

Verónica A Jiménez

List of Publications by Year in descending order

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63
papers

743
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567144

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64
all docs

64
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64
times ranked

1044
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#	ARTICLE	IF	CITATIONS
1	Complete basis set calculations on the tautomerism and protonation of triazoles and tetrazole. <i>Computational and Theoretical Chemistry</i> , 2006, 775, 1-7.	1.5	43
2	PAMAM-grafted TiO ₂ nanotubes as novel versatile materials for drug delivery applications. <i>Materials Science and Engineering C</i> , 2016, 65, 164-171.	3.8	38
3	Gold catalysts supported on TiO ₂ -nanotubes for the selective hydrogenation of p -substituted nitrobenzenes. <i>Molecular Catalysis</i> , 2018, 447, 21-27.	1.0	38
4	Partially PEGylated PAMAM dendrimers as solubility enhancers of Silybin. <i>Pharmaceutical Development and Technology</i> , 2018, 23, 689-696.	1.1	32
5	Molecular modeling simulation studies reveal new potential inhibitors against HPV E6 protein. <i>PLoS ONE</i> , 2019, 14, e0213028.	1.1	31
6	Cytotoxicity and in vivo plasma kinetic behavior of surface-functionalized PAMAM dendrimers. <i>Nanomedicine: Nanotechnology, Biology, and Medicine</i> , 2018, 14, 2227-2234.	1.7	27
7	Novel amides and Schiff's bases derived from 1,3,4-oxadiazole derivatives: synthesis and mesomorphic behaviour. <i>Liquid Crystals</i> , 2009, 36, 301-317.	0.9	26
8	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. <i>Macromolecular Chemistry and Physics</i> , 2015, 216, 1689-1701.	1.1	25
9	Theoretical calculations on the tautomerism of uric acid in gas phase and aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2005, 755, 209-214.	1.5	21
10	Association of Methotrexate with Native and PEGylated PAMAM-G4 Dendrimers: Effect of the PEGylation Degree on the Drug-Loading Capacity and Preferential Binding Sites. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4-12.	1.2	21
11	Esters derived from 7-decanoyloxychromone-3-carboxylic acid: synthesis and mesomorphic properties. <i>Liquid Crystals</i> , 2003, 30, 1319-1325.	0.9	18
12	Methotrexate Complexation with Native and PEGylated PAMAM-G4: Effect of the PEGylation Degree on the Drug Loading Capacity and Release Kinetics. <i>Macromolecular Chemistry and Physics</i> , 2016, 217, 605-613.	1.1	18
13	Scaling trend in diffusion coefficients of low generation G0-G3 PAMAM dendrimers in aqueous solution at high and neutral pH. <i>Structural Chemistry</i> , 2012, 23, 123-128.	1.0	17
14	<i>In Silico</i> Design of Novel Mutant Anti-MUC1 Aptamers for Targeted Cancer Therapy. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 786-793.	2.5	17
15	Computational study on the carbonylation reaction of acetohydroxyacid synthase: New approach on the role of the HETHP ⁺ intermediate. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1774-1788.	1.5	16
16	Inhibition of the Ethanol-induced Potentiation of $\hat{1}$ Glycine Receptor by a Small Peptide That Interferes with $\hat{2}$ Binding. <i>Journal of Biological Chemistry</i> , 2012, 287, 40713-40721.	1.6	16
17	Hartree-Fock and Density Functional Theory Study of $\hat{1}$ -Cyclodextrin Conformers. <i>Journal of Physical Chemistry A</i> , 2008, 112, 678-685.	1.1	14
18	A QM/MM approach on the structural and stereoelectronic factors governing glycosylation by GTF-SI from <i>Streptococcus mutans</i> . <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 2438-2447.	1.5	14

