

Maria Cristina Menziani

List of Publications by Year in descending order

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177
papers

5,722
citations

66315

42
h-index

106281

65
g-index

180
all docs

180
docs citations

180
times ranked

5554
citing authors

#	ARTICLE	IF	CITATIONS
1	Biasing crystallization in fused silica: An assessment of optimal metadynamics parameters. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	3
2	Novel Petâ€Degrading Enzymes: Structureâ€Function from a Computational Perspective. <i>ChemBioChem</i> , 2021, 22, 2032-2050.	1.3	16
3	Improved empirical force field for multicomponent oxide glasses and crystals. <i>Physical Review Materials</i> , 2021, 5, .	0.9	12
4	Development and Application of a ReaxFF Reactive Force Field for Cerium Oxide/Water Interfaces. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5693-5708.	1.1	8
5	Exploring the crystallization path of lithium disilicate through metadynamics simulations. <i>Physical Review Materials</i> , 2021, 5, .	0.9	8
6	Toward the understanding of crystallization, mechanical properties and reactivity of multicomponent bioactive glasses. <i>Acta Materialia</i> , 2021, 213, 116977.	3.8	14
7	Exploring Translocator Protein (TSPO) Medicinal Chemistry: An Approach for Targeting Radionuclides and Boron Atoms to Mitochondria. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 9649-9676.	2.9	2
8	Computational Insight on the Interaction of Common Blood Proteins with Gold Nanoparticles. <i>International Journal of Molecular Sciences</i> , 2021, 22, 8722.	1.8	4
9	Disclosing the Interaction of Gold Nanoparticles with Al ²⁺ (1â€40) Monomers through Replica Exchange Molecular Dynamics Simulations. <i>International Journal of Molecular Sciences</i> , 2021, 22, 26.	1.8	21
10	O ₂ Activation over Ag-Decorated CeO ₂ (111) and TiO ₂ (110) Surfaces: A Theoretical Comparative Investigation. <i>Journal of Physical Chemistry C</i> , 2020, 124, 25917-25930.	1.5	19
11	Insights into the Effect of Curcumin and (â€)-Epigallocatechin-3-Gallate on the Aggregation of Al ²⁺ (1â€40) Monomers by Means of Molecular Dynamics. <i>International Journal of Molecular Sciences</i> , 2020, 21, 5462.	1.8	18
12	Disclosing crystal nucleation mechanism in lithium disilicate glass through molecular dynamics simulations and free-energy calculations. <i>Scientific Reports</i> , 2020, 10, 17867.	1.6	18
13	Computational Insights into the Binding of Monolayer-Capped Gold Nanoparticles onto Amyloid- β^2 Fibrils. <i>ACS Chemical Neuroscience</i> , 2020, 11, 3153-3160.	1.7	22
14	Structural origins of the Mixed Alkali Effect in Alkali Aluminosilicate Glasses: Molecular Dynamics Study and its Assessment. <i>Scientific Reports</i> , 2020, 10, 2906.	1.6	36
15	Unraveling the complexity of amyloid polymorphism using gold nanoparticles and cryo-EM. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 6866-6874.	3.3	54
16	Multiscale Molecular Dynamics Simulation of Multiple Protein Adsorption on Gold Nanoparticles. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3539.	1.8	36
17	DARPin ₉₋₂₉ -Targeted Mini Gold Nanorods Specifically Eliminate HER2-Overexpressing Cancer Cells. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 34645-34651.	4.0	18
18	H ₂ Dissociation and Water Evolution on Silver-Decorated CeO ₂ (111): A Hybrid Density Functional Theory Investigation. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25668-25679.	1.5	9

