# Chaok Seok

List of Publications by Year
in descending order



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|---|---|---|---|
| 106 papers | 6,399 citations | 109137 35 h-index | 76769 74 g-index |
| 113 all docs | 113 docs citations | 113 times ranked | 7898 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | GalaxyRefine: protein structure refinement driven by side-chain repacking. Nucleic Acids Research, 2013, 41, W384-W388. | 6.5 | 735 |
| 2 | GalaxyWEB server for protein structure prediction and refinement. Nucleic Acids Research, 2012, 40, W294-W297. | 6.5 | 603 |
| 3 | 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. | 2.3 | 416 |
| 4 | Pulsating Tubules from Noncovalent Macrocycles. Science, 2012, 337, 1521-1526. | 6.0 | 298 |
| 5 | Using quaternions to calculate RMSD. Journal of Computational Chemistry, 2004, 25, 1849-1857. | 1.5 | 296 |
| 6 | A kinematic view of loop closure. Journal of Computational Chemistry, 2004, 25, 510-528. | 1.5 | 265 |
| 7 | 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. | 1.2 | 240 |
| 8 | GalaxyPepDock: a proteinâ€“peptide docking tool based on interaction similarity and energy optimization. Nucleic Acids Research, 2015, 43, W431-W435. | 6.5 | 236 |
| 9 | Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348. | 1.5 | 148 |
| 10 | Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302. | 2.0 | 131 |
| 11 | GalaxyHomomer: a web server for protein homo-oligomer structure prediction from a monomer sequence or structure. Nucleic Acids Research, 2017, 45, W320-W324. | 6.5 | 102 |
| 12 | The FALC-Loop web server for protein loop modeling. Nucleic Acids Research, 2011, 39, W210-W214. | 6.5 | 101 |
| 13 | Blind prediction of homoâ€and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221. | 1.5 | 99 |
| 14 | GalaxyRefineComplex: Refinement of protein-protein complex model structures driven by interface repacking. Scientific Reports, 2016, 6, 32153. | 1.6 | 94 |
| 15 | Protein loop modeling by using fragment assembly and analytical loop closure. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3428-3436. | 1.5 | 90 |
| 16 | Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987. | 1.5 | 87 |
| 17 | GalaxyTBM: template-based modeling by building a reliable core and refining unreliable local regions. BMC Bioinformatics, 2012, 13, 198. | 1.2 | 86 |
| 18 | The challenge of modeling protein assemblies: the CASP12â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2018, 86, 257-273. | 1.5 | 85 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | GalaxySite: ligand-binding-site prediction by using molecular docking. Nucleic Acids Research, 2014, 42, W210-W214. | 6.5 | 80 |
| 20 | Effective protein model structure refinement by loop modeling and overall relaxation. Proteins: Structure, Function and Bioinformatics, 2016, 84, 293-301. | 1.5 | 79 |
| 21 | Protein Loop Modeling Using a New Hybrid Energy Function and Its Application to Modeling in Inaccurate Structural Environments. PLoS ONE, 2014, 9, e113811. | 1.1 | 78 |
| 22 | The flexibility in the proline ring couples to the protein backbone. Protein Science, 2005, 14, 1011-1018. | 3.1 | 77 |
| 23 | Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823. | 1.5 | 73 |
| 24 | GalaxyRefine2: simultaneous refinement of inaccurate local regions and overall protein structure. Nucleic Acids Research, 2019, 47, W451-W455. | 6.5 | 66 |
| 25 | Refinement of unreliable local regions in templateâ€based protein models. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1974-1986. | 1.5 | 62 |
| 26 | 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. | 2.3 | 62 |
| 27 | GalaxyDock2: Proteinâ€“ligand docking using betaâ€complex and global optimization. Journal of Computational Chemistry, 2013, 34, 2647-2656. | 1.5 | 60 |
| 28 | GalaxyDock: Proteinâ€“Ligand Docking with Flexible Protein Side-chains. Journal of Chemical Information and Modeling, 2012, 52, 3225-3232. | 2.5 | 59 |
