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	Sampling of Protein Conformational Space Using Hybrid Simulations: A Critical Assessment of Recent Methods. Frontiers in Molecular Biosciences, 2022, 9, 832847.	3.5	14
2	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
3	Revealing the activation mechanism of autoinhibited RalF by integrated simulation and experimental approaches. Scientific Reports, 2021, 11, 10059.	3.3	5
4	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
5	Unexpected Gating Behaviour of an Engineered Potassium Channel Kir. Frontiers in Molecular Biosciences, 2021, 8, 691901.	3.5	3
6	Insights into the substrate binding mechanism of SULT1A1 through molecular dynamics with excited normal modes simulations. Scientific Reports, 2021, 11, 13129.	3.3	16
7	Concerted conformational dynamics and water movements in the ghrelin G protein-coupled receptor. ELife, 2021, 10, .	6.0	5
8	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
9	New Structural insights into Kir channel gating from molecular simulations, HDX-MS and functional studies. Scientific Reports, 2020, 10, 8392.	3.3	10
10	Nucleotide-Specific Autoinhibition of Full-Length K-Ras4B Identified by Extensive Conformational Sampling. Frontiers in Molecular Biosciences, 2020, 7, 145.	3.5	11
11	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
12	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
13	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
14	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
15	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
16	Structural Dynamics of DPP-4 and Its Influence on the Projection of Bioactive Ligands. Molecules, 2018, 23, 490.	3.8	25
17	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
18	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

#	Article	IF	Citations
19	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
20	Binding of phenothiazines into allosteric hydrophobic pocket of human thioredoxin 1. European Biophysics Journal, 2016, 45, 279-286.	2.2	3
21	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
22	Conformational Equilibrium of CDK/Cyclin Complexes by Molecular Dynamics with Excited Normal Modes. Biophysical Journal, 2015, 109, 1179-1189.	0.5	21
23	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
24	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
25	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
26	Dynamic Motion and Communication in the Streptococcal C1 Phage Lysin, PlyC. PLoS ONE, 2015, 10, e0140219.	2.5	3
27	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
28	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
29	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
30	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
31	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
32	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
33	An Atomistic View of Microtubule Stabilization by GTP. Structure, 2013, 21, 833-843.	3.3	8
34	Relation between flexibility and positively selected HIVâ€1 protease mutants against inhibitors. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2680-2691.	2.6	13
35	GANM: A proteinâ€“ligand docking approach based on genetic algorithm and normal modes. Applied Mathematics and Computation, 2012, 219, 511-520.	2.2	5
36	Hybrid approaches to molecular simulation. Current Opinion in Structural Biology, 2012, 22, 386-393.	5.7	11

#	Article	IF	Citations
37	Influence of Ligand Chirality on the Catalytic Efficiency of Human 3-Phosphoglycerate Kinase. Biophysical Journal, 2011, 100, 395a.	0.5	0
38	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
39	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
40	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
41	Vibrational Softening of a Protein on Ligand Binding. Journal of Physical Chemistry B, 2011, 115, 6811-6817.	2.6	39
42	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
43	Receptor Flexibility in Ligand Docking and Virtual Screening. , 2011, , 99-117.		2
44	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
45	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
46	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
47	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
48	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
49	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
50	Substrate Binding Directs the Functional Hinge Bending Motion of Human 3-Phosphoglycerate Kinase. Biophysical Journal, 2009, 96, 84a.	0.5	0
51	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
52	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
53	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
54	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

#	Article	IF	Citations
55	CO migration pathways in cytochrome P450camstudied by molecular dynamics simulations. Protein Science, 2007, 16, 781-794.	7.6	10
56	Odorant Binding and Conformational Dynamics in the Odorant-binding Protein. Journal of Biological Chemistry, 2006, 281, 29929-29937.	3.4	46
57	Conformational heterogeneity and low-frequency vibrational modes of proteins. Physical Chemistry Chemical Physics, 2006, 8, 5543.	2.8	26
58	Normal mode analysis as a prerequisite for drug design: Application to matrix metalloproteinases inhibitors. FEBS Letters, 2006, 580, 5130-5136.	2.8	58
59	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
60	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
61	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
62	Integrating Three Views of Arf1 Activation Dynamics. Journal of Molecular Biology, 2004, 337, 969-983.	4.2	8
63	New Insights into the Allosteric Mechanism of Human Hemoglobin from Molecular Dynamics Simulations. Biophysical Journal, 2002, 82, 3224-3245.	0.5	50
64	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
65	Theoretical modeling of the heme group with a hybrid QM/MM method. Journal of Computational Chemistry, 2000, 21, 282-294.	3.3	39
66	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
67	Tertiary and quaternary conformational changes in aspartate transcarbamylase: a normal mode study. Proteins: Structure, Function and Bioinformatics, 1999, 34, 96-112.	2.6	61
68	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
69	Conformational dynamics and enzyme activity. Biochimie, 1998, 80, 33-42.	2.6	78
70	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
71	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
72	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

