Chaok Seok

List of Publications by Year in Descending Order

108 papers	4,360 citations	32 h-index	64 g-index
113 ext. papers	5,537 ext. citations	6.1 avg, IF	5.75 L-index

#	Paper	IF	Citations
108	A pGpG-specific phosphodiesterase regulates cyclic di-GMP signaling in Vibrio cholerae.. *Journal of Biological Chemistry*, **2022**, 101626	5.4	1
107	Structural basis of neuropeptide Y signaling through Y1 receptor.. *Nature Communications*, **2022**, 13, 853	17.4	1
106	GalaxyDomDock: An Ab Initio Domain–domain Docking Web Server for Multi-domain Protein Structure Prediction. *Journal of Molecular Biology*, **2022**, 167508	6.5	0
105	MOLGENGO: Finding Novel Molecules with Desired Electronic Properties by Capitalizing on Their Global Optimization. *ACS Omega*, **2021**, 6, 27454-27465	3.9	1
104	Structure, Dynamics, Receptor Binding, and Antibody Binding of the Fully Glycosylated Full-Length SARS-CoV-2 Spike Protein in a Viral Membrane. *Journal of Chemical Theory and Computation*, **2021**, 17, 2479-2487	6.4	26
103	GalaxyWater-wKGB: Prediction of Water Positions on Protein Structure Using wKGB Statistical Potential. *Journal of Chemical Information and Modeling*, **2021**, 61, 2283-2293	6.1	4
102	GalaxyHeteromer: protein heterodimer structure prediction by template-based and ab initio docking. *Nucleic Acids Research*, **2021**, 49, W237-W241	20.1	4
101	Protein oligomer structure prediction using GALAXY in CASP14. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1844-1851	4.2	0
100	Assessment of protein model structure accuracy estimation in CASP14: Old and new challenges. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1940-1948	4.2	10
99	Modeling SARS-CoV-2 proteins in the CASP-commons experiment. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1987-1996	4.2	8
98	Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1800-1823	4.2	17
97	Discovery of a transdermally deliverable pentapeptide for activating AdipoR1 to promote hair growth. *EMBO Molecular Medicine*, **2021**, 13, e13790	12	2
96	Accurate protein structure prediction: what comes next?. *Biodesign*, **2021**, 9, 47-50	0	4
95	Dynamic Interactions of Fully Glycosylated SARS-CoV-2 Spike Protein with Various Antibodies. *Journal of Chemical Theory and Computation*, **2021**, 17, 6559-6569	6.4	2
94	Symmetry-related residues as promising hotspots for the evolution of oligomeric enzymes. *Chemical Science*, **2021**, 12, 5091-5101	9.4	3
93	GalaxySagittarius: Structure- and Similarity-Based Prediction of Protein Targets for Druglike Compounds. *Journal of Chemical Information and Modeling*, **2020**, 60, 3246-3254	6.1	9
92	Aldehyde-alcohol dehydrogenase undergoes structural transition to form extended spirosomes for substrate channeling. *Communications Biology*, **2020**, 3, 298	6.7	6

