Maria Cristina Menziani

List of Publications by Year
in descending order

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	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
2	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
3	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
4	Molecular Dynamics Studies of Stressâ^'Strain Behavior of Silica Glass under a Tensile Load. Chemistry of Materials, 2008, 20, 4356-4366.	3.2	121
5	Evidence of Catalase Mimetic Activity in Ce³⁺/Ce⁴⁺ Doped Bioactive Glasses. Journal of Physical Chemistry B, 2015, 119, 4009-4019.	1.2	119
6	Blue copper proteins: A comparative analysis of their molecular interaction properties. Protein Science, 2000, 9, 1439-1454.	3.1	109
7	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
8	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
9	Qualitative and Quantitative Structureâ^'Property Relationships Analysis of Multicomponent Potential Bioglasses. Journal of Physical Chemistry B, 2005, 109, 4989-4998.	1.2	98
10	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
11	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
12	Site-Selective Surface-Enhanced Raman Detection of Proteins. ACS Nano, 2017, 11, 918-926.	7.3	85
13	Computational simulations of solid state NMR spectra: a new era in structure determination of oxide glasses. RSC Advances, 2013, 3, 10550.	1.7	81
14	Electrostatic Analysis and Brownian Dynamics Simulation of the Association of Plastocyanin and Cytochrome F. Biophysical Journal, 2001, 81, 3090-3104.	0.2	80
15	Quantitative Structureâ^'Property Relationships of Potentially Bioactive Fluoro Phospho-silicate Glasses. Journal of Physical Chemistry B, 2009, 113, 10331-10338.	1.2	80
16	Fluorine Environment in Bioactive Glasses: ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 2038-2045.	1.2	79
17	Synthesis, Characterization, and Molecular Dynamics Simulation Of Na2Oâ^'CaOâ^'SiO2â^'ZnO Glasses. Journal of Physical Chemistry B, 2002, 106, 9753-9760.	1.2	76
18	Competitive Binding of Proteins to Gold Nanoparticles Disclosed by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 22172-22180.	1.5	76

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19	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
20	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
21	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
22	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
23	Multinuclear NMR of CaSiO3 glass: simulation from first-principles. Physical Chemistry Chemical Physics, 2010, 12, 6054.	1.3	71
24	Void size distribution in MD-modelled silica glass structures. Journal of Non-Crystalline Solids, 2006, 352, 285-296.	1.5	70
25	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
26	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
27	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
28	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
29	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
30	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
31	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
32	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
33	Properties of Zinc Releasing Surfaces for Clinical Applications. Journal of Biomaterials Applications, 2008, 22, 505-526.	1.2	52
34	Understanding Aggregation-Induced Emission in Molecular Crystals: Insights from Theory. Journal of Physical Chemistry C, 2017, 121, 5747-5752.	1.5	52
35	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
36	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

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37	A closer look into the ubiquitin corona on gold nanoparticles by computational studies. New Journal of Chemistry, 2015, 39, 2474-2482.	1.4	49
38	The binding of benzenesulfonamides to carbonic anhydrase enzyme. A molecular mechanics study and quantitative structure-activity relationships. Journal of Medicinal Chemistry, 1989, 32, 951-956.	2.9	45
39	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
40	Elastic and dynamical properties of alkali-silicate glasses from computer simulations techniques. Theoretical Chemistry Accounts, 2008, 120, 557-564.	0.5	44
41	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
42	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
43	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
44	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
45	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
46	Ab InitioModeling and Molecular Dynamics Simulation of the Î±1b-Adrenergic Receptor Activation. Methods, 1998, 14, 302-317.	1.9	38
47	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
48	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
49	Synthesis, Characterization, and Selective Delivery of DARPinâ€“Gold Nanoparticle Conjugates to Cancer Cells. Bioconjugate Chemistry, 2017, 28, 2569-2574.	1.8	37
50	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
51	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:mat DFG flip mechanism by accelerated molecular dynamics. Bioorganic and Medicinal Chemistry, 2010, 18, 6805-6812.	1.4	36
52	Multiscale Molecular Dynamics Simulation of Multiple Protein Adsorption on Gold Nanoparticles. International Journal of Molecular Sciences, 2019, 20, 3539.	1.8	36
53	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
54	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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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	A DFT Approach to the Surface-Enhanced Raman Scattering of 4-Cyanopyridine Adsorbed on Silver Nanoparticles. Nanomaterials, 2019, 9, 1211.	1.9	33
57	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
58	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
59	An ab initio parameterized interatomic force field for hydroxyapatite. Journal of Materials Chemistry, 2007, 17, 2061.	6.7	32
60	A computational multiscale strategy to the study of amorphous materials. Theoretical Chemistry Accounts, 2007, 117, 933-942.	0.5	32
61	Theoretical study of the electrostatically driven step of receptor-G protein recognition. , 1999, 37, 145-156.		31
62	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
63	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
64	Theoretical versus empirical molecular descriptors in monosubstituted benzenes. Chemometrics and Intelligent Laboratory Systems, 1992, 14, 209-224.	1.8	28
65	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
66	Î±1-Adrenoceptor subtype selectivity: Molecular modelling and theoretical quantitative structureâ€”affinity relationships. Bioorganic and Medicinal Chemistry, 1997, 5, 809-816.	1.4	27
67	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
68	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
69	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
70	Molecular dynamics simulations of sodium silicate glasses: Optimization and limits of the computational procedure. Computational Materials Science, 2010, 47, 739-751.	1.4	26
71	Modeling emission features of salicylidene aniline molecular crystals: A QM/QMâ€™ approach. Journal of Computational Chemistry, 2016, 37, 861-870.	1.5	26
72	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

