Miguel Machuqueiro

List of Publications by Citations

74 papers	1,844 citations	22 h-index	40 g-index
102 ext. papers	2,288 ext. citations	6.2 avg, IF	5.06 L-index

#	Paper	IF	Citations
74	Zn-Proline catalyzed direct aldol reaction in aqueous media. *Chemical Communications*, **2003**, 1090-1091	5.8	165
73	The multi-factorial nature of clinical multidrug resistance in cancer. *Drug Resistance Updates*, **2019**, 46, 100645	23.2	155
72	Constant-pH molecular dynamics with ionic strength effects: protonation-conformation coupling in decalysine. *Journal of Physical Chemistry B*, **2006**, 110, 2927-33	3.4	93
71	A Selective Direct Aldol Reaction in Aqueous Media Catalyzed byZinc□Proline. *European Journal of Organic Chemistry*, **2005**, 2005, 5268-5276	3.2	90
70	Zinc-proline catalyzed pathway for the formation of sugars. *Chemical Communications*, **2004**, 1540-1	5.8	88
69	Constant-pH molecular dynamics simulations reveal a □rich form of the human prion protein. *Journal of Physical Chemistry B*, **2010**, 114, 12692-700	3.4	77
68	On the use of different dielectric constants for computing individual and pairwise terms in poisson-boltzmann studies of protein ionization equilibrium. *Journal of Physical Chemistry B*, **2005**, 109, 14691-706	3.4	75
67	Improvement of conventional anti-cancer drugs as new tools against multidrug resistant tumors. *Drug Resistance Updates*, **2020**, 50, 100682	23.2	72
66	Acidic range titration of HEWL using a constant-pH molecular dynamics method. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 289-98	4.2	66
65	Molecular dynamics at constant pH and reduction potential: application to cytochrome c(3). *Journal of the American Chemical Society*, **2009**, 131, 12586-94	16.4	51
64	Is the prediction of pKa values by constant-pH molecular dynamics being hindered by inherited problems?. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 3437-47	4.2	50
63	The pH-dependent conformational states of kyotorphin: a constant-pH molecular dynamics study. *Biophysical Journal*, **2007**, 92, 1836-45	2.9	44
62	pK(a) Values of Titrable Amino Acids at the Water/Membrane Interface. *Journal of Chemical Theory and Computation*, **2016**, 12, 930-4	6.4	42
61	Targeting Type 2 Diabetes with C-Glucosyl Dihydrochalcones as Selective Sodium Glucose Co-Transporter 2 (SGLT2) Inhibitors: Synthesis and Biological Evaluation. *Journal of Medicinal Chemistry*, **2017**, 60, 568-579	8.3	35
60	Reversibility of prion misfolding: insights from constant-pH molecular dynamics simulations. *Journal of Physical Chemistry B*, **2012**, 116, 8812-21	3.4	33
59	Apple tree branches derived activated carbons for the removal of □blocker atenolol. *Chemical Engineering Journal*, **2018**, 345, 669-678	14.7	32
58	Differential targeting of membrane lipid domains by caffeic acid and its ester derivatives. *Free Radical Biology and Medicine*, **2018**, 115, 232-245	7.8	31