91	Developing a Fully Glycosylated Full-Length SARS-CoV-2 Spike Protein Model in a Viral Membrane. *Journal of Physical Chemistry B*, **2020**, 124, 7128-7137	3.4	131
90	Developing a Fully-glycosylated Full-length SARS-CoV-2 Spike Protein Model in a Viral Membrane **2020**,		4
89	Structure prediction of biological assemblies using GALAXY in CAPRI rounds 38-45. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 1009-1017	4.2	2
88	Sclerostin inhibits Wnt signaling through tandem interaction with two LRP6 ectodomains. *Nature Communications*, **2020**, 11, 5357	17.4	18
87	Prediction of Molecular Electronic Transitions Using Random Forests. *Journal of Chemical Information and Modeling*, **2020**, 60, 5984-5994	6.1	14
86	Modeling Protein Homo-Oligomer Structures with GalaxyHomomer Web Server. *Methods in Molecular Biology*, **2020**, 2165, 127-137	1.4	0
85	GalaxyTongDock: Symmetric and asymmetric ab initio protein-protein docking web server with improved energy parameters. *Journal of Computational Chemistry*, **2019**, 40, 2413-2417	3.5	20
84	GalaxyRefine2: simultaneous refinement of inaccurate local regions and overall protein structure. *Nucleic Acids Research*, **2019**, 47, W451-W455	20.1	31
83	GalaxyDock3: Protein-ligand docking that considers the full ligand conformational flexibility. *Journal of Computational Chemistry*, **2019**, 40, 2739-2748	3.5	8
82	Assessment of protein model structure accuracy estimation in CASP13: Challenges in the era of deep learning. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 1351-1360	4.2	28
81	Prediction of protein oligomer structures using GALAXY in CASP13. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 1233-1240	4.2	6
80	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 1200-1221	4.2	58
79	Structural Basis for the Enantioselectivity of Esterase Est-Y29 toward (S)-Ketoprofen. *ACS Catalysis*, **2019**, 9, 755-767	13.1	8
78	Novel Compound Heterozygote Mutation in IL10RA in a Patient With Very Early-Onset Inflammatory Bowel Disease. *Inflammatory Bowel Diseases*, **2019**, 25, 498-509	4.5	3
77	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. *Scientific Reports*, **2018**, 8, 9939	4.9	16
76	Biophysical and functional characterization of Norrin signaling through Frizzled4. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 8787-8792	11.5	20
75	Simultaneous refinement of inaccurate local regions and overall structure in the CASP12 protein model refinement experiment. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86 Suppl 1, 168-176	4.2	12
74	The challenge of modeling protein assemblies: the CASP12-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86 Suppl 1, 257-273	4.2	56

73	GalaxyGPCRloop: Template-Based and Ab Initio Structure Sampling of the Extracellular Loops of G-Protein-Coupled Receptors. *Journal of Chemical Information and Modeling*, **2018**, 58, 1234-1243	6.1	3
72	Cover Image, Volume 85, Issue 3. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, C4-C4	4.2	
71	Benchmarking predictions of allostery in liver pyruvate kinase in CAGI4. *Human Mutation*, **2017**, 38, 1123-1131	4.1	12
70	Absolute binding free energies for octa-acids and guests in SAMPL5 : Evaluating binding free energies for octa-acid and guest complexes in the SAMPL5 blind challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 107-118	4.2	15
69	GalaxyDock BP2 score: a hybrid scoring function for accurate protein-ligand docking. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 653-666	4.2	30
68	Template-based modeling and ab initio refinement of protein oligomer structures using GALAXY in CAPRI round 30. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 399-407	4.2	9
67	Absolute binding free energy calculations of CBClip host-guest systems in the SAMPL5 blind challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 71-85	4.2	9
66	GalaxyHomomer: a web server for protein homo-oligomer structure prediction from a monomer sequence or structure. *Nucleic Acids Research*, **2017**, 45, W320-W324	20.1	63
65	Cell-cell adhesion in metazoans relies on evolutionarily conserved features of the □catenin□□catenin-binding interface. *Journal of Biological Chemistry*, **2017**, 292, 16477-16490	5.4	6
64	Template-Based Prediction of Protein-Peptide Interactions by Using GalaxyPepDock. *Methods in Molecular Biology*, **2017**, 1561, 37-47	1.4	9
63	GalaxyRefineComplex: Refinement of protein-protein complex model structures driven by interface repacking. *Scientific Reports*, **2016**, 6, 32153	4.9	55
62	Galaxy7TM: flexible GPCR-ligand docking by structure refinement. *Nucleic Acids Research*, **2016**, 44, W502-W506	20.1	25
61	Effective protein model structure refinement by loop modeling and overall relaxation. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 293-301	4.2	54
60	Crystal Structure of Streptococcus pyogenes Cas1 and Its Interaction with Csn2 in the Type II CRISPR-Cas System. *Structure*, **2016**, 24, 70-79	5.2	18
59	Evaluation of GalaxyDock Based on the Community Structure-Activity Resource 2013 and 2014 Benchmark Studies. *Journal of Chemical Information and Modeling*, **2016**, 56, 988-95	6.1	9
58	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 323-48	4.2	111
57	Binding Site Prediction of Proteins with Organic Compounds or Peptides Using GALAXY Web Servers. *Methods in Molecular Biology*, **2016**, 1414, 33-45	1.4	4
56	Measured and predicted affinities of binding and relative potencies to activate the AhR of PAHs and their alkylated analogues. *Chemosphere*, **2015**, 139, 23-9	8.4	27