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19	A DFT Approach to the Surface-Enhanced Raman Scattering of 4-Cyanopyridine Adsorbed on Silver Nanoparticles. <i>Nanomaterials</i> , 2019, 9, 1211.	1.9	33
20	Reducibility of Ag- and Cu-Modified Ultrathin Epitaxial Cerium Oxide Films. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13702-13711.	1.5	6
21	Nanoreactors for the multi-functionalization of poly-histidine fragments. <i>New Journal of Chemistry</i> , 2019, 43, 6834-6837.	1.4	8
22	Functionalization of protein hexahistidine tags by functional nanoreactors. <i>New Journal of Chemistry</i> , 2019, 43, 17946-17953.	1.4	3
23	An atomic-level look at the structure-property relationship of cerium-doped glasses using classical molecular dynamics. <i>Journal of Non-Crystalline Solids</i> , 2018, 498, 331-337.	1.5	9
24	Computational Insight into the Effect of Natural Compounds on the Destabilization of Preformed Amyloid- β (1-40) Fibrils. <i>Molecules</i> , 2018, 23, 1320.	1.7	28
25	Curcumin derivatives and A β ² -fibrillar aggregates: An interactions study for diagnostic/therapeutic purposes in neurodegenerative diseases. <i>Bioorganic and Medicinal Chemistry</i> , 2018, 26, 4288-4300.	1.4	29
26	Assessment of Density Functional Approximations for Highly Correlated Oxides: The Case of CeO ₂ and Ce ₂ O ₃ . <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4914-4927.	2.3	27
27	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5747-5752.	1.5	52
28	Site-Selective Surface-Enhanced Raman Detection of Proteins. <i>ACS Nano</i> , 2017, 11, 918-926.	7.3	85
29	Computational Insight into the Interaction of Cytochrome C with Wet and PVP-Coated Ag Surfaces. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9532-9540.	1.2	18
30	Structure of active cerium sites within bioactive glasses. <i>Journal of the American Ceramic Society</i> , 2017, 100, 5086-5095.	1.9	16
31	Synthesis, Characterization, and Selective Delivery of DARPIn-Gold Nanoparticle Conjugates to Cancer Cells. <i>Bioconjugate Chemistry</i> , 2017, 28, 2569-2574.	1.8	37
32	Modeling emission features of salicylidene aniline molecular crystals: A QM/QM approach. <i>Journal of Computational Chemistry</i> , 2016, 37, 861-870.	1.5	26
33	What Can We Learn from Atomistic Simulations of Bioactive Glasses?. <i>Advanced Structured Materials</i> , 2016, , 119-145.	0.3	2
34	Optical properties of the dibenzothiazolylphenol molecular crystals through ONIOM calculations: the effect of the electrostatic embedding scheme. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	14
35	Assessment of the basis set effect on the structural and electronic properties of organic-protected gold nanoclusters. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	6
36	Phenylindanone isomers as divergent modulators of p38 MAP kinase. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2016, 26, 5160-5163.	1.0	3

