Roman Osman

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/11414200/publications.pdf

Version: 2024-02-01

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	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
2	Lactisole Interacts with the Transmembrane Domains of Human T1R3 to Inhibit Sweet Taste. Journal of Biological Chemistry, 2005, 280, 15238-15246.	3.4	262
3	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
4	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
5	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
6	Î¼ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. Nucleic Acids Research, 2014, 42, 12272-12283.	14.5	186
7	The Heterodimeric Sweet Taste Receptor has Multiple Potential Ligand Binding Sites. Current Pharmaceutical Design, 2006, 12, 4591-4600.	1.9	155
8	Theoretical study on the deoxyribose radicals formed by hydrogen abstraction. Journal of the American Chemical Society, 1994, 116, 232-238.	13.7	130
9	Unfolded state of polyalanine is a segmented polyproline II helix. Proteins: Structure, Function and Bioinformatics, 2004, 55, 493-501.	2.6	94
10	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
11	On the mechanism of action of superoxide dismutase: a theoretical study. Journal of the American Chemical Society, 1984, 106, 5710-5714.	13.7	77
12	Essential dynamics of DNA containing a cis.syn cyclobutane thymine dimer lesion. Nucleic Acids Research, 1998, 26, 1939-1946.	14.5	69
13	Characterization of the Binding Site of Aspartame in the Human Sweet Taste Receptor. Chemical Senses, 2015, 40, 577-586.	2.0	64
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	Minireview: Insights into G Protein-Coupled Receptor Function Using Molecular Models. Endocrinology, 2001, 142, 2-10.	2.8	46
16	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
17	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
18	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

#	Article	IF	Citations
19	CASSCF Investigation of Electronic Excited States of 2-Aminopurine. Journal of Physical Chemistry A, 2001, 105, 190-197.	2.5	35
20	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
21	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
22	Structures of Two Melanoma-Associated Antigens Suggest Allosteric Regulation of Effector Binding. PLoS ONE, 2016, 11, e0148762.	2.5	26
23	Calculation of the Free Energy and Cooperativity of Protein Folding. PLoS ONE, 2007, 2, e446.	2.5	25
24	Theoretical Studies of Hydrogen Abstraction from 2-Propanol by OH Radical. Journal of Physical Chemistry A, 1997, 101, 926-936.	2.5	24
25	Identifying a Small Molecule Blocking Antigen Presentation in Autoimmune Thyroiditis. Journal of Biological Chemistry, 2016, 291, 4079-4090.	3.4	23
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	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
28	Tg.2098 is a major human thyroglobulin T-cell epitope. Journal of Autoimmunity, 2010, 35, 45-51.	6.5	21
29	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
30	Probing the General Base Catalysis in the First Step ofBamHI Action by Computer Simulationsâ€. Biochemistry, 2001, 40, 15017-15023.	2.5	20
31	Unwinding of the Substrate Transmembrane Helix inÂIntramembrane Proteolysis. Biophysical Journal, 2018, 114, 1579-1589.	0.5	20
32	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
33	Molecular structure of the hydroperoxyl anion (HOâ^'2). Journal of Chemical Physics, 1984, 80, 5684-5686.	3.0	16
34	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
35	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
36	Origin of the sequence-dependent polyproline II structure in unfolded peptides. Proteins: Structure, Function and Bioinformatics, 2005, 61, 769-776.	2.6	15

#	Article	IF	Citations
37	Gas Phase Absorption Spectrum and Cross Sections of Vinylperoxy (C2H3O2) Radical. Journal of Physical Chemistry A, 1997, 101, 4879-4886.	2.5	12
38	Cepharanthine blocks TSH receptor peptide presentation by HLA-DR3: Therapeutic implications to Gravesâ€™ disease. Journal of Autoimmunity, 2020, 108, 102402.	6.5	12
39	Models for Active Sites of Metalloenzymes: Comparison of Zinc and Beryllium Containing Complexes. Israel Journal of Chemistry, 1980, 19, 149-153.	2.3	11
40	Retro-inverso D-peptides as a novel targeted immunotherapy for Type 1 diabetes. Journal of Autoimmunity, 2020, 115, 102543.	6.5	10
41	Effect of Local Environment and Protein on the Mechanism of Action of Superoxide Dismutase. Enzyme, 1986, 36, 32-43.	0.7	8
42	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
43	Thermodynamic basis of selectivity in guideâ€¢targetâ€•mismatched rna interference. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1283-1298.	2.6	6
44	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
45	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
46	Molecular Models of Sweet Taste Receptors Provide Insights into Function. ACS Symposium Series, 2008, , 117-132.	0.5	3
47	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
48	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
49	Making Sense of the Sweet Taste Receptor. ACS Symposium Series, 2008, , 48-64.	0.5	1
50	Modeling Duplex DNA Oligonucleotides with Modified Pyrimidine Bases. ACS Symposium Series, 1997, , 312-328.	0.5	0
51	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
52	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
53	Simulations of Molecular Mechanisms in Radiation Damage to DNA. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1995, , 349-363.	0.2	0