Pemra Doruker

List of Publications by Year
in descending order

71	2,916	147801 31	175258 52
papers	citations	h-index	g-index

73	73	73	2378
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Bridging the Gap Between Atomistic and Coarse-Grained Models of Polymers: Status and Perspectives. Advances in Polymer Science, 2000, , 41-156.	0.8	336
2	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to ?-amylase inhibitor. Proteins: Structure, Function and Bioinformatics, 2000, 40, 512-524.	2.6	260
3	Dynamics of large proteins through hierarchical levels of coarse-grained structures. Journal of Computational Chemistry, 2002, 23, 119-127.	3.3	224
4	Reverse Mapping of Coarse-Grained Polyethylene Chains from the Second Nearest Neighbor Diamond Lattice to an Atomistic Model in Continuous Space. Macromolecules, 1997, 30, 5520-5526.	4.8	101
5	ProDy 2.0: increased scale and scope after 10 years of protein dynamics modelling with Python. Bioinformatics, 2021, 37, 3657-3659.	4.1	93
6	Simulation of Polyethylene Thin Films on a High Coordination Lattice. Macromolecules, 1998, 31, 1418-1426.	4.8	86
7	Intrinsic dynamics is evolutionarily optimized to enable allosteric behavior. Current Opinion in Structural Biology, 2020, 62, 14-21.	5.7	85
8	Functional Motions of Influenza Virus Hemagglutinin: A Structure-Based Analytical Approach. Biophysical Journal, 2002, 82, 569-581.	0.5	77
9	Molecular simulations of small gas diffusion and solubility in copolymers of styrene. Polymer, 2003, 44, 3607-3620.	3.8	70
10	Mathematical description of ethanol fermentation by immobilised Saccharomyces cerevisiae. Process Biochemistry, 1998, 33, 763-771.	3.7	69
11	Mobility of the Surface and Interior of Thin Films Composed of Amorphous Polyethylene. Macromolecules, 1999, 32, 194-198.	4.8	64
12	Effect of Cooperative Hydrogen Bonding in Azoâ''Hydrazone Tautomerism of Azo Dyes. Journal of Physical Chemistry A, 2007, 111, 13506-13514.	2.5	62
13	The ribosome structure controls and directs mRNA entry, translocation and exit dynamics. Physical Biology, 2008, 5, 046005.	1.8	61
14	Mixed levels of coarse-graining of large proteins using elastic network model succeeds in extracting the slowest motions. Polymer, 2004, 45, 649-657.	3.8	55
15	Functional motions can be extracted from on-lattice construction of protein structures. Proteins: Structure, Function and Bioinformatics, 2003, 53, 174-181.	2.6	53
16	Conformational Transition Pathways Explored by Monte Carlo Simulation Integrated with Collective Modes. Biophysical Journal, 2008, 95, 5862-5873.	0.5	53
17	Loop Motions of Triosephosphate Isomerase Observed with Elastic Networks. Biochemistry, 2006, 45, 1173-1182.	2.5	52
18	Molecular dynamics simulations on constraint metal binding peptides. Polymer, 2005, 46, 4307-4313.	3.8	47