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37	The antioxidant properties of Ce-containing bioactive glass nanoparticles explained by Molecular Dynamics simulations. <i>Biomedical Glasses</i> , 2016, 2, .	2.4	9
38	The effect of composition on structural, thermal, redox and bioactive properties of Ce-containing glasses. <i>Materials and Design</i> , 2016, 97, 73-85.	3.3	43
39	Electronic and optical properties of the Au ₂₂ [1,8-bis(diphenylphosphino) octane] ₆ nanoclusters disclosed by DFT and TD-DFT calculations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	12
40	Calcium environment in silicate and aluminosilicate glasses probed by ⁴³ Ca MQMAS NMR experiments and MD-GIPAW calculations. <i>Solid State Nuclear Magnetic Resonance</i> , 2015, 68-69, 31-36.	1.5	37
41	Evidence of Catalase Mimetic Activity in Ce ³⁺ /Ce ⁴⁺ Doped Bioactive Glasses. <i>Journal of Physical Chemistry B</i> , 2015, 119, 4009-4019.	1.2	119
42	Computational Modeling of Silicate Glasses: A Quantitative Structure-Property Relationship Perspective. <i>Springer Series in Materials Science</i> , 2015, , 113-135.	0.4	15
43	Influence of Silver Doping on the Photoluminescence of Protected Ag _n Au ₂₅ Nanoclusters: A Time-Dependent Density Functional Theory Investigation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10766-10775.	1.5	40
44	Competitive Binding of Proteins to Gold Nanoparticles Disclosed by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 22172-22180.	1.5	76
45	Dynamics of Fracture in Silica and Soda-Silicate Glasses: From Bulk Materials to Nanowires. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25499-25507.	1.5	25
46	A closer look into the ubiquitin corona on gold nanoparticles by computational studies. <i>New Journal of Chemistry</i> , 2015, 39, 2474-2482.	1.4	49
47	DFT and TD-DFT Assessment of the Structural and Optoelectronic Properties of an Organic-Ag ₁₄ Nanocluster. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5088-5098.	1.1	31
48	Computational Protocol for Modeling Thermochromic Molecular Crystals: Salicylidene Aniline As a Case Study. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5577-5585.	2.3	44
49	Arylsulfonyl Groups: The Best Cyclization Auxiliaries for the Preparation of ATRC β -Lactams can be Acidolytically Removed. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 6734-6745.	1.2	15
50	Dendrimeric tetravalent ligands for the serotonin-gated ion channel. <i>Chemical Communications</i> , 2014, 50, 8582.	2.2	16
51	Oxalyl dihydrazide polymorphism: a periodic dispersion-corrected DFT and MP2 investigation. <i>CrystEngComm</i> , 2014, 16, 102-109.	1.3	23
52	Unraveling the Polymorphism of [(p-cymene)Ru(η^5 -INA)Cl ₂] through Dispersion-Corrected DFT and NMR GIPAW Calculations. <i>Inorganic Chemistry</i> , 2014, 53, 7926-7935.	1.9	11
53	Assessment of Exchange-Correlation Functionals in Reproducing the Structure and Optical Gap of Organic-Protected Gold Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2014, 118, 7532-7544.	1.5	51
54	On the opto-electronic properties of phosphine and thiolate-protected undecagold nanoclusters. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18749-18758.	1.3	19

