

# Pemra Doruker

## List of Publications by Year in descending order

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71  
papers

2,916  
citations

147801

31  
h-index

175258

52  
g-index

73  
all docs

73  
docs citations

73  
times ranked

2378  
citing authors

#	ARTICLE	IF	CITATIONS
1	Sampling of Protein Conformational Space Using Hybrid Simulations: A Critical Assessment of Recent Methods. <i>Frontiers in Molecular Biosciences</i> , 2022, 9, 832847.	3.5	14
2	Precise druggability of the PTH type 1 receptor. <i>Nature Chemical Biology</i> , 2022, 18, 272-280.	8.0	11
3	Activation and Speciation Mechanisms in Class A GPCRs. <i>Journal of Molecular Biology</i> , 2022, 434, 167690.	4.2	4
4	<i>ProDy</i> 2.0: increased scale and scope after 10 years of protein dynamics modelling with Python. <i>Bioinformatics</i> , 2021, 37, 3657-3659.	4.1	93
5	Editorial: Understanding Protein Dynamics, Binding and Allostery for Drug Design. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 681364.	3.5	2
6	ClustENMD: efficient sampling of biomolecular conformational space at atomic resolution. <i>Bioinformatics</i> , 2021, 37, 3956-3958.	4.1	11
7	Intrinsic dynamics is evolutionarily optimized to enable allosteric behavior. <i>Current Opinion in Structural Biology</i> , 2020, 62, 14-21.	5.7	85
8	Towards gaining sight of multiscale events: utilizing network models and normal modes in hybrid methods. <i>Current Opinion in Structural Biology</i> , 2020, 64, 34-41.	5.7	32
9	Essential site scanning analysis: A new approach for detecting sites that modulate the dispersion of protein global motions. <i>Computational and Structural Biotechnology Journal</i> , 2020, 18, 1577-1586.	4.1	35
10	Allosteric interactions in the parathyroid hormone GPCR-arrestin complex formation. <i>Nature Chemical Biology</i> , 2020, 16, 1096-1104.	8.0	38
11	Modulation of Toroidal Proteins Dynamics in Favor of Functional Mechanisms upon Ligand Binding. <i>Biophysical Journal</i> , 2020, 118, 1782-1794.	0.5	9
12	Protein-Ligand Complexes as Constrained Dynamical Systems. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2352-2358.	5.4	10
13	Ligand-binding affinity of alternative conformers of human $\beta_2$ -adrenergic receptor in the presence of intracellular loop 3 (ICL3) and their potential use in virtual screening studies. <i>Chemical Biology and Drug Design</i> , 2019, 93, 883-899.	3.2	9
14	RESPEC Incorporates Residue Specificity and the Ligand Effect into the Elastic Network Model. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5347-5355.	2.6	16
15	Conformational dynamics of bacterial trigger factor in apo and ribosome-bound states. <i>PLoS ONE</i> , 2017, 12, e0176262.	2.5	9
16	Ligand Docking to Intermediate and Close-To-Bound Conformers Generated by an Elastic Network Model Based Algorithm for Highly Flexible Proteins. <i>PLoS ONE</i> , 2016, 11, e0158063.	2.5	18
17	ClustENM: ENM-Based Sampling of Essential Conformational Space at Full Atomic Resolution. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4549-4562.	5.3	43
18	Investigation of allosteric coupling in human $\beta_2$ -adrenergic receptor in the presence of intracellular loop 3. <i>BMC Structural Biology</i> , 2016, 16, 9.	2.3	18

