Joel B Alderete

List of Publications by Year
in descending order

113 papers	1,653 citations	279798 23 h-index	434195 31 g-index
113 all docs	113 docs citations	113 times ranked	2222 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.	2.6	5
2	Mesoporous mixed oxides prepared by hard template methodology as novel drug delivery carriers for methotrexate. Journal of Drug Delivery Science and Technology, 2022, 73, 103483.	3.0	3
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.	4.4	5
4	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.	9.3	3
5	Rational Design of Novel Glycomimetic Peptides for E-Selectin Targeting. Journal of Chemical Information and Modeling, 2021, 61, 2463-2474.	5.4	5
6	In Silico Design of Novel Mutant Anti-MUC1 Aptamers for Targeted Cancer Therapy. Journal of Chemical Information and Modeling, 2020, 60, 786-793.	5.4	17
7	Polyamidoamine-based nanovector for the efficient delivery of methotrexate to U87 glioma cells. Nanomedicine, 2020, 15, 2771-2784.	3.3	9
8	Visible-light-responsive folate-conjugated titania and alumina nanotubes for photodynamic therapy applications. Journal of Materials Science, 2020, 55, 6976-6991.	3.7	5
9	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.	3.1	8
10	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.	5.4	6
11	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.	2.8	7
12	Molecular modeling simulation studies reveal new potential inhibitors against HPV E6 protein. PLoS ONE, 2019, 14, e0213028.	2.5	31
13	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.	2.6	6
14	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.	2.8	14
15	Gold catalysts supported on TiO 2 -nanotubes for the selective hydrogenation of p -substituted nitrobenzenes. Molecular Catalysis, 2018, 447, 21-27.	2.0	38
16	Cytotoxicity, genotoxicity and uptake detection of folic acid-functionalized green upconversion nanoparticles Y2O3/Er3+, Yb3+ as biolabels for cancer cells. Journal of Materials Science, 2018, 53, 6665-6680.	3.7	17
17	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.	3.2	7
18	Upconversion rare earth nanoparticles functionalized with folic acid for bioimaging of MCF-7 breast cancer cells. Journal of Materials Research, 2018, 33, 191-200.	2.6	14

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19	Effect of pH on Eosin Y/PAMAM interactions studied from absorption spectroscopy and molecular dynamics simulations. Journal of Luminescence, 2018, 199, 258-265.	3.1	11
20	Partially PEGylated PAMAM dendrimers as solubility enhancers of Silybin. Pharmaceutical Development and Technology, 2018, 23, 689-696.	2.4	32
21	Cytotoxicity and in vivo plasma kinetic behavior of surface-functionalized PAMAM dendrimers. Nanomedicine: Nanotechnology, Biology, and Medicine, 2018, 14, 2227-2234.	3.3	27
22	Prevention of Synaptic Alterations and Neurotoxic Effects of PAMAM Dendrimers by Surface Functionalization. Nanomaterials, 2018, 8, 7.	4.1	30
23	Rhodium(i) diphenylphosphine complexes supported on porous organic polymers as efficient and recyclable catalysts for alkene hydrogenation. RSC Advances, 2017, 7, 3398-3407.	3.6	9
24	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.	3.7	12
25	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.	3.2	3
26	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.	2.9	11
27	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.	2.6	21
28	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.	3.2	8
29	A Novel Synthesis of Gold Nanoparticles Supported on Hybrid Polymer/Metal Oxide as Catalysts for p-Chloronitrobenzene Hydrogenation. Journal of Chemistry, 2017, 2017, 1-9.	1.9	11
30	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.	2.2	18
31	PAMAMâ€Conjugated Alumina Nanotubes as Novel Noncytotoxic Nanocarriers with Enhanced Drug Loading and Releasing Performances. Macromolecular Chemistry and Physics, 2016, 217, 1712-1722.	2.2	11
32	PAMAM-grafted TiO2 nanotubes as novel versatile materials for drug delivery applications. Materials Science and Engineering C, 2016, 65, 164-171.	7.3	38
33	Mechanism of PAMAM Dendrimers Internalization in Hippocampal Neurons. Molecular Pharmaceutics, 2016, 13, 3395-3403.	4.6	24
34	Maleic anhydride hydrogenation to succinic anhydride over mesoporous Ni/TiO2 catalysts: Effects of Ni loading and temperature. Journal of Molecular Catalysis A, 2016, 423, 441-448.	4.8	26
35	Discovery of New Eâ€Selectin Inhibitors by Virtual Screening, Fluorescence Binding Assays, and STD NMR Experiments. ChemMedChem, 2016, 11, 1008-1014.	3.2	5
36	Heterogeneous hydrogenation of nitroaromatic compounds on gold catalysts: Influence of titanium substitution in MCM-41 mesoporous supports. Applied Catalysis A: General, 2016, 517, 110-119.	4.3	17