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55	Computational interpretation of ^{23}Na MQMAS NMR spectra: A comprehensive investigation of the Na environment in silicate glasses. <i>Chemical Physics Letters</i> , 2014, 612, 56-61.	1.2	34
56	Synthesis and structure-activity relationship studies in serotonin 5-HT ₄ receptor ligands based on a benzo[de][2,6]naphthridine scaffold. <i>European Journal of Medicinal Chemistry</i> , 2014, 82, 36-46.	2.6	15
57	Probing silicon and aluminium chemical environments in silicate and aluminosilicate glasses by solid state NMR spectroscopy and accurate first-principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2014, 125, 170-185.	1.6	72
58	Approaching the 5-HT ₃ receptor heterogeneity by computational studies of the transmembrane and intracellular domains. <i>Journal of Computer-Aided Molecular Design</i> , 2013, 27, 491-509.	1.3	0
59	Study of the Structural Role of Gallium and Aluminum in 45S5 Bioactive Glasses by Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 4142-4150.	1.2	68
60	New insights into the bioactivity of $\text{SiO}_2\text{-CaO}$ and $\text{SiO}_2\text{-CaO-P}_2\text{O}_5$ sol-gel glasses by molecular dynamics simulations. <i>Journal of Sol-Gel Science and Technology</i> , 2013, 67, 208-219.	1.1	18
61	Local versus Average Structure in $\text{LaSrAl}_3\text{O}_7$: A NMR and DFT Investigation. <i>Journal of Physical Chemistry C</i> , 2013, 117, 23451-23458.	1.5	20
62	Exploring a potential palonosetron allosteric binding site in the 5-HT ₃ receptor. <i>Bioorganic and Medicinal Chemistry</i> , 2013, 21, 7523-7528.	1.4	14
63	Computational simulations of solid state NMR spectra: a new era in structure determination of oxide glasses. <i>RSC Advances</i> , 2013, 3, 10550.	1.7	81
64	Novel route to chaetomelic acid A and analogues: Serendipitous discovery of a more competent FTase inhibitor. <i>Bioorganic and Medicinal Chemistry</i> , 2013, 21, 348-358.	1.4	8
65	First-principles simulations of the ^{27}Al and ^{17}O solid-state NMR spectra of the $\text{CaAl}_2\text{Si}_3\text{O}_{10}$ glass. <i>Highlights in Theoretical Chemistry</i> , 2013, , 87-97.	0.0	0
66	A first step towards the understanding of the 5-HT ₃ receptor subunit heterogeneity from a computational point of view. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12625.	1.3	6
67	Unambiguous Description of the Oxygen Environment in Multicomponent Aluminosilicate Glasses from ^{17}O Solid State NMR Computational Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2012, 116, 14599-14609.	1.5	59
68	The structure of fluoride-containing bioactive glasses: new insights from first-principles calculations and solid state NMR spectroscopy. <i>Journal of Materials Chemistry</i> , 2012, 22, 12599.	6.7	88
69	The extracellular subunit interface of the 5-HT ₃ receptors: a computational alanine scanning mutagenesis study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2012, 30, 280-298.	2.0	6
70	On the ability of periodic dispersion-corrected DFT calculations to predict molecular crystal polymorphism in para-diiodobenzene. <i>Chemical Physics Letters</i> , 2012, 541, 12-15.	1.2	18
71	Computational Insights into ADAMTS4, ADAMTS5 and MMP13 Inhibitor Selectivity. <i>Molecular Informatics</i> , 2012, 31, 421-430.	1.4	2
72	First-principles simulations of the ^{27}Al and ^{17}O solid-state NMR spectra of the $\text{CaAl}_2\text{Si}_3\text{O}_{10}$ glass. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	34

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73	Modeling the Binding Affinity of p38 $\hat{\pm}$ MAP Kinase Inhibitors by Partial Least Squares Regression. <i>Chemical Biology and Drug Design</i> , 2012, 80, 455-470.	1.5	1
74	Bivalent Ligands for the Serotonin 5-HT ₃ Receptor. <i>ACS Medicinal Chemistry Letters</i> , 2011, 2, 571-576.	1.3	14
75	Fluorine Environment in Bioactive Glasses: <i>ab Initio</i> Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2038-2045.	1.2	79
76	Insights into MAPK $\hat{\pm}$ DFG flip mechanism by accelerated molecular dynamics. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 6805-6812.	1.4	36
77	Computational analysis of ligand recognition sites of homo- and heteropentameric 5-HT ₃ receptors. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 4746-4760.	2.6	14
78	New Insights into the Atomic Structure of 45S5 Bioglass by Means of Solid-State NMR Spectroscopy and Accurate First-Principles Simulations. <i>Chemistry of Materials</i> , 2010, 22, 5644-5652.	3.2	131
79	Molecular dynamics simulations of sodium silicate glasses: Optimization and limits of the computational procedure. <i>Computational Materials Science</i> , 2010, 47, 739-751.	1.4	26
80	Multinuclear NMR of CaSiO ₃ glass: simulation from first-principles. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6054.	1.3	71
81	Extension of the AMBER force-field for the study of large nitroxides in condensed phases: an <i>ab initio</i> parameterization. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11697.	1.3	74
82	Progress Towards the Identification of New Aggrecanase Inhibitors. <i>Current Medicinal Chemistry</i> , 2009, 16, 2395-2415.	1.2	22
83	Quantitative Structure $\hat{\sim}$ Property Relationships of Potentially Bioactive Fluoro Phospho-silicate Glasses. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10331-10338.	1.2	80
84	Computational Insight into the Effect of CaO/MgO Substitution on the Structural Properties of Phospho-Silicate Bioactive Glasses. <i>Journal of Physical Chemistry C</i> , 2009, 113, 15723-15730.	1.5	99
85	Elastic and dynamical properties of alkali-silicate glasses from computer simulations techniques. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 557-564.	0.5	44
86	Role of Magnesium in Soda-Lime Glasses: Insight into Structural, Transport, and Mechanical Properties through Computer Simulations. <i>Journal of Physical Chemistry C</i> , 2008, 112, 11034-11041.	1.5	89
87	Accurate First-Principle Prediction of ²⁹ Si and ¹⁷ O NMR Parameters in SiO ₂ Polymorphs: The Cases of Zeolites Sigma-2 and Ferrierite. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 2130-2140.	2.3	27
88	FFSiOH: a New Force Field for Silica Polymorphs and Their Hydroxylated Surfaces Based on Periodic B3LYP Calculations. <i>Chemistry of Materials</i> , 2008, 20, 2522-2531.	3.2	68
89	Molecular Dynamics Studies of Stress $\hat{\sim}$ Strain Behavior of Silica Glass under a Tensile Load. <i>Chemistry of Materials</i> , 2008, 20, 4356-4366.	3.2	121
90	Medium-range order in phospho-silicate bioactive glasses: Insights from MAS-NMR spectra, chemical durability experiments and molecular dynamics simulations. <i>Journal of Non-Crystalline Solids</i> , 2008, 354, 84-89.	1.5	54

