Arthur J Olson

List of Publications by Citations

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69 papers	39,569 citations	33 h-index	70 g-index
70 ext. papers	46,601 ext. citations	6 avg, IF	7.7 L-index

#	Paper	IF	Citations
69	AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *Journal of Computational Chemistry*, **2010**, 31, 455-61	3.5	11670
68	AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. *Journal of Computational Chemistry*, **2009**, 30, 2785-91	3.5	11655
67	Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function **1998**, 19, 1639-1662		7548
66	A semiempirical free energy force field with charge-based desolvation. *Journal of Computational Chemistry*, **2007**, 28, 1145-52	3.5	1602
65	Automated docking of flexible ligands: applications of AutoDock. *Journal of Molecular Recognition*, **1996**, 9, 1-5	2.6	1057
64	Automated docking of substrates to proteins by simulated annealing. *Proteins: Structure, Function and Bioinformatics*, **1990**, 8, 195-202	4.2	943
63	Distributed automated docking of flexible ligands to proteins: parallel applications of AutoDock 2.4. *Journal of Computer-Aided Molecular Design*, **1996**, 10, 293-304	4.2	796
62	Computational protein-ligand docking and virtual drug screening with the AutoDock suite. *Nature Protocols*, **2016**, 11, 905-19	18.8	719
61	Structural symmetry and protein function. *Annual Review of Biophysics and Biomolecular Structure*, **2000**, 29, 105-53		671
60	Proteome-wide covalent ligand discovery in native biological systems. *Nature*, **2016**, 534, 570-4	50.4	406
59	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	4.2	341
58	Virtual Screening with AutoDock: Theory and Practice. *Expert Opinion on Drug Discovery*, **2010**, 5, 597-607	6.2	326
57	AutoDock4(Zn): an improved AutoDock force field for small-molecule docking to zinc metalloproteins. *Journal of Chemical Information and Modeling*, **2014**, 54, 2371-9	6.1	152
56	A force field with discrete displaceable waters and desolvation entropy for hydrated ligand docking. *Journal of Medicinal Chemistry*, **2012**, 55, 623-38	8.3	150
55	AutoDockFR: Advances in Protein-Ligand Docking with Explicitly Specified Binding Site Flexibility. *PLoS Computational Biology*, **2015**, 11, e1004586	5	129
54	Covalent docking using autodock: Two-point attractor and flexible side chain methods. *Protein Science*, **2016**, 25, 295-301	6.3	114
53	Automated prediction of ligand-binding sites in proteins. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 1506-17	4.2	94

52	Chemical mimicry of viral capsid self-assembly. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 20731-6	11.5	92
51	cellPACK: a virtual mesoscope to model and visualize structural systems biology. *Nature Methods*, **2015**, 12, 85-91	21.6	89
50	Automated docking in crystallography: analysis of the substrates of aconitase. *Proteins: Structure, Function and Bioinformatics*, **1993**, 17, 1-10	4.2	71
49	Illustrate: Software for Biomolecular Illustration. *Structure*, **2019**, 27, 1716-1720.e1	5.2	57
48	A dynamic model of HIV integrase inhibition and drug resistance. *Journal of Molecular Biology*, **2010** , 397, 600-15	6.5	52
47	Development of a New Type of Protease Inhibitors, Efficacious against FIV and HIV Variants. *Journal of the American Chemical Society*, **1999**, 121, 1145-1155	16.4	51
46	Importance of factor VIIa Gla-domain residue Arg-36 for recognition of the macromolecular substrate factor X Gla-domain. *Biochemistry*, **1999**, 38, 1957-66	3.2	48
45	Blind prediction of HIV integrase binding from the SAMPL4 challenge. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 327-45	4.2	46
44	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, 271-9	4.2	46
43	Virtual screening of integrase inhibitors by large scale binding free energy calculations: the SAMPL4 challenge. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 475-90	4.2	45
42	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, 976-88	3.4	45
41	Perspectives on Structural Molecular Biology Visualization: From Past to Present. *Journal of Molecular Biology*, **2018**, 430, 3997-4012	6.5	44
40	Modelling of factor Xa-inhibitor complexes: a computational flexible docking approach. *Proteins: Structure, Function and Bioinformatics*, **1999**, 34, 173-83	4.2	41
39	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 protein-ligand binding challenge. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 429-441	4.2	38
38	Challenges in structural approaches to cell modeling. *Journal of Molecular Biology*, **2016**, 428, 2943-64	6.5	36
37	Dense Array of Spikes on HIV-1 Virion Particles. *Journal of Virology*, **2017**, 91,	6.6	35
36	A virtual screen discovers novel, fragment-sized inhibitors of Mycobacterium tuberculosis InhA. *Journal of Chemical Information and Modeling*, **2015**, 55, 645-59	6.1	30
35	Viral evolution in response to the broad-based retroviral protease inhibitor TL-3. *Journal of Virology* , **2001**, 75, 9502-8	6.6	28

