JiÅÃ- ÄŒernÃ½

List of Publications by Year
in descending order

88 papers	5,464 citations	172207 29 h-index	79541 73 g-index
91 all docs	91 docs citations	91 times ranked	6337 citing authors

#	Article	IF	Citations
1	Benchmark database of accurate (MP2 and CCSD(T) complete basis set limit) interaction energies of small model complexes, DNA base pairs, and amino acid pairs. Physical Chemistry Chemical Physics, 2006, 8, 1985-1993.	1.3	1,635
2	Density functional theory augmented with an empirical dispersion term. Interaction energies and geometries of 80 noncovalent complexes compared withab initioquantum mechanics calculations. Journal of Computational Chemistry, 2007, 28, 555-569.	1.5	620
3	Non-covalent interactions in biomacromolecules. Physical Chemistry Chemical Physics, 2007, 9, 5291.	1.3	391
4	Scaled MP3 Nonâ€Covalent Interaction Energies Agree Closely with Accurate CCSD(T) Benchmark Data. ChemPhysChem, 2009, 10, 282-289.	1.0	232
5	Structure, Function, and Pharmacology of NMDA Receptor Channels. Physiological Research, 2014, 63, S191-S203.	0.4	216
6	On the Structure and Geometry of Biomolecular Binding Motifs (Hydrogen-Bonding, Stacking, Xâˆ'HÂ·Â·Â·Ï€): WFT and DFT Calculations. Journal of Chemical Theory and Computation, 2010, 6, 66-80.	2.3	175
7	Mitochondrial Targeting of Vitamin E Succinate Enhances Its Pro-apoptotic and Anti-cancer Activity via Mitochondrial Complex II. Journal of Biological Chemistry, 2011, 286, 3717-3728.	1.6	171
8	Quantum Chemical Benchmark Energy and Geometry Database for Molecular Clusters and Complex Molecular Systems (www.begdb.com): A Users Manual and Examples. Collection of Czechoslovak Chemical Communications, 2008, 73, 1261-1270.	1.0	144
9	The X3LYP extended density functional accurately describes H-bonding but fails completely for stacking. Physical Chemistry Chemical Physics, 2005, 7, 1624-1626.	1.3	141
10	Toward Designed Singlet Fission: Electronic States and Photophysics of 1,3-Diphenylisobenzofuran. Journal of Physical Chemistry A, 2010, 114, 1457-1473.	1.1	98
11	Selective Disruption of Respiratory Supercomplexes as a New Strategy to Suppress Her2^{high} Breast Cancer. Antioxidants and Redox Signaling, 2017, 26, 84-103.	2.5	93
12	Double-Helical â†' Ladder Structural Transition in the B-DNA is Induced by a Loss of Dispersion Energy. Journal of the American Chemical Society, 2008, 130, 16055-16059.	6.6	81
13	Protein flexibility in the light of structural alphabets. Frontiers in Molecular Biosciences, 2015, 2, 20.	1.6	71
14	Resolution of Identity Density Functional Theory Augmented with an Empirical Dispersion Term (RI-DFT-D):Â A Promising Tool for Studying Isolated Small Peptides. Journal of Physical Chemistry A, 2007, 111, 1146-1154.	1.1	66
15	Mitochondrial Targeting of Metformin Enhances Its Activity against Pancreatic Cancer. Molecular Cancer Therapeutics, 2016, 15, 2875-2886.	1.9	65
16	Bordetella adenylate cyclase toxin is a unique ligand of the integrin complement receptor 3. ELife, 2015, 4, e10766.	2.8	65
17	Block of NMDA receptor channels by endogenous neurosteroids: implications for the agonist induced conformational states of the channel vestibule. Scientific Reports, 2015, 5, 10935.	1.6	52
18	Bioinformatic analysis of the protein/DNA interface. Nucleic Acids Research, 2014, 42, 3381-3394.	6.5	51