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91	Elucidation of the Structural Role of Fluorine in Potentially Bioactive Glasses by Experimental and Computational Investigation. <i>Journal of Physical Chemistry B</i> , 2008, 112, 12730-12739.	1.2	107
92	Properties of Zinc Releasing Surfaces for Clinical Applications. <i>Journal of Biomaterials Applications</i> , 2008, 22, 505-526.	1.2	52
93	A Combined Experimental-Computational Strategy for the Design, Synthesis and Characterization of Bioactive Zinc-Silicate Glasses. <i>Key Engineering Materials</i> , 2008, 377, 211-224.	0.4	3
94	An ab initio parameterized interatomic force field for hydroxyapatite. <i>Journal of Materials Chemistry</i> , 2007, 17, 2061.	6.7	32
95	Insight into Elastic Properties of Binary Alkali Silicate Glasses; Prediction and Interpretation through Atomistic Simulation Techniques. <i>Chemistry of Materials</i> , 2007, 19, 3144-3154.	3.2	125
96	Crystallization Kinetics of Bioactive Glasses in the $ZnO\sim Na_2O\sim CaO\sim SiO_2$ System. <i>Journal of Physical Chemistry A</i> , 2007, 111, 8401-8408.	1.1	20
97	A computational multiscale strategy to the study of amorphous materials. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 933-942.	0.5	32
98	Density of multicomponent silica-based potential bioglasses: Quantitative structure-property relationships (QSPR) analysis. <i>Journal of the European Ceramic Society</i> , 2007, 27, 499-504.	2.8	14
99	A New Self-Consistent Empirical Interatomic Potential Model for Oxides, Silicates, and Silica-Based Glasses. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11780-11795.	1.2	471
100	Towards a quantitative rationalization of multicomponent glass properties by means of molecular dynamics simulations. <i>Molecular Simulation</i> , 2006, 32, 1045-1055.	0.9	20
101	Void size distribution in MD-modelled silica glass structures. <i>Journal of Non-Crystalline Solids</i> , 2006, 352, 285-296.	1.5	70
102	Molecular Interactions Between Human Cytochrome P450 1A2 and Flavone Derivatives. <i>Medicinal Chemistry</i> , 2006, 2, 401-406.	0.7	0
103	Theoretical quantitative structure-activity relationships of flavone ligands interacting with cytochrome P450 1A1 and 1A2 isozymes. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 4366-4374.	1.4	39
104	A Computational Tool for the Prediction of Crystalline Phases Obtained from Controlled Crystallization of Glasses. <i>Journal of Physical Chemistry B</i> , 2005, 109, 21586-21592.	1.2	32
105	A computational protocol to probe the role of solvation effects on the reduction potential of azurin mutants. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 262-269.	1.5	10
106	Qualitative and Quantitative Structure-Property Relationships Analysis of Multicomponent Potential Bioglasses. <i>Journal of Physical Chemistry B</i> , 2005, 109, 4989-4998.	1.2	98
107	Further Studies on the Interaction of the 5-Hydroxytryptamine ₃ (5-HT ₃) Receptor with Arylpiperazine Ligands. Development of a New 5-HT ₃ Receptor Ligand Showing Potent Acetylcholinesterase Inhibitory Properties. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 3564-3575.	2.9	64
108	Computational Insight into Anti-mutagenic Properties of CYP1A Flavonoid Ligands. <i>Medicinal Chemistry</i> , 2005, 1, 355-360.	0.7	0

