Maria Natlia Dias Soeiro Cordeiro

List of Publications by Citations

339 papers	7,175 citations	42 h-index	61 g-index
367 ext. papers	8,140 ext. citations	4.3 avg, IF	6.52 L-index

#	Paper	IF	Citations
339	Phenolic acid derivatives with potential anticancer properties--a structure-activity relationship study. Part 1: methyl, propyl and octyl esters of caffeic and gallic acids. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 3581-9	3.4	251
338	Quinoxaline, its derivatives and applications: A State of the Art review. *European Journal of Medicinal Chemistry*, **2015**, 97, 664-72	6.8	221
337	Applications of 2D descriptors in drug design: a DRAGON tale. *Current Topics in Medicinal Chemistry*, **2008**, 8, 1628-55	3	136
336	Computational tool for risk assessment of nanomaterials: novel QSTR-perturbation model for simultaneous prediction of ecotoxicity and cytotoxicity of uncoated and coated nanoparticles under multiple experimental conditions. *Environmental Science & Technology*, **2014**, 48, 14686-94	10.3	106
335	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. *Drug Discovery Today*, **2014**, 19, 1069-80	8.8	103
334	Intrinsic Structure and Dynamics of the Water/Nitrobenzene Interface. *Journal of Physical Chemistry C*, **2007**, 111, 17612-17626	3.8	102
333	Computer-aided nanotoxicology: assessing cytotoxicity of nanoparticles under diverse experimental conditions by using a novel QSTR-perturbation approach. *Nanoscale*, **2014**, 6, 10623-30	7.7	100
332	Influence of step sites in the molecular mechanism of the water gas shift reaction catalyzed by copper. *Journal of Catalysis*, **2009**, 268, 131-141	7.3	88
331	Computational ecotoxicology: simultaneous prediction of ecotoxic effects of nanoparticles under different experimental conditions. *Environment International*, **2014**, 73, 288-94	12.9	84
330	Density functional theory study of the water dissociation on platinum surfaces: general trends. *Journal of Physical Chemistry A*, **2014**, 118, 5832-40	2.8	82
329	A Critical Assessment of Methods for the Intrinsic Analysis of Liquid Interfaces. 1. Surface Site Distributions. *Journal of Physical Chemistry C*, **2010**, 114, 11169-11179	3.8	81
328	Descriptors controlling the catalytic activity of metallic surfaces toward water splitting. *Journal of Catalysis*, **2010**, 276, 92-100	7.3	74
327	Molecular Dynamics Simulation of the Water/2-Heptanone Liquid-Liquid Interface. *Journal of Physical Chemistry B*, **1999**, 103, 6290-6299	3.4	70
326	Rational drug design for anti-cancer chemotherapy: multi-target QSAR models for the in silico discovery of anti-colorectal cancer agents. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 4848-55	3.4	65
325	Beta-nitrostyrene derivatives as potential antibacterial agents: a structure-property-activity relationship study. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 4078-88	3.4	65
324	Probing the toxicity of nanoparticles: a unified in silico machine learning model based on perturbation theory. *Nanotoxicology*, **2017**, 11, 891-906	5.3	64
323	Molecularly imprinted polymer-based electrochemical sensors for environmental analysis. *Biosensors and Bioelectronics*, **2021**, 172, 112719	11.8	63