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19	Ubiquinone-binding site mutagenesis reveals the role of mitochondrial complex II in cell death initiation. Cell Death and Disease, 2015, 6, e1749-e1749.	2.7	47
20	The Amino Group in Adenine: MP2 and CCSD(T) Complete Basis Set Limit Calculations of the Planarization Barrier and DFT/B3LYP Study of the Anharmonic Frequencies of Adenine. Journal of Physical Chemistry B, 2008, 112, 16734-16740.	1.2	46
21	Preferential Inhibition of Tonically over Phasically Activated NMDA Receptors by Pregnane Derivatives. Journal of Neuroscience, 2016, 36, 2161-2175.	1.7	44
22	Surface Expression, Function, and Pharmacology of Disease-Associated Mutations in the Membrane Domain of the Human GluN2B Subunit. Frontiers in Molecular Neuroscience, 2018, 11, 110.	1.4	41
23	Thermodynamic Penalty Arising from Burial of a Ligand Polar Group Within a Hydrophobic Pocket of a Protein Receptor. Journal of Molecular Biology, 2006, 362, 994-1003.	2.0	39
24	Local dynamics of proteins and DNA evaluated from crystallographicBfactors. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2413-2419.	2.5	38
25	Rigid Duplex Î±-Cyclodextrin Reversibly Connected With Disulfide Bonds. Synthesis and Inclusion Complexes. Journal of Organic Chemistry, 2009, 74, 1082-1092.	1.7	36
26	State of the art theoretical study and comparison to experiment for the phenolâ¯argon complex. Journal of Chemical Physics, 2008, 128, 114319.	1.2	33
27	Human interleukinâ€23 receptor antagonists derived from an albuminâ€binding domain scaffold inhibit ILâ€23â€dependent ex vivo expansion of ILâ€17â€producing Tâ€cells. Proteins: Structure, Function and Bioinformatics, 2014, 82, 975-989.	1.5	31
28	Theoretical study of the ground and excited states of 7-methyl guanine and 9-methyl guanine: comparison with experiment. Physical Chemistry Chemical Physics, 2006, 8, 3059-3065.	1.3	30
29	Chemical Cross-Linking and H/D Exchange for Fast Refinement of Protein Crystal Structure. Analytical Chemistry, 2012, 84, 867-870.	3.2	30
30	Novel highâ€affinity binders of human interferon gamma derived from albuminâ€binding domain of protein G. Proteins: Structure, Function and Bioinformatics, 2012, 80, 774-789.	1.5	30
31	A unified dinucleotide alphabet describing both RNA and DNA structures. Nucleic Acids Research, 2020, 48, 6367-6381.	6.5	30
32	A Novel Anti-CD 18 mAb Recognizes an Activation-Related Epitope and Induces a High-Affinity Conformation in Leukocyte Integrins. Immunobiology, 2001, 203, 687-698.	0.8	29
33	Dispersion Interactions Govern the Strong Thermal Stability of a Protein. Chemistry - A European Journal, 2007, 13, 9022-9027.	1.7	29
34	Density-Functional, Density-Functional Tight-Binding, and Wave Function Calculations on Biomolecular Systemsâ€. Journal of Physical Chemistry A, 2007, 111, 5642-5647.	1.1	27
35	Competition between stacking and hydrogen bonding: theoretical study of the phenolâ¯Ar cation and neutral complex and comparison to experiment. Physical Chemistry Chemical Physics, 2008, 10, 2780.	1.3	26
36	CD9 and CD81 Interactions and Their Structural Modelling in Sperm Prior to Fertilization. International Journal of Molecular Sciences, 2018, 19, 1236.	1.8	26

