David Perahia

List of Publications by Year
in descending order

126	4,439	76326	123424
papers	citations	40 h-index	61 g-index

132	132	132	3274
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Evaluation of the configurational entropy for proteins: application to molecular dynamics simulations of an Î±-helix. Macromolecules, 1984, 17, 1370-1374.	4.8	244
2	Internal and interfacial dielectric properties of cytochrome c from molecular dynamics in aqueous solution.. Proceedings of the National Academy of Sciences of the United States of America, 1995, 92, 1082-1086.	7.1	210
3	Molecular dynamics of an Â-helical polypeptide: Temperature dependence and deviation from harmonic behavior. Proceedings of the National Academy of Sciences of the United States of America, 1982, 79, 1346-1350.	7.1	127
4	Hydration scheme of uracil and cytosine. Theoretica Chimica Acta, 1978, 48, 29-36.	0.8	123
5	Microscopic Dielectric Properties of Cytochrome c from Molecular Dynamics Simulations in Aqueous Solution. Journal of the American Chemical Society, 1995, 117, 7987-8000.	13.7	116
6	Motions in Hemoglobin Studied by Normal Mode Analysis and Energy Minimization: Evidence for the Existence of Tertiary T-like, Quaternary R-like Intermediate Structures. Journal of Molecular Biology, 1996, 258, 393-410.	4.2	97
7	Microscopic theory of the dielectric properties of proteins. Biophysical Journal, 1991, 59, 670-690.	0.5	94
8	Computation of low-frequency normal modes in macromolecules: Improvements to the method of diagonalization in a mixed basis and application to hemoglobin. Computers & Chemistry, 1995, 19, 241-246.	1.2	94
9	Success of the PCILO method and failure of the CNDO/2 method for predicting conformations in some conjugated systems. Chemical Physics Letters, 1973, 19, 73-75.	2.6	84
10	Targeting STAT1 by myricetin and delphinidin provides efficient protection of the heart from ischemia/reperfusionâ€induced injury. FEBS Letters, 2009, 583, 531-541.	2.8	80
11	Conformational dynamics and enzyme activity. Biochimie, 1998, 80, 33-42.	2.6	78
12	Molecular orbital calculations on the conformation of polypeptides and proteins IV. The conformation of the prolyl and hydroxyprolyl residues. Journal of Theoretical Biology, 1970, 29, 275-291.	1.7	77
13	Molecular orbital calculations on the conformation of nucleic acids and their constituents. Theoretica Chimica Acta, 1973, 30, 31-44.	0.8	77
14	Diagonalization in a mixed basis: A method to compute low-frequency normal modes for large macromolecules. Biopolymers, 1993, 33, 599-611.	2.4	72
15	Molecular orbital calculations on the conformation of nucleic acids and their constituents. Nucleic Acids and Protein Synthesis, 1972, 269, 1-14.	1.7	70
16	Ghrelin receptor conformational dynamics regulate the transition from a preassembled to an active receptor:Gq complex. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 1601-1606.	7.1	69
17	How to choose relevant multiple receptor conformations for virtual screening: a test case of Cdk2 and normal mode analysis. European Biophysics Journal, 2010, 39, 1365-1372.	2.2	68
18	On searching neighbors in computer simulations of macromolecular systems. Journal of Computational Chemistry, 1984, 5, 272-279.	3.3	67