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37	Substrate ionization energy influences the epoxidation of m-substituted styrenes catalyzed by chloroperoxidase from Caldariomyces fumago. Catalysis Communications, 2016, 77, 52-54.	3.3	7
38	Biocatalytic Performance of Chloroperoxidase from Caldariomyces fumago Immobilized onto TiO2 Based Supports. Topics in Catalysis, 2016, 59, 387-393.	2.8	8
39	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.	2.2	25
40	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.	3.5	6
41	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.	3.5	7
42	Enhancement of operational stability of chloroperoxidase from Caldariomyces fumago by immobilization onto mesoporous supports and the use of co-solvents. Journal of Molecular Catalysis B: Enzymatic, 2015, 116, 1-8.	1.8	16
43	Ceanothane and oleanane-type triterpenes from Talguenea quinquenervia have insecticidal activity against Cydia pomonella, Tenebrio molitor and Drosophila melanogaster. Industrial Crops and Products, 2015, 74, 759-766.	5.2	15
44	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.	2.2	13
45	Drug-dendrimer supramolecular complexation studied from molecular dynamics simulations and NMR spectroscopy. Structural Chemistry, 2014, 25, 1443-1455.	2.0	13
46	Prediction model based on decision tree analysis for laccase mediators. Enzyme and Microbial Technology, 2013, 52, 68-76.	3.2	32
47	Unusual activation during peroxidase reaction of a cytochrome c variant. Journal of Molecular Catalysis B: Enzymatic, 2013, 85-86, 187-192.	1.8	5
48	Aspergillus niger catalyzes the synthesis of flavonoids from chalcones. Biocatalysis and Biotransformation, 2013, 31, 160-167.	2.0	17
49	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.	2.0	17
50	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.	1.8	2
51	Structure activity relationship, acute toxicity and cytotoxicity of antimycobacterial neolignan analogues. Journal of Pharmacy and Pharmacology, 2011, 63, 936-942.	2.4	4
52	Enzymatic fructosylation of aromatic and aliphatic alcohols by Bacillus subtilis levansucrase: Reactivity of acceptors. Journal of Molecular Catalysis B: Enzymatic, 2011, 70, 41-48.	1.8	23
53	Enhancing oxidation activity and stability of iso-1-cytochrome c and chloroperoxidase by immobilization in nanostructured supports. Journal of Molecular Catalysis B: Enzymatic, 2011, 70, 81-87.	1.8	27
54	On the inhibition of AHAS by chlorimuron ethyl: A theoretical study. Chemical Physics Letters, 2011, 516, 239-243.	2.6	3

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55	Density-functional study on the equilibria in the ThDP activation. Journal of Molecular Modeling, 2011, 17, 2735-2739.	1.8	7
56	A QM/MM study on the last two steps of the catalytic cycle of acetohydroxyacid synthase. Computational and Theoretical Chemistry, 2011, 966, 159-166.	2.5	11
57	Colorectal cancer chemoprevention by 2 Î²â€cyclodextrin inclusion compounds of auraptene and 4â€²â€geranyloxyferulic acid. International Journal of Cancer, 2010, 126, 830-840.	5.1	67
58	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.	2.6	16
59	Bioreduction of Some Common Carbonylic Compounds Mediated by Yeasts. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 2010, 65, 1-9.	1.4	2
60	Stereoselective oxidation of R-(+)-limonene by chloroperoxidase from Caldariomyces fumago. Green Chemistry, 2008, 10, 647.	9.0	38
61	Hartreeâ^'Fock and Density Functional Theory Study of Î±-Cyclodextrin Conformers. Journal of Physical Chemistry A, 2008, 112, 678-685.	2.5	14
62	Biotransformation of Indole Derivatives by Mycelial Cultures. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 2008, 63, 82-84.	1.4	4
63	Synthesis and mesomorphic properties of 3â€(4â€nâ€alkyloxyarylaminomethylene)chromanâ€2,4â€diones. Liquid Crystals, 2008, 35, 157-162.	2.2	13
64	Correlation Models for the Inclusion Complexation of Aliphatic Compounds with Î±- and Î²-Cyclodextrins. Supramolecular Chemistry, 2008, 20, 317-325.	1.2	2
65	Production of Exopolysaccharides by a Submerged Culture of an Entomopathogenic Fungus, Paecilomyces sp.. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 2007, 62, 576-578.	1.4	2
66	Structural Studies of Native Paecilomyces sp. Exopolysaccharide. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 2007, 62, 623-626.	1.4	2
67	New anionic cobalt complexes using highly hindered bis-amides with varying donor abilities as ligands. Dalton Transactions, 2007, , 2135-2144.	3.3	13
68	Biotransformation of 5Î±-hydroxy-14-eudesm-11-en-3-one by Rhizopus nigricans, Cunninghamella elegans and Mucor plumbeus. Journal of Molecular Catalysis B: Enzymatic, 2007, 48, 23-27.	1.8	12
69	Biotransformation of Tryptophan by Liquid Medium Culture of Psilocybe coprophila (Basidiomycetes). Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 2006, 61, 806-808.	1.4	0
70	DFT derived solvation models for organic compounds in alkane solvents. Chemical Physics, 2006, 325, 220-224.	1.9	4
71	Complete basis set calculations on the tautomerism and protonation of triazoles and tetrazole. Computational and Theoretical Chemistry, 2006, 775, 1-7.	1.5	43
72	â€œOn the complexation of allopurinol with Î²-cyclodextrinâ€• Structural Chemistry, 2006, 17, 217-223.	2.0	3

