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	Exploring Dihydroflavonolâ€4â€Reductase Reactivity and Selectivity by QM/MMâ€MD Simulations. ChemBioChem, 2022, 23, .	2.6	4
2	Novel scaffold of natural compound eliciting sweet taste revealed by machine learning. Food Chemistry, 2020, 324, 126864.	8.2	18
3	Allosteric Modulation Mechanism of the mGluR₅ Transmembrane Domain. Journal of Chemical Information and Modeling, 2019, 59, 2871-2878.	5.4	12
4	Conserved Residues Control the T1R3-Specific Allosteric Signaling Pathway of the Mammalian Sweet-Taste Receptor. Chemical Senses, 2019, 44, 303-310.	2.0	8
5	Bornyl-diphosphate synthase from Lavandula angustifolia: A major monoterpene synthase involved in essential oil quality. Phytochemistry, 2017, 137, 24-33.	2.9	42
6	The anatomy of mammalian sweet taste receptors. Proteins: Structure, Function and Bioinformatics, 2017, 85, 332-341.	2.6	41
7	Sweetness prediction of natural compounds. Food Chemistry, 2017, 221, 1421-1425.	8.2	47
8	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
9	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
10	<scp>G</scp> proteinâ€coupled odorant receptors: From sequence to structure. Protein Science, 2015, 24, 1543-1548.	7.6	69
11	Discrimination between Olfactory Receptor Agonists and Nonâ€agonists. Chemistry - A European Journal, 2014, 20, 10227-10230.	3.3	23
12	Molecular Features Underlying the Chemoreception of Odorant Binding Proteins and Olfactory Receptors. Insights from Molecular Modeling and Biophysical Data. , 2014, , 519-523.		0
13	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
14	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	3.3	149
15	Kinetics and thermodynamics of gas diffusion in a NiFe hydrogenase. Proteins: Structure, Function and Bioinformatics, 2012, 80, 677-682.	2.6	10
16	Molecular Features Underlying the Perception of Astringency as Probed by Molecular Modeling. Molecular Informatics, 2011, 30, 410-414.	2.5	1
17	Prediction and Calculation of Proteinâ€“Protein Binding Affinities and Mutation Effects. , 2010, , 295-317.		0
18	Chiroptical Properties of Amino Acids: A Density Functional Theory Study. Symmetry, 2010, 2, 935-949.	2.2	22

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19	Theoretical investigations of the role played by quercetinase enzymes upon the flavonoids oxygenolysis mechanism. Physical Chemistry Chemical Physics, 2009, 11, 1491.	2.8	14
20	Molecular simulations enlighten the binding mode of quercetin to lipoxygenaseâ€3. Proteins: Structure, Function and Bioinformatics, 2008, 73, 290-298.	2.6	7
21	Deciphering the Selectivity of Bombyx mori Pheromone Binding Protein for Bombykol over Bombykal: A Theoretical Approach. ChemPhysChem, 2008, 9, 2785-2793.	2.1	4
22	Electronic description of four flavonoids revisited by DFT method. Computational and Theoretical Chemistry, 2008, 856, 38-45.	1.5	56
23	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
24	Binding free energy prediction in strongly hydrophobic biomolecular systems. Physical Chemistry Chemical Physics, 2007, 9, 5761.	2.8	25
25	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
26	Mechanistic events underlying odorant binding protein chemoreception. Proteins: Structure, Function and Bioinformatics, 2007, 67, 448-458.	2.6	24
27	Molecular simulations bring new insights into flavonoid/quercetinase interaction modes. Proteins: Structure, Function and Bioinformatics, 2007, 67, 961-970.	2.6	14
28	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
29	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
30	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
31	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
32	Oxygenolysis of Flavonoid Compounds: DFT Description of the Mechanism for Quercetin. ChemPhysChem, 2004, 5, 1726-1733.	2.1	40
33	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
34	Insights in the Peptide Hydrolysis Mechanism by Thermolysin: A Theoretical QM/MM study. Journal of Molecular Modeling, 2000, 6, 527-538.	1.8	86
35	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
36	Thermochemistry of Oxygen Transfer between Rhenium and Phosphine Complexes. A Density Functional Studyâ€. Organometallics, 1999, 18, 5044-5056.	2.3	31

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37	Olefin Epoxidation by Methyltrioxorhenium: A Density Functional Study on Energetics and Mechanisms. Angewandte Chemie - International Edition, 1998, 37, 2211-2214.	13.8	70
38	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
39	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
40	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