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73	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
74	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
75	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
76	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
77	Oxalyl dihydrazide polymorphism: a periodic dispersion-corrected DFT and MP2 investigation. CrystEngComm, 2014, 16, 102-109.	1.3	23
78	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
79	Progress Towards the Identification of New Aggrecanase Inhibitors. Current Medicinal Chemistry, 2009, 16, 2395-2415.	1.2	22
80	Computational Insights into the Binding of Monolayer-Capped Gold Nanoparticles onto Amyloid-Î² Fibrils. ACS Chemical Neuroscience, 2020, 11, 3153-3160.	1.7	22
81	Quantitative structure-activity analysis in dihydropteroate synthase inhibition of sulfones. Comparison with sulfanilamides. Journal of Medicinal Chemistry, 1987, 30, 459-464.	2.9	21
82	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
83	Conformational analysis, molecular modeling and quantitative structure-activity relationship studies of 2,4-diamino-6,7-dimethoxy-2-substituted quinazoline Î±1-adrenergic antagonists. Computational and Theoretical Chemistry, 1991, 251, 307-318.	1.5	20
84	Molecular modelling and quantitative structure- activity relationship analysis using theoretical descriptors of 1,4-benzodioxan (WB-4101) related compounds Î±1-adrenergic antagonists. Computational and Theoretical Chemistry, 1992, 276, 327-340.	1.5	20
85	Molecular dynamics simulations of m3-muscarinic receptor activation and QSAR analysis. Bioorganic and Medicinal Chemistry, 1995, 3, 1465-1477.	1.4	20
86	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
87	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
88	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
89	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
90	Towards a quantitative rationalization of multicomponent glass properties by means of molecular dynamics simulations. Molecular Simulation, 2006, 32, 1045-1055.	0.9	20

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91	Crystallization Kinetics of Bioactive Glasses in the ZnOâˆ’Na₂Oâˆ’CaOâˆ’SiO₂ System. Journal of Physical Chemistry A, 2007, 111, 8401-8408.	1.1	20
92	Local versus Average Structure in LaSrAl₃O₇: A NMR and DFT Investigation. Journal of Physical Chemistry C, 2013, 117, 23451-23458.	1.5	20
93	On the opto-electronic properties of phosphine and thiolate-protected undecagold nanoclusters. Physical Chemistry Chemical Physics, 2014, 16, 18749-18758.	1.3	19
94	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
95	The heuristic-direct approach to quantitative structure-activity relationship analysis. Computational and Theoretical Chemistry, 1993, 285, 147-153.	1.5	18
96	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
97	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
98	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
99	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
100	DARPin_9-29-Targeted Mini Gold Nanorods Specifically Eliminate HER2-Overexpressing Cancer Cells. ACS Applied Materials & Interfaces, 2019, 11, 34645-34651.	4.0	18
101	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
102	Disclosing crystal nucleation mechanism in lithium disilicate glass through molecular dynamics simulations and free-energy calculations. Scientific Reports, 2020, 10, 17867.	1.6	18
103	Molecular orbital study of the nitrogen basicity of prazosin analogues in relation to their Î±1-adrenoceptor binding affinity. Computational and Theoretical Chemistry, 1991, 233, 343-351.	1.5	16
104	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
105	Molecular Dynamics Simulations of Alumina Addition in Sodium Silicate Glasses. Molecular Simulation, 2000, 24, 157-165.	0.9	16
106	Dendrimeric tetravalent ligands for the serotonin-gated ion channel. Chemical Communications, 2014, 50, 8582.	2.2	16
107	Structure of active cerium sites within bioactive glasses. Journal of the American Ceramic Society, 2017, 100, 5086-5095.	1.9	16
108	Novel Petâ€Đegrading Enzymes: Structureâ€Function from a Computational Perspective. ChemBioChem, 2021, 22, 2032-2050.	1.3	16