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73	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
74	The role of charge transfer interactions in the inclusion complexation of anionic guests with Î±-cyclodextrin. Tetrahedron, 2005, 61, 5449-5456.	1.9	13
75	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
76	Synthesis and tautomeric studies of enamines from 1-(n-Hexyl)-3-methyl-2-pyrazolin-5-one. Journal of the Brazilian Chemical Society, 2005, 16, .	0.6	9
77	Properties of thermotropic liquid crystals induced by hydrogen bonding between pyridylâ€1,2,4â€oxadiazole derivatives and benzoic acid, 4â€chlorobenzoic acid or 4â€methylbenzoic acid. Liquid Crystals, 2005, 32, 573-577.	2.2	46
78	New supramolecular liquid crystals induced by hydrogen bonding between pyridylâ€1,2,4â€oxadiazole derivatives and 2,5â€thiophene dicarboxylic acid. Liquid Crystals, 2005, 32, 449-455.	2.2	35
79	PHYSICO-CHEMICAL CHARACTERIZATION OF THE INCLUSION COMPLEX BETWEEN A 2-PROPEN-1-AMINE DERIVATIVE AND b-CYCLODEXTRIN. Journal of the Chilean Chemical Society, 2005, 50, .	1.2	2
80	Quantum-connectivity descriptors in modeling solubility of environmentally important organic compounds. Journal of Computational Chemistry, 2004, 25, 1787-1796.	3.3	24
81	Aggregation State and QSPR Models. The Solubility of Herbicides as a Case Study.. ChemInform, 2004, 35, no.	0.0	0
82	Elucidation of inclusion compounds between Î²-cyclodextrin/local anaesthetics structure: a theoretical and experimental study using differential scanning calorimetry and molecular mechanics. Computational and Theoretical Chemistry, 2004, 678, 63-66.	1.5	23
83	On the Aggregation State and QSPR Models. The Solubility of Herbicides as a Case Study. Journal of Chemical Information and Computer Sciences, 2004, 44, 958-963.	2.8	4
84	Synthesis and mesomorphic properties of esters derived from Schiff's bases containing 1,3,4-thiadiazole. Liquid Crystals, 2004, 31, 1531-1537.	2.2	30
85	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
86	Prediction of Henryâ€²s Law Constants of Triazine Derived Herbicides from Quantum Chemical Continuum Solvation Models.. ChemInform, 2003, 34, no.	0.0	0
87	A Simple QSPR Model for Predicting Soil Sorption Coefficients of Polar and Nonpolar Organic Compounds from Molecular Formula. Journal of Chemical Information and Computer Sciences, 2003, 43, 1928-1932.	2.8	16
88	Esters derived from 7-decanoyloxychromone-3-carboxylic acid: synthesis and mesomorphic properties. Liquid Crystals, 2003, 30, 1319-1325.	2.2	18
89	Prediction of Henry's Law Constants of Triazine Derived Herbicides from Quantum Chemical Continuum Solvation Models. Journal of Chemical Information and Computer Sciences, 2003, 43, 1226-1230.	2.8	11
90	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.	2.2	13