57	Unfolding the conformational behavior of peptide dendrimers: insights from molecular dynamics simulations. *Journal of the American Chemical Society*, **2011**, 133, 5042-52	16.4	30
56	Isorhamnetin derivatives and piscidic acid for hypercholesterolemia: cholesterol permeability, HMG-CoA reductase inhibition, and docking studies. *Archives of Pharmacal Research*, **2017**, 40, 1278-1286	6.1	29
55	A simulated intermediate state for folding and aggregation provides insights into N6 2-microglobulin amyloidogenic behavior. *PLoS Computational Biology*, **2014**, 10, e1003606	5	28
54	Conformational study of GSH and GSSG using constant-pH molecular dynamics simulations. *Journal of Physical Chemistry B*, **2013**, 117, 7507-17	3.4	24
53	Constant-pH MD Simulations of DMPA/DMPC Lipid Bilayers. *Journal of Chemical Theory and Computation*, **2015**, 11, 5973-9	6.4	23
52	Constant-pH MD Simulations of an Oleic Acid Bilayer. *Journal of Chemical Theory and Computation*, **2015**, 11, 2367-76	6.4	22
51	Proactive response to tackle the threat of emerging drugs: Synthesis and toxicity evaluation of new cathinones. *Forensic Science International*, **2018**, 290, 146-156	2.6	22
50	Protonation of DMPC in a Bilayer Environment Using a Linear Response Approximation. *Journal of Chemical Theory and Computation*, **2014**, 10, 2176-84	6.4	22
49	Influence of activated carbons porous structure on iopamidol adsorption. *Carbon*, **2014**, 77, 607-615	10.4	21
48	The Lysosomotropic Activity of Hydrophobic Weak Base Drugs is Mediated via Their Intercalation into the Lysosomal Membrane. *Cells*, **2020**, 9,	7.9	20
47	Structural effects of pH and deacylation on surfactant protein C in an organic solvent mixture: a constant-pH MD study. *Journal of Chemical Information and Modeling*, **2013**, 53, 2979-89	6.1	19
46	Membrane-induced conformational changes of kyotorphin revealed by molecular dynamics simulations. *Journal of Physical Chemistry B*, **2010**, 114, 11659-67	3.4	19
45	Membrane-Induced p K Shifts in wt-pHLIP and Its L16H Variant. *Journal of Chemical Theory and Computation*, **2018**, 14, 3289-3297	6.4	18
44	Zinc mediated methyl transfer from trimethyl phosphate to chelating and non-chelating alkyl thiols. Model for Zn-dependent methyltransferases. *Journal of Inorganic Biochemistry*, **2003**, 94, 193-6	4.2	18
43	Charge parametrization of the DvH-c3 heme group: validation using constant-(pH,E) molecular dynamics simulations. *Journal of Physical Chemistry B*, **2013**, 117, 70-82	3.4	17
42	Treatment of Ionic Strength in Biomolecular Simulations of Charged Lipid Bilayers. *Journal of Chemical Theory and Computation*, **2014**, 10, 5483-92	6.4	17
41	Indenyl ring slippage in crown thioether complexes [IndMo(CO)2L]+ and C-S activation of trithiacyclononane: experimental and theoretical studies. *Dalton Transactions*, **2011**, 40, 10513-25	4.3	17
40	The Impact of Using Single Atomistic Long-Range Cutoff Schemes with the GROMOS 54A7 Force Field. *Journal of Chemical Theory and Computation*, **2018**, 14, 5823-5833	6.4	16

39	Exploring the Structural Properties of Positively Charged Peptide Dendrimers. *Journal of Physical Chemistry B*, **2016**, 120, 11323-11330	3.4	15
38	Bioactivities of (Gentianaceae) Decoctions: Antioxidant Activity, Enzyme Inhibition and Docking Studies. *Molecules*, **2019**, 24,	4.8	15
37	Sugar-based bactericides targeting phosphatidylethanolamine-enriched membranes. *Nature Communications*, **2018**, 9, 4857	17.4	15
36	Antiacetylcholinesterase activity and docking studies with chlorogenic acid, cynarin and arzanol from Helichrysum stoechas (Lamiaceae). *Medicinal Chemistry Research*, **2017**, 26, 2942-2950	2.2	14
35	Biomolecular Simulations of Halogen Bonds with a GROMOS Force Field. *Journal of Chemical Theory and Computation*, **2018**, 14, 5383-5392	6.4	14
34	PypKa: A Flexible Python Module for Poisson-Boltzmann-Based p Calculations. *Journal of Chemical Information and Modeling*, **2020**, 60, 4442-4448	6.1	13
33	Hydrogen peroxide regulates cell adhesion through the redox sensor RPSA. *Free Radical Biology and Medicine*, **2016**, 90, 145-57	7.8	12
32	Constant-pH Molecular Dynamics Study of Kyotorphin in an Explicit Bilayer. *Biophysical Journal*, **2015**, 108, 2282-90	2.9	11
31	Role of Counterions in Constant-pH Molecular Dynamics Simulations of PAMAM Dendrimers. *ACS Omega*, **2018**, 3, 2001-2009	3.9	11
30	Insights on the Mechanism of Action of INH-C as an Antitubercular Prodrug. *Molecular Pharmaceutics*, **2017**, 14, 4597-4605	5.6	10
29	A tale of two tails: The importance of unstructured termini in the aggregation pathway of β-microglobulin. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 2045-2057	4.2	10
28	Molecular details of INH-C10 binding to wt KatG and Its S315T mutant. *Molecular Pharmaceutics*, **2015**, 12, 898-909	5.6	10
27	The Catalase Activity of Catalase-Peroxidases Is Modulated by Changes in the pK of the Distal Histidine. *Biochemistry*, **2017**, 56, 2271-2281	3.2	9
26	Bioactivities of decoctions from Plectranthus species related to their traditional use on the treatment of digestive problems and alcohol intoxication. *Journal of Ethnopharmacology*, **2018**, 220, 147-154	5	8
25	Molybdenum(ii) complexes with p-substituted BIAN ligands: synthesis, characterization, biological activity and computational study. *Dalton Transactions*, **2019**, 48, 8449-8463	4.3	7
24	A pH Replica Exchange Scheme in the Stochastic Titration Constant-pH MD Method. *Journal of Chemical Theory and Computation*, **2019**, 15, 3108-3116	6.4	7
23	Unraveling the Conformational Determinants of Peptide Dendrimers Using Molecular Dynamics Simulations. *Macromolecules*, **2013**, 46, 9427-9436	5.5	7
22	Structuring Peptide Dendrimers through pH Modulation and Substrate Binding. *Journal of Physical Chemistry B*, **2016**, 120, 10138-10152	3.4	7