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19	Mutation D816V Alters the Internal Structure and Dynamics of c-KIT Receptor Cytoplasmic Region: Implications for Dimerization and Activation Mechanisms. PLoS Computational Biology, 2011, 7, e1002068.	3.2	67
20	Intramolecular dielectric screening in proteins. Journal of Molecular Biology, 1991, 218, 859-886.	4.2	66
21	Hydration scheme of the purine and pyrimidine bases and base-pairs of the nucleic acids. Theoretica Chimica Acta, 1979, 50, 317-325.	0.8	63
22	Tertiary and quaternary conformational changes in aspartate transcarbamylase: a normal mode study. Proteins: Structure, Function and Bioinformatics, 1999, 34, 96-112.	2.6	61
23	An ab initio study of the effect of the 3d orbitals of phosphorus on the properties of the phosphate group. Theoretica Chimica Acta, 1975, 40, 47-60.	0.8	59
24	Molecular orbital calculations on the conformation of nucleic acids and their constituents. IV. Conformations about the exocyclic C(4â€²)-C(5â€²) bond. Nucleic Acids and Protein Synthesis, 1972, 287, 211-231.	1.7	58
25	Normal mode analysis as a prerequisite for drug design: Application to matrix metalloproteinases inhibitors. FEBS Letters, 2006, 580, 5130-5136.	2.8	58
26	The molecular electrostatic potential of the B-DNA helix. VL The regions of the base pairs in poly (dG.dC) and poly (dA.dT). Nucleic Acids Research, 1979, 6, 3821-3830.	14.5	57
27	Insight into the apoptosis-inducing action of Î±-bisabolol towards malignant tumor cells: Involvement of lipid rafts and Bid. Archives of Biochemistry and Biophysics, 2008, 476, 113-123.	3.0	57
28	Use of the overlap multipole expansion for approximating molecular electrostatic potentials. International Journal of Quantum Chemistry, 1979, 15, 121-129.	2.0	55
29	Molecular electrostatic potential of the B-DNA helix. I. Region of the guanine-cytosine base pair. International Journal of Quantum Chemistry, 1979, 16, 395-403.	2.0	54
30	Cation-binding to biomolecules. Theoretica Chimica Acta, 1977, 43, 207-214.	0.8	53
31	Exploring Free Energy Landscapes of Large Conformational Changes: Molecular Dynamics with Excited Normal Modes. Journal of Chemical Theory and Computation, 2015, 11, 2755-2767.	5.3	52
32	Molecular orbital calculations on the conformation of nucleic acids and their constituents. Nucleic Acids and Protein Synthesis, 1974, 340, 299-313.	1.7	51
33	Normal modes of symmetric protein assemblies. Application to the tobacco mosaic virus protein disk. Biophysical Journal, 1992, 61, 410-427.	0.5	51
34	Analysis of the Low Frequency Normal Modes of the T-state of Aspartate Transcarbamylase. Journal of Molecular Biology, 1996, 257, 1070-1087.	4.2	51
35	New Insights into the Allosteric Mechanism of Human Hemoglobin from Molecular Dynamics Simulations. Biophysical Journal, 2002, 82, 3224-3245.	0.5	50
36	Odorant Binding and Conformational Dynamics in the Odorant-binding Protein. Journal of Biological Chemistry, 2006, 281, 29929-29937.	3.4	46

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37	Molecular orbital calculations on the conformation of polypeptides and proteins. Theoretica Chimica Acta, 1970, 18, 44-56.	0.8	44
38	Molecular orbital calculations on the conformation of polypeptides and proteins. Journal of Theoretical Biology, 1971, 31, 269-285.	1.7	43
39	Hydration scheme of the complementary base-pairs of DNA. FEBS Letters, 1978, 91, 213-215.	2.8	42
40	Analysis of the Low-frequency Normal Modes of the R State of Aspartate Transcarbamylase and a Comparison with the T State Modes. Journal of Molecular Biology, 1996, 261, 490-506.	4.2	42
41	Collective motions in Glucosamine-6-phosphate Synthase: Influence of Ligand Binding and role in Ammonia Channelling and Opening of the Fructose-6-Phosphate Binding Site. Journal of Molecular Biology, 2009, 385, 653-664.	4.2	42
42	Cation-binding to biomolecules. Theoretica Chimica Acta, 1976, 42, 23-31.	0.8	40
43	Human thrombospondinâ€™s (TSP-1) C-terminal domain opens to interact with the CD-47 receptor: A molecular modeling study. Archives of Biochemistry and Biophysics, 2008, 478, 103-109.	3.0	40
44	Motions of an ?-helical polypeptide: Comparison of molecular and harmonic dynamics. Biopolymers, 1990, 29, 645-677.	2.4	39
45	A method to explore transition paths in macromolecules. Applications to hemoglobin and phosphoglycerate kinase. Computer Physics Communications, 1995, 91, 263-273.	7.5	39
46	Theoretical modeling of the heme group with a hybrid QM/MM method. Journal of Computational Chemistry, 2000, 21, 282-294.	3.3	39
47	Vibrational Softening of a Protein on Ligand Binding. Journal of Physical Chemistry B, 2011, 115, 6811-6817.	2.6	39
48	A Concerted Mechanism for Opening the GDP Binding Pocket and Release of the Nucleotide in Hetero-Trimeric G-Proteins. Journal of Molecular Biology, 2011, 411, 298-312.	4.2	37
49	The molecular electrostatic potentials of the complementary base pairs of DNA. Theoretica Chimica Acta, 1978, 48, 263-266.	0.8	35
50	Cofactor-dependent conformational heterogeneity of GAD65 and its role in autoimmunity and neurotransmitter homeostasis. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E2524-E2529.	7.1	34
51	Polar fluctuations in proteins: molecular-dynamic studies of cytochrome c in aqueous solution. Faraday Discussions, 1996, 103, 71.	3.2	33
52	Molecular orbital calculations on the conformation of polypeptides and proteins. II. Conformational energy maps and stereochemical rotational states of aromatic residues. Biopolymers, 1971, 10, 107-128.	2.4	32
53	Activation of the Ghrelin Receptor is Described by a Privileged Collective Motion: A Model for Constitutive and Agonist-induced Activation of a Sub-class A G-Protein Coupled Receptor (GPCR). Journal of Molecular Biology, 2010, 395, 769-784.	4.2	32
54	Free Energy Profiles along Consensus Normal Modes Provide Insight into HIV-1 Protease Flap Opening. Journal of Chemical Theory and Computation, 2011, 7, 2348-2352.	5.3	32

