Leslie A Kuhn

List of Publications by Year
in descending order

43	3,241	279487	329751
papers	citations	23 h-index	37 g-index

47	47	47	3479
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Machine Learning to Identify Flexibility Signatures of Class A GPCR Inhibition. Biomolecules, 2020, 10, 454.	1.8	21
2	Deciphering the three-domain architecture in schlafens and the structures and roles of human schlafen12 and serpinB12 in transcriptional regulation. Journal of Molecular Graphics and Modelling, 2019, 90, 59-76.	1.3	9
3	Automated Inference of Chemical Discriminants of Biological Activity. Methods in Molecular Biology, 2018, 1762, 307-338.	0.4	7
4	Proteinâ€“ligand interfaces are polarized: discovery of a strong trend for intermolecular hydrogen bonds to favor donors on the protein side with implications for predicting and designing ligand complexes. Journal of Computer-Aided Molecular Design, 2018, 32, 511-528.	1.3	36
5	Enabling the hypothesis-driven prioritization of ligand candidates in big databases: Screenlamp and its application to GPCR inhibitor discovery for invasive species control. Journal of Computer-Aided Molecular Design, 2018, 32, 415-433.	1.3	8
6	Schlafen 12 Interaction with SerpinB12 and Deubiquitylases Drives Human Enterocyte Differentiation. Cellular Physiology and Biochemistry, 2018, 48, 1274-1290.	1.1	27
7	Inhibition of pressure-activated cancer cell adhesion by FAK-derived peptides. Oncotarget, 2017, 8, 98051-98067.	0.8	6
8	Translocator Protein 18 kDa (TSPO): An Old Protein with New Functions?. Biochemistry, 2016, 55, 2821-2831.	1.2	96
9	Genome of the Asian longhorned beetle (Anoplophora glabripennis), a globally significant invasive species, reveals key functional and evolutionary innovations at the beetleâ€“plant interface. Genome Biology, 2016, 17, 227.	3.8	244
10	Detecting the native ligand orientation by interfacial rigidity: SiteInterlock. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1888-1901.	1.5	10
11	CholMine: Determinants and Prediction of Cholesterol and Cholate Binding Across Nonhomologous Protein Structures. Journal of Chemical Information and Modeling, 2015, 55, 747-759.	2.5	4
12	Structural Determinants Allowing Transferase Activity in SENSITIVE TO FREEZING 2, Classified as a Family I Glycosyl Hydrolase. Journal of Biological Chemistry, 2014, 289, 26089-26106.	1.6	23
13	The P-loop region of Schlafen 3 acts within the cytosol to induce differentiation of human Caco-2 intestinal epithelial cells. Biochimica Et Biophysica Acta - Molecular Cell Research, 2014, 1843, 3029-3037.	1.9	19
14	Ring-Substituted Î±-Arylalanines for Probing Substituent Effects on the Isomerization Reaction Catalyzed by an Aminomutase. ACS Catalysis, 2014, 4, 3077-3090.	5.5	10
15	Computational Prediction and in Vitro Analysis of Potential Physiological Ligands of the Bile Acid Binding Site in Cytochrome c Oxidase. Biochemistry, 2013, 52, 6995-7006.	1.2	13
16	Characterization of the ADRP Fatty Acid Binding Site: A Fluorescence Binding and Circular Dichroic Study. FASEB Journal, 2013, 27, 856.5.	0.2	0
17	Educating Students for an Interdisciplinary World. FASEB Journal, 2013, 27, 215.3.	0.2	0
18	ArtSurf. , 2012, , .		2

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19	Scoring ligand similarity in structureâ€based virtual screening. Journal of Molecular Recognition, 2009, 22, 280-292.	1.1	32
20	StoneHinge: Hinge prediction by network analysis of individual protein structures. Protein Science, 2009, 18, 359-371.	3.1	44
21	HingeMaster: Normal mode hinge prediction approach and integration of complementary predictors. Proteins: Structure, Function and Bioinformatics, 2008, 73, 299-319.	1.5	38
22	Using structural analysis to generate parasiteâ€selective monoclonal antibodies. Protein Science, 2008, 17, 983-989.	3.1	5
23	Target Flexibility: An Emerging Consideration in Drug Discovery and Design. Journal of Medicinal Chemistry, 2008, 51, 6237-6255.	2.9	280
24	Structural basis for the enantiospecificities ofR- andS-specific phenoxypropionate/Î±-ketoglutarate dioxygenases. Protein Science, 2006, 15, 1356-1368.	3.1	15
25	Discovering New Classes of BrugiaÂmalayi Asparaginyl-tRNA Synthetase Inhibitors and Relating Specificity to Conformational Change. Journal of Computer-Aided Molecular Design, 2006, 20, 159-178.	1.3	46
26	Side-chain flexibility in protein-ligand binding: The minimal rotation hypothesis. Protein Science, 2005, 14, 1104-1114.	3.1	157
27	FLEXIBILITY IN BIOMOLECULES. , 2005, , 97-112.		5
28	Change in protein flexibility upon complex formation: Analysis of Ras-Raf using molecular dynamics and a molecular framework approach. Proteins: Structure, Function and Bioinformatics, 2004, 56, 322-337.	1.5	106
29	Modeling correlated main-chain motions in proteins for flexible molecular recognition. Proteins: Structure, Function and Bioinformatics, 2004, 57, 243-261.	1.5	72
30	Sampling protein conformations and pathways. Journal of Computational Chemistry, 2004, 25, 1133-1148.	1.5	58
31	Protein unfolding: Rigidity lost. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 3540-3545.	3.3	255
32	Flexible and Rigid Regions in Proteins. , 2002, , 357-384.		17
33	Identifying protein folding cores from the evolution of flexible regions during unfolding. Journal of Molecular Graphics and Modelling, 2002, 21, 195-207.	1.3	113
34	Distilling the essential features of a protein surface for improving protein-ligand docking, scoring, and virtual screening. Journal of Computer-Aided Molecular Design, 2002, 16, 883-902.	1.3	90
35	Protein flexibility predictions using graph theory. Proteins: Structure, Function and Bioinformatics, 2001, 44, 150-165.	1.5	670
36	One site fits both: a model for the ternary complex of folate + NADPH in R67 dihydrofolate reductase, a D2 symmetric enzyme. Journal of Computer-Aided Molecular Design, 2001, 15, 1035-1052.	1.3	18

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37	Protein flexibility and dynamics using constraint theory. Journal of Molecular Graphics and Modelling, 2001, 19, 60-69.	1.3	109
38	Virtual screening with solvation and ligand-induced complementarity. Journal of Computer - Aided Molecular Design, 2000, 20, 171-190.	1.0	138
39	FLEXIBILITY AND CRITICAL HYDROGEN BONDS IN CYTOCHROME C. , 1999, , 191-202.		6
40	Screening a peptidyl database for potential ligands to proteins with side-chain flexibility. Proteins: Structure, Function and Bioinformatics, 1998, 33, 74-87.	1.5	108
41	Cluster analysis of consensus water sites in thrombin and trypsin shows conservation between serine proteases and contributions to ligand specificity. Protein Science, 1998, 7, 2054-2064.	3.1	76
42	Predicting conserved water-mediated and polar ligand interactions in proteins using a K-nearest-neighbors genetic algorithm. Journal of Molecular Biology, 1997, 265, 445-464.	2.0	168
43	Atomic and residue hydrophilicity in the context of folded protein structures. Proteins: Structure, Function and Bioinformatics, 1995, 23, 536-547.	1.5	78