Maria Cristina Menziani

List of Publications by Year
in descending order

177 papers	5,722 citations	76031 42 h-index	120465 65 g-index
180 all docs	180 docs citations	180 times ranked	6283 citing authors

#	Article	IF	Citations
1	Biasing crystallization in fused silica: An assessment of optimal metadynamics parameters. Journal of Chemical Physics, 2022, 156, .	1.2	3
2	Novel Petâ€Degrading Enzymes: Structureâ€Function from a Computational Perspective. ChemBioChem, 2021, 22, 2032-2050.	1.3	16
3	Improved empirical force field for multicomponent oxide glasses and crystals. Physical Review Materials, 2021, 5, .	0.9	12
4	Development and Application of a ReaxFF Reactive Force Field for Cerium Oxide/Water Interfaces. Journal of Physical Chemistry A, 2021, 125, 5693-5708.	1.1	8
5	Exploring the crystallization path of lithium disilicate through metadynamics simulations. Physical Review Materials, 2021, 5, .	0.9	8
6	Toward the understanding of crystallization, mechanical properties and reactivity of multicomponent bioactive glasses. Acta Materialia, 2021, 213, 116977.	3.8	14
7	Exploring Translocator Protein (TSPO) Medicinal Chemistry: An Approach for Targeting Radionuclides and Boron Atoms to Mitochondria. Journal of Medicinal Chemistry, 2021, 64, 9649-9676.	2.9	2
8	Computational Insight on the Interaction of Common Blood Proteins with Gold Nanoparticles. International Journal of Molecular Sciences, 2021, 22, 8722.	1.8	4
9	Disclosing the Interaction of Gold Nanoparticles with AÎ²(1â€“40) Monomers through Replica Exchange Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2021, 22, 26.	1.8	21
10	O₂ Activation over Ag-Decorated CeO₂(111) and TiO₂(110) Surfaces: A Theoretical Comparative Investigation. Journal of Physical Chemistry C, 2020, 124, 25917-25930.	1.5	19
11	Insights into the Effect of Curcumin and (â€“)-Epigallocatechin-3-Gallate on the Aggregation of AÎ²(1â€“40) Monomers by Means of Molecular Dynamics. International Journal of Molecular Sciences, 2020, 21, 5462.	1.8	18
12	Disclosing crystal nucleation mechanism in lithium disilicate glass through molecular dynamics simulations and free-energy calculations. Scientific Reports, 2020, 10, 17867.	1.6	18
13	Computational Insights into the Binding of Monolayer-Capped Gold Nanoparticles onto Amyloid-Î² Fibrils. ACS Chemical Neuroscience, 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. Scientific Reports, 2020, 10, 2906.	1.6	36
15	Unraveling the complexity of amyloid polymorphism using gold nanoparticles and cryo-EM. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 6866-6874.	3.3	54
16	Multiscale Molecular Dynamics Simulation of Multiple Protein Adsorption on Gold Nanoparticles. International Journal of Molecular Sciences, 2019, 20, 3539.	1.8	36
17	DARPin_9-29-Targeted Mini Gold Nanorods Specifically Eliminate HER2-Overexpressing Cancer Cells. ACS Applied Materials & Interfaces, 2019, 11, 34645-34651.	4.0	18
18	H₂ Dissociation and Water Evolution on Silver-Decorated CeO₂(111): A Hybrid Density Functional Theory Investigation. Journal of Physical Chemistry C, 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. Nanomaterials, 2019, 9, 1211.	1.9	33
20	Reducibility of Ag- and Cu-Modified Ultrathin Epitaxial Cerium Oxide Films. Journal of Physical Chemistry C, 2019, 123, 13702-13711.	1.5	6
21	Nanoreactors for the multi-functionalization of poly-histidine fragments. New Journal of Chemistry, 2019, 43, 6834-6837.	1.4	8