55	High-resolution protein-protein docking by global optimization: recent advances and future challenges. *Current Opinion in Structural Biology*, **2015**, 35, 24-31	8.1	30
54	Factors affecting redox potential and differential sensitivity of SoxR to redox-active compounds. *Molecular Microbiology*, **2015**, 97, 808-21	4.1	13
53	GalaxyPepDock: a protein-peptide docking tool based on interaction similarity and energy optimization. *Nucleic Acids Research*, **2015**, 43, W431-5	20.1	149
52	Potential Application of Alchemical Free Energy Simulations to Discriminate GPCR Ligand Efficacy. *Journal of Chemical Theory and Computation*, **2015**, 11, 1255-66	6.4	8
51	Blind prediction of interfacial water positions in CAPRI. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 620-32	4.2	43
50	GalaxySite: ligand-binding-site prediction by using molecular docking. *Nucleic Acids Research*, **2014**, 42, W210-4	20.1	55
49	Structure of vaccinia virus A46, an inhibitor of TLR4 signaling pathway, shows the conformation of VIPER motif. *Protein Science*, **2014**, 23, 906-14	6.3	11
48	Protein loop modeling using a new hybrid energy function and its application to modeling in inaccurate structural environments. *PLoS ONE*, **2014**, 9, e113811	3.7	54
47	New molecular interaction of IIA(Ntr) and HPr from Burkholderia pseudomallei identified by X-ray crystallography and docking studies. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1499-508	4.2	2
46	GalaxyDock2: protein-ligand docking using beta-complex and global optimization. *Journal of Computational Chemistry*, **2013**, 34, 2647-56	3.5	44
45	Alternative zinc-binding sites explain the redox sensitivity of zinc-containing anti-sigma factors. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1644-52	4.2	6
44	What stabilizes close arginine pairing in proteins?. *Physical Chemistry Chemical Physics*, **2013**, 15, 5844-53	3.6	30
43	GalaxyGemini: a web server for protein homo-oligomer structure prediction based on similarity. *Bioinformatics*, **2013**, 29, 1078-80	7.2	30
42	GalaxyRefine: Protein structure refinement driven by side-chain repacking. *Nucleic Acids Research*, **2013**, 41, W384-8	20.1	403
41	Switchable Nanoporous Sheets by the Aqueous Self-Assembly of Aromatic Macrobicycles. *Angewandte Chemie*, **2013**, 125, 6554-6557	3.6	21
40	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1980-7	4.2	78
39	Discovery, design and synthesis of Y-shaped peroxisome proliferator-activated receptor agonists as potent anti-obesity agents in vivo. *European Journal of Medicinal Chemistry*, **2012**, 53, 190-202	6.8	10
38	GalaxyDock: protein-ligand docking with flexible protein side-chains. *Journal of Chemical Information and Modeling*, **2012**, 52, 3225-32	6.1	44

