactions with the host. Virology, 2015, 479-480, 508-517.	2.4	103
15	Relative Binding Enthalpies from Molecular Dynamics Simulations Using a Direct Method. Journal of Chemical Theory and Computation, 2014, 10, 2759-2768.	5.3	16
16	Differential recognition of sykâ€binding sites by each of the two phosphotyrosineâ€binding pockets of the Vav SH2 domain. Biopolymers, 2013, 99, 897-907.	2.4	11
17	Detection of Long-Range Concerted Motions in Protein by a Distance Covariance. Journal of Chemical Theory and Computation, 2012, 8, 3009-3014.	5.3	16
18	αC Helix as a Switch in the Conformational Transition of Src/CDK-like Kinase Domains. Journal of Physical Chemistry B. 2012. 116. 4465-4475.	2.6	49

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19	Unrestrained Computation of Free Energy along a Path. Journal of Physical Chemistry B, 2012, 116, 11046-11055.	2.6	28
20	Long-distance correlations of rhinovirus capsid dynamics contribute to uncoating and antiviral activity. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 5271-5276.	7.1	35
21	Two Closely Spaced Tyrosines Regulate NFAT Signaling in B Cells via Syk Association with Vav. Molecular and Cellular Biology, 2011, 31, 2984-2996.	2.3	25
22	Constraining Binding Hot Spots: NMR and Molecular Dynamics Simulations Provide a Structural Explanation for Enthalpyâ^'Entropy Compensation in SH2â^'Ligand Binding. Journal of the American Chemical Society, 2010, 132, 11058-11070.	13.7	42
23	An electrostatic network and longâ€range regulation of Src kinases. Protein Science, 2008, 17, 1871-1880.	7.6	54
24	Tyr130 phosphorylation triggers Syk release from antigen receptor by long-distance conformational uncoupling. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 11760-11765.	7.1	53
25	Src kinase activation: A switched electrostatic network. Protein Science, 2006, 15, 1051-1062.	7.6	71
26	Exchange-transferred NOE spectroscopy and bound ligand structure determination. Current Opinion in Structural Biology, 2003, 13, 581-588.	5.7	177
27	Docking multiple conformations of a flexible ligand into a protein binding site using NMR restraints. Proteins: Structure, Function and Bioinformatics, 2002, 46, 295-307.	2.6	24
28	Intermolecular relaxation has little effect on intra-peptide exchange-transferred NOE intensities. Journal of Biomolecular NMR, 2002, 22, 303-315.	2.8	6
29	Insights into Protein Compressibility from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2001, 105, 715-724.	2.6	57
30	Theoretical studies of viral capsid proteins. Current Opinion in Structural Biology, 2000, 10, 170-173.	5.7	42
31	Accuracy of bound peptide structures determined by exchange transferred nuclear Overhauser data: a simulation study. Journal of Biomolecular NMR, 2000, 17, 17-32.	2.8	20
32	Substrate Recognition by the Lyn Protein-tyrosine Kinase. Journal of Biological Chemistry, 2000, 275, 16174-16182.	3.4	23
33	NMR structure of phospho-tyrosine signaling complexes. , 1999, 19, 295-305.		6
34	Molecular dynamics investigation of the effect of an antiviral compound on human rhinovirus. Protein Science, 1999, 8, 2281-2289.	7.6	20
35	Catalysis by Entropic Guidance from Enzymesâ€. Biochemistry, 1996, 35, 15129-15133.	2.5	41