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109	Molecular mechanics and quantum chemical qsar analysis in carbonic anhydrase-heterocyclic sulfonamide interactions. Structural Chemistry, 1992, 3, 215-219.	1.0	15
110	Arylsulfonyl Groups: The Best Cyclization Auxiliaries for the Preparation of ATRC Î³â€Ł actams can be Acidolytically Removed. European Journal of Organic Chemistry, 2014, 2014, 6734-6745.	1.2	15
111	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
112	Computational Modeling of Silicate Glasses: A Quantitative Structure-Property Relationship Perspective. Springer Series in Materials Science, 2015, , 113-135.	0.4	15
113	QSAR Analysis in 2,4-Diamino-6,7-dimethoxy Quinoline Derivatives Ã¢Â€Â“ ÃŽÂ±1-Adrenoceptor Antagonists Ã¢Â€Â“ Using the Partial Least Squares (PLS) Method and Theoretical Molecular Descriptors. QSAR and Combinatorial Science, 1990, 9, 340-345.	1.4	14
114	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
115	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
116	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
117	Development of an IL-6 antagonist peptide that induces apoptosis in 7TD1 cells. Peptides, 2003, 24, 1207-1220.	1.2	14
118	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
119	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
120	Bivalent Ligands for the Serotonin 5-HT₃ Receptor. ACS Medicinal Chemistry Letters, 2011, 2, 571-576.	1.3	14
121	Exploring a potential palonosetron allosteric binding site in the 5-HT3 receptor. Bioorganic and Medicinal Chemistry, 2013, 21, 7523-7528.	1.4	14
122	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
123	Toward the understanding of crystallization, mechanical properties and reactivity of multicomponent bioactive glasses. Acta Materialia, 2021, 213, 116977.	3.8	14
124	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
125	Rational drug design: binding free energy differences of carbonic anhydrase inhibitors. Journal of the Chemical Society Chemical Communications, 1989, , 853.	2.0	12
126	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

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127	Improved empirical force field for multicomponent oxide glasses and crystals. Physical Review Materials, 2021, 5, .	0.9	12
128	Quantitative structure-activity relationships in dihydropteroate synthase inhibition by multisubstituted sulfones. Design and synthesis of some new derivatives with improved potency. Journal of Medicinal Chemistry, 1989, 32, 2396-2399.	2.9	11
129	Theoretical quantitative structure-activity analysis of quinuclidine-based muscarinic cholinergic receptor ligands. Computational and Theoretical Chemistry, 1993, 283, 63-71.	1.5	11
130	Prototropic molecular forms and theoretical descriptors in QSAR analysis. Computational and Theoretical Chemistry, 1995, 333, 1-17.	1.5	11
131	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
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	Unraveling the Polymorphism of [(p-cymene)Ru(ºN-INA)Cl₂] through Dispersion-Corrected DFT and NMR GIPAW Calculations. Inorganic Chemistry, 2014, 53, 7926-7935.	1.9	11
134	Crystal and molecular structure of bis(2-amino-5-methyl-1,3,4-thiadiazole-N 3)dibromomercury(II). A spectroscopic study and INDO calculations. Journal of the Chemical Society Dalton Transactions, 1988, , 1075.	1.1	10
135	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
136	Theoretical investigation of IL-6 multiprotein receptor assembly. , 1997, 29, 528-548.		9
137	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
138	The antioxidant properties of Ce-containing bioactive glass nanoparticles explained by Molecular Dynamics simulations. Biomedical Glasses, 2016, 2, .	2.4	9
139	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
140	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
141	Title is missing!. Journal of Solution Chemistry, 2001, 30, 149-169.	0.6	8
142	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
143	Nanoreactors for the multi-functionalization of poly-histidine fragments. New Journal of Chemistry, 2019, 43, 6834-6837.	1.4	8
144	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

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145	Exploring the crystallization path of lithium disilicate through metadynamics simulations. Physical Review Materials, 2021, 5, .	0.9	8
146	Electronic and electrostatic aspects of carbonic anhydrase inhibition by sulphonamides. Computational and Theoretical Chemistry, 1992, 256, 217-229.	1.5	7
147	The ad hoc supermolecule approach to receptor ligand design. Computational and Theoretical Chemistry, 2000, 503, 1-16.	1.5	7
148	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
149	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
150	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
151	Reducibility of Ag- and Cu-Modified Ultrathin Epitaxial Cerium Oxide Films. Journal of Physical Chemistry C, 2019, 123, 13702-13711.	1.5	6
152	Multinuclear NMR and vibrational spectroscopy studies of the substituent effects in benzensulphonamide inhibitors of the enzyme carbonic anhydrase. Journal of Molecular Structure, 1988, 175, 37-42.	1.8	5
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