#	Article	IF	Citations
19	Focused Functional Dynamics of Supramolecules by Use of a Mixed-Resolution Elastic Network Model. Biophysical Journal, 2009, 97, 1178-1187.	0.5	46
20	ClustENM: ENM-Based Sampling of Essential Conformational Space at Full Atomic Resolution. Journal of Chemical Theory and Computation, 2016, 12, 4549-4562.	5.3	43
21	Molecular simulations of gas transport in nitrile rubber and styrene butadiene rubber. Polymer, 2006, 47, 7835-7845.	3.8	42
22	Collective dynamics of the ribosomal tunnel revealed by elastic network modeling. Proteins: Structure, Function and Bioinformatics, 2009, 75, 837-845.	2.6	42
23	A Docking Study Using Atomistic Conformers Generated via Elastic Network Model for Cyclosporin A/Cyclophilin A Complex. Journal of Biomolecular Structure and Dynamics, 2009, 27, 13-25.	3.5	42
24	Coupling between Catalytic Loop Motions and Enzyme Global Dynamics. PLoS Computational Biology, 2012, 8, e1002705.	3.2	42
25	Role of water on unfolding kinetics of helical peptides studied by molecular dynamics simulations. Biophysical Journal, 1997, 72, 2445-2456.	0.5	41
26	A second generation of mapping/reverse mapping of coarse-grained and fully atomistic models of polymer melts. Macromolecular Theory and Simulations, 1999, 8, 463-478.	1.4	40
27	Simulation of an amorphous polyethylene nanofiber on a high coordination lattice. Macromolecular Theory and Simulations, 2000, 9, 1-13.	1.4	39
28	Allosteric interactions in the parathyroid hormone GPCRâ€“arrestin complex formation. Nature Chemical Biology, 2020, 16, 1096-1104.	8.0	38
29	Segregation of Chain Ends Is a Weak Contributor to Increased Mobility at Free Polymer Surfaces. Journal of Physical Chemistry B, 1999, 103, 178-183.	2.6	36
30	Dimerization Affects Collective Dynamics of Triosephosphate Isomerase. Biochemistry, 2008, 47, 1358-1368.	2.5	35
31	Essential site scanning analysis: A new approach for detecting sites that modulate the dispersion of protein global motions. Computational and Structural Biotechnology Journal, 2020, 18, 1577-1586.	4.1	35
32	Collective Dynamics of Large Proteins from Mixed Coarse-Grained Elastic Network Model. QSAR and Combinatorial Science, 2005, 24, 443-448.	1.4	33
33	Towards gaining sight of multiscale events: utilizing network models and normal modes in hybrid methods. Current Opinion in Structural Biology, 2020, 64, 34-41.	5.7	32
34	Effect of absorbed water on oxygen transport in EVOH matrices. A molecular dynamics study. Polymer, 2004, 45, 3555-3564.	3.8	30
35	How an Inhibitor Bound to Subunit Interface Alters Triosephosphate Isomerase Dynamics. Biophysical Journal, 2015, 109, 1169-1178.	0.5	28
36	Effect of intracellular loop 3 on intrinsic dynamics of human Î²2-adrenergic receptor. BMC Structural Biology, 2013, 13, 29.	2.3	25

#	Article	IF	Citations
37	Important fluctuation dynamics of large protein structures are preserved upon coarse-grained renormalization. International Journal of Quantum Chemistry, 2002, 90, 822-837.	2.0	23
38	Application of time series analysis on molecular dynamics simulations of proteins: A study of different conformational spaces by principal component analysis. Journal of Chemical Physics, 2004, 121, 4759-4769.	3.0	22
39	Collective Motions of RNA Polymerases. Analysis of Core Enzyme, Elongation Complex and Holoenzyme. Journal of Biomolecular Structure and Dynamics, 2004, 22, 267-280.	3.5	22
40	Features of Large Hinge-Bending Conformational Transitions. Prediction of Closed Structure from Open State. Biophysical Journal, 2014, 106, 2656-2666.	0.5	21
41	Rotational isomeric state models for polyoxyethylene and polythiaethylene on a high coordination lattice. Journal of Chemical Physics, 1996, 104, 8742-8749.	3.0	20
42	Dynamics of bulk polyethylene on a high coordination lattice. Macromolecular Symposia, 1998, 133, 47-70.	0.7	19
43	Ligand Docking to Intermediate and Close-To-Bound Conformers Generated by an Elastic Network Model Based Algorithm for Highly Flexible Proteins. PLoS ONE, 2016, 11, e0158063.	2.5	18
44	Investigation of allosteric coupling in human Î²2-adrenergic receptor in the presence of intracellular loop 3. BMC Structural Biology, 2016, 16, 9.	2.3	18
45	RESPEC Incorporates Residue Specificity and the Ligand Effect into the Elastic Network Model. Journal of Physical Chemistry B, 2018, 122, 5347-5355.	2.6	16
46	Effect of Surface Roughness on Structure and Dynamics in Thin Films. Macromolecular Theory and Simulations, 2001, 10, 363-367.	1.4	15
47	Collective Dynamics ofEcoRI-DNA Complex by Elastic Network Model and Molecular Dynamics Simulations. Journal of Biomolecular Structure and Dynamics, 2006, 24, 1-15.	3.5	15
48	Sampling of Protein Conformational Space Using Hybrid Simulations: A Critical Assessment of Recent Methods. Frontiers in Molecular Biosciences, 2022, 9, 832847.	3.5	14
49	Cooperative Fluctuations Point to the Dimerization Interface of P53 Core Domain. Biophysical Journal, 2006, 91, 421-432.	0.5	13
50	Blind Dockings of Benzothiazoles to Multiple Receptor Conformations of Triosephosphate Isomerase from Trypanosoma cruzi and Human. Molecular Informatics, 2011, 30, 986-995.	2.5	12
51	Collective deformations in proteins determined by a mode analysis of molecular dynamics trajectories. Polymer, 2002, 43, 431-439.	3.8	11
52	Simulation of polyethylene thin films composed of various chain lengths. Polymer, 2002, 43, 425-430.	3.8	11
53	ClustENMD: efficient sampling of biomolecular conformational space at atomic resolution. Bioinformatics, 2021, 37, 3956-3958.	4.1	11
54	Precise druggability of the PTH type 1 receptor. Nature Chemical Biology, 2022, 18, 272-280.	8.0	11