322	DFT Study of the CO Oxidation on the Au(321) Surface. *Journal of Physical Chemistry C*, **2008**, 112, 17291-17302	3.7	61
321	A systematic molecular simulation study of ionic liquid surfaces using intrinsic analysis methods. *Physical Chemistry Chemical Physics*, **2012**, 14, 5200-13	3.6	60
320	On the theoretical understanding of the unexpected O2 activation by nanoporous gold. *Chemical Communications*, **2011**, 47, 8403-5	5.8	60
319	Adsorption of Atomic and Molecular Oxygen on the Au(321) Surface: DFT Study. *Journal of Physical Chemistry C*, **2007**, 111, 17311-17321	3.8	59
318	Long-term follow-up of breast capsule contracture rates in cosmetic and reconstructive cases. *Plastic and Reconstructive Surgery*, **2010**, 126, 769-778	2.7	57
317	A Critical Assessment of Methods for the Intrinsic Analysis of Liquid Interfaces: 2. Density Profiles. *Journal of Physical Chemistry C*, **2010**, 114, 18656-18663	3.8	56
316	Chemoinformatics in anti-cancer chemotherapy: multi-target QSAR model for the in silico discovery of anti-breast cancer agents. *European Journal of Pharmaceutical Sciences*, **2012**, 47, 273-9	5.1	55
315	Application of the replacement method as a novel variable selection strategy in QSAR. 1. Carcinogenic potential. *Chemometrics and Intelligent Laboratory Systems*, **2006**, 81, 180-187	3.8	55
314	Enabling the Discovery and Virtual Screening of Potent and Safe Antimicrobial Peptides. Simultaneous Prediction of Antibacterial Activity and Cytotoxicity. *ACS Combinatorial Science*, **2016**, 18, 490-8	3.9	52
313	Probing the Environmental Toxicity of Deep Eutectic Solvents and Their Components: An In Silico Modeling Approach. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 10649-10660	8.3	51
312	Synthesis and QSAR study of the anticancer activity of some novel indane carbocyclic nucleosides. *Bioorganic and Medicinal Chemistry*, **2003**, 11, 4999-5006	3.4	51
311	Density functional theory model study of size and structure effects on water dissociation by platinum nanoparticles. *Journal of Chemical Physics*, **2012**, 137, 034701	3.9	49
310	Quantitative structure carcinogenicity relationship for detecting structural alerts in nitroso-compounds. *Toxicology and Applied Pharmacology*, **2007**, 221, 189-202	4.6	49
309	Toward the prediction of the activity of antioxidants: experimental and theoretical study of the gas-phase acidities of flavonoids. *Journal of the American Society for Mass Spectrometry*, **2004**, 15, 848-61	3.5	49
308	Molecular Dynamics Study of the Transfer of Iodide across Two Liquid/Liquid Interfaces. *Journal of Physical Chemistry B*, **1999**, 103, 8930-8939	3.4	49
307	Two new parameters based on distances in a receiver operating characteristic chart for the selection of classification models. *Journal of Chemical Information and Modeling*, **2011**, 51, 2746-59	6.1	48
306	Evaluation of the lipophilic properties of opioids, amphetamine-like drugs, and metabolites through electrochemical studies at the interface between two immiscible solutions. *Analytical Biochemistry*, **2007**, 361, 236-43	3.1	48
305	Computational modeling in nanomedicine: prediction of multiple antibacterial profiles of nanoparticles using a quantitative structure-activity relationship perturbation model. *Nanomedicine* , **2015**, 10, 193-204	5.6	47