37	Pulsating tubules from noncovalent macrocycles. *Science*, **2012**, 337, 1521-6	33.3	250
36	GalaxyWEB server for protein structure prediction and refinement. *Nucleic Acids Research*, **2012**, 40, W294-7	20.1	335
35	GalaxyTBM: template-based modeling by building a reliable core and refining unreliable local regions. *BMC Bioinformatics*, **2012**, 13, 198	3.6	64
34	Refinement of unreliable local regions in template-based protein models. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1974-86	4.2	47
33	Contribution of Counterion Entropy to the Salt-Induced Transition Between B-DNA and Z-DNA. *Bulletin of the Korean Chemical Society*, **2012**, 33, 3719-3726	1.2	2
32	Transmembrane signaling of chemotaxis receptor tar: insights from molecular dynamics simulation studies. *Biophysical Journal*, **2011**, 100, 2955-63	2.9	32
31	Community-wide assessment of protein-interface modeling suggests improvements to design methodology. *Journal of Molecular Biology*, **2011**, 414, 289-302	6.5	114
30	De novo protein structure prediction by dynamic fragment assembly and conformational space annealing. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2403-17	4.2	46
29	Refinement of protein termini in template-based modeling using conformational space annealing. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2725-34	4.2	19
28	LigDockCSA: protein-ligand docking using conformational space annealing. *Journal of Computational Chemistry*, **2011**, 32, 3226-32	3.5	29
27	The FALC-Loop web server for protein loop modeling. *Nucleic Acids Research*, **2011**, 39, W210-4	20.1	72
26	Cooperativity and specificity of Cys2His2 zinc finger protein-DNA interactions: a molecular dynamics simulation study. *Journal of Physical Chemistry B*, **2010**, 114, 7662-71	3.4	33
25	Transition between B-DNA and Z-DNA: free energy landscape for the B-Z junction propagation. *Journal of Physical Chemistry B*, **2010**, 114, 9872-81	3.4	24
24	Self-Dissociating Tubules from Helical Stacking of Noncovalent Macrocycles. *Angewandte Chemie*, **2010**, 122, 8649-8653	3.6	17
23	Protein loop modeling by using fragment assembly and analytical loop closure. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 3428-36	4.2	77
22	Strength of Calpha-H...O=C hydrogen bonds in transmembrane proteins. *Journal of Physical Chemistry B*, **2008**, 112, 1041-8	3.4	35
21	A statistical rescoring scheme for protein-ligand docking: Consideration of entropic effect. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 1074-83	4.2	24
20	Protein Loop Modeling Using Fragment Assembly. *Journal of the Korean Physical Society*, **2008**, 52, 1137-1142	0.64	6

19	Use of the Weighted Histogram Analysis Method for the Analysis of Simulated and Parallel Tempering Simulations. *Journal of Chemical Theory and Computation*, **2007**, 3, 26-41	6.4	367
18	Resultants and loop closure. *International Journal of Quantum Chemistry*, **2006**, 106, 176-189	2.1	39
17	The flexibility in the proline ring couples to the protein backbone. *Protein Science*, **2005**, 14, 1011-8	6.3	68
16	Rotational superposition and least squares: the SVD and quaternions approaches yield identical results. Reply to the preceding comment by G. Kneller. *Journal of Computational Chemistry*, **2005**, 26, 1663-5	3.5	12
15	Analytic density-functional self-consistent-field theory of diblock copolymers near patterned surfaces. *Journal of Chemical Physics*, **2004**, 120, 7174-82	3.9	10
14	A kinematic view of loop closure. *Journal of Computational Chemistry*, **2004**, 25, 510-28	3.5	206
13	Using quaternions to calculate RMSD. *Journal of Computational Chemistry*, **2004**, 25, 1849-57	3.5	239
12	MOPED: method for optimizing physical energy parameters using decoys. *Journal of Computational Chemistry*, **2003**, 24, 89-97	3.5	18
11	Parameter optimization for the Gaussian model of protein folding. *Polymer*, **2002**, 43, 495-501	3.9	5
10	Polymer melts and polymer solutions near patterned surfaces. *Journal of Chemical Physics*, **2000**, 112, 6443-6451	3.9	19
9	Polymer blends near patterned surfaces. *Journal of Chemical Physics*, **2000**, 112, 6452-6460	3.9	16
8	Bulk and surface nucleation of the order-disorder transition in. *Journal of Physics Condensed Matter*, **1998**, 10, 45-60	1.8	6
7	Nucleation in n-alkanes: A density-functional approach. *Journal of Chemical Physics*, **1998**, 109, 7982-7990	3.9	31
6	Mechanism of Ag+ ordering in AgI. *Physical Review B*, **1998**, 58, 5146-5148	3.3	8
5	Insertion-duplication mutagenesis in Streptococcus pneumoniae: targeting fragment length is a critical parameter in use as a random insertion tool. *Applied and Environmental Microbiology*, **1998**, 64, 4796-802	4.8	33
4	Order - disorder transition in : a density functional approach. *Journal of Physics Condensed Matter*, **1997**, 9, 87-102	1.8	10
3	Phase transitions in AgI. *Physical Review B*, **1997**, 56, 11485-11492	3.3	20
2	Structure, Dynamics, Receptor Binding, and Antibody Binding of Fully-glycosylated Full-length SARS-CoV-2 Spike Protein in a Viral Membrane		1

1 GalaxyWater-CNN: Prediction of Water Positions on the Protein Structure by a 3D-Convolutional Neural Network. *Journal of Chemical Information and Modeling*, 6.1 1