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19	Microcystins Detection Methods: A Focus on Recent Advances Using Molecularly Imprinted Polymers. <i>Analytical Chemistry</i> , 2022, 94, 464-478.	3.2	14
20	Hydrogen-bonded complexes between mesogenic heterocyclic Schiff's bases and mesogenic 4-nonyloxybenzoic acid: mesomorphic behaviour, FTIR study and PM3 semi-empirical calculations. <i>Liquid Crystals</i> , 2003, 30, 297-304.	0.9	13
21	The role of charge transfer interactions in the inclusion complexation of anionic guests with β -cyclodextrin. <i>Tetrahedron</i> , 2005, 61, 5449-5456.	1.0	13
22	Inclusion Complexation of Phenol Derivatives with a β -Cyclodextrin Based Polymer. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2005, 53, 63-68.	1.6	13
23	Complexation of Mefenamic Acid by Low-Generation PAMAM Dendrimers: Insight from NMR Spectroscopy Studies and Molecular Dynamics Simulations. <i>Macromolecular Chemistry and Physics</i> , 2014, 215, 372-383.	1.1	13
24	Drug-dendrimer supramolecular complexation studied from molecular dynamics simulations and NMR spectroscopy. <i>Structural Chemistry</i> , 2014, 25, 1443-1455.	1.0	13
25	Polyamido amine (PAMAM)-grafted magnetic nanotubes as emerging platforms for the delivery and sustained release of silibinin. <i>Journal of Materials Science</i> , 2017, 52, 9269-9281.	1.7	12
26	A QM/MM study on the last two steps of the catalytic cycle of acetohydroxyacid synthase. <i>Computational and Theoretical Chemistry</i> , 2011, 966, 159-166.	1.1	11
27	PAMAM-Conjugated Alumina Nanotubes as Novel Noncytotoxic Nanocarriers with Enhanced Drug Loading and Releasing Performances. <i>Macromolecular Chemistry and Physics</i> , 2016, 217, 1712-1722.	1.1	11
28	Structural insight into the role of Gln293Met mutation on the Peloruside A/Laulimalide association with β -tubulin from molecular dynamics simulations, binding free energy calculations and weak interactions analysis. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 643-652.	1.3	11
29	Effect of pH on Eosin Y/PAMAM interactions studied from absorption spectroscopy and molecular dynamics simulations. <i>Journal of Luminescence</i> , 2018, 199, 258-265.	1.5	11
30	Determination of the Association Constant of 6-Thiopurine and Chitosan Grafted β -Cyclodextrin. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2003, 47, 71-75.	1.6	9
31	Polyamidoamine-based nanovector for the efficient delivery of methotrexate to U87 glioma cells. <i>Nanomedicine</i> , 2020, 15, 2771-2784.	1.7	9
32	Inhibitory Activities on Mammalian Central Nervous System Receptors and Computational Studies of Three Sesquiterpene Lactones from <i>Coriaria ruscifolia</i> subsp. <i>ruscifolia</i> . <i>Chemical and Pharmaceutical Bulletin</i> , 2011, 59, 161-165.	0.6	8
33	Binding free energy calculations on α -selectin complexes with oligosaccharide analogs. <i>Chemical Biology and Drug Design</i> , 2017, 89, 114-123.	1.5	8
34	Host-guest complexation of curcumin and coumarin 6 with PAMAM-OH: Insight from fluorescence spectroscopy and molecular dynamics simulations. <i>Journal of Luminescence</i> , 2020, 222, 117182.	1.5	8
35	Synthesis and properties of new liquid crystals derivatives of 2,7-diethynyl-9,9-dihexylfluorene. <i>Liquid Crystals</i> , 2012, 39, 847-856.	0.9	7
36	Structural basis for drug resistance conferred by β -tubulin mutations: a molecular modeling study on native and mutated tubulin complexes with epothilone B. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 2530-2540.	2.0	7