304	Model for high-throughput screening of multitarget drugs in chemical neurosciences: synthesis, assay, and theoretic study of rasagiline carbamates. *ACS Chemical Neuroscience*, **2013**, 4, 1393-403	5.7	47
303	What does an ionic liquid surface really look like? Unprecedented details from molecular simulations. *Physical Chemistry Chemical Physics*, **2011**, 13, 21230-2	3.6	47
302	Speeding up Early Drug Discovery in Antiviral Research: A Fragment-Based in Silico Approach for the Design of Virtual Anti-Hepatitis C Leads. *ACS Combinatorial Science*, **2017**, 19, 501-512	3.9	44
301	Improved Force Field Model for the Deep Eutectic Solvent Ethaline: Reliable Physicochemical Properties. *Journal of Physical Chemistry B*, **2016**, 120, 10124-10137	3.4	44
300	DFT study of the adsorption of D-(L-)cysteine on flat and chiral stepped gold surfaces. *Langmuir*, **2013**, 29, 8856-64	4	44
299	Predicting multiple ecotoxicological profiles in agrochemical fungicides: a multi-species chemoinformatic approach. *Ecotoxicology and Environmental Safety*, **2012**, 80, 308-13	7	44
298	Multi-target drug discovery in anti-cancer therapy: fragment-based approach toward the design of potent and versatile anti-prostate cancer agents. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 6239-44	3.4	44
297	Molecular dynamics study of the interface between water and 2-nitrophenyl octyl ether. *Journal of Physical Chemistry B*, **2008**, 112, 2415-29	3.4	42
296	Computational chemistry approach for the early detection of drug-induced idiosyncratic liver toxicity. *Journal of Computational Chemistry*, **2008**, 29, 533-49	3.5	42
295	Fragment-based in silico modeling of multi-target inhibitors against breast cancer-related proteins. *Molecular Diversity*, **2017**, 21, 511-523	3.1	41
294	QSAR-Co: An Open Source Software for Developing Robust Multitasking or Multitarget Classification-Based QSAR Models. *Journal of Chemical Information and Modeling*, **2019**, 59, 2538-2544	6.1	40
293	Desirability-based methods of multiobjective optimization and ranking for global QSAR studies. Filtering safe and potent drug candidates from combinatorial libraries. *ACS Combinatorial Science*, **2008**, 10, 897-913		40
292	Desirability-based multiobjective optimization for global QSAR studies: application to the design of novel NSAIDs with improved analgesic, antiinflammatory, and ulcerogenic profiles. *Journal of Computational Chemistry*, **2008**, 29, 2445-59	3.5	40
291	Generalized Brønsted–Evans–Polanyi relationships and descriptors for O–H bond cleavage of organic molecules on transition metal surfaces. *Journal of Catalysis*, **2014**, 313, 24-33	7.3	39
290	Simultaneous virtual prediction of anti-Escherichia coli activities and ADMET profiles: A chemoinformatic complementary approach for high-throughput screening. *ACS Combinatorial Science*, **2014**, 16, 78-84	3.9	39
289	Combining QSAR classification models for predictive modeling of human monoamine oxidase inhibitors. *European Journal of Medicinal Chemistry*, **2013**, 59, 75-90	6.8	39
288	TOPS-MODE model of multiplexing neuroprotective effects of drugs and experimental-theoretic study of new 1,3-rasagiline derivatives potentially useful in neurodegenerative diseases. *Bioorganic and Medicinal Chemistry*, **2013**, 21, 1870-9	3.4	39
287	Structure-function relationships in ABCG2: insights from molecular dynamics simulations and molecular docking studies. *Scientific Reports*, **2017**, 7, 15534	4.9	39

