Gert-Jan Bekker

List of Publications by Year
in descending order

25 papers	1,348 citations	567281 15 h-index	642732 23 g-index
27 all docs	27 docs citations	27 times ranked	1923 citing authors

#	Article	IF	Citations
1	Protein Data Bank Japan: Celebrating our 20th anniversary during a global pandemic as the Asian hub of three dimensional macromolecular structural data. Protein Science, 2022, 31, 173-186.	7.6	28
2	Dynamical Methods to Study Interaction in Proteins Facilitating Molecular Understanding of Cancer. , 2022, , 2231-2247.		0
3	Structural basis of mutants of <scp>PET</scp>â€degrading enzyme from Saccharomonospora viridis<scp>AHK190</scp> with high activity and thermal stability. Proteins: Structure, Function and Bioinformatics, 2021, 89, 502-511.	2.6	17
4	Cutinases from thermophilic bacteria (actinomycetes): From identification to functional and structural characterization. Methods in Enzymology, 2021, 648, 159-185.	1.0	8
5	Dynamic Docking Using Multicanonical Molecular Dynamics: Simulating Complex Formation at the Atomistic Level. Methods in Molecular Biology, 2021, 2266, 187-202.	0.9	8
6	Cryptic-site binding mechanism of medium-sized Bcl-xL inhibiting compounds elucidated by McMD-based dynamic docking simulations. Scientific Reports, 2021, 11, 5046.	3.3	11
7	Exploring ligand binding pathways on proteins using hypersound-accelerated molecular dynamics. Nature Communications, 2021, 12, 2793.	12.8	24
8	Accurate Binding Configuration Prediction of a G-Protein-Coupled Receptor to Its Antagonist Using Multicanonical Molecular Dynamics-Based Dynamic Docking. Journal of Chemical Information and Modeling, 2021, 61, 5161-5171.	5.4	10
9	N-Terminal-Driven Binding Mechanism of an Antigen Peptide to Human Leukocyte Antigen-A*2402 Elucidated by Multicanonical Molecular Dynamic-Based Dynamic Docking and Path Sampling Simulations. Journal of Physical Chemistry B, 2021, 125, 13376-13384.	2.6	7
10	The Biological Structure Model Archive (BSM-Arc): an archive for in silico models and simulations. Biophysical Reviews, 2020, 12, 371-375.	3.2	40
11	Mutual population-shift driven antibody-peptide binding elucidated by molecular dynamics simulations. Scientific Reports, 2020, 10, 1406.	3.3	32
12	Exhaustive search of the configurational space of heatâ€shock protein 90 with its inhibitor by multicanonical molecular dynamics based dynamic docking. Journal of Computational Chemistry, 2020, 41, 1606-1615.	3.3	20
13	Folding thermodynamics of PET-hydrolyzing enzyme Cut190 depending on Ca2+ concentration. Journal of Thermal Analysis and Calorimetry, 2019, 135, 2655-2663.	3.6	31
14	Metal binding to cutinase-like enzyme from Saccharomonospora viridis AHK190 and its effects on enzyme activity and stability. Journal of Biochemistry, 2019, 166, 149-156.	1.7	6
15	Dynamic Docking of a Medium-Sized Molecule to Its Receptor by Multicanonical MD Simulations. Journal of Physical Chemistry B, 2019, 123, 2479-2490.	2.6	22
16	Thermal stability of singleâ€domain antibodies estimated by molecular dynamics simulations. Protein Science, 2019, 28, 429-438.	7.6	38
17	Protein Data Bank: the single global archive for 3D macromolecular structure data. Nucleic Acids Research, 2019, 47, D520-D528.	14.5	671
18	PDBx/mmCIF Format Mandatory for Protein Data Bank Deposition. Nihon Kessho Gakkaishi, 2019, 61, 159-160.	0.0	1

#	Article	IF	Citations
19	Structural and thermodynamic characterization of endo-1,3-Î²-glucanase: Insights into the substrate recognition mechanism. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2018, 1866, 415-425.	2.3	17
20	New tools and functions in dataâ€out activities at Protein Data Bank Japan (PDBj). Protein Science, 2018, 27, 95-102.	7.6	90
21	Structural Dynamics of the PET-Degrading Cutinase-like Enzyme from Saccharomonospora viridis AHK190 in Substrate-Bound States Elucidates the Ca²⁺-Driven Catalytic Cycle. Biochemistry, 2018, 57, 5289-5300.	2.5	59
22	Accurate Prediction of Complex Structure and Affinity for a Flexible Protein Receptor and Its Inhibitor. Journal of Chemical Theory and Computation, 2017, 13, 2389-2399.	5.3	43
23	Protein Data Bank Japan (PDBj): updated user interfaces, resource description framework, analysis tools for large structures. Nucleic Acids Research, 2017, 45, D282-D288.	14.5	108
24	Molmil: a molecular viewer for the PDB and beyond. Journal of Cheminformatics, 2016, 8, 42.	6.1	56
25	The new PDBj web Interface : Customizable, Modern and User-friendly(PDBj: Protein Data Bank) Tj ETQq1 1 0.784314 rgBT /Overlock 10	0.1	0