Arthur J Olson

List of Publications by Year
in descending order

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70 papers	58,823 citations	126708 33 h-index	118652 62 g-index
70 all docs	70 docs citations	70 times ranked	55832 citing authors

#	Article	IF	Citations
1	AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. Journal of Computational Chemistry, 2010, 31, 455-461.	1.5	21,573
2	AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. Journal of Computational Chemistry, 2009, 30, 2785-2791.	1.5	16,850
3	Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function. , 1998, 19, 1639-1662.		8,897
4	A semiempirical free energy force field with charge-based desolvation. Journal of Computational Chemistry, 2007, 28, 1145-1152.	1.5	1,854
5	Computational proteinâ€“ligand docking and virtual drug screening with the AutoDock suite. Nature Protocols, 2016, 11, 905-919.	5.5	1,370
6	Automated docking of flexible ligands: Applications of autodock. , 1996, 9, 1-5.		1,284
7	Automated docking of substrates to proteins by simulated annealing. Proteins: Structure, Function and Bioinformatics, 1990, 8, 195-202.	1.5	1,109
8	Distributed automated docking of flexible ligands to proteins: Parallel applications of AutoDock 2.4. Journal of Computer-Aided Molecular Design, 1996, 10, 293-304.	1.3	907
9	Structural Symmetry and Protein Function. Annual Review of Biophysics and Biomolecular Structure, 2000, 29, 105-153.	18.3	806
10	Proteome-wide covalent ligand discovery in native biological systems. Nature, 2016, 534, 570-574.	13.7	651
11	Virtual screening with AutoDock: theory and practice. Expert Opinion on Drug Discovery, 2010, 5, 597-607.	2.5	462
12	Automated docking to multiple target structures: Incorporation of protein mobility and structural water heterogeneity in AutoDock. Proteins: Structure, Function and Bioinformatics, 2002, 46, 34-40.	1.5	394
13	AutoDockFR: Advances in Protein-Ligand Docking with Explicitly Specified Binding Site Flexibility. PLoS Computational Biology, 2015, 11, e1004586.	1.5	287
14	AutoDock4_{Zn}: An Improved AutoDock Force Field for Small-Molecule Docking to Zinc Metalloproteins. Journal of Chemical Information and Modeling, 2014, 54, 2371-2379.	2.5	218
15	A Force Field with Discrete Displaceable Waters and Desolvation Entropy for Hydrated Ligand Docking. Journal of Medicinal Chemistry, 2012, 55, 623-638.	2.9	216
16	Covalent docking using autodock: Twoâ€point attractor and flexible side chain methods. Protein Science, 2016, 25, 295-301.	3.1	170
17	Automated prediction of ligandâ€binding sites in proteins. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1506-1517.	1.5	134
18	cellPACK: a virtual mesoscope to model and visualize structural systems biology. Nature Methods, 2015, 12, 85-91.	9.0	130

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19	Chemical mimicry of viral capsid self-assembly. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 20731-20736.	3.3	98
20	Illustrate: Software for Biomolecular Illustration. Structure, 2019, 27, 1716-1720.e1.	1.6	87
21	The <scp>AutoDock</scp> suite at 30. Protein Science, 2021, 30, 31-43.	3.1	85
22	Automated docking in crystallography: Analysis of the substrates of aconitase. Proteins: Structure, Function and Bioinformatics, 1993, 17, 1-10.	1.5	84
23	Perspectives on Structural Molecular Biology Visualization: From Past to Present. Journal of Molecular Biology, 2018, 430, 3997-4012.	2.0	64
24	A Dynamic Model of HIV Integrase Inhibition and Drug Resistance. Journal of Molecular Biology, 2010, 397, 600-615.	2.0	63
25	Development of a New Type of Protease Inhibitors, Efficacious against FIV and HIV Variants. Journal of the American Chemical Society, 1999, 121, 1145-1155.	6.6	56
26	Distinguishing Binders from False Positives by Free Energy Calculations: Fragment Screening Against the Flap Site of HIV Protease. Journal of Physical Chemistry B, 2015, 119, 976-988.	1.2	54
27	Virtual screening of integrase inhibitors by large scale binding free energy calculations: the SAMPL4 challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 475-490.	1.3	53
28	Blind prediction of HIV integrase binding from the SAMPL4 challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 327-345.	1.3	53
29	Dense Array of Spikes on HIV-1 Virion Particles. Journal of Virology, 2017, 91, .	1.5	53
30	Importance of Factor VIIa Gla-Domain Residue Arg-36 for Recognition of the Macromolecular Substrate Factor X Gla-Domainâ€. Biochemistry, 1999, 38, 1957-1966.	1.2	52
31	Challenges in structural approaches to cell modeling. Journal of Molecular Biology, 2016, 428, 2943-2964.	2.0	51
32	Analysis of a data set of paired uncomplexed protein structures: New metrics for side-chain flexibility and model evaluation. Proteins: Structure, Function and Bioinformatics, 2001, 43, 271-279.	1.5	50
33	Modelling of Factor Xa-inhibitor complexes: a computational flexible docking approach. , 1999, 34, 173-183.		48
34	Virtual screening with AutoDock Vina and the common pharmacophore engine of a low diversity library of fragments and hits against the three allosteric sites of HIV integrase: participation in the SAMPL4 proteinâ€“ligand binding challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 429-441.	1.3	44
35	Building Structural Models of a Whole Mycoplasma Cell. Journal of Molecular Biology, 2022, 434, 167351.	2.0	40
36	Instant Construction and Visualization of Crowded Biological Environments. IEEE Transactions on Visualization and Computer Graphics, 2018, 24, 862-872.	2.9	36