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19	How an Inhibitor Bound to Subunit Interface Alters Triosephosphate Isomerase Dynamics. <i>Biophysical Journal</i> , 2015, 109, 1169-1178.	0.5	28
20	Features of Large Hinge-Bending Conformational Transitions. Prediction of Closed Structure from Open State. <i>Biophysical Journal</i> , 2014, 106, 2656-2666.	0.5	21
21	Effect of intracellular loop 3 on intrinsic dynamics of human $\beta_2$ -adrenergic receptor. <i>BMC Structural Biology</i> , 2013, 13, 29.	2.3	25
22	Substrate Effect on Catalytic Loop and Global Dynamics of Triosephosphate Isomerase. <i>Entropy</i> , 2013, 15, 1085-1099.	2.2	4
23	Coupling between Catalytic Loop Motions and Enzyme Global Dynamics. <i>PLoS Computational Biology</i> , 2012, 8, e1002705.	3.2	42
24	Blind Dockings of Benzothiazoles to Multiple Receptor Conformations of Triosephosphate Isomerase from <i>Trypanosoma cruzi</i> and Human. <i>Molecular Informatics</i> , 2011, 30, 986-995.	2.5	12
25	Effect of ligand binding on the intraminimum dynamics of proteins. <i>Journal of Computational Chemistry</i> , 2011, 32, 483-496.	3.3	10
26	Collective dynamics of the ribosomal tunnel revealed by elastic network modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 837-845.	2.6	42
27	Focused Functional Dynamics of Supramolecules by Use of a Mixed-Resolution Elastic Network Model. <i>Biophysical Journal</i> , 2009, 97, 1178-1187.	0.5	46
28	A Docking Study Using Atomistic Conformers Generated via Elastic Network Model for Cyclosporin A/Cyclophilin A Complex. <i>Journal of Biomolecular Structure and Dynamics</i> , 2009, 27, 13-25.	3.5	42
29	Conformational Transition Pathways Explored by Monte Carlo Simulation Integrated with Collective Modes. <i>Biophysical Journal</i> , 2008, 95, 5862-5873.	0.5	53
30	Dimerization Affects Collective Dynamics of Triosephosphate Isomerase. <i>Biochemistry</i> , 2008, 47, 1358-1368.	2.5	35
31	The ribosome structure controls and directs mRNA entry, translocation and exit dynamics. <i>Physical Biology</i> , 2008, 5, 046005.	1.8	61
32	Elastic Network Models of Coarse-Grained Proteins Are Effective for Studying the Structural Control Exerted over Their Dynamics. , 2008, , 237-254.		3
33	Mimicking Protein Dynamics by the Integration of Elastic Network Model with Time Series Analysis. <i>International Journal of High Performance Computing Applications</i> , 2007, 21, 59-65.	3.7	1
34	Effect of Cooperative Hydrogen Bonding in Azo $\rightleftharpoons$ Hydrazone Tautomerism of Azo Dyes. <i>Journal of Physical Chemistry A</i> , 2007, 111, 13506-13514.	2.5	62
35	Collective Dynamics of EcoRI-DNA Complex by Elastic Network Model and Molecular Dynamics Simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2006, 24, 1-15.	3.5	15
36	Cooperative Fluctuations Point to the Dimerization Interface of P53 Core Domain. <i>Biophysical Journal</i> , 2006, 91, 421-432.	0.5	13

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37	Loop Motions of Triosephosphate Isomerase Observed with Elastic Networks. <i>Biochemistry</i> , 2006, 45, 1173-1182.	2.5	52
38	Molecular simulations of gas transport in nitrile rubber and styrene butadiene rubber. <i>Polymer</i> , 2006, 47, 7835-7845.	3.8	42
39	Molecular dynamics simulations on constraint metal binding peptides. <i>Polymer</i> , 2005, 46, 4307-4313.	3.8	47
40	Collective Dynamics of Large Proteins from Mixed Coarse-Grained Elastic Network Model. <i>QSAR and Combinatorial Science</i> , 2005, 24, 443-448.	1.4	33
41	Hierarchical structure of the energy landscape of proteins revisited by time series analysis. I. Mimicking protein dynamics in different time scales. <i>Journal of Chemical Physics</i> , 2005, 123, 144910.	3.0	7
42	Hierarchical structure of the energy landscape of proteins revisited by time series analysis. II. Investigation of explicit solvent effects. <i>Journal of Chemical Physics</i> , 2005, 123, 144911.	3.0	8
43	Application of time series analysis on molecular dynamics simulations of proteins: A study of different conformational spaces by principal component analysis. <i>Journal of Chemical Physics</i> , 2004, 121, 4759-4769.	3.0	22
44	Time series analysis of collective motions in proteins. <i>Journal of Chemical Physics</i> , 2004, 120, 1072-1088.	3.0	10
45	Mixed levels of coarse-graining of large proteins using elastic network model succeeds in extracting the slowest motions. <i>Polymer</i> , 2004, 45, 649-657.	3.8	55
46	Effect of absorbed water on oxygen transport in EVOH matrices. A molecular dynamics study. <i>Polymer</i> , 2004, 45, 3555-3564.	3.8	30
47	Collective Motions of RNA Polymerases. Analysis of Core Enzyme, Elongation Complex and Holoenzyme. <i>Journal of Biomolecular Structure and Dynamics</i> , 2004, 22, 267-280.	3.5	22
48	Molecular simulations of small gas diffusion and solubility in copolymers of styrene. <i>Polymer</i> , 2003, 44, 3607-3620.	3.8	70
49	Functional motions can be extracted from on-lattice construction of protein structures. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 53, 174-181.	2.6	53
50	Simulations of Thin Films and Fibers of Amorphous Polymers. , 2002, , 117-126.		1
51	Functional Motions of Influenza Virus Hemagglutinin: A Structure-Based Analytical Approach. <i>Biophysical Journal</i> , 2002, 82, 569-581.	0.5	77
52	Dynamics of large proteins through hierarchical levels of coarse-grained structures. <i>Journal of Computational Chemistry</i> , 2002, 23, 119-127.	3.3	224
53	Important fluctuation dynamics of large protein structures are preserved upon coarse-grained renormalization. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 822-837.	2.0	23
54	Collective deformations in proteins determined by a mode analysis of molecular dynamics trajectories. <i>Polymer</i> , 2002, 43, 431-439.	3.8	11