#	Article	IF	Citations
55	Solvent effect on translational diffusivity and orientational mobility of polymers in solution: A molecular dynamics study. Journal of Chemical Physics, 1993, 99, 2235-2246.	3.0	10
56	Time series analysis of collective motions in proteins. Journal of Chemical Physics, 2004, 120, 1072-1088.	3.0	10
57	Effect of ligand binding on the intraminimum dynamics of proteins. Journal of Computational Chemistry, 2011, 32, 483-496.	3.3	10
58	Proteinâ€“Ligand Complexes as Constrained Dynamical Systems. Journal of Chemical Information and Modeling, 2019, 59, 2352-2358.	5.4	10
59	Ligandâ€binding affinity of alternative conformers of human Î² 2 â€adrenergic receptor in the presence of intracellular loop 3 (ICL 3) and their potential use in virtual screening studies. Chemical Biology and Drug Design, 2019, 93, 883-899.	3.2	9
60	Modulation of Toroidal Proteins Dynamics in Favor of Functional Mechanisms upon Ligand Binding. Biophysical Journal, 2020, 118, 1782-1794.	0.5	9
61	Conformational dynamics of bacterial trigger factor in apo and ribosome-bound states. PLoS ONE, 2017, 12, e0176262.	2.5	9
62	Hierarchical structure of the energy landscape of proteins revisited by time series analysis. II. Investigation of explicit solvent effects. Journal of Chemical Physics, 2005, 123, 144911.	3.0	8
63	Hierarchical structure of the energy landscape of proteins revisited by time series analysis. I. Mimicking protein dynamics in different time scales. Journal of Chemical Physics, 2005, 123, 144910.	3.0	7
64	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to Î±â€amylase inhibitor. Proteins: Structure, Function and Bioinformatics, 2000, 40, 512-524.	2.6	7
65	Substrate Effect on Catalytic Loop and Global Dynamics of Triosephosphate Isomerase. Entropy, 2013, 15, 1085-1099.	2.2	4
66	Activation and Speciation Mechanisms in Class A GPCRs. Journal of Molecular Biology, 2022, 434, 167690.	4.2	4
67	Elastic Network Models of Coarse-Grained Proteins Are Effective for Studying the Structural Control Exerted over Their Dynamics. , 2008, , 237-254.		3
68	Editorial: Understanding Protein Dynamics, Binding and Allostery for Drug Design. Frontiers in Molecular Biosciences, 2021, 8, 681364.	3.5	2
69	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to Î±-amylase inhibitor. , 0, .		2
70	Simulations of Thin Films and Fibers of Amorphous Polymers. , 2002, , 117-126.		1
71	Mimicking Protein Dynamics by the Integration of Elastic Network Model with Time Series Analysis. International Journal of High Performance Computing Applications, 2007, 21, 59-65.	3.7	1