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109	Computational approaches to structural and functional analysis of plastocyanin and other blue copper proteins. <i>Cellular and Molecular Life Sciences</i> , 2004, 61, 1123-1142.	2.4	24
110	A combined experimental and computational approach to $(\text{Na}_2\text{O})_{1-x}\text{CaO}\cdot(\text{ZnO})_x\cdot 2\text{SiO}_2$ glasses characterization. <i>Journal of Non-Crystalline Solids</i> , 2004, 345-346, 710-714.	1.5	22
111	Design, Synthesis, Structural Studies, Biological Evaluation, and Computational Simulations of Novel Potent AT1 Angiotensin II Receptor Antagonists Based on the 4-Phenylquinoline Structure. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 2574-2586.	2.9	75
112	Seeking for binding determinants of the prion protein to human plasminogen. <i>Molecular Physics</i> , 2003, 101, 2763-2773.	0.8	1
113	Development of an IL-6 antagonist peptide that induces apoptosis in 7TD1 cells. <i>Peptides</i> , 2003, 24, 1207-1220.	1.2	14
114	Synthesis, Biological Evaluation, and Receptor Docking Simulations of 2-[(Acylamino)ethyl]-1,4-benzodiazepines as μ -Opioid Receptor Agonists Endowed with Antinociceptive and Antiamnesic Activity. <i>Journal of Medicinal Chemistry</i> , 2003, 46, 3853-3864.	2.9	32
115	Modelling the metabolic action of human and rat CYP1A2 and its relationship with the carcinogenicity of heterocyclic amines. <i>Molecular Physics</i> , 2003, 101, 2731-2741.	0.8	4
116	Experimental Versus Computer Simulation Analysis of Zirconia Containing Glasses. <i>Key Engineering Materials</i> , 2002, 206-213, 2101-2104.	0.4	0
117	Synthesis, Characterization, and Molecular Dynamics Simulation Of $\text{Na}_2\text{O}\cdot\text{CaO}\cdot\text{SiO}_2\cdot\text{ZnO}$ Glasses. <i>Journal of Physical Chemistry B</i> , 2002, 106, 9753-9760.	1.2	76
118	Novel Potent 5-HT ₃ Receptor Ligands Based on the Pyrrolidone Structure: Synthesis, Biological Evaluation, and Computational Rationalization of the Ligand-Receptor Interaction Modalities. <i>Bioorganic and Medicinal Chemistry</i> , 2002, 10, 779-801.	1.4	36
119	Novel potent 5-HT ₃ receptor ligands based on the pyrrolidone structure. effects of the quaternization of the basic nitrogen on the interaction with 5-HT ₃ receptor. <i>Bioorganic and Medicinal Chemistry</i> , 2002, 10, 2681-2691.	1.4	9
120	Theoretical descriptors for the quantitative rationalisation of plastocyanin mutant functional properties. <i>Journal of Computer-Aided Molecular Design</i> , 2002, 16, 501-509.	1.3	3
121	Mapping and Fitting the Peripheral Benzodiazepine Receptor Binding Site by Carboxamide Derivatives. Comparison of Different Approaches to Quantitative Ligand-Receptor Interaction Modeling. <i>Journal of Medicinal Chemistry</i> , 2001, 44, 1134-1150.	2.9	68
122	Electrostatic Analysis and Brownian Dynamics Simulation of the Association of Plastocyanin and Cytochrome F. <i>Biophysical Journal</i> , 2001, 81, 3090-3104.	0.2	80
123	Influence of Small Additions of Al ₂ O ₃ on the Properties of the $\text{Na}_2\text{O}\cdot 3\text{SiO}_2$ Glass. <i>Journal of Physical Chemistry B</i> , 2001, 105, 919-927.	1.2	25
124	Control of Metalloprotein Reduction Potential: The Role of Electrostatic and Solvation Effects Probed on Plastocyanin Mutants. <i>Biochemistry</i> , 2001, 40, 6422-6430.	1.2	44
125	A computational model of the 5-HT ₃ receptor extracellular domain: search for ligand binding sites. <i>Theoretical Chemistry Accounts</i> , 2001, 106, 98-104.	0.5	14
126	Title is missing!. <i>Journal of Solution Chemistry</i> , 2001, 30, 149-169.	0.6	8