#	Article	IF	Citations
73	Polar fluctuations in proteins: molecular-dynamic studies of cytochrome c in aqueous solution. Faraday Discussions, 1996, 103, 71.	3.2	33
74	Low frequency motions in phosphoglycerate kinase. A normal mode analysis. Chemical Physics, 1996, 204, 327-336.	1.9	27
75	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
76	A method to explore transition paths in macromolecules. Applications to hemoglobin and phosphoglycerate kinase. Computer Physics Communications, 1995, 91, 263-273.	7.5	39
77	Dielectric properties of proteins from simulations: tools and techniques. Computer Physics Communications, 1995, 91, 291-303.	7.5	15
78	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
79	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
80	A freeâ€energy simulation study of a bacterial collagenase inhibitor. International Journal of Peptide and Protein Research, 1994, 43, 384-392.	0.1	3
81	Diagonalization in a mixed basis: A method to compute low-frequency normal modes for large macromolecules. Biopolymers, 1993, 33, 599-611.	2.4	72
82	Normal modes of symmetric protein assemblies. Application to the tobacco mosaic virus protein disk. Biophysical Journal, 1992, 61, 410-427.	0.5	51
83	Microscopic theory of the dielectric properties of proteins. Biophysical Journal, 1991, 59, 670-690.	0.5	94
84	Intramolecular dielectric screening in proteins. Journal of Molecular Biology, 1991, 218, 859-886.	4.2	66
85	Normal Mode Analysis of Large Symmetric Assemblies of Macromolecules. AIP Conference Proceedings, 1991, , .	0.4	1
86	Motions of an ?-helical polypeptide: Comparison of molecular and harmonic dynamics. Biopolymers, 1990, 29, 645-677.	2.4	39
87	The effects of ligands on the conformation of phosphoglycerate kinase: Fluorescence anisotropy decay and theoretical interpretation. Biopolymers, 1990, 30, 1151-1160.	2.4	14
88	Introduction of internal cysteines as conformational probes in yeast phosphoglycerate kinase. Protein Engineering, Design and Selection, 1990, 3, 199-204.	2.1	15
89	Flexibility and folding of phosphoglycerate kinase. Biochimie, 1990, 72, 417-429.	2.6	19
90	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

#	Article	IF	Citations
91	On searching neighbors in computer simulations of macromolecular systems. Journal of Computational Chemistry, 1984, 5, 272-279.	3.3	67
92	Evaluation of the configurational entropy for proteins: application to molecular dynamics simulations of an Î±-helix. Macromolecules, 1984, 17, 1370-1374.	4.8	244
93	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
94	The molecular electrostatic potential of the B-DNA helix. Theoretica Chimica Acta, 1979, 51, 349-357.	0.8	30
95	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
96	The molecular electrostatic potential of the B-DNA helix. Theoretica Chimica Acta, 1979, 50, 351-354.	0.8	26
97	Use of the overlap multipole expansion for approximating molecular electrostatic potentials. International Journal of Quantum Chemistry, 1979, 15, 121-129.	2.0	55
98	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
99	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
100	The molecular electrostatic potentials of the complementary base pairs of DNA. Theoretica Chimica Acta, 1978, 48, 263-266.	0.8	35
101	Hydration scheme of uracil and cytosine. Theoretica Chimica Acta, 1978, 48, 29-36.	0.8	123
102	Hydration scheme of the complementary base-pairs of DNA. FEBS Letters, 1978, 91, 213-215.	2.8	42
103	Cation-binding to biomolecules. Theoretica Chimica Acta, 1977, 43, 207-214.	0.8	53
104	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
105	Cation-binding to biomolecules. Theoretica Chimica Acta, 1976, 42, 23-31.	0.8	40
106	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
107	Molecular orbital calculations on the conformation of nucleic acids and their constituents. Nucleic Acids and Protein Synthesis, 1974, 349, 189-203.	1.7	17
108	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.	1.7	23

#	Article	IF	Citations
109	Molecular orbital calculations on the conformation of nucleic acids and their constituents. Nucleic Acids and Protein Synthesis, 1974, 340, 299-313.	1.7	51
110	Molecular orbital calculations on the conformation of nucleic acids and their constituents. Theoretica Chimica Acta, 1973, 30, 31-44.	0.8	77
111	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
112	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
113	Molecular orbital studies on the conformation of the terminal aminoacyladenosine moieties of tRNA. FEBS Letters, 1972, 23, 332-336.	2.8	2
114	Molecular orbital calculations on the conformation of nucleic acids and their constituents. Nucleic Acids and Protein Synthesis, 1972, 269, 1-14.	1.7	70
115	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
116	A Molecular Orbital probe into the conformation of ATP. Biochemical and Biophysical Research Communications, 1972, 47, 1284-1289.	2.1	15
117	The conformational energy map for the disulphide bridge in proteins. Biochemical and Biophysical Research Communications, 1971, 43, 65-68.	2.1	19
118	Molecular orbital calculations on the conformation of polypeptides and proteins. Theoretica Chimica Acta, 1971, 22, 11-22.	0.8	8
119	Molecular orbital calculations on the conformation of polypeptides and proteins. Journal of Theoretical Biology, 1971, 31, 269-285.	1.7	43
120	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
121	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
122	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
123	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
124	Molecular orbital calculations on the conformation of polypeptides and proteins. Theoretica Chimica Acta, 1970, 18, 44-56.	0.8	44
125	Molecular orbital calculations on the conformation of polypeptides and proteins. Theoretica Chimica Acta, 1970, 19, 121-134.	0.8	17
126	Editorial: Integrative Structural Biology of Proteins and Macromolecular Assemblies: Bridging Experiments and Simulations. Frontiers in Molecular Biosciences, 0, 9, .	3.5	0