22	Functionalization of protein hexahistidine tags by functional nanoreactors. New Journal of Chemistry, 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. Journal of Non-Crystalline Solids, 2018, 498, 331-337.	1.5	9
24	Computational Insight into the Effect of Natural Compounds on the Destabilization of Preformed Amyloid-Î²(1â€“40) Fibrils. Molecules, 2018, 23, 1320.	1.7	28
25	Curcumin derivatives and AÎ²-fibrillar aggregates: An interactionsâ€™ study for diagnostic/therapeutic purposes in neurodegenerative diseases. Bioorganic and Medicinal Chemistry, 2018, 26, 4288-4300.	1.4	29
26	Assessment of Density Functional Approximations for Highly Correlated Oxides: The Case of CeO₂ and Ce₂O₃. Journal of Chemical Theory and Computation, 2018, 14, 4914-4927.	2.3	27
27	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. Journal of Physical Chemistry C, 2017, 121, 5747-5752.	1.5	52
28	Site-Selective Surface-Enhanced Raman Detection of Proteins. ACS Nano, 2017, 11, 918-926.	7.3	85
29	Computational Insight into the Interaction of Cytochrome C with Wet and PVP-Coated Ag Surfaces. Journal of Physical Chemistry B, 2017, 121, 9532-9540.	1.2	18
30	Structure of active cerium sites within bioactive glasses. Journal of the American Ceramic Society, 2017, 100, 5086-5095.	1.9	16
31	Synthesis, Characterization, and Selective Delivery of DARPinâ€“Gold Nanoparticle Conjugates to Cancer Cells. Bioconjugate Chemistry, 2017, 28, 2569-2574.	1.8	37
32	Modeling emission features of salicylidene aniline molecular crystals: A QM/QMâ€™ approach. Journal of Computational Chemistry, 2016, 37, 861-870.	1.5	26
33	What Can We Learn from Atomistic Simulations of Bioactive Glasses?. Advanced Structured Materials, 2016, , 119-145.	0.3	2
34	Optical properties of the dibenzothiazolylphenol molecular crystals through ONIOM calculations: the effect of the electrostatic embedding scheme. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	14
35	Assessment of the basis set effect on the structural and electronic properties of organic-protected gold nanoclusters. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	6
36	Phenylindenone isomers as divergent modulators of p38Î± MAP kinase. Bioorganic and Medicinal Chemistry Letters, 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. Biomedical Glasses, 2016, 2, .	2.4	9
38	The effect of composition on structural, thermal, redox and bioactive properties of Ce-containing glasses. Materials and Design, 2016, 97, 73-85.	3.3	43
39	Electronic and optical properties of the Au22[1,8-bis(diphenylphosphino) octane]6 nanoclusters disclosed by DFT and TD-DFT calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	12
40	Calcium environment in silicate and aluminosilicate glasses probed by 43Ca MQMAS NMR experiments and MD-GIPAW calculations. Solid State Nuclear Magnetic Resonance, 2015, 68-69, 31-36.	1.5	37
41	Evidence of Catalase Mimetic Activity in Ce³⁺/Ce⁴⁺ Doped Bioactive Glasses. Journal of Physical Chemistry B, 2015, 119, 4009-4019.	1.2	119
42	Computational Modeling of Silicate Glasses: A Quantitative Structure-Property Relationship Perspective. Springer Series in Materials Science, 2015, , 113-135.	0.4	15
43	Influence of Silver Doping on the Photoluminescence of Protected Ag_nAu_{25â€“n} Nanoclusters: A Time-Dependent Density Functional Theory Investigation. Journal of Physical Chemistry C, 2015, 119, 10766-10775.	1.5	40
44	Competitive Binding of Proteins to Gold Nanoparticles Disclosed by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 22172-22180.	1.5	76
45	Dynamics of Fracture in Silica and Soda-Silicate Glasses: From Bulk Materials to Nanowires. Journal of Physical Chemistry C, 2015, 119, 25499-25507.	1.5	25