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37	The LILI Motif of M3-S2 Linkers Is a Component of the NMDA Receptor Channel Gate. Frontiers in Molecular Neuroscience, 2018, 11, 113.	1.4	25
38	Complete Basis Set Extrapolation and Hybrid Schemes for Geometry Gradients of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2011, 7, 3924-3934.	2.3	24
39	A DNA structural alphabet provides new insight into DNA flexibility. Acta Crystallographica Section D: Structural Biology, 2018, 74, 52-64.	1.1	23
40	Loss of Dispersion Energy Changes the Stability and Folding/Unfolding Equilibrium of the Trp-Cage Protein. Journal of Physical Chemistry B, 2009, 113, 5657-5660.	1.2	21
41	Germline SUCLG2 Variants in Patients With Pheochromocytoma and Paraganglioma. Journal of the National Cancer Institute, 2022, 114, 130-138.	3.0	21
42	Design of composite inhibitors targeting glutamate carboxypeptidase <scp>II</scp>: the importance of effector functionalities. FEBS Journal, 2016, 283, 130-143.	2.2	20
43	p19-targeted ABD-derived protein variants inhibit IL-23 binding and exert suppressive control over IL-23-stimulated expansion of primary human IL-17+ T-cells. Autoimmunity, 2017, 50, 102-113.	1.2	20
44	Engineered Lactococcus lactis Secreting IL-23 Receptor-Targeted REX Protein Blockers for Modulation of IL-23/Th17-Mediated Inflammation. Microorganisms, 2019, 7, 152.	1.6	20
45	Site of Action of Brain Neurosteroid Pregnenolone Sulfate at the N-Methyl-D-Aspartate Receptor. Journal of Neuroscience, 2020, 40, 5922-5936.	1.7	18
46	Automatic workflow for the classification of local DNA conformations. BMC Bioinformatics, 2013, 14, 205.	1.2	17
47	p19-Targeting ILP Protein Blockers of IL-23/Th-17 Pro-Inflammatory Axis Displayed on Engineered Bacteria of Food Origin. International Journal of Molecular Sciences, 2018, 19, 1933.	1.8	16
48	NMDA Receptor Opening and Closingâ€"Transitions of a Molecular Machine Revealed by Molecular Dynamics. Biomolecules, 2019, 9, 546.	1.8	15
49	Effect of Noncovalent Interactions on Conformers of the n-Butylbenzene Monomer Studied by Mass Analyzed Threshold Ionization Spectroscopy and Basis-set Convergent ab initio Computations. Journal of Physical Chemistry A, 2008, 112, 5866-5871.	1.1	14
50	Structural characterization of P1â€²-diversified urea-based inhibitors of glutamate carboxypeptidase II. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 2340-2345.	1.0	14
51	Addressing the Compartmentalization of Specific Integrin Heterodimers in Mouse Sperm. International Journal of Molecular Sciences, 2019, 20, 1004.	1.8	13
52	Structural alphabets for conformational analysis of nucleic acids available at dnatco.datmos.org. Acta Crystallographica Section D: Structural Biology, 2020, 76, 805-813.	1.1	13
53	Increasing Affinity of Interferon-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="M1"><mml:mrow><mml:mi mathvariant="bold">Î³</mml:mi></mml:mrow></mml:math>Receptor 1 to Interferon-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="M2"><mml:mrow><mml:mi mathvariant="bold">Î³</mml:mi></mml:mrow></mml:math>by Computer-Aided Design. BioMed Research International, 2013, 2013, 1-12.	0.9	12
54	Crystal structure of human interferon-Î³ receptor 2 reveals the structural basis for receptor specificity. Acta Crystallographica Section D: Structural Biology, 2016, 72, 1017-1025.	1.1	12

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55	DNATCO: assignment of DNA conformers at dnatco.org. Nucleic Acids Research, 2016, 44, W284-W287.	6.5	12
56	Palmitoylation Controls NMDA Receptor Function and Steroid Sensitivity. Journal of Neuroscience, 2021, 41, 2119-2134.	1.7	12
57	Study of the Origin of the Hindered Rotation of an Aryl Ring in Chromium Aminocarbene Complexes Bearing an Aromatic Ring Attached to the Carbene Carbon Atom. Organometallics, 2006, 25, 5540-5548.	1.1	11
58	Cationâ€“Ï€ complexes between alkali metal cation andpara-halogenophenols. Structures, binding energies and thermodynamic properties: DFT study and CCSD(T) complete basis set limit calculations. Molecular Physics, 2006, 104, 2317-2325.	0.8	10
59	Spectral shifts and structures of phenolâ‹¯Arn clusters. Physical Chemistry Chemical Physics, 2011, 13, 6077.	1.3	9
60	Affinity of vitamin E analogues for the ubiquinone complex II site correlates with their toxicity to cancer cells. Molecular Nutrition and Food Research, 2011, 55, 1543-1551.	1.5	9
61	A DNA Structural Alphabet Distinguishes Structural Features of DNA Bound to Regulatory Proteins and in the Nucleosome Core Particle. Genes, 2017, 8, 278.	1.0	9
62	ABD-Derived Protein Blockers of Human IL-17 Receptor A as Non-IgG Alternatives for Modulation of IL-17-Dependent Pro-Inflammatory Axis. International Journal of Molecular Sciences, 2018, 19, 3089.	1.8	9
63	Expression and distribution of CD151 as a partner of alpha6 integrin in male germ cells. Scientific Reports, 2020, 10, 4374.	1.6	9
64	WatAA: Atlas of Protein Hydration. Exploring synergies between data mining and ab initio calculations. Physical Chemistry Chemical Physics, 2017, 19, 17094-17102.	1.3	8
65	Protein Binder (ProBi) as a New Class of Structurally Robust Non-Antibody Protein Scaffold for Directed Evolution. Viruses, 2021, 13, 190.	1.5	7
66	Reprogramming of leukemic cell metabolism through the naphthoquinonic compound Quambalarine B. Oncotarget, 2017, 8, 103137-103153.	0.8	6
67	Proteins mimicking epitope of HIV-1 virus neutralizing antibody induce virus-neutralizing sera in mice. EBioMedicine, 2019, 47, 247-256.	2.7	6
68	Pregnaneâ€based steroids are novel positive NMDA receptor modulators that may compensate for the effect of lossâ€ofâ€function diseaseâ€associated GRIN mutations. British Journal of Pharmacology, 2022, 179, 3970-3990.	2.7	6
69	Energy barriers between H-bonded and stacked structures of 9-methyladenineâ‹¯1-methylthymine and 9-methylguanineâ‹¯1-methylcytosine complexes. Chemical Communications, 2010, 46, 383-385.	2.2	5
70	Redesigning Protein Cavities as a Strategy for Increasing Affinity in Protein-Protein Interaction: Interferon-Î³Receptor 1 as a Model. BioMed Research International, 2015, 2015, 1-12.	0.9	5
71	A Hybrid Hamiltonian for the Accelerated Sampling along Experimental Restraints. International Journal of Molecular Sciences, 2019, 20, 370.	1.8	5
72	Molecular dynamics simulations provide structural insight into binding of cyclic dinucleotides to human STING protein. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10250-10264.	2.0	5