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37	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. <i>Chemical Biology and Drug Design</i> , 2018, 91, 1042-1055.	1.5	7
38	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 <i>Streptococcus mutans</i> . <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 6269-6276.	1.5	7
39	Modulation of glucan-enzyme interactions by domain V in GTF-SI from <i>Streptococcus mutans</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 74-80.	1.5	7
40	Quantum-Chemical Study on the Bioactive Conformation of Epothilones. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 2176-2190.	2.5	6
41	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. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 789-803.	2.0	6
42	Reversal of Ethanol-induced Intoxication by a Novel Modulator of $\text{G}\beta\gamma$ Protein Potentiation of the Glycine Receptor. <i>Journal of Biological Chemistry</i> , 2016, 291, 18791-18798.	1.6	6
43	Molecular modeling study on the differential microtubule-stabilizing effect in singly- and doubly-bonded complexes with peloruside A and paclitaxel. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 668-678.	1.5	6
44	Catalytic Role of Gln202 in the Carbonylation Reaction Mechanism of Yeast AHAS: A QM/MM Study. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 915-922.	2.5	6
45	Mechanism-Based Rational Discovery and <i>In Vitro</i> Evaluation of Novel Microtubule Stabilizing Agents with Non-Taxol-Competitive Activity. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3204-3213.	2.5	6
46	NanoMIPs Design for Fucose and Mannose Recognition: A Molecular Dynamics Approach. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2048-2061.	2.5	6
47	Discovery of New E-Selectin Inhibitors by Virtual Screening, Fluorescence Binding Assays, and STD NMR Experiments. <i>ChemMedChem</i> , 2016, 11, 1008-1014.	1.6	5
48	Copper metallic nanoparticles capped with PEGylated PAMAM-G3 dendrimers for the catalytic reduction of low solubility nitroarenes of pharmaceutical interest. <i>Catalysis Today</i> , 2021, 372, 27-35.	2.2	5
49	Visible-light-responsive folate-conjugated titania and alumina nanotubes for photodynamic therapy applications. <i>Journal of Materials Science</i> , 2020, 55, 6976-6991.	1.7	5
50	Rational Design of Novel Glycomimetic Peptides for E-Selectin Targeting. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2463-2474.	2.5	5
51	Polyamidoamine dendrimers of the third generation-chlorin e6 nanoconjugates: Nontoxic hybrid polymers with photodynamic activity. <i>Journal of Applied Polymer Science</i> , 2022, 139, 51835.	1.3	5
52	On the Microtubule-Stabilizing Properties of a Tau Oligopeptide. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5682-5691.	2.5	5
53	Convenient synthesis and characterization of molecules containing multiple β -keto ester units. <i>Tetrahedron Letters</i> , 2012, 53, 4984-4988.	0.7	4
54	Interdimeric Curvature in Tubulin-Tubulin Complexes Delineates the Microtubule-Destabilizing Properties of Plocabulin. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4076-4084.	2.5	4

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55	“On the complexation of allopurinol with β -cyclodextrin”. Structural Chemistry, 2006, 17, 217-223.	1.0	3
56	Theoretical approach to the out-of-plane deformation of 1,3-disubstituted azulenes. Structural Chemistry, 2009, 20, 677-684.	1.0	3
57	Molecular modeling study on the tubulin-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
58	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
59	Correlation Models for the Inclusion Complexation of Aliphatic Compounds with α - and β -Cyclodextrins. Supramolecular Chemistry, 2008, 20, 317-325.	1.5	2
60	Diffusion coefficients of first-generation polyamidoamine dendrimer and its β -cyclodextrin conjugate in aqueous solution by means of molecular dynamics simulations. Monatshefte für Chemie, 2012, 143, 29-35.	0.9	2
61	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
62	INNOVATIVE USE OF A TABLET DEVICE TO DELIVER INSTRUCTION IN UNDERGRADUATE CHEMISTRY LECTURES. Quimica Nova, 2015, , .	0.3	1
63	Stereospecific Inhibition of Ethanol Potentiation on Glycine Receptor by M554 Stereoisomers. Journal of Chemical Information and Modeling, 2020, 60, 6634-6641.	2.5	0