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37	Art and Science of the Cellular Mesoscale. Trends in Biochemical Sciences, 2020, 45, 472-483.	3.7	36
38	A Virtual Screen Discovers Novel, Fragment-Sized Inhibitors of Mycobacterium tuberculosis InhA. Journal of Chemical Information and Modeling, 2015, 55, 645-659.	2.5	35
39	Structural studies of FIV and HIV-1 proteases complexed with an efficient inhibitor of FIV protease. , 2000, 38, 29-40.		32
40	Small Molecule Regulation of Protein Conformation by Binding in the Flap of HIV Protease. ACS Chemical Biology, 2013, 8, 1223-1231.	1.6	30
41	Viral Evolution in Response to the Broad-Based Retroviral Protease Inhibitor TL-3. Journal of Virology, 2001, 75, 9502-9508.	1.5	28
42	Automated Docking and the Search for HIV Protease Inhibitors. SAR and QSAR in Environmental Research, 1998, 8, 273-285.	1.0	24
43	Lattice Models of Bacterial Nucleoids. Journal of Physical Chemistry B, 2018, 122, 5441-5447.	1.2	23
44	A New Class of Allosteric HIV-1 Integrase Inhibitors Identified by Crystallographic Fragment Screening of the Catalytic Core Domain. Journal of Biological Chemistry, 2016, 291, 23569-23577.	1.6	20
45	CellPAINT: Turnkey Illustration of Molecular Cell Biology. Frontiers in Bioinformatics, 2021, 1, .	1.0	20
46	Icosahedral virus structures and the protein data bank. Journal of Biological Chemistry, 2021, 296, 100554.	1.6	17
47	A Self-Assisting Protein Folding Model for Teaching Structural Molecular Biology. Structure, 2017, 25, 671-678.	1.6	16
48	Intrabacterial Metabolism Obscures the Successful Prediction of an InhA Inhibitor of Mycobacterium tuberculosis. ACS Infectious Diseases, 2019, 5, 2148-2163.	1.8	16
49	Novel Intersubunit Interaction Critical for HIV-1 Core Assembly Defines a Potentially Targetable Inhibitor Binding Pocket. MBio, 2019, 10, .	1.8	13
50	Biomolecular visualization using AVS. Journal of Molecular Graphics, 1995, 13, 271-282.	1.7	12
51	Pococurante (Poc): An ENU-Induced Missense Mutation of MyD88 with Selective Effects on TLR Signal Transduction.. Blood, 2004, 104, 649-649.	0.6	11
52	Transmembrane ?-helices in the gap junction membrane channel: Systematic search of packing models based on the pair potential function. Microscopy Research and Technique, 2001, 52, 344-351.	1.2	10
53	Building self-avoiding lattice models of proteins using a self-consistent field optimization. , 1996, 26, 1-8.		9
54	Structural basis for drug and substrate specificity exhibited by FIV encoding a chimeric FIV/HIV protease. Acta Crystallographica Section D: Biological Crystallography, 2011, 67, 540-548.	2.5	9

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55	A Study on Docking Mode of HIV Protease and Their Inhibitors.. Journal of Chemical Software, 2001, 7, 103-114.	0.2	9
56	Adjusting potential energy functions for lattice models of chain molecules. , 1996, 25, 379-388.		8
57	Automated docking of flexible ligands: Applications of autodock. , 1996, 9, 1.		7
58	Visualizing The Future of Molecular Graphics. SAR and QSAR in Environmental Research, 1998, 8, 233-247.	1.0	6
59	Novel GABA-AT inhibitors: QSAR and docking based virtual screening of phenyl substituted Î²-phenyl ethylidene hydrazine analogues. Medicinal Chemistry Research, 2011, 20, 1482-1489.	1.1	6
60	Computational Challenges of Structure-Based Approaches Applied to HIV. Current Topics in Microbiology and Immunology, 2015, 389, 31-51.	0.7	6
61	Massive-Scale Binding Free Energy Simulations of HIV Integrase Complexes Using Asynchronous Replica Exchange Framework Implemented on the IBM WCG Distributed Network. Journal of Chemical Information and Modeling, 2019, 59, 1382-1397.	2.5	6
62	Parallel Generation and Visualization of Bacterial Genome Structures. Computer Graphics Forum, 2019, 38, 57-68.	1.8	6
63	Structure-based virtual screening workflow to identify antivirals targeting HIV-1 capsid. Journal of Computer-Aided Molecular Design, 2022, 36, 193-203.	1.3	6
64	Lattice modeling: Accuracy of energy calculations. Journal of Computational Chemistry, 1996, 17, 1025-1032.	1.5	5
65	Fragment-Based Analysis of Ligand Dockings Improves Classification of Actives. Journal of Chemical Information and Modeling, 2016, 56, 1597-1607.	2.5	4
66	Integrative modeling of the HIV-1 ribonucleoprotein complex. PLoS Computational Biology, 2019, 15, e1007150.	1.5	4
67	Flap-site Fragment Restores Back Wild-type Behaviour in Resistant Form of HIV Protease. Molecular Informatics, 2018, 37, 1800053.	1.4	2
68	Modelling of Factor Xa-inhibitor complexes: a computational flexible docking approach. , 1999, 34, 173.		2
69	Transmembrane Î±â€helices in the gap junction membrane channel: Systematic search of packing models based on the pair potential function. Microscopy Research and Technique, 2001, 52, 344-351.	1.2	1
70	Identification of novel Î²â€secretase inhibitors through the inclusion of protein flexibility in virtual screening calculations. FASEB Journal, 2008, 22, 791.8.	0.2	1