46	A closer look into the ubiquitin corona on gold nanoparticles by computational studies. New Journal of Chemistry, 2015, 39, 2474-2482.	1.4	49
47	DFT and TD-DFT Assessment of the Structural and Optoelectronic Properties of an Organicâ€“Ag₁₄ Nanocluster. Journal of Physical Chemistry A, 2015, 119, 5088-5098.	1.1	31
48	Computational Protocol for Modeling Thermochromic Molecular Crystals: Salicylidene Aniline As a Case Study. Journal of Chemical Theory and Computation, 2014, 10, 5577-5585.	2.3	44
49	Arylsulfonyl Groups: The Best Cyclization Auxiliaries for the Preparation of ATRC Î³â€Ł-lactams can be Acidolytically Removed. European Journal of Organic Chemistry, 2014, 2014, 6734-6745.	1.2	15
50	Dendrimeric tetravalent ligands for the serotonin-gated ion channel. Chemical Communications, 2014, 50, 8582.	2.2	16
51	Oxalyl dihydrazide polymorphism: a periodic dispersion-corrected DFT and MP2 investigation. CrystEngComm, 2014, 16, 102-109.	1.3	23
52	Unraveling the Polymorphism of [(p-cymene)Ru(Îº²N-INA)Cl₂] through Dispersion-Corrected DFT and NMR GIPAW Calculations. Inorganic Chemistry, 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. Journal of Physical Chemistry C, 2014, 118, 7532-7544.	1.5	51
54	On the opto-electronic properties of phosphine and thiolate-protected undecagold nanoclusters. Physical Chemistry Chemical Physics, 2014, 16, 18749-18758.	1.3	19

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55	Computational interpretation of 23Na MQMAS NMR spectra: A comprehensive investigation of the Na environment in silicate glasses. Chemical Physics Letters, 2014, 612, 56-61.	1.2	34
56	Synthesis and structureâ€“activity relationship studies in serotonin 5-HT4 receptor ligands based on a benzo[de][2,6]naphthridine scaffold. European Journal of Medicinal Chemistry, 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. Geochimica Et Cosmochimica Acta, 2014, 125, 170-185.	1.6	72
58	Approaching the 5-HT3 receptor heterogeneity by computational studies of the transmembrane and intracellular domains. Journal of Computer-Aided Molecular Design, 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. Journal of Physical Chemistry B, 2013, 117, 4142-4150.	1.2	68
60	New insights into the bioactivity of SiO2â€“CaO and SiO2â€“CaOâ€“P2O5 solâ€“gel glasses by molecular dynamics simulations. Journal of Sol-Gel Science and Technology, 2013, 67, 208-219.	1.1	18
61	Local versus Average Structure in LaSrAl₃O₇: A NMR and DFT Investigation. Journal of Physical Chemistry C, 2013, 117, 23451-23458.	1.5	20
62	Exploring a potential palonosetron allosteric binding site in the 5-HT3 receptor. Bioorganic and Medicinal Chemistry, 2013, 21, 7523-7528.	1.4	14
63	Computational simulations of solid state NMR spectra: a new era in structure determination of oxide glasses. RSC Advances, 2013, 3, 10550.	1.7	81
64	Novel route to chaetomellic acid A and analogues: Serendipitous discovery of a more competent FTase inhibitor. Bioorganic and Medicinal Chemistry, 2013, 21, 348-358.	1.4	8
65	First-principles simulations of the 27Al and 17O solid-state NMR spectra of the CaAl2Si3O10 glass. Highlights in Theoretical Chemistry, 2013, , 87-97.	0.0	0
66	A first step towards the understanding of the 5-HT3 receptor subunit heterogeneity from a computational point of view. Physical Chemistry Chemical Physics, 2012, 14, 12625.	1.3	6
