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List of Publications by Year
in descending order

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53 papers	2,848 citations	279798 23 h-index	197818 49 g-index
54 all docs	54 docs citations	54 times ranked	2720 citing authors

#	Article	IF	Citations
1	Cepharanthine Blocks the Presentation of Thyroid & Islet Peptides in a Novel Humanized Autoimmune Polyglandular Syndrome Type 3 Variant (APS3v) Mouse Model. Journal of the Endocrine Society, 2021, 5, A874-A875.	0.2	0
2	Cepharanthine Blocks Presentation of Thyroid and Islet Peptides in a Novel Humanized Autoimmune Diabetes and Thyroiditis Mouse Model. Frontiers in Immunology, 2021, 12, 796552.	4.8	5
3	In silico design and molecular basis for the selectivity of Olinone toward the first over the second bromodomain of BRD4. Proteins: Structure, Function and Bioinformatics, 2020, 88, 414-430.	2.6	16
4	Retro-inverso D-peptides as a novel targeted immunotherapy for Type 1 diabetes. Journal of Autoimmunity, 2020, 115, 102543.	6.5	10
5	Cepharanthine blocks TSH receptor peptide presentation by HLA-DR3: Therapeutic implications to Gravesâ€™ disease. Journal of Autoimmunity, 2020, 108, 102402.	6.5	12
6	Unwinding of the Substrate Transmembrane Helix inÂIntramembrane Proteolysis. Biophysical Journal, 2018, 114, 1579-1589.	0.5	20
7	Flexible peptide recognition by HLA-DR triggers specific autoimmune T-cell responses in autoimmune thyroiditis and diabetes. Journal of Autoimmunity, 2017, 76, 1-9.	6.5	27
8	The role of protein â€œStability patchesâ€•in molecular recognition: A case study of the human growth hormoneâ€•receptor complex. Journal of Computational Chemistry, 2016, 37, 913-919.	3.3	3
9	Identifying a Small Molecule Blocking Antigen Presentation in Autoimmune Thyroiditis. Journal of Biological Chemistry, 2016, 291, 4079-4090.	3.4	23
10	Structures of Two Melanoma-Associated Antigens Suggest Allosteric Regulation of Effector Binding. PLoS ONE, 2016, 11, e0148762.	2.5	26
11	Characterization of the Binding Site of Aspartame in the Human Sweet Taste Receptor. Chemical Senses, 2015, 40, 577-586.	2.0	64
12	Î¼ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. Nucleic Acids Research, 2014, 42, 12272-12283.	14.5	186
13	Thermodynamic basis of selectivity in guideâ€•targetâ€•mismatched rna interference. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1283-1298.	2.6	6
14	Shared molecular amino acid signature in the HLA-DR peptide binding pocket predisposes to both autoimmune diabetes and thyroiditis. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 16899-16903.	7.1	63
15	A systematic molecular dynamics study of nearest-neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA. Nucleic Acids Research, 2010, 38, 299-313.	14.5	349
16	Tg.2098 is a major human thyroglobulin T-cell epitope. Journal of Autoimmunity, 2010, 35, 45-51.	6.5	21
17	Employing a Recombinant HLA-DR3 Expression System to Dissect Major Histocompatibility Complex II-Thyroglobulin Peptide Dynamism. Journal of Biological Chemistry, 2009, 284, 34231-34243.	3.4	30
18	Molecular amino acid signatures in the MHC class II peptide-binding pocket predispose to autoimmune thyroiditis in humans and in mice. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 14034-14039.	7.1	89