| 29 | De novo protein structure prediction by dynamic fragment assembly and conformational space annealing. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2403-2417. | 1.5 | 54 |
| 30 | 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. | 1.5 | 54 |
| 31 | Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632. | 1.5 | 50 |
| 32 | Resultants and loop closure. International Journal of Quantum Chemistry, 2006, 106, 176-189. | 1.0 | 49 |
| 33 | Assessment of protein model structure accuracy estimation in <scp>CASP14</scp>: Old and new challenges. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1940-1948. | 1.5 | 48 |
| 34 | GalaxyDock BP2 score: a hybrid scoring function for accurate proteinâ€“ligand docking. Journal of Computer-Aided Molecular Design, 2017, 31, 653-666. | 1.3 | 44 |
| 35 | Sclerostin inhibits Wnt signaling through tandem interaction with two LRP6 ectodomains. Nature Communications, 2020, 11, 5357. | 5.8 | 44 |
| 36 | GalaxyTongDock: Symmetric and asymmetric ab initio proteinâ€“protein docking web server with improved energy parameters. Journal of Computational Chemistry, 2019, 40, 2413-2417. | 1.5 | 41 |

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|---|---|---|---|
| 37 | LigDockCSA: Proteinâ€“ligand docking using conformational space annealing. Journal of Computational Chemistry, 2011, 32, 3226-3232. | 1.5 | 40 |
| 38 | What stabilizes close arginine pairing in proteins?. Physical Chemistry Chemical Physics, 2013, 15, 5844. | 1.3 | 40 |
| 39 | Strength of CÎ±â^'HÂ·Â·Â·OC Hydrogen Bonds in Transmembrane Proteins. Journal of Physical Chemistry B, 2008, 112, 1041-1048. | 1.2 | 39 |
| 40 | Insertion-Duplication Mutagenesis inStreptococcus pneumoniae: Targeting Fragment Length Is a Critical Parameter in Use as a Random Insertion Tool. Applied and Environmental Microbiology, 1998, 64, 4796-4802. | 1.4 | 39 |
| 41 | GalaxyGemini: a web server for protein homo-oligomer structure prediction based on similarity. Bioinformatics, 2013, 29, 1078-1080. | 1.8 | 38 |
| 42 | High-resolution proteinâ€“protein docking by global optimization: recent advances and future challenges. Current Opinion in Structural Biology, 2015, 35, 24-31. | 2.6 | 36 |
| 43 | Cooperativity and Specificity of Cys2His2 Zinc Finger Proteinâ^'DNA Interactions: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2010, 114, 7662-7671. | 1.2 | 35 |
| 44 | Nucleation in n-alkanes: A density-functional approach. Journal of Chemical Physics, 1998, 109, 7982-7990. | 1.2 | 34 |
| 45 | Transmembrane Signaling of Chemotaxis Receptor Tar: Insights from Molecular Dynamics Simulation Studies. Biophysical Journal, 2011, 100, 2955-2963. | 0.2 | 33 |
| 46 | Galaxy7TM: flexible GPCRâ€“ligand docking by structure refinement. Nucleic Acids Research, 2016, 44, W502-W506. | 6.5 | 33 |
| 47 | 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. | 3.3 | 30 |
| 48 | Prediction of Molecular Electronic Transitions Using Random Forests. Journal of Chemical Information and Modeling, 2020, 60, 5984-5994. | 2.5 | 30 |
| 49 | A statistical rescoring scheme for proteinâ€“ligand docking: Consideration of entropic effect. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1074-1083. | 1.5 | 29 |
| 50 | Measured and predicted affinities of binding and relative potencies to activate the AhR of PAHs and their alkylated analogues. Chemosphere, 2015, 139, 23-29. | 4.2 | 28 |
| 51 | GalaxySagittarius: Structure- and Similarity-Based Prediction of Protein Targets for Druglike Compounds. Journal of Chemical Information and Modeling, 2020, 60, 3246-3254. | 2.5 | 27 |
| 52 | Transition between B-DNA and Z-DNA: Free Energy Landscape for the Bâ^'Z Junction Propagation. Journal of Physical Chemistry B, 2010, 114, 9872-9881. | 1.2 | 26 |
| 53 | Refinement of protein termini in templateâ€based modeling using conformational space annealing. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2725-2734. | 1.5 | 25 |
| 54 | Accurate protein structure prediction: what comes next?. Biodesign, 2021, 9, 47-50. | 0.2 | 25 |