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55	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
56	Unfolding of hen egg lysozyme by molecular dynamics simulations at 300K: Insight into the role of the interdomain interface. Proteins: Structure, Function and Bioinformatics, 2000, 41, 58-74.	2.6	31
57	Consensus modes, a robust description of protein collective motions from multiple-minima normal mode analysisâ€"application to the HIV-1 protease. Physical Chemistry Chemical Physics, 2010, 12, 2850.	2.8	31
58	The molecular electrostatic potential of the B-DNA helix. Theoretica Chimica Acta, 1979, 51, 349-357.	0.8	30
59	Low frequency motions in phosphoglycerate kinase. A normal mode analysis. Chemical Physics, 1996, 204, 327-336.	1.9	27
60	The molecular electrostatic potential of the B-DNA helix. Theoretica Chimica Acta, 1979, 50, 351-354.	0.8	26
61	Internal cavities and ligand passageways in human hemoglobin characterized by molecular dynamics simulations. Biochimica Et Biophysica Acta - General Subjects, 2005, 1724, 385-393.	2.4	26
62	Conformational heterogeneity and low-frequency vibrational modes of proteins. Physical Chemistry Chemical Physics, 2006, 8, 5543.	2.8	26
63	Molecular orbital calculations on the conformation of polypeptides and proteins. V. Conformational energy maps and stereochemical rotational states of aliphatic residues. Biopolymers, 1971, 10, 491-511.	2.4	25
64	Structural Dynamics of DPP-4 and Its Influence on the Projection of Bioactive Ligands. Molecules, 2018, 23, 490.	3.8	25
65	Molecular orbital calculations on the conformation of phosphodiesters An extended correlation between the geometry and the conformation of the phosphate group. Nucleic Acids and Protein Synthesis, 1976, 435, 282-289.	1.7	24
66	Study of the fast-reacting cysteines in phosphoglycerate kinase using chemical modification and site-directed mutagenesis. FEBS Journal, 1989, 185, 419-423.	0.2	24
67	Molecular orbital calculations on the conformation of nucleic acids and their constituents XI. The backbone structure of (3â€²â€“5â€²) and (2â€²â€“5â€²)-linked diribose monophosphates with different sugar puckers. Nucleic Acids and Protein Synthesis, 1974, 353, 16-27.	0.7	23
68	Molecular dynamics of the FixJ receiver domain: movement of the Î²4-Î±4 loop correlates with the in and out flip of Phe101. Protein Science, 2008, 11, 2622-2630.	7.6	22
69	Sampling of conformational ensemble for virtual screening using molecular dynamics simulations and normal mode analysis. Future Medicinal Chemistry, 2015, 7, 2317-2331.	2.3	22
70	Conformational Equilibrium of CDK/Cyclin Complexes by Molecular Dynamics with Excited Normal Modes. Biophysical Journal, 2015, 109, 1179-1189.	0.5	21
71	Substrate binding modifies the hinge bending characteristics of human 3â€phosphoglycerate kinase: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2009, 77, 319-329.	2.6	20
72	The conformational energy map for the disulphide bridge in proteins. Biochemical and Biophysical Research Communications, 1971, 43, 65-68.	2.1	19