67	Unambiguous Description of the Oxygen Environment in Multicomponent Aluminosilicate Glasses from ¹⁷O Solid State NMR Computational Spectroscopy. Journal of Physical Chemistry C, 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. Journal of Materials Chemistry, 2012, 22, 12599.	6.7	88
69	The extracellular subunit interface of the 5-HT₃receptors: a computational alanine scanning mutagenesis study. Journal of Biomolecular Structure and Dynamics, 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. Chemical Physics Letters, 2012, 541, 12-15.	1.2	18
71	Computational Insights into ADAMTS4, ADAMTS5 and MMP13 Inhibitor Selectivity. Molecular Informatics, 2012, 31, 421-430.	1.4	2
72	First-principles simulations of the 27Al and 17O solid-state NMR spectra of the CaAl2Si3O10 glass. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	34

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73	Modeling the Binding Affinity of p38Î± MAP Kinase Inhibitors by Partial Least Squares Regression. Chemical Biology and Drug Design, 2012, 80, 455-470.	1.5	1
74	Bivalent Ligands for the Serotonin 5-HT₃ Receptor. ACS Medicinal Chemistry Letters, 2011, 2, 571-576.	1.3	14
75	Fluorine Environment in Bioactive Glasses: ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 2038-2045.	1.2	79
76	Insights into MAPK <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si44.gif" overflow="scroll"><mml:mrow><mml:mtext>p</mml:mtext><mml:mn>38</mml:mn><mml:mi>Î±</mml:mi></mml:mrow></mml:math> DFG flip mechanism by accelerated molecular dynamics. Bioorganic and Medicinal Chemistry, 2010, 18, 6805-6812.	1.4	36
77	Computational analysis of ligand recognition sites of homo- and heteropentameric 5-HT3 receptors. European Journal of Medicinal Chemistry, 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. Chemistry of Materials, 2010, 22, 5644-5652.	3.2	131
79	Molecular dynamics simulations of sodium silicate glasses: Optimization and limits of the computational procedure. Computational Materials Science, 2010, 47, 739-751.	1.4	26
80	Multinuclear NMR of CaSiO3 glass: simulation from first-principles. Physical Chemistry Chemical Physics, 2010, 12, 6054.	1.3	71
81	Extension of the AMBER force-field for the study of large nitroxides in condensed phases: an ab initio parameterization. Physical Chemistry Chemical Physics, 2010, 12, 11697.	1.3	74
82	Progress Towards the Identification of New Aggrecanase Inhibitors. Current Medicinal Chemistry, 2009, 16, 2395-2415.	1.2	22
83	Quantitative Structureâ^'Property Relationships of Potentially Bioactive Fluoro Phospho-silicate Glasses. Journal of Physical Chemistry B, 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. Journal of Physical Chemistry C, 2009, 113, 15723-15730.	1.5	99
85	Elastic and dynamical properties of alkali-silicate glasses from computer simulations techniques. Theoretical Chemistry Accounts, 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. Journal of Physical Chemistry C, 2008, 112, 11034-11041.	1.5	89
87	Accurate First-Principle Prediction of ²⁹Si and ¹⁷O NMR Parameters in SiO₂ Polymorphs: The Cases of Zeolites Sigma-2 and Ferrierite. Journal of Chemical Theory and Computation, 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. Chemistry of Materials, 2008, 20, 2522-2531.	3.2	68
89	Molecular Dynamics Studies of Stressâ^'Strain Behavior of Silica Glass under a Tensile Load. Chemistry of Materials, 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. Journal of Non-Crystalline Solids, 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. Journal of Physical Chemistry B, 2008, 112, 12730-12739.	1.2	107
