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List of Publications by Year
in descending order

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63	743	567144	677027
papers	citations	15 h-index	22 g-index

64	64	64	1044
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Polyamidoamine dendrimers of the third generationâ€“chlorin e6 nanoconjugates: Nontoxic hybrid polymers with photodynamic activity. Journal of Applied Polymer Science, 2022, 139, 51835.	1.3	5
2	Microcystins Detection Methods: A Focus on Recent Advances Using Molecularly Imprinted Polymers. Analytical Chemistry, 2022, 94, 464-478.	3.2	14
3	Copper metallic nanoparticles capped with PEGylated PAMAM-G3 dendrimers for the catalytic reduction of low solubility nitroarenes of pharmaceutical interest. Catalysis Today, 2021, 372, 27-35.	2.2	5
4	NanoMIPs Design for Fucose and Mannose Recognition: A Molecular Dynamics Approach. Journal of Chemical Information and Modeling, 2021, 61, 2048-2061.	2.5	6
5	Efficient and recyclable gold nanoparticles as catalysts for the cleaner production of 4-morpholinoanilines used as pharmaceutical building blocks. Journal of Cleaner Production, 2021, 290, 125761.	4.6	3
6	Rational Design of Novel Glycomimetic Peptides for E-Selectin Targeting. Journal of Chemical Information and Modeling, 2021, 61, 2463-2474.	2.5	5
7	On the Microtubule-Stabilizing Properties of a Tau Oligopeptide. Journal of Chemical Information and Modeling, 2021, 61, 5682-5691.	2.5	5
8	In Silico Design of Novel Mutant Anti-MUC1 Aptamers for Targeted Cancer Therapy. Journal of Chemical Information and Modeling, 2020, 60, 786-793.	2.5	17
9	Rational Design and In Vitro Evaluation of Novel Peptides Binding to Neuroligin-1 for Synaptic Targeting. Journal of Chemical Information and Modeling, 2020, 60, 995-1004.	2.5	2
10	Catalytic Role of Gln202 in the Carboligation Reaction Mechanism of Yeast AHAS: A QM/MM Study. Journal of Chemical Information and Modeling, 2020, 60, 915-922.	2.5	6
11	Interdimeric Curvature in Tubulinâ€“Tubulin Complexes Delineates the Microtubule-Destabilizing Properties of Plocabulin. Journal of Chemical Information and Modeling, 2020, 60, 4076-4084.	2.5	4
12	Polyamidoamine-based nanovector for the efficient delivery of methotrexate to U87 glioma cells. Nanomedicine, 2020, 15, 2771-2784.	1.7	9
13	Stereospecific Inhibition of Ethanol Potentiation on Glycine Receptor by M554 Stereoisomers. Journal of Chemical Information and Modeling, 2020, 60, 6634-6641.	2.5	0
14	Visible-light-responsive folate-conjugated titania and alumina nanotubes for photodynamic therapy applications. Journal of Materials Science, 2020, 55, 6976-6991.	1.7	5
15	Host-guest complexation of curcumin and coumarin 6 with PAMAM-OH: Insight from fluorescence spectroscopy and molecular dynamics simulations. Journal of Luminescence, 2020, 222, 117182.	1.5	8
16	Mechanism-Based Rational Discovery and In Vitro Evaluation of Novel Microtubule Stabilizing Agents with Non-Taxol-Competitive Activity. Journal of Chemical Information and Modeling, 2020, 60, 3204-3213.	2.5	6
17	The role of conserved arginine in the GH70 family: a computational study of the structural features and their implications on the catalytic mechanism of GTF-SI from Streptoccocus mutans. Organic and Biomolecular Chemistry, 2019, 17, 6269-6276.	1.5	7
18	Molecular modeling simulation studies reveal new potential inhibitors against HPV E6 protein. PLoS ONE, 2019, 14, e0213028.	1.1	31