34	Small molecule regulation of protein conformation by binding in the Flap of HIV protease. *ACS Chemical Biology*, **2013**, 8, 1223-31	4.9	27
33	Structural studies of FIV and HIV-1 proteases complexed with an efficient inhibitor of FIV protease. *Proteins: Structure, Function and Bioinformatics*, **2000**, 38, 29-40	4.2	27
32	Automated docking and the search for HIV protease inhibitors. *SAR and QSAR in Environmental Research*, **1998**, 8, 273-85	3.5	23
31	Instant Construction and Visualization of Crowded Biological Environments. *IEEE Transactions on Visualization and Computer Graphics*, **2018**, 24, 862-872	4	22
30	The AutoDock suite at 30. *Protein Science*, **2021**, 30, 31-43	6.3	21
29	Lattice Models of Bacterial Nucleoids. *Journal of Physical Chemistry B*, **2018**, 122, 5441-5447	3.4	16
28	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	5.4	15
27	Art and Science of the Cellular Mesoscale. *Trends in Biochemical Sciences*, **2020**, 45, 472-483	10.3	14
26	A Self-Assisting Protein Folding Model for Teaching Structural Molecular Biology. *Structure*, **2017**, 25, 671-678	5.2	12
25	Novel Intersubunit Interaction Critical for HIV-1 Core Assembly Defines a Potentially Targetable Inhibitor Binding Pocket. *MBio*, **2019**, 10,	7.8	11
24	Biomolecular visualization using AVS. *Journal of Molecular Graphics*, **1995**, 13, 271-82, 299		11
23	Structural basis for drug and substrate specificity exhibited by FIV encoding a chimeric FIV/HIV protease. *Acta Crystallographica Section D: Biological Crystallography*, **2011**, 67, 540-8		9
22	Transmembrane alpha-helices in the gap junction membrane channel: systematic search of packing models based on the pair potential function. *Microscopy Research and Technique*, **2001**, 52, 344-51	2.8	8
21	Building self-avoiding lattice models of proteins using a self-consistent field optimization. *Proteins: Structure, Function and Bioinformatics*, **1996**, 26, 1-8	4.2	8
20	A Study on Docking Mode of HIV Protease and Their Inhibitors.. *Journal of Chemical Software*, **2001**, 7, 103-114		8
19	CellPAINT: Turnkey Illustration of Molecular Cell Biology. *Frontiers in Bioinformatics*, **2021**, 1,		7
18	Computational challenges of structure-based approaches applied to HIV. *Current Topics in Microbiology and Immunology*, **2015**, 389, 31-51	3.3	6
17	Adjusting potential energy functions for lattice models of chain molecules. *Proteins: Structure, Function and Bioinformatics*, **1996**, 25, 379-88	4.2	6

16	Automated docking of flexible ligands: Applications of autodock **1996**, 9, 1		6
15	Intrabacterial Metabolism Obscures the Successful Prediction of an InhA Inhibitor of. *ACS Infectious Diseases*, **2019**, 5, 2148-2163	5.5	5
14	Novel GABA-AT inhibitors: QSAR and docking based virtual screening of phenyl substituted □phenyl ethylidene hydrazine analogues. *Medicinal Chemistry Research*, **2011**, 20, 1482-1489	2.2	5
13	Visualizing the future of molecular graphics. *SAR and QSAR in Environmental Research*, **1998**, 8, 233-47	3.5	5
12	Building Structural Models of a Whole Mycoplasma Cell. *Journal of Molecular Biology*, **2021**, 434, 167351	6.5	5
11	Parallel Generation and Visualization of Bacterial Genome Structures. *Computer Graphics Forum*, **2019**, 38, 57-68	2.4	4
10	Integrative modeling of the HIV-1 ribonucleoprotein complex. *PLoS Computational Biology*, **2019**, 15, e1007150	5	3
9	Lattice modeling: Accuracy of energy calculations. *Journal of Computational Chemistry*, **1996**, 17, 1025-1032	3.3	3
8	Fragment-Based Analysis of Ligand Dockings Improves Classification of Actives. *Journal of Chemical Information and Modeling*, **2016**, 56, 1597-607	6.1	3
7	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	6.1	3
6	Icosahedral virus structures and the protein data bank. *Journal of Biological Chemistry*, **2021**, 296, 100554	5.4	3
5	Modelling of Factor Xa-inhibitor complexes: a computational flexible docking approach **1999**, 34, 173		2
4	Flap-site Fragment Restores Back Wild-type Behaviour in Resistant Form of HIV Protease. *Molecular Informatics*, **2018**, 37, e1800053	3.8	1
3	Identification of novel □secretase inhibitors through the inclusion of protein flexibility in virtual screening calculations. *FASEB Journal*, **2008**, 22, 791.8	0.9	1
2	Transmembrane □helices in the gap junction membrane channel: Systematic search of packing models based on the pair potential function **2001**, 52, 344		1
1	Structure-based virtual screening workflow to identify antivirals targeting HIV-1 capsid.. *Journal of Computer-Aided Molecular Design*, **2022**, 36, 193	4.2	1