92	Properties of Zinc Releasing Surfaces for Clinical Applications. Journal of Biomaterials Applications, 2008, 22, 505-526.	1.2	52
93	A Combined Experimental-Computational Strategy for the Design, Synthesis and Characterization of Bioactive Zinc-Silicate Glasses. Key Engineering Materials, 2008, 377, 211-224.	0.4	3
94	An ab initio parameterized interatomic force field for hydroxyapatite. Journal of Materials Chemistry, 2007, 17, 2061.	6.7	32
95	Insight into Elastic Properties of Binary Alkali Silicate Glasses; Prediction and Interpretation through Atomistic Simulation Techniques. Chemistry of Materials, 2007, 19, 3144-3154.	3.2	125
96	Crystallization Kinetics of Bioactive Glasses in the ZnOâ^'Na₂Oâ^'CaOâ^'SiO₂ System. Journal of Physical Chemistry A, 2007, 111, 8401-8408.	1.1	20
97	A computational multiscale strategy to the study of amorphous materials. Theoretical Chemistry Accounts, 2007, 117, 933-942.	0.5	32
98	Density of multicomponent silica-based potential bioglasses: Quantitative structure-property relationships (QSPR) analysis. Journal of the European Ceramic Society, 2007, 27, 499-504.	2.8	14
99	A New Self-Consistent Empirical Interatomic Potential Model for Oxides, Silicates, and Silica-Based Glasses. Journal of Physical Chemistry B, 2006, 110, 11780-11795.	1.2	471
100	Towards a quantitative rationalization of multicomponent glass properties by means of molecular dynamics simulations. Molecular Simulation, 2006, 32, 1045-1055.	0.9	20
101	Void size distribution in MD-modelled silica glass structures. Journal of Non-Crystalline Solids, 2006, 352, 285-296.	1.5	70
102	Molecular Interactions Between Human Cytochrome P450 1A2 and Flavone Derivatives. Medicinal Chemistry, 2006, 2, 401-406.	0.7	0
103	Theoretical quantitative structureâ€"activity relationships of flavone ligands interacting with cytochrome P450 1A1 and 1A2 isozymes. Bioorganic and Medicinal Chemistry, 2005, 13, 4366-4374.	1.4	39
104	A Computational Tool for the Prediction of Crystalline Phases Obtained from Controlled Crystallization of Glasses. Journal of Physical Chemistry B, 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. Proteins: Structure, Function and Bioinformatics, 2005, 62, 262-269.	1.5	10
106	Qualitative and Quantitative Structureâ^'Property Relationships Analysis of Multicomponent Potential Bioglasses. Journal of Physical Chemistry B, 2005, 109, 4989-4998.	1.2	98
107	Further Studies on the Interaction of the 5-Hydroxytryptamine3(5-HT3) Receptor with Arylpiperazine Ligands. Development of a New 5-HT3Receptor Ligand Showing Potent Acetylcholinesterase Inhibitory Properties. Journal of Medicinal Chemistry, 2005, 48, 3564-3575.	2.9	64
108	Computational Insight into Anti-mutagenic Properties of CYP1A Flavonoid Ligands. Medicinal Chemistry, 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. Cellular and Molecular Life Sciences, 2004, 61, 1123-1142.	2.4	24
110	A combined experimental and computational approach to (Na2O)1â^'xÂ·CaOÂ·(ZnO)xÂ·2SiO2 glasses characterization. Journal of Non-Crystalline Solids, 2004, 345-346, 710-714.	1.5	22
111	Design, Synthesis, Structural Studies, Biological Evaluation, and Computational Simulations of Novel Potent AT1Angiotensin II Receptor Antagonists Based on the 4-Phenylquinoline Structure. Journal of Medicinal Chemistry, 2004, 47, 2574-2586.	2.9	75
112	Seeking for binding determinants of the prion protein to human plasminogen. Molecular Physics, 2003, 101, 2763-2773.	0.8	1
113	Development of an IL-6 antagonist peptide that induces apoptosis in 7TD1 cells. Peptides, 2003, 24, 1207-1220.	1.2	14