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73	Flexibility and folding of phosphoglycerate kinase. Biochimie, 1990, 72, 417-429.	2.6	19
74	A New Strategy for Atomic Flexible Fitting in Cryo-EM Maps by Molecular Dynamics with Excited Normal Modes (MDeNM-EMfit). Journal of Chemical Information and Modeling, 2020, 60, 2419-2423.	5.4	18
75	Molecular orbital calculations on the conformation of polypeptides and proteins. Theoretica Chimica Acta, 1970, 19, 121-134.	0.8	17
76	Molecular orbital calculations on the conformation of nucleic acids and their constituents. Nucleic Acids and Protein Synthesis, 1974, 349, 189-203.	1.7	17
77	Molecular orbital calculations on the conformation of nucleic acids and their constituents VI. Conformation about the exocyclic C(4â€²)-C(5â€²) bond in Î±-nucleosides. Nucleic Acids and Protein Synthesis, 1973, 299, 497-499.	1.7	16
78	Insights into the substrate binding mechanism of SULT1A1 through molecular dynamics with excited normal modes simulations. Scientific Reports, 2021, 11, 13129.	3.3	16
79	A Molecular Orbital probe into the conformation of ATP. Biochemical and Biophysical Research Communications, 1972, 47, 1284-1289.	2.1	15
80	Introduction of internal cysteines as conformational probes in yeast phosphoglycerate kinase. Protein Engineering, Design and Selection, 1990, 3, 199-204.	2.1	15
81	Dielectric properties of proteins from simulations: tools and techniques. Computer Physics Communications, 1995, 91, 291-303.	7.5	15
82	Binding sites and hydrophobic pockets in Human Thioredoxin 1 determined by normal mode analysis. Journal of Structural Biology, 2013, 184, 293-300.	2.8	15
83	The effects of ligands on the conformation of phosphoglycerate kinase: Fluorescence anisotropy decay and theoretical interpretation. Biopolymers, 1990, 30, 1151-1160.	2.4	14
84	Direct interaction of natural and synthetic catechins with signal transducer activator of transcription 1 affects both its phosphorylation and activity. FEBS Journal, 2014, 281, 724-738.	4.7	14
85	The allosteric activation mechanism of a phospholipase A2-like toxin from Bothrops jararacussu venom: a dynamic description. Scientific Reports, 2020, 10, 16252.	3.3	14
86	Sampling of Protein Conformational Space Using Hybrid Simulations: A Critical Assessment of Recent Methods. Frontiers in Molecular Biosciences, 2022, 9, 832847.	3.5	14
87	Relation between flexibility and positively selected HIVâ€1 protease mutants against inhibitors. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2680-2691.	2.6	13
88	Use of normal modes for structural modeling of proteins: the case study of rat heme oxygenase 1. European Biophysics Journal, 2008, 37, 1157-1165.	2.2	11
89	Hybrid approaches to molecular simulation. Current Opinion in Structural Biology, 2012, 22, 386-393.	5.7	11
90	Conformational restriction of Gâ€proteins Coupled Receptors (GPCRs) upon complexation to Gâ€proteins: A putative activation mode of GPCRs?. FEBS Letters, 2013, 587, 2656-2661.	2.8	11

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91	Complexes of a Znâ€metalloenzyme binding site with hydroxamateâ€containing ligands. A case for detailed benchmarkings of polarizable molecular mechanics/dynamics potentials when the experimental binding structure is unknown. Journal of Computational Chemistry, 2016, 37, 2770-2782.	3.3	11
92	Nucleotide-Specific Autoinhibition of Full-Length K-Ras4B Identified by Extensive Conformational Sampling. Frontiers in Molecular Biosciences, 2020, 7, 145.	3.5	11
93	Ab initio calculations predict a very low barrier for the rotation of the axial ligand in Fe(P)(Im). Chemical Physics Letters, 2002, 353, 379-382.	2.6	10
94	A DFT study on the relative affinity for oxygen of the Î± and Î² subunits of hemoglobin. Journal of Computational Chemistry, 2006, 27, 1446-1453.	3.3	10
95	CO migration pathways in cytochrome P450camstudied by molecular dynamics simulations. Protein Science, 2007, 16, 781-794.	7.6	10
96	Effects of pH and aggregation in the human prion conversion into scrapie form: a study using molecular dynamics with excited normal modes. European Biophysics Journal, 2018, 47, 583-590.	2.2	10
97	New Structural insights into Kir channel gating from molecular simulations, HDX-MS and functional studies. Scientific Reports, 2020, 10, 8392.	3.3	10
98	Polarizable molecular mechanics studies of <scp>Cu(I)/Zn(II)</scp> superoxide dismutase: Bimetallic binding site and structured waters. Journal of Computational Chemistry, 2014, 35, 2096-2106.	3.3	9
99	A novel molecular mechanism to explain mutations of the HCV protease associated with resistance against covalently bound inhibitors. Virus Research, 2019, 274, 197778.	2.2	9
100	Molecular orbital calculations on the conformation of polypeptides and proteins. Theoretica Chimica Acta, 1971, 22, 11-22.	0.8	8
101	Molecular orbital calculations on the conformation of polypeptides and proteins. VIII. The conformational energy maps and stereochemical rotational slates of the asparaginyl, glutaminyl aspartyl and glutamyl residues. Biopolymers, 1971, 10, 1649-1660.	2.4	8
102	Integrating Three Views of Arf1 Activation Dynamics. Journal of Molecular Biology, 2004, 337, 969-983.	4.2	8
103	An Atomistic View of Microtubule Stabilization by GTP. Structure, 2013, 21, 833-843.	3.3	8
104	In vitro and in silico studies reveal capsid-mutant Porcine circovirus 2b with novel cytopathogenic and structural characteristics. Virus Research, 2018, 251, 22-33.	2.2	7
105	1.2â€…Ã… Refinement of the Kunitz-Type Domain from the Î±3 Chain of Human Type VI Collagen. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 306-312.	2.5	5
106	GANM: A proteinâ€“ligand docking approach based on genetic algorithm and normal modes. Applied Mathematics and Computation, 2012, 219, 511-520.	2.2	5
107	Unveiling functional motions based on point mutations in biased signaling systems: A normal mode study on nerve growth factor bound to TrkA. PLoS ONE, 2020, 15, e0231542.	2.5	5
108	Revealing the activation mechanism of autoinhibited RalF by integrated simulation and experimental approaches. Scientific Reports, 2021, 11, 10059.	3.3	5