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127	The ad hoc supermolecule approach to receptor ligand design. Computational and Theoretical Chemistry, 2000, 503, 1-16.	1.5	7
128	Theoretical investigation of substrate specificity for cytochromes P450 IA2, P450 IID6 and P450 IIIA4. Journal of Computer-Aided Molecular Design, 2000, 14, 93-116.	1.3	59
129	Blue copper proteins: A comparative analysis of their molecular interaction properties. Protein Science, 2000, 9, 1439-1454.	3.1	109
130	Molecular Dynamics Simulations of Alumina Addition in Sodium Silicate Glasses. Molecular Simulation, 2000, 24, 157-165.	0.9	16
131	Relevance of theoretical molecular descriptors in quantitative structure-activity relationship analysis of α -1-adrenergic receptor antagonists. Bioorganic and Medicinal Chemistry, 1999, 7, 2437-2451.	1.4	23
132	Field experiments to study evaporation from a saturated bare soil. Physics and Chemistry of the Earth, 1999, 24, 813-818.	0.3	11
133	Theoretical study of the electrostatically driven step of receptor-G protein recognition. , 1999, 37, 145-156.		31
134	Synthesis, Pharmacological Evaluation, and Structure-Activity Relationship and Quantitative Structure-Activity Relationship Studies on Novel Derivatives of 2,4-Diamino-6,7-dimethoxyquinazoline α -1-Adrenoceptor Antagonists. Journal of Medicinal Chemistry, 1999, 42, 427-437.	2.9	20
135	Novel Potent and Selective Central 5-HT ₃ Receptor Ligands Provided with Different Intrinsic Efficacy. 2. Molecular Basis of the Intrinsic Efficacy of Arylpiperazine Derivatives at the Central 5-HT ₃ Receptors. Journal of Medicinal Chemistry, 1999, 42, 1556-1575.	2.9	37
136	Theoretical descriptors in quantitative structure-affinity and selectivity relationship study of potent N ₄ -substituted arylpiperazine 5-HT _{1A} receptor antagonists. Bioorganic and Medicinal Chemistry, 1998, 6, 535-550.	1.4	20
137	Computer Modeling of Size and Shape Descriptors of α -1-Adrenergic Receptor Antagonists and Quantitative Structure-Affinity/Selectivity Relationships. Methods, 1998, 14, 239-254.	1.9	14
138	Ab Initio Modeling and Molecular Dynamics Simulation of the α -1b-Adrenergic Receptor Activation. Methods, 1998, 14, 302-317.	1.9	38
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