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19	Molecular modeling study on the differential microtubuleâ€stabilizing effect in singlyâ€and doublyâ€bonded complexes with peloruside A and paclitaxel. Proteins: Structure, Function and Bioinformatics, 2019, 87, 668-678.	1.5	6
20	Modulation of glucanâ€enzyme interactions by domain V in GTFâ€SI from Streptococcus mutans. Proteins: Structure, Function and Bioinformatics, 2019, 87, 74-80.	1.5	7
21	A QM/MM approach on the structural and stereoelectronic factors governing glycosylation by GTF-SI fromStreptococcus mutans. Organic and Biomolecular Chemistry, 2018, 16, 2438-2447.	1.5	14
22	Gold catalysts supported on TiO 2 -nanotubes for the selective hydrogenation of p -substituted nitrobenzenes. Molecular Catalysis, 2018, 447, 21-27.	1.0	38
23	Modulation of lateral and longitudinal interdimeric interactions in microtubule models by Laulimalide and Peloruside A association: A molecular modeling approach on the mechanism of microtubule stabilizing agents. Chemical Biology and Drug Design, 2018, 91, 1042-1055.	1.5	7
24	Effect of pH on Eosin Y/PAMAM interactions studied from absorption spectroscopy and molecular dynamics simulations. Journal of Luminescence, 2018, 199, 258-265.	1.5	11
25	Partially PEGylated PAMAM dendrimers as solubility enhancers of Silybin. Pharmaceutical Development and Technology, 2018, 23, 689-696.	1.1	32
26	Cytotoxicity and in vivo plasma kinetic behavior of surface-functionalized PAMAM dendrimers. Nanomedicine: Nanotechnology, Biology, and Medicine, 2018, 14, 2227-2234.	1.7	27
27	Polyamido amine (PAMAM)-grafted magnetic nanotubes as emerging platforms for the delivery and sustained release of silibinin. Journal of Materials Science, 2017, 52, 9269-9281.	1.7	12
28	Molecular modeling study on the tubulinâ€binding modes of epothilone derivatives: Insight into the structural basis for epothilones activity. Chemical Biology and Drug Design, 2017, 90, 1247-1259.	1.5	3
29	Structural insight into the role of Gln293Met mutation on the Peloruside A/Laulimalide association with Î±Î²-tubulin from molecular dynamics simulations, binding free energy calculations and weak interactions analysis. Journal of Computer-Aided Molecular Design, 2017, 31, 643-652.	1.3	11
30	Association of Methotrexate with Native and PEGylated PAMAM-G4 Dendrimers: Effect of the PEGylation Degree on the Drug-Loading Capacity and Preferential Binding Sites. Journal of Physical Chemistry B, 2017, 121, 4-12.	1.2	21
31	Binding free energy calculations on Eâ€selectin complexes with <scp>sL</scp>e^x oligosaccharide analogs. Chemical Biology and Drug Design, 2017, 89, 114-123.	1.5	8
32	Methotrexate Complexation with Native and PEGylated PAMAMâ€G4: Effect of the PEGylation Degree on the Drug Loading Capacity and Release Kinetics. Macromolecular Chemistry and Physics, 2016, 217, 605-613.	1.1	18
33	PAMAMâ€Conjugated Alumina Nanotubes as Novel Noncytotoxic Nanocarriers with Enhanced Drug Loading and Releasing Performances. Macromolecular Chemistry and Physics, 2016, 217, 1712-1722.	1.1	11
34	PAMAM-grafted TiO2 nanotubes as novel versatile materials for drug delivery applications. Materials Science and Engineering C, 2016, 65, 164-171.	3.8	38
35	Reversal of Ethanol-induced Intoxication by a Novel Modulator of GÎ²Î³ Protein Potentiation of the Glycine Receptor. Journal of Biological Chemistry, 2016, 291, 18791-18798.	1.6	6
36	Discovery of New Eâ€Selectin Inhibitors by Virtual Screening, Fluorescence Binding Assays, and STD NMR Experiments. ChemMedChem, 2016, 11, 1008-1014.	1.6	5