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| 55 | Modeling SARSâ€CoVâ€2 proteins in the CASPâ€commons experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1987-1996. | 1.5 | 24 |
| 56 | Phase transitions in AgI. Physical Review B, 1997, 56, 11485-11492. | 1.1 | 23 |
| 57 | Polymer melts and polymer solutions near patterned surfaces. Journal of Chemical Physics, 2000, 112, 6443-6451. | 1.2 | 22 |
| 58 | Switchable Nanoporous Sheets by the Aqueous Selfâ€Assembly of Aromatic Macrobicycles. Angewandte Chemie, 2013, 125, 6554-6557. | 1.6 | 22 |
| 59 | Crystal Structure of Streptococcus pyogenes Cas1 and Its Interaction with Csn2 in the Type II CRISPR-Cas System. Structure, 2016, 24, 70-79. | 1.6 | 21 |
| 60 | Template-Based Prediction of Protein-Peptide Interactions by Using GalaxyPepDock. Methods in Molecular Biology, 2017, 1561, 37-47. | 0.4 | 20 |
| 61 | Structural basis of neuropeptide Y signaling through Y1 receptor. Nature Communications, 2022, 13, 853. | 5.8 | 20 |
| 62 | An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. Scientific Reports, 2018, 8, 9939. | 1.6 | 19 |
| 63 | Polymer blends near patterned surfaces. Journal of Chemical Physics, 2000, 112, 6452-6460. | 1.2 | 18 |
| 64 | MOPED: Method for optimizing physical energy parameters using decoys. Journal of Computational Chemistry, 2003, 24, 89-97. | 1.5 | 18 |
| 65 | Factors affecting redox potential and differential sensitivity of <scp>SoxR</scp> to redoxâ€active compounds. Molecular Microbiology, 2015, 97, 808-821. | 1.2 | 18 |
| 66 | Benchmarking predictions of allostery in liver pyruvate kinase in CAGI4. Human Mutation, 2017, 38, 1123-1131. | 1.1 | 17 |
| 67 | GalaxyWater-CNN: Prediction of Water Positions on the Protein Structure by a 3D-Convolutional Neural Network. Journal of Chemical Information and Modeling, 2022, 62, 3157-3168. | 2.5 | 17 |
| 68 | Absolute binding free energies for octa-acids and guests in SAMPL5. Journal of Computer-Aided Molecular Design, 2017, 31, 107-118. | 1.3 | 16 |
| 69 | Aldehyde-alcohol dehydrogenase undergoes structural transition to form extended spirosomes for substrate channeling. Communications Biology, 2020, 3, 298. | 2.0 | 16 |
| 70 | GalaxyDock3: Proteinâ€“ligand docking that considers the full ligand conformational flexibility. Journal of Computational Chemistry, 2019, 40, 2739-2748. | 1.5 | 15 |
| 71 | Simultaneous refinement of inaccurate local regions and overall structure in the CASP12 protein model refinement experiment. Proteins: Structure, Function and Bioinformatics, 2018, 86, 168-176. | 1.5 | 14 |
| 72 | Structural Basis for the Enantioselectivity of Esterase Est-Y29 toward (S)-Ketoprofen. ACS Catalysis, 2019, 9, 755-767. | 5.5 | 14 |

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| 73 | Discovery, design and synthesis of Y-shaped peroxisome proliferator-activated receptor Î´ agonists as potent anti-obesity agents inÂvivo. European Journal of Medicinal Chemistry, 2012, 53, 190-202. | 2.6 | 13 |
| 74 | Structure of vaccinia virus A46, an inhibitor of TLR4 signaling pathway, shows the conformation of VIPER motif. Protein Science, 2014, 23, 906-914. | 3.1 | 13 |
| 75 | Potential Application of Alchemical Free Energy Simulations to Discriminate GPCR Ligand Efficacy. Journal of Chemical Theory and Computation, 2015, 11, 1255-1266. | 2.3 | 13 |
| 76 | Absolute binding free energy calculations of CBClip hostâ€“guest systems in the SAMPL5 blind challenge. Journal of Computer-Aided Molecular Design, 2017, 31, 71-85. | 1.3 | 13 |
| 77 | Dynamic Interactions of Fully Glycosylated SARS-CoV-2 Spike Protein with Various Antibodies. Journal of Chemical Theory and Computation, 2021, 17, 6559-6569. | 2.3 | 13 |
| 78 | Order - disorder transition in : a density functional approach. Journal of Physics Condensed Matter, 1997, 9, 87-102. | 0.7 | 12 |
| 79 | 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, 1663-1665. | 1.5 | 12 |
| 80 | GalaxyHeteromer: protein heterodimer structure prediction by template-based and ab initio docking. Nucleic Acids Research, 2021, 49, W237-W241. | 6.5 | 11 |
