Serge Antonczak

List of Publications by Year
in descending order

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40 papers	1,244 citations	361413 20 h-index	361022 35 g-index
42 all docs	42 docs citations	42 times ranked	1642 citing authors

#	Article	IF	Citations
1	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	3.3	149
2	DFT Study of Quercetin Activated Forms Involved in Antiradical, Antioxidant, and Prooxidant Biological Processes. Journal of Agricultural and Food Chemistry, 2007, 55, 903-911.	5.2	98
3	Insights in the Peptide Hydrolysis Mechanism by Thermolysin: A Theoretical QM/MM study. Journal of Molecular Modeling, 2000, 6, 527-538.	1.8	86
4	Modeling of Peptide Hydrolysis by Thermolysin. A Semiempirical and QM/MM Study. Journal of the American Chemical Society, 1998, 120, 8825-8833.	13.7	76
5	Olefin Epoxidation by Methyltrioxorhenium: A Density Functional Study on Energetics and Mechanisms. Angewandte Chemie - International Edition, 1998, 37, 2211-2214.	13.8	70
6	<scp>G</scp> proteinâ€coupled odorant receptors: From sequence to structure. Protein Science, 2015, 24, 1543-1548.	7.6	69
7	Electronic description of four flavonoids revisited by DFT method. Computational and Theoretical Chemistry, 2008, 856, 38-45.	1.5	56
8	The Hydrolysis Mechanism of Formamide Revisited: Comparison Between ab initio, Semiempirical and DFT Results. Journal of Molecular Modeling, 1997, 3, 434-442.	1.8	48
9	Sweetness prediction of natural compounds. Food Chemistry, 2017, 221, 1421-1425.	8.2	47
10	A three-dimensional construction of the active site (region 507â€“749) of human neutral endopeptidase (EC.3.4.24.11). Protein Engineering, Design and Selection, 1999, 12, 141-149.	2.1	46
11	Bornyl-diphosphate synthase from Lavandula angustifolia: A major monoterpene synthase involved in essential oil quality. Phytochemistry, 2017, 137, 24-33.	2.9	42
12	Evidence by Site-Directed Mutagenesis That Arginine 203 of Thermolysin and Arginine 717 of Neprilysin (Neutral Endopeptidase) Play Equivalent Critical Roles in Substrate Hydrolysis and Inhibitor Binding. Biochemistry, 1997, 36, 13938-13945.	2.5	41
13	The anatomy of mammalian sweet taste receptors. Proteins: Structure, Function and Bioinformatics, 2017, 85, 332-341.	2.6	41
14	Oxygenolysis of Flavonoid Compounds: DFT Description of the Mechanism for Quercetin. ChemPhysChem, 2004, 5, 1726-1733.	2.1	40
15	Thermochemistry of Oxygen Transfer between Rhenium and Phosphine Complexes. A Density Functional Studyâ€. Organometallics, 1999, 18, 5044-5056.	2.3	31
16	Binding free energy prediction in strongly hydrophobic biomolecular systems. Physical Chemistry Chemical Physics, 2007, 9, 5761.	2.8	25
17	Mechanistic events underlying odorant binding protein chemoreception. Proteins: Structure, Function and Bioinformatics, 2007, 67, 448-458.	2.6	24
18	Discrimination between Olfactory Receptor Agonists and Nonâ€agonists. Chemistry - A European Journal, 2014, 20, 10227-10230.	3.3	23

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19	Chiroptical Properties of Amino Acids: A Density Functional Theory Study. Symmetry, 2010, 2, 935-949.	2.2	22
20	Molecular dynamics studies of odorant binding protein free of ligand and complexed to pyrazine and octenol. Computational and Theoretical Chemistry, 2006, 763, 165-174.	1.5	20
21	Intramolecular Allyl Transfer Reaction from Allyl Ether to Aldehyde Groups: Experimental and Theoretical Studies. Chemistry - A European Journal, 2002, 8, 664-672.	3.3	18
22	Novel scaffold of natural compound eliciting sweet taste revealed by machine learning. Food Chemistry, 2020, 324, 126864.	8.2	18
23	Molecular simulations reveal a new entry site in quercetin 2,3-dioxygenase. A pathway for dioxygen?. Proteins: Structure, Function and Bioinformatics, 2006, 64, 845-850.	2.6	14
24	Molecular simulations bring new insights into flavonoid/quercetinase interaction modes. Proteins: Structure, Function and Bioinformatics, 2007, 67, 961-970.	2.6	14
25	Theoretical investigations of the role played by quercetinase enzymes upon the flavonoids oxygenolysis mechanism. Physical Chemistry Chemical Physics, 2009, 11, 1491.	2.8	14
26	Molecular dynamics simulation of hepatitis C virus IRES IIId domain: structural behavior, electrostatic and energetic analysis. Journal of Molecular Modeling, 2004, 10, 60-68.	1.8	13
27	Allosteric Modulation Mechanism of the mGluR₅ Transmembrane Domain. Journal of Chemical Information and Modeling, 2019, 59, 2871-2878.	5.4	12
28	Closing loop base pairs in RNA loopâ€“loop complexes: structural behavior, interaction energy and solvation analysis through molecular dynamics simulations. Journal of Molecular Modeling, 2004, 10, 408-417.	1.8	11
29	Fine-tuning of microsolvation and hydrogen bond interaction regulates substrate channelling in the course of flavonoid biosynthesis. Physical Chemistry Chemical Physics, 2016, 18, 10337-10345.	2.8	11
30	Cerium(IV)-mediated oxidation of flavonol with relevance to flavonol 2,4-dioxygenase. Direct evidence for spin delocalization in the flavonoxy radical. Journal of Inorganic Biochemistry, 2007, 101, 893-899.	3.5	10
31	Kinetics and thermodynamics of gas diffusion in a NiFe hydrogenase. Proteins: Structure, Function and Bioinformatics, 2012, 80, 677-682.	2.6	10
32	Update of the ATTRACT force field for the prediction of protein-protein binding affinity. Journal of Computational Chemistry, 2017, 38, 1887-1890.	3.3	9
33	O2 Migration Rates in [NiFe] Hydrogenases. A Joint Approach Combining Free-Energy Calculations and Kinetic Modeling. Journal of Physical Chemistry B, 2014, 118, 676-681.	2.6	8
34	Conserved Residues Control the T1R3-Specific Allosteric Signaling Pathway of the Mammalian Sweet-Taste Receptor. Chemical Senses, 2019, 44, 303-310.	2.0	8
35	Molecular simulations enlighten the binding mode of quercetin to lipoxygenaseâ€3. Proteins: Structure, Function and Bioinformatics, 2008, 73, 290-298.	2.6	7
36	Deciphering the Selectivity of Bombyx mori Pheromone Binding Protein for Bombykol over Bombykal: A Theoretical Approach. ChemPhysChem, 2008, 9, 2785-2793.	2.1	4

#	Article	IF	Citations
37	Exploring Dihydroflavonolâ€4â€Reductase Reactivity and Selectivity by QM/MMâ€MD Simulations. ChemBioChem, 2022, 23, .	2.6	4
38	Molecular Features Underlying the Perception of Astringency as Probed by Molecular Modeling. Molecular Informatics, 2011, 30, 410-414.	2.5	1
39	Prediction and Calculation of Proteinâ€“Protein Binding Affinities and Mutation Effects. , 2010, , 295-317.		0
40	Molecular Features Underlying the Chemoreception of Odorant Binding Proteins and Olfactory Receptors. Insights from Molecular Modeling and Biophysical Data. , 2014, , 519-523.		0