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37	Effect of PEGylation on the Structure and Drug Loading Capacity of PAMAM-G4 Dendrimers: A Molecular Modeling Approach on the Complexation of 5-Fluorouracil with Native and PEGylated PAMAM-G4. Macromolecular Chemistry and Physics, 2015, 216, 1689-1701.	1.1	25
38	Structural insight into epothilones antitumor activity based on the conformational preferences and tubulin binding modes of epothilones A and B obtained from molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2015, 33, 789-803.	2.0	6
39	Structural basis for drug resistance conferred by Î²-tubulin mutations: a molecular modeling study on native and mutated tubulin complexes with epothilone B. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2530-2540.	2.0	7
40	INNOVATIVE USE OF A TABLET DEVICE TO DELIVER INSTRUCTION IN UNDERGRADUATE CHEMISTRY LECTURES. Quimica Nova, 2015, , .	0.3	1
41	Complexation of Mefenamic Acid by Lowâ€Generation PAMAM Dendrimers: Insight from NMR Spectroscopy Studies and Molecular Dynamics Simulations. Macromolecular Chemistry and Physics, 2014, 215, 372-383.	1.1	13
42	Drug-dendrimer supramolecular complexation studied from molecular dynamics simulations and NMR spectroscopy. Structural Chemistry, 2014, 25, 1443-1455.	1.0	13
43	Inhibition of the Ethanol-induced Potentiation of Î±1 Glycine Receptor by a Small Peptide That Interferes with GÎ²Î³ Binding. Journal of Biological Chemistry, 2012, 287, 40713-40721.	1.6	16
44	Convenient synthesis and characterization of molecules containing multiple Î²-keto ester units. Tetrahedron Letters, 2012, 53, 4984-4988.	0.7	4
45	Synthesis and properties of new liquid crystals derivatives of 2,7-diethynyl-9,9-dihexylfluorene. Liquid Crystals, 2012, 39, 847-856.	0.9	7
46	Scaling trend in diffusion coefficients of low generation G0â€“G3 PAMAM dendrimers in aqueous solution at high and neutral pH. Structural Chemistry, 2012, 23, 123-128.	1.0	17
47	Diffusion coefficients of first-generation polyamidoamine dendrimer and its Î²-cyclodextrin conjugate in aqueous solution by means of molecular dynamics simulations. Monatshefte FÃ¼r Chemie, 2012, 143, 29-35.	0.9	2
48	Inhibitory Activities on Mammalian Central Nervous System Receptors and Computational Studies of Three Sesquiterpene Lactones from Coriaria ruscifolia subsp. ruscifolia. Chemical and Pharmaceutical Bulletin, 2011, 59, 161-165.	0.6	8
49	A QM/MM study on the last two steps of the catalytic cycle of acetohydroxyacid synthase. Computational and Theoretical Chemistry, 2011, 966, 159-166.	1.1	11
50	Computational study on the carboligation reaction of acetohidroxyacid synthase: New approach on the role of the HEThDP^{â^’} intermediate. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1774-1788.	1.5	16
51	Quantum-Chemical Study on the Bioactive Conformation of Epothilones. Journal of Chemical Information and Modeling, 2010, 50, 2176-2190.	2.5	6
52	Theoretical approach to the out-of-plane deformation of 1,3-disubstituted azulenes. Structural Chemistry, 2009, 20, 677-684.	1.0	3
53	Novel amides and Schiff's bases derived from 1,3,4-oxadiazole derivatives: synthesis and mesomorphic behaviour. Liquid Crystals, 2009, 36, 301-317.	0.9	26
54	Hartreeâ^’Fock and Density Functional Theory Study of Î±-Cyclodextrin Conformers. Journal of Physical Chemistry A, 2008, 112, 678-685.	1.1	14

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55	Correlation Models for the Inclusion Complexation of Aliphatic Compounds with Î±- and Î²-Cyclodextrins. Supramolecular Chemistry, 2008, 20, 317-325.	1.5	2
56	Complete basis set calculations on the tautomerism and protonation of triazoles and tetrazole. Computational and Theoretical Chemistry, 2006, 775, 1-7.	1.5	43
57	â€œOn the complexation of allopurinol with Î²-cyclodextrinâ€• Structural Chemistry, 2006, 17, 217-223.	1.0	3
58	Theoretical calculations on the tautomerism of uric acid in gas phase and aqueous solution. Computational and Theoretical Chemistry, 2005, 755, 209-214.	1.5	21
59	The role of charge transfer interactions in the inclusion complexation of anionic guests with Î±-cyclodextrin. Tetrahedron, 2005, 61, 5449-5456.	1.0	13
60	Inclusion Complexation of Phenol Derivatives with a Î²-Cyclodextrin Based Polymer. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2005, 53, 63-68.	1.6	13
61	Determination of the Association Constant of 6-Thiopurine and Chitosan GraftedÂ-Cyclodextrin. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2003, 47, 71-75.	1.6	9
62	Esters derived from 7-decanoyloxychromone-3-carboxylic acid: synthesis and mesomorphic properties. Liquid Crystals, 2003, 30, 1319-1325.	0.9	18
63	Hydrogen-bonded complexes between mesogenic heterocyclic Schiff's bases and mesogenic 4- n -nonyloxybenzoic acid: mesomorphic behaviour, FTIR study and PM3 semi-empirical calculations. Liquid Crystals, 2003, 30, 297-304.	0.9	13