21	The Early Phase of β2m Aggregation: An Integrative Computational Study Framed on the D76N Mutant and the ΔN6 Variant. *Biomolecules*, **2019**, 9,	5.9	6
20	Tuning the Bioactivity of Tensioactive Deoxy Glycosides to Structure: Antibacterial Activity Versus Selective Cholinesterase Inhibition Rationalized by Molecular Docking. *European Journal of Organic Chemistry*, **2013**, 2013, 1448-1459	3.2	6
19	Why a diaminopyrrolic tripodal receptor binds mannosides in acetonitrile but not in water?. *Beilstein Journal of Organic Chemistry*, **2014**, 10, 1513-23	2.5	6
18	Improved GROMOS 54A7 Charge Sets for Phosphorylated Tyr, Ser, and Thr to Deal with pH-Dependent Binding Phenomena. *Journal of Chemical Theory and Computation*, **2020**, 16, 6368-6376	6.4	6
17	The role of electrostatics in TrxR electron transfer mechanism: A computational approach. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 1836-1843	4.2	6
16	Designing new antitubercular isoniazid derivatives with improved reactivity and membrane trafficking abilities. *Biomedicine and Pharmacotherapy*, **2021**, 144, 112362	7.5	5
15	Novel "ruthenium cyclopentadienyl"-peptide conjugate complexes against human FGFR(+) breast cancer. *Dalton Transactions*, **2020**, 49, 5974-5987	4.3	5
14	Evaluation of EGCG Loading Capacity in DMPC Membranes. *Langmuir*, **2019**, 35, 6771-6781	4	3
13	Network biology and artificial intelligence drive the understanding of the multidrug resistance phenotype in cancer.. *Drug Resistance Updates*, **2022**, 60, 100811	23.2	3
12	Key Factors for Activated Carbon Adsorption of Pharmaceutical Compounds from Wastewaters: A Multivariate Modelling Approach. *Water (Switzerland)*, **2022**, 14, 166	3	3
11	Glucosylpolyphenols as Inhibitors of Aβ-Induced Fyn Kinase Activation and Tau Phosphorylation: Synthesis, Membrane Permeability, and Exploratory Target Assessment within the Scope of Type 2 Diabetes and Alzheimer's Disease. *Journal of Medicinal Chemistry*, **2020**, 63, 11663-11690	8.3	3
10	Cu-binding to S100B triggers polymerization of disulfide cross-linked tetramers with enhanced chaperone activity against amyloid-β aggregation. *Chemical Communications*, **2021**, 57, 379-382	5.8	2
9	Dynamical Rearrangement of Human Epidermal Growth Factor Receptor 2 upon Antibody Binding: Effects on the Dimerization. *Biomolecules*, **2019**, 9,	5.9	1
8	Computational Analysis of the Interactions between the S100B Extracellular Chaperone and Its Amyloid β Peptide Client. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
7	Improved Protocol to Tackle the pH Effects on Membrane-Inserting Peptides. *Journal of Chemical Theory and Computation*, **2021**, 17, 3830-3840	6.4	1
6	pKPDB: a Protein Data Bank extension database of pKa and pI theoretical values. *Bioinformatics*, **2021**,	7.2	1
5	Identification of Pan-Assay INterference compoundS (PAINS) Using an MD-Based Protocol. *Methods in Molecular Biology*, **2021**, 2315, 263-271	1.4	1
4	pK Calculations in Membrane Proteins from Molecular Dynamics Simulations. *Methods in Molecular Biology*, **2021**, 2315, 185-195	1.4	1

3	Mutant p53 reactivator SLMP53-2 hinders ultraviolet B radiation-induced skin carcinogenesis. *Pharmacological Research*, **2021**, 106026	10.2	0
2	In Silico End-to-End Protein-Ligand Interaction Characterization Pipeline: The Case of SARS-CoV-2. *ACS Synthetic Biology*, **2021**, 10, 3209-3235	5.7	0
1	Predicting stable binding modes from simulated dimers of the D76N mutant of 2-microglobulin. *Computational and Structural Biotechnology Journal*, **2021**, 19, 5160-5169	6.8	0