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19	Molecular Models of Sweet Taste Receptors Provide Insights into Function. ACS Symposium Series, 2008, , 117-132.	0.5	3
20	Making Sense of the Sweet Taste Receptor. ACS Symposium Series, 2008, , 48-64.	0.5	1
21	Calculation of the Free Energy and Cooperativity of Protein Folding. PLoS ONE, 2007, 2, e446.	2.5	25
22	The Heterodimeric Sweet Taste Receptor has Multiple Potential Ligand Binding Sites. Current Pharmaceutical Design, 2006, 12, 4591-4600.	1.9	155
23	Origin of the sequence-dependent polyproline II structure in unfolded peptides. Proteins: Structure, Function and Bioinformatics, 2005, 61, 769-776.	2.6	15
24	Lactisole Interacts with the Transmembrane Domains of Human T1R3 to Inhibit Sweet Taste. Journal of Biological Chemistry, 2005, 280, 15238-15246.	3.4	262
25	Identification of the Cyclamate Interaction Site within the Transmembrane Domain of the Human Sweet Taste Receptor Subunit T1R3. Journal of Biological Chemistry, 2005, 280, 34296-34305.	3.4	191
26	Agonist-Induced Conformational Changes in Thyrotropin-Releasing Hormone Receptor Type I:Â Disulfide Cross-Linking and Molecular Modeling Approaches. Biochemistry, 2005, 44, 2419-2431.	2.5	22
27	Molecular Dynamics Simulations of the 136 Unique Tetranucleotide Sequences of DNA Oligonucleotides. II: Sequence Context Effects on the Dynamical Structures of the 10 Unique Dinucleotide Steps. Biophysical Journal, 2005, 89, 3721-3740.	0.5	216
28	A Model of Inverse Agonist Action at Thyrotropin-Releasing Hormone Receptor Type 1: Role of a Conserved Tryptophan in Helix 6. Molecular Pharmacology, 2004, 66, 1192-1200.	2.3	16
29	Unfolded state of polyalanine is a segmented polyproline II helix. Proteins: Structure, Function and Bioinformatics, 2004, 55, 493-501.	2.6	94
30	Molecular Dynamics Simulations of the 136 Unique Tetranucleotide Sequences of DNA Oligonucleotides. I. Research Design and Results on d(CpG) Steps. Biophysical Journal, 2004, 87, 3799-3813.	0.5	245
31	MC-PHS: A Monte Carlo Implementation of the Primary Hydration Shell for Protein Folding and Design. Biophysical Journal, 2003, 84, 805-815.	0.5	21
32	Quantum mechanical investigation of the electronic structure and spectral properties of 6,8-dimethylisoxanthopterin. International Journal of Quantum Chemistry, 2002, 88, 28-33.	2.0	3
33	Probing the General Base Catalysis in the First Step ofBamHI Action by Computer Simulationsâ€. Biochemistry, 2001, 40, 15017-15023.	2.5	20
34	CASSCF Investigation of Electronic Excited States of 2-Aminopurine. Journal of Physical Chemistry A, 2001, 105, 190-197.	2.5	35
35	Minireview: Insights into G Protein-Coupled Receptor Function Using Molecular Models. Endocrinology, 2001, 142, 2-10.	2.8	46
36	Application of the Primary Hydration Shell Approach to Locally Enhanced Sampling Simulated Annealing: Computer Simulation of Thyrotropin-Releasing Hormone in Water. Biophysical Journal, 2000, 79, 66-79.	0.5	8

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37	Theoretical Studies of Ribose and Its Radicals Produced by Hydrogen Abstraction from Ring Carbons. Journal of Physical Chemistry A, 1999, 103, 592-600.	2.5	20
38	Essential dynamics of DNA containing a cis.syn cyclobutane thymine dimer lesion. Nucleic Acids Research, 1998, 26, 1939-1946.	14.5	69
39	A Hydrophobic Cluster between Transmembrane Helices 5 and 6 Constrains the Thyrotropin-Releasing Hormone Receptor in an Inactive Conformation. Molecular Pharmacology, 1998, 54, 968-978.	2.3	43
40	Modeling Duplex DNA Oligonucleotides with Modified Pyrimidine Bases. ACS Symposium Series, 1997, , 312-328.	0.5	0
41	Theoretical Studies of Hydrogen Abstraction from 2-Propanol by OH Radical. Journal of Physical Chemistry A, 1997, 101, 926-936.	2.5	24
42	Gas Phase Absorption Spectrum and Cross Sections of Vinylperoxy (C2H3O2) Radical. Journal of Physical Chemistry A, 1997, 101, 4879-4886.	2.5	12
43	Role of the Extracellular Loops of the Thyrotropin-Releasing Hormone Receptor:Â Evidence for an Initial Interaction with Thyrotropin-Releasing Hormoneâ€. Biochemistry, 1997, 36, 15670-15676.	2.5	45
44	A Refined Model of the Thyrotropin-Releasing Hormone (TRH) Receptor Binding Pocket. Experimental Analysis and Energy Minimization of the Complex between TRH and TRH Receptor. Biochemistry, 1996, 35, 7643-7650.	2.5	45
45	Simulations of Molecular Mechanisms in Radiation Damage to DNA. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1995, , 349-363.	0.2	0
46	Theoretical study on the deoxyribose radicals formed by hydrogen abstraction. Journal of the American Chemical Society, 1994, 116, 232-238.	13.7	130
47	Effect of Local Environment and Protein on the Mechanism of Action of Superoxide Dismutase. Enzyme, 1986, 36, 32-43.	0.7	8
48	Molecular structure of the hydroperoxyl anion (HOâ^'2). Journal of Chemical Physics, 1984, 80, 5684-5686.	3.0	16
49	On the mechanism of action of superoxide dismutase: a theoretical study. Journal of the American Chemical Society, 1984, 106, 5710-5714.	13.7	77
50	On the use of minimal valence basis sets with the coreless Hartreeâ€“Fock effective potential. Journal of Chemical Physics, 1980, 73, 5191-5196.	3.0	18
51	Models for Active Sites of Metalloenzymes: Comparison of Zinc and Beryllium Containing Complexes. Israel Journal of Chemistry, 1980, 19, 149-153.	2.3	11
52	Theoretical models for molecular mechanisms in biological systems: Tryptamine congeners acting on an LSD-Serotonin receptor. International Journal of Quantum Chemistry, 1978, 14, 449-461.	2.0	0
53	Models for molecular mechanisms in drug-receptor interactions. Serotonin and 5-hydroxyindole complexes with imidazolium cation. International Journal of Quantum Chemistry, 1977, 12, 253-268.	2.0	2