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55	Simulation of polyethylene thin films composed of various chain lengths. <i>Polymer</i> , 2002, 43, 425-430.	3.8	11
56	Effect of Surface Roughness on Structure and Dynamics in Thin Films. <i>Macromolecular Theory and Simulations</i> , 2001, 10, 363-367.	1.4	15
57	Simulation of an amorphous polyethylene nanofiber on a high coordination lattice. <i>Macromolecular Theory and Simulations</i> , 2000, 9, 1-13.	1.4	39
58	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to $\alpha$ -amylase inhibitor. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 40, 512-524.	2.6	260
59	Bridging the Gap Between Atomistic and Coarse-Grained Models of Polymers: Status and Perspectives. <i>Advances in Polymer Science</i> , 2000, , 41-156.	0.8	336
60	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to $\alpha$ -amylase inhibitor. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 40, 512-524.	2.6	7
61	A second generation of mapping/reverse mapping of coarse-grained and fully atomistic models of polymer melts. <i>Macromolecular Theory and Simulations</i> , 1999, 8, 463-478.	1.4	40
62	Mobility of the Surface and Interior of Thin Films Composed of Amorphous Polyethylene. <i>Macromolecules</i> , 1999, 32, 194-198.	4.8	64
63	Segregation of Chain Ends Is a Weak Contributor to Increased Mobility at Free Polymer Surfaces. <i>Journal of Physical Chemistry B</i> , 1999, 103, 178-183.	2.6	36
64	Mathematical description of ethanol fermentation by immobilised <i>Saccharomyces cerevisiae</i> . <i>Process Biochemistry</i> , 1998, 33, 763-771.	3.7	69
65	Simulation of Polyethylene Thin Films on a High Coordination Lattice. <i>Macromolecules</i> , 1998, 31, 1418-1426.	4.8	86
66	Dynamics of bulk polyethylene on a high coordination lattice. <i>Macromolecular Symposia</i> , 1998, 133, 47-70.	0.7	19
67	Reverse Mapping of Coarse-Grained Polyethylene Chains from the Second Nearest Neighbor Diamond Lattice to an Atomistic Model in Continuous Space. <i>Macromolecules</i> , 1997, 30, 5520-5526.	4.8	101
68	Role of water on unfolding kinetics of helical peptides studied by molecular dynamics simulations. <i>Biophysical Journal</i> , 1997, 72, 2445-2456.	0.5	41
69	Rotational isomeric state models for polyoxyethylene and polythiaethylene on a high coordination lattice. <i>Journal of Chemical Physics</i> , 1996, 104, 8742-8749.	3.0	20
70	Solvent effect on translational diffusivity and orientational mobility of polymers in solution: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1993, 99, 2235-2246.	3.0	10
71	Dynamics of proteins predicted by molecular dynamics simulations and analytical approaches: Application to $\alpha$ -amylase inhibitor. , 0, .		2