114	Synthesis, Biological Evaluation, and Receptor Docking Simulations of 2-[(Acylamino)ethyl]-1,4-benzodiazepines as Î¹-Opioid Receptor Agonists Endowed with Antinociceptive and Antiamnesic Activity. Journal of Medicinal Chemistry, 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. Molecular Physics, 2003, 101, 2731-2741.	0.8	4
116	Experimental Versus Computer Simulation Analysis of Zirconia Containing Glasses. Key Engineering Materials, 2002, 206-213, 2101-2104.	0.4	0
117	Synthesis, Characterization, and Molecular Dynamics Simulation Of Na2Oâ^'CaOâ^'SiO2â^'ZnO Glasses. Journal of Physical Chemistry B, 2002, 106, 9753-9760.	1.2	76
118	Novel Potent 5-HT3 Receptor Ligands Based on the Pyrrolidone Structure: Synthesis, Biological Evaluation, and Computational Rationalization of the Ligandâ€"Receptor Interaction Modalities. Bioorganic and Medicinal Chemistry, 2002, 10, 779-801.	1.4	36
119	Novel potent 5-HT3 receptor ligands based on the pyrrolidone structure. effects of the quaternization of the basic nitrogen on the interaction with 5-HT3 receptor. Bioorganic and Medicinal Chemistry, 2002, 10, 2681-2691.	1.4	9
120	Theoretical descriptors for the quantitative rationalisation of plastocyanin mutant functional propertiess. Journal of Computer-Aided Molecular Design, 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 Ligandâ^'Receptor Interaction Modeling. Journal of Medicinal Chemistry, 2001, 44, 1134-1150.	2.9	68
122	Electrostatic Analysis and Brownian Dynamics Simulation of the Association of Plastocyanin and Cytochrome F. Biophysical Journal, 2001, 81, 3090-3104.	0.2	80
123	Influence of Small Additions of Al2O3 on the Properties of the Na2OÂ·3SiO2 Glass. Journal of Physical Chemistry B, 2001, 105, 919-927.	1.2	25
124	Control of Metalloprotein Reduction Potential:Â The Role of Electrostatic and Solvation Effects Probed on Plastocyanin Mutantsâ€. Biochemistry, 2001, 40, 6422-6430.	1.2	44
125	A computational model of the 5-HT 3 receptor extracellular domain: search for ligand binding sites. Theoretical Chemistry Accounts, 2001, 106, 98-104.	0.5	14
126	Title is missing!. Journal of Solution Chemistry, 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 structureâ€“activity relationship analysis of Î±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 Structureâ^'Activity Relationship and Quantitative Structureâ^'Activity Relationship Studies on Novel Derivatives of 2,4-Diamino-6,7-dimethoxyquinazoline Î±1-Adrenoceptor Antagonists. Journal of Medicinal Chemistry, 1999, 42, 427-437.	2.9	20
135	Novel Potent and Selective Central 5-HT3Receptor Ligands Provided with Different Intrinsic Efficacy. 2. Molecular Basis of the Intrinsic Efficacy of Arylpiperazine Derivatives at the Central 5-HT3Receptors. Journal of Medicinal Chemistry, 1999, 42, 1556-1575.	2.9	37
136	Theoretical descriptors in quantitative structureâ€“affinity and selectivity relationship study of potent N4-substituted arylpiperazine 5-HT1A receptor antagonists. Bioorganic and Medicinal Chemistry, 1998, 6, 535-550.	1.4	20
137	Computer Modeling of Size and Shape Descriptors of Î±1-Adrenergic Receptor Antagonists and Quantitative Structureâ€“Affinity/Selectivity Relationships. Methods, 1998, 14, 239-254.	1.9	14
138	Ab InitioModeling and Molecular Dynamics Simulation of the Î±1b-Adrenergic Receptor Activation. Methods, 1998, 14, 302-317.	1.9	38
