

# Gert-Jan Bekker

## List of Publications by Year in descending order

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Version: 2024-02-01

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: the single global archive for 3D macromolecular structure data. <i>Nucleic Acids Research</i> , 2019, 47, D520-D528.	14.5	671
2	Protein Data Bank Japan (PDBj): updated user interfaces, resource description framework, analysis tools for large structures. <i>Nucleic Acids Research</i> , 2017, 45, D282-D288.	14.5	108
3	New tools and functions in data activities at Protein Data Bank Japan (PDBj). <i>Protein Science</i> , 2018, 27, 95-102.	7.6	90
4	Structural Dynamics of the PET-Degrading Cutinase-like Enzyme from <i>Saccharomonospora viridis</i> AHK190 in Substrate-Bound States Elucidates the Ca <sup>2+</sup> -Driven Catalytic Cycle. <i>Biochemistry</i> , 2018, 57, 5289-5300.	2.5	59
5	Molmil: a molecular viewer for the PDB and beyond. <i>Journal of Cheminformatics</i> , 2016, 8, 42.	6.1	56
6	Accurate Prediction of Complex Structure and Affinity for a Flexible Protein Receptor and Its Inhibitor. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2389-2399.	5.3	43
7	The Biological Structure Model Archive (BSM-Arc): an archive for in silico models and simulations. <i>Biophysical Reviews</i> , 2020, 12, 371-375.	3.2	40
8	Thermal stability of single domain antibodies estimated by molecular dynamics simulations. <i>Protein Science</i> , 2019, 28, 429-438.	7.6	38
9	Mutual population-shift driven antibody-peptide binding elucidated by molecular dynamics simulations. <i>Scientific Reports</i> , 2020, 10, 1406.	3.3	32
10	Folding thermodynamics of PET-hydrolyzing enzyme Cut190 depending on Ca <sup>2+</sup> concentration. <i>Journal of Thermal Analysis and Calorimetry</i> , 2019, 135, 2655-2663.	3.6	31
11	Protein Data Bank Japan: Celebrating our 20th anniversary during a global pandemic as the Asian hub of three dimensional macromolecular structural data. <i>Protein Science</i> , 2022, 31, 173-186.	7.6	28
12	Exploring ligand binding pathways on proteins using hypersound-accelerated molecular dynamics. <i>Nature Communications</i> , 2021, 12, 2793.	12.8	24
13	Dynamic Docking of a Medium-Sized Molecule to Its Receptor by Multicanonical MD Simulations. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2479-2490.	2.6	22
14	Exhaustive search of the configurational space of heat shock protein 90 with its inhibitor by multicanonical molecular dynamics based dynamic docking. <i>Journal of Computational Chemistry</i> , 2020, 41, 1606-1615.	3.3	20
15	Structural and thermodynamic characterization of endo-1,3- $\beta$ -glucanase: Insights into the substrate recognition mechanism. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2018, 1866, 415-425.	2.3	17
16	Structural basis of mutants of PET-degrading enzyme from <i>Saccharomonospora viridis</i> AHK190 with high activity and thermal stability. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 502-511.	2.6	17
17	Cryptic-site binding mechanism of medium-sized Bcl-xL inhibiting compounds elucidated by McMD-based dynamic docking simulations. <i>Scientific Reports</i> , 2021, 11, 5046.	3.3	11
18	Accurate Binding Configuration Prediction of a G-Protein-Coupled Receptor to Its Antagonist Using Multicanonical Molecular Dynamics-Based Dynamic Docking. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5161-5171.	5.4	10

#	ARTICLE	IF	CITATIONS
19	Cutinases from thermophilic bacteria (actinomycetes): From identification to functional and structural characterization. <i>Methods in Enzymology</i> , 2021, 648, 159-185.	1.0	8
20	Dynamic Docking Using Multicanonical Molecular Dynamics: Simulating Complex Formation at the Atomistic Level. <i>Methods in Molecular Biology</i> , 2021, 2266, 187-202.	0.9	8
21	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. <i>Journal of Physical Chemistry B</i> , 2021, 125, 13376-13384.	2.6	7
22	Metal binding to cutinase-like enzyme from <i>Saccharomonospora viridis</i> AHK190 and its effects on enzyme activity and stability. <i>Journal of Biochemistry</i> , 2019, 166, 149-156.	1.7	6
23	PDBx/mmCIF Format Mandatory for Protein Data Bank Deposition. <i>Nihon Kessho Gakkaishi</i> , 2019, 61, 159-160.	0.0	1
24	The new PDBj web Interface : Customizable, Modern and User-friendly(PDBj: Protein Data Bank) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 54</i>	0.1	0
25	Dynamical Methods to Study Interaction in Proteins Facilitating Molecular Understanding of Cancer. , 2022, , 2231-2247.		0