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91	Symmetric esters derived from 1,3,4-oxadiazole: synthesis, mesomorphic properties and structural study by semi-empirical calculations. Liquid Crystals, 2002, 29, 1375-1382.	2.2	22
92	Predicting Gas Chromatographic Retention Time of Polychlorinated Dibenzo-p-Dioxins from Molecular Structure. Zeitschrift Fur Physikalische Chemie, 2002, 216, .	2.8	2
93	On the Calculation of Henry's Law Constants of Chlorinated Benzenes in Water from Semiempirical Quantum Chemical Methods. Journal of Chemical Information and Computer Sciences, 2002, 42, 559-563.	2.8	12
94	Synthesis, mesomorphic properties and structural study by semi-empirical calculations of amides containing the 1,3,4-thiadiazole unit. Liquid Crystals, 2002, 29, 647-652.	2.2	19
95	Characterisation and properties of the inclusion complex of 24-epibrassinolide with Î²-cyclodextrin. Plant Growth Regulation, 2002, 37, 233-240.	3.4	10
96	Azo compounds and Schiff 's bases derived from 5-(4-pyridyl)-2-amino-1,3,4-thiadiazole: synthesis, mesomorphic properties and structural study by semi-empirical calculations. Liquid Crystals, 2001, 28, 1659-1666.	2.2	36
97	Prediction of infinite dilution activity coefficients of chlorinated organic compounds in aqueous solution from quantum-chemical descriptors. Journal of Computational Chemistry, 2001, 22, 1851-1856.	3.3	5
98	Title is missing!. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2000, 37, 67-74.	1.6	25
99	New Schiff's bases containing 1,3,4-thiadiazole and 1,3,4-oxadiazole units: a study of the effect of the heterocyclic ring and the position of the lateral alkoxy group on liquid crystalline properties. Liquid Crystals, 2000, 27, 995-1000.	2.2	49
100	Inclusion complex of the antiviral drug acyclovir with cyclodextrin in aqueous solution and in solid phase. Quimica Nova, 2000, 23, 749-752.	0.3	51
101	NMR AND DFT STUDY ON THE PROTOTROPIC TAUTOMERISM OF 3-METHYL-5-PYRAZOLONE. Journal of the Chilean Chemical Society, 2000, 45, .	0.1	2
102	SYNTHESIS AND TAUTOMERISM OF NEW 1-n-ALKYL-5-PYRAZOLONE DERIVATIVES. Journal of the Chilean Chemical Society, 1999, 44, .	0.1	6
103	Theoretical study of the tautomerism of 8-azaadenine. Journal of Physical Organic Chemistry, 1998, 11, 392-396.	1.9	14
104	Aqueous solvation effect on the tautomerism of 8-azapurine. Computational and Theoretical Chemistry, 1996, 365, 63-69.	1.5	11
105	Ab initio SCRF study of the tautomeric equilibrium of 2-thiopyrimidine. Chemical Physics Letters, 1995, 232, 61-66.	2.6	10
106	Aqueous solvation effect on the prototropic tautomerism of 2-thiocytosine. Journal of Physical Organic Chemistry, 1995, 8, 395-399.	1.9	11
107	MO studies on the prototropic tautomerism and protonation of 2-thiopurine. Computational and Theoretical Chemistry, 1995, 334, 223-228.	1.5	7
108	The vibrational spectra of some 2-mercaptopyrimidine complexes of mercury(II). Spectrochimica Acta Part A: Molecular Spectroscopy, 1994, 50, 371-374.	0.1	8

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109	MO calculations of solvent effects on the prototropic tautomerism of 6-thiopurine. Computational and Theoretical Chemistry, 1994, 309, 137-141.	1.5	12
110	AM1 studies on the prototropic tautomerism of 6-thioguanine. Computational and Theoretical Chemistry, 1993, 283, 283-287.	1.5	16
111	A semiempirical study of the prototropic tautomerism of hypoxanthine. Molecular Engineering, 1992, 2, 29-36.	0.2	3
112	Semiempirical molecular orbital calculations on the prototropic tautomerism of 2-thiocytosine. Computational and Theoretical Chemistry, 1991, 251, 195-204.	1.5	12
113	Semi-empirical molecular orbital calculations on pyrimidine-2-thiol and pyrimidine-2-thione: prototropic tautomerism. Computational and Theoretical Chemistry, 1991, 231, 257-265.	1.5	16