| 81 | Analytic density-functional self-consistent-field theory of diblock copolymers near patterned surfaces. Journal of Chemical Physics, 2004, 120, 7174-7182. | 1.2 | 10 |
| 82 | Templateâ€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. | 1.5 | 10 |
| 83 | 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. | 2.5 | 10 |
| 84 | A pGpG-specific phosphodiesterase regulates cyclic di-GMP signaling in Vibrio cholerae. Journal of Biological Chemistry, 2022, 298, 101626. | 1.6 | 10 |
| 85 | Evaluation of GalaxyDock Based on the Community Structureâ€“Activity Resource 2013 and 2014 Benchmark Studies. Journal of Chemical Information and Modeling, 2016, 56, 988-995. | 2.5 | 9 |
| 86 | Cellâ€“cell adhesion in metazoans relies on evolutionarily conserved features of the Î±-cateninÂ·Î²-cateninâ€“binding interface. Journal of Biological Chemistry, 2017, 292, 16477-16490. | 1.6 | 9 |
| 87 | GalaxyWater-wKGB: Prediction of Water Positions on Protein Structure Using wKGB Statistical Potential. Journal of Chemical Information and Modeling, 2021, 61, 2283-2293. | 2.5 | 9 |
| 88 | A benchmark study of machine learning methods for molecular electronic transition: Treeâ€based ensemble learning versus graph neural network. Bulletin of the Korean Chemical Society, 2022, 43, 328-335. | 1.0 | 9 |
| 89 | Mechanism ofAg+ordering in AgI. Physical Review B, 1998, 58, 5146-5148. | 1.1 | 8 |
| 90 | Discovery of a transdermally deliverable pentapeptide for activating AdipoR1 to promote hair growth. EMBO Molecular Medicine, 2021, 13, e13790. | 3.3 | 7 |

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|---|---|---|---|
| 91 | Protein Loop Modeling Using Fragment Assembly. Journal of the Korean Physical Society, 2008, 52, 1137-1142. | 0.3 | 7 |
| 92 | Bulk and surface nucleation of the order-disorder transition in. Journal of Physics Condensed Matter, 1998, 10, 45-60. | 0.7 | 6 |
| 93 | Parameter optimization for the Gaussian model of protein folding. Polymer, 2002, 43, 495-501. | 1.8 | 6 |
| 94 | Alternative zincâ€binding sites explain the redox sensitivity of zincâ€containing antiâ€sigma factors. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1644-1652. | 1.5 | 6 |
| 95 | Prediction of protein oligomer structures using GALAXY in CASP13. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1233-1240. | 1.5 | 6 |
| 96 | Novel Compound Heterozygote Mutation in IL10RA in a Patient With Very Early-Onset Inflammatory Bowel Disease. Inflammatory Bowel Diseases, 2019, 25, 498-509. | 0.9 | 6 |
| 97 | Structure prediction of biological assemblies using GALAXY in CAPRI rounds 38â€45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1009-1017. | 1.5 | 5 |
| 98 | Symmetry-related residues as promising hotspots for the evolution of de novo oligomeric enzymes. Chemical Science, 2021, 12, 5091-5101. | 3.7 | 5 |
| 99 | GalaxyDomDock: An Ab Initio Domainâ€“domain Docking Web Server for Multi-domain Protein Structure Prediction. Journal of Molecular Biology, 2022, 434, 167508. | 2.0 | 5 |
| 100 | Binding Site Prediction of Proteins with Organic Compounds or Peptides Using GALAXY Web Servers. Methods in Molecular Biology, 2016, 1414, 33-45. | 0.4 | 4 |
| 101 | Protein oligomer structure prediction using GALAXY in CASP14. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1844-1851. | 1.5 | 4 |
| 102 | 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. | 1.0 | 3 |
| 103 | MOLGENGO: Finding Novel Molecules with Desired Electronic Properties by Capitalizing on Their Global Optimization. ACS Omega, 2021, 6, 27454-27465. | 1.6 | 3 |
| 104 | New molecular interaction of IIA<sup>Ntr</sup> and HPr from Burkholderia pseudomallei identified by Xâ€ray crystallography and docking studies. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1499-1508. | 1.5 | 2 |
| 105 | Modeling Protein Homo-Oligomer Structures with GalaxyHomomer Web Server. Methods in Molecular Biology, 2020, 2165, 127-137. | 0.4 | 2 |
| 106 | Cover Image, Volume 85, Issue 3. Proteins: Structure, Function and Bioinformatics, 2017, 85, C4. | 1.5 | 0 |