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	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
2	Germline SUCLG2 Variants in Patients With Pheochromocytoma and Paraganglioma. Journal of the National Cancer Institute, 2022, 114, 130-138.	3.0	21
3	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
4	Motif orientation matters: Structural characterization of TEAD1 recognition of genomic DNA. Structure, 2021, 29, 345-356.e8.	1.6	2
5	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
6	Palmitoylation Controls NMDA Receptor Function and Steroid Sensitivity. Journal of Neuroscience, 2021, 41, 2119-2134.	1.7	12
7	Novel Germline SUCLG2 Mutations in Patients With Pheochromocytoma and Paraganglioma. Journal of the Endocrine Society, 2021, 5, A168-A169.	0.1	0
8	Protein Binder (ProBi) as a New Class of Structurally Robust Non-Antibody Protein Scaffold for Directed Evolution. Viruses, 2021, 13, 190.	1.5	7
9	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
10	A unified dinucleotide alphabet describing both RNA and DNA structures. Nucleic Acids Research, 2020, 48, 6367-6381.	6.5	30
11	Expression and distribution of CD151 as a partner of alpha6 integrin in male germ cells. Scientific Reports, 2020, 10, 4374.	1.6	9
12	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
13	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
14	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
15	NMDA Receptor Opening and Closingâ€”Transitions of a Molecular Machine Revealed by Molecular Dynamics. Biomolecules, 2019, 9, 546.	1.8	15
16	Proteins mimicking epitope of HIV-1 virus neutralizing antibody induce virus-neutralizing sera in mice. EBioMedicine, 2019, 47, 247-256.	2.7	6
17	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
18	Addressing the Compartmentalization of Specific Integrin Heterodimers in Mouse Sperm. International Journal of Molecular Sciences, 2019, 20, 1004.	1.8	13

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19	A Hybrid Hamiltonian for the Accelerated Sampling along Experimental Restraints. International Journal of Molecular Sciences, 2019, 20, 370.	1.8	5
20	Structural alphabets for conformational analysis of nucleic acids. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e102-e102.	0.0	0
21	Function, Expression, and Pharmacology of Disease-Associated Mutations of NMDA Receptors. Biophysical Journal, 2018, 114, 309a.	0.2	0
22	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
23	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
24	The crystal structure of XdpB, the bacterial old yellow enzyme, in an FMN-free form. PLoS ONE, 2018, 13, e0195299.	1.1	4
25	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
26	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
27	CD9 and CD81 Interactions and Their Structural Modelling in Sperm Prior to Fertilization. International Journal of Molecular Sciences, 2018, 19, 1236.	1.8	26
28	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
29	A DNA structural alphabet provides new insight into DNA flexibility. Acta Crystallographica Section D: Structural Biology, 2018, 74, 52-64.	1.1	23
30	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
31	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
32	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
33	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
34	Reprogramming of leukemic cell metabolism through the naphthoquinonic compound Quambalarine B. Oncotarget, 2017, 8, 103137-103153.	0.8	6
35	DNA structural alphabet opens ways to understand proteinâ€“DNA interactions. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C450-C450.	0.0	0
36	Mitochondrial Targeting of Metformin Enhances Its Activity against Pancreatic Cancer. Molecular Cancer Therapeutics, 2016, 15, 2875-2886.	1.9	65

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37	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
38	Threshold ionization spectroscopic investigation of supersonic jet-cooled, laser-desorbed Tryptophan. Chemical Physics Letters, 2016, 657, 142-147.	1.2	1
39	DNATCO: assignment of DNA conformers at dnatco.org. Nucleic Acids Research, 2016, 44, W284-W287.	6.5	12
40	Design of composite inhibitors targeting glutamate carboxypeptidase <scp>II</scp>: the importance of effector functionalities. FEBS Journal, 2016, 283, 130-143.	2.2	20
41	Preferential Inhibition of Tonically over Phasically Activated NMDA Receptors by Pregnane Derivatives. Journal of Neuroscience, 2016, 36, 2161-2175.	1.7	44
42	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
43	Protein flexibility in the light of structural alphabets. Frontiers in Molecular Biosciences, 2015, 2, 20.	1.6	71
44	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
45	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
46	Bordetella adenylate cyclase toxin is a unique ligand of the integrin complement receptor 3. ELife, 2015, 4, e10766.	2.8	65
47	Bioinformatic analysis of the protein/DNA interface. Nucleic Acids Research, 2014, 42, 3381-3394.	6.5	51
48	Local dynamics of proteins and DNA evaluated from crystallographicBfactors. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2413-2419.	2.5	38
49	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
50	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
51	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
52	Structure, Function, and Pharmacology of NMDA Receptor Channels. Physiological Research, 2014, 63, S191-S203.	0.4	216
53	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
54	Automatic workflow for the classification of local DNA conformations. BMC Bioinformatics, 2013, 14, 205.	1.2	17

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55	Design and Testing of High-Affinity Mutants of Interferon Gamma Receptor 1. Biophysical Journal, 2013, 104, 558a.	0.2	0
56	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
57	Chemical Cross-Linking and H/D Exchange for Fast Refinement of Protein Crystal Structure. Analytical Chemistry, 2012, 84, 867-870.	3.2	30
58	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
59	Spectral shifts and structures of phenolâ‹¯Arn clusters. Physical Chemistry Chemical Physics, 2011, 13, 6077.	1.3	9
60	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
61	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
62	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
63	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
64	On the Structure and Geometry of Biomolecular Binding Motifs (Hydrogen-Bonding, Stacking, Xâ‹¯HÂ·Â·Â·Ï€): WFT and DFT Calculations. Journal of Chemical Theory and Computation, 2010, 6, 66-80.	2.3	175
65	Toward Designed Singlet Fission: Electronic States and Photophysics of 1,3-Diphenylisobenzofuran. Journal of Physical Chemistry A, 2010, 114, 1457-1473.	1.1	98
66	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
67	Scaled MP3 Nonâ€Covalent Interaction Energies Agree Closely with Accurate CCSD(T) Benchmark Data. ChemPhysChem, 2009, 10, 282-289.	1.0	232
68	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
69	Rigid Duplex Î±-Cyclodextrin Reversibly Connected With Disulfide Bonds. Synthesis and Inclusion Complexes. Journal of Organic Chemistry, 2009, 74, 1082-1092.	1.7	36
70	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
71	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
72	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

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73	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
74	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
75	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
76	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
77	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
78	Non-covalent interactions in biomacromolecules. Physical Chemistry Chemical Physics, 2007, 9, 5291.	1.3	391
79	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
80	Dispersion Interactions Govern the Strong Thermal Stability of a Protein. Chemistry - A European Journal, 2007, 13, 9022-9027.	1.7	29
81	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
82	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
83	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
84	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
85	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
86	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
87	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
88	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