139	Novel Potent and Selective Central 5-HT3Receptor Ligands Provided with Different Intrinsic Efficacy. 1. Mapping the Central 5-HT3Receptor Binding Site by Arylpiperazine Derivatives. Journal of Medicinal Chemistry, 1998, 41, 728-741.	2.9	73
140	Conformational analysis and theoretical quantitative size and shape-affinity relationships of N4-protonated N1-arylpiperazine 5-HT1A serotoninergic ligands. Computational and Theoretical Chemistry, 1997, 397, 129-145.	1.5	11
141	Mapping the Peripheral Benzodiazepine Receptor Binding Site by Conformationally Restrained Derivatives of 1-(2-Chlorophenyl)-N-methyl-N-(1-methylpropyl)-3-isoquinolinecarboxamide (PK11195). Journal of Medicinal Chemistry, 1997, 40, 2910-2921.	2.9	51
142	Î±1-Adrenoceptor subtype selectivity: Molecular modelling and theoretical quantitative structureâ€”affinity relationships. Bioorganic and Medicinal Chemistry, 1997, 5, 809-816.	1.4	27
143	Theoretical investigation of IL-6 multiprotein receptor assembly. , 1997, 29, 528-548.		9
144	Synthesis, Biological Evaluation, and Quantitative Receptor Docking Simulations of 2-[(Acylamino)ethyl]-1,4-benzodiazepines as Novel Tifluadom-like Ligands with High Affinity and Selectivity for Îº-Opioid Receptors1. Journal of Medicinal Chemistry, 1996, 39, 860-872.	2.9	42

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145	Computational simulations of stem-cell factor/c-Kit receptor interaction. , 1996, 26, 42-54.		2
146	Molecular structure and dynamics of some potent 5-HT 3 receptor antagonists. Insight into the interaction with the receptor. Bioorganic and Medicinal Chemistry, 1996, 4, 1255-1269.	1.4	20
147	Molecular dynamics simulations of m3-muscarinic receptor activation and QSAR analysis. Bioorganic and Medicinal Chemistry, 1995, 3, 1465-1477.	1.4	20
148	Theoretical quantitative structure-activity relationship analysis of congeneric and non-congeneric Î±1-adrenoceptor antagonists: a chemometric study. Computational and Theoretical Chemistry, 1995, 331, 79-93.	1.5	26
149	Quantitative structure-affinity/selectivity relationship analysis on three-dimensional models of the complexes between the ETA and ETB receptors and C-terminal endothelin hexapeptide antagonists. Computational and Theoretical Chemistry, 1995, 333, 243-248.	1.5	5
150	Comparative molecular dynamics study of the seven-helix bundle arrangement of G-protein coupled receptors. Computational and Theoretical Chemistry, 1995, 333, 49-69.	1.5	18
151	Prototropic molecular forms and theoretical descriptors in QSAR analysis. Computational and Theoretical Chemistry, 1995, 333, 1-17.	1.5	11
152	Computer simulations of signal transduction mechanism in Î±1B-adrenergic and m3-muscarinic receptors. Protein Engineering, Design and Selection, 1995, 8, 557-564.	1.0	20
153	Theoretical quantitative structureâ€"activity relationship analysis on three dimensional models of ligandâ€"m1 muscarinic receptor complexes. Bioorganic and Medicinal Chemistry, 1994, 2, 195-211.	1.4	23
154	The heuristic-direct approach to theoretical quantitative structure-activity relationship analysis of Î±1-adrenoceptor ligands. Computational and Theoretical Chemistry, 1994, 314, 265-276.	1.5	13
155	Theoretical quantitative size and shape activity and selectivity analyses of 5-HT1A serotonin and Î±1-adrenergic receptor ligands. Computational and Theoretical Chemistry, 1994, 305, 101-110.	1.5	16
156	Theoretical quantitative structure-activity analysis and pharmacophore modelling of selective non-congeneric Î±1a-adrenergic antagonists. Computational and Theoretical Chemistry, 1993, 280, 283-290.	1.5	14
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