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73	The crystal structure of XdpB, the bacterial old yellow enzyme, in an FMN-free form. PLoS ONE, 2018, 13, e0195299.	1.1	4
74	Retro operation on the Trp-cage miniprotein sequence produces an unstructured molecule capable of folding similar to the original only upon 2,2,2-trifluoroethanol addition. Protein Engineering, Design and Selection, 2014, 27, 463-472.	1.0	3
75	Enriched Conformational Sampling of DNA and Proteins with a Hybrid Hamiltonian Derived from the Protein Data Bank. International Journal of Molecular Sciences, 2018, 19, 3405.	1.8	3
76	Effect of Noncovalent Interactions on the n-ButylbenzeneÂ·Â·Â·Ar Cluster Studied by Mass Analyzed Threshold Ionization Spectroscopy and ab initio Computations. Journal of Physical Chemistry A, 2008, 112, 5872-5877.	1.1	2
77	Motif orientation matters: Structural characterization of TEAD1 recognition of genomic DNA. Structure, 2021, 29, 345-356.e8.	1.6	2
78	Myomedin scaffold variants targeted to 10E8 HIV-1 broadly neutralizing antibody mimic gp41 epitope and elicit HIV-1 virus-neutralizing sera in mice. Virulence, 2021, 12, 1271-1287.	1.8	2
79	Local dynamics of proteins and DNA evaluated from crystallographic B-factors. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1513-C1513.	0.0	2
80	Structural variability of CG-rich DNA 18-mers accommodating double Tâ€“T mismatches. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1233-1243.	1.1	2
81	Threshold ionization spectroscopic investigation of supersonic jet-cooled, laser-desorbed Tryptophan. Chemical Physics Letters, 2016, 657, 142-147.	1.2	1
82	Evidence for the Association between the Intronic Haplotypes of Ionotropic Glutamate Receptors and First-Episode Schizophrenia. Journal of Personalized Medicine, 2021, 11, 1250.	1.1	1
83	How to fragment a polypeptide? An ab initio computational study of pair interactions between amino acids and ligand-amino acids in proteins. Collection of Czechoslovak Chemical Communications, 2011, 76, 605-618.	1.0	0
84	Design and Testing of High-Affinity Mutants of Interferon Gamma Receptor 1. Biophysical Journal, 2013, 104, 558a.	0.2	0
85	Function, Expression, and Pharmacology of Disease-Associated Mutations of NMDA Receptors. Biophysical Journal, 2018, 114, 309a.	0.2	0
86	Novel Germline SUCLG2 Mutations in Patients With Pheochromocytoma and Paraganglioma. Journal of the Endocrine Society, 2021, 5, A168-A169.	0.1	0
87	DNA structural alphabet opens ways to understand proteinâ€“DNA interactions. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C450-C450.	0.0	0
88	Structural alphabets for conformational analysis of nucleic acids. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e102-e102.	0.0	0