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109	Concerted conformational dynamics and water movements in the ghrelin G protein-coupled receptor. ELife, 2021, 10, .	6.0	5
110	A freeâ€energy simulation study of a bacterial collagenase inhibitor. International Journal of Peptide and Protein Research, 1994, 43, 384-392.	0.1	3
111	Recovery of the wild type atomic flexibility in the HIV-1 protease double mutants. Journal of Molecular Graphics and Modelling, 2015, 59, 107-116.	2.4	3
112	Binding of phenothiazines into allosteric hydrophobic pocket of human thioredoxin 1. European Biophysics Journal, 2016, 45, 279-286.	2.2	3
113	Long-Term, Open-Label, Safety Study of Edivoxetine Monotherapy in Children and Adolescents with Attention-Deficit/Hyperactivity Disorder. Journal of Child and Adolescent Psychopharmacology, 2017, 27, 700-707.	1.3	3
114	Unexpected Gating Behaviour of an Engineered Potassium Channel Kir. Frontiers in Molecular Biosciences, 2021, 8, 691901.	3.5	3
115	Dynamic Motion and Communication in the Streptococcal C1 Phage Lysin, PlyC. PLoS ONE, 2015, 10, e0140219.	2.5	3
116	Molecular orbital studies on the conformation of the terminal aminoacyladenosine moieties of tRNA. FEBS Letters, 1972, 23, 332-336.	2.8	2
117	Ligand chirality effects on the dynamics of human 3-phosphoglycerate kinase: Comparison between d- and l-nucleotides. Archives of Biochemistry and Biophysics, 2011, 511, 88-100.	3.0	2
118	Receptor Flexibility in Ligand Docking and Virtual Screening. , 2011, , 99-117.		2
119	Normal Mode Analysis of Large Symmetric Assemblies of Macromolecules. AIP Conference Proceedings, 1991, , .	0.4	1
120	Addressing the Issues of Non-isotropy and Non-additivity in the Development of Quantum Chemistry-Grounded Polarizable Molecular Mechanics. Challenges and Advances in Computational Chemistry and Physics, 2015, , 1-49.	0.6	1
121	Substrate Binding Directs the Functional Hinge Bending Motion of Human 3-Phosphoglycerate Kinase. Biophysical Journal, 2009, 96, 84a.	0.5	0
122	Influence of Ligand Chirality on the Catalytic Efficiency of Human 3-Phosphoglycerate Kinase. Biophysical Journal, 2011, 100, 395a.	0.5	0
123	Multimolecular complexes of the phosphodiester anion with Zn(II) or Mg(II) and water moleculesâ€"Preliminary validations of a polarizable potential by ab initio quantum chemistry. Journal of Computational Chemistry, 2021, 42, 1430-1446.	3.3	0
124	All-Atom Normal Mode Calculations of Large Molecular Systems Using Iterative Methods. Chapman & Hall/CRC Mathematical and Computational Biology Series, 2005, , 17-39.	0.1	0
125	Integrative Study of the Structural and Dynamical Properties of a KirBac3.1 Mutant: Functional Implication of a Highly Conserved Tryptophan in the Transmembrane Domain. International Journal of Molecular Sciences, 2022, 23, 335.	4.1	0
126	Editorial: Integrative Structural Biology of Proteins and Macromolecular Assemblies: Bridging Experiments and Simulations. Frontiers in Molecular Biosciences, 0, 9, .	3.5	0