286	First Multitarget Chemo-Bioinformatic Model To Enable the Discovery of Antibacterial Peptides against Multiple Gram-Positive Pathogens. *Journal of Chemical Information and Modeling*, **2016**, 56, 588-98	6.1	38
285	The Role of Preadsorbed Atomic Hydrogen in the NO Dissociation on a Zigzag Stepped Gold Surface: A DFT Study. *Journal of Physical Chemistry C*, **2009**, 113, 8864-8877	3.8	38
284	Molecular simulation of silica/surfactant self-assembly in the synthesis of periodic mesoporous silicas. *Journal of the American Chemical Society*, **2007**, 129, 15414-5	16.4	38
283	Multi-target inhibitors for proteins associated with Alzheimer: in silico discovery using fragment-based descriptors. *Current Alzheimer Research*, **2013**, 10, 117-24	3	38
282	Mechanistic Study of Carbon Monoxide Methanation over Pure and Rhodium- or Ruthenium-Doped Nickel Catalysts. *Journal of Physical Chemistry C*, **2015**, 119, 16537-16551	3.8	37
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280	Quantum and simulation studies of X(H2O)n systems. *Electrochimica Acta*, **1999**, 45, 659-673	6.7	37
279	RutheniumPlatinum Catalysts and Direct Methanol Fuel Cells (DMFC): A Review of Theoretical and Experimental Breakthroughs. *Catalysts*, **2017**, 7, 47	4	36
278	Quantitative structure-carcinogenicity relationship for detecting structural alerts in nitroso compounds: species, rat; sex, female; route of administration, gavage. *Chemical Research in Toxicology*, **2008**, 21, 633-42	4	36
277	Unified multi-target approach for the rational in silico design of anti-bladder cancer agents. *Anti-Cancer Agents in Medicinal Chemistry*, **2013**, 13, 791-800	2.2	36
276	Multitasking models for quantitative structure-biological effect relationships: current status and future perspectives to speed up drug discovery. *Expert Opinion on Drug Discovery*, **2015**, 10, 245-56	6.2	35
275	Simultaneous modeling of antimycobacterial activities and ADMET profiles: a chemoinformatic approach to medicinal chemistry. *Current Topics in Medicinal Chemistry*, **2013**, 13, 1656-65	3	35
274	Molecular dynamics simulation of the early stages of the synthesis of periodic mesoporous silica. *Journal of Physical Chemistry B*, **2009**, 113, 708-18	3.4	35
273	3D-MEDNEs: an alternative "in silico" technique for chemical research in toxicology. 2. quantitative proteome-toxicity relationships (QPTR) based on mass spectrum spiral entropy. *Chemical Research in Toxicology*, **2008**, 21, 619-32	4	35
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271	Physical properties at the base for the development of an all-atom force field for ethylene glycol. *Journal of Physical Chemistry B*, **2011**, 115, 3013-9	3.4	34
270	Probing the anticancer activity of nucleoside analogues: a QSAR model approach using an internally consistent training set. *Journal of Medicinal Chemistry*, **2007**, 50, 1537-45	8.3	34
269	Dermic diffusion and stratum corneum: a state of the art review of mathematical models. *Journal of Controlled Release*, **2014**, 177, 74-83	11.7	33

268	Influence of Ion Size and Charge in Ion Transfer Processes Across a Liquid|Liquid Interface. *Journal of Physical Chemistry B*, **2000**, 104, 2278-2286	3.4	33
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266	De novo computational design of compounds virtually displaying potent antibacterial activity and desirable in vitro ADMET profiles. *Medicinal Chemistry Research*, **2017**, 26, 2345-2356	2.2	32
265	Chemoinformatics for medicinal chemistry: in silico model to enable the discovery of potent and safer anti-cocci agents. *Future Medicinal Chemistry*, **2014**, 6, 2013-28	4.1	32
264	Calibration sets and the accuracy of vibrational scaling factors: a case study with the X3LYP hybrid functional. *Journal of Chemical Physics*, **2010**, 133, 114109	3.9	32
263	Gas-phase molecular structure and energetics of anionic silicates. *Geochimica Et Cosmochimica Acta*, **2008**, 72, 4421-4439	5.5	32
262	Towards the discovery of a novel class of monoamine oxidase inhibitors: structure-property-activity and docking studies on chromone amides. *ChemMedChem*, **2011**, 6, 628-32	3.7	30
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258	Salt separation from water using graphene oxide nanochannels: A molecular dynamics simulation study. *Desalination*, **2019**, 460, 1-14	10.3	29
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255	Chemoinformatics for rational discovery of safe antibacterial drugs: simultaneous predictions of biological activity against streptococci and toxicological profiles in laboratory animals. *Bioorganic and Medicinal Chemistry*, **2013**, 21, 2727-32	3.4	29
254	Fragment-based QSAR model toward the selection of versatile anti-sarcoma leads. *European Journal of Medicinal Chemistry*, **2011**, 46, 5910-6	6.8	29
253	New Workflow for QSAR Model Development from Small Data Sets: Small Dataset Curator and Small Dataset Modeler. Integration of Data Curation, Exhaustive Double Cross-Validation, and a Set of Optimal Model Selection Techniques. *Journal of Chemical Information and Modeling*, **2019**, 59, 4070-4076	6.1	28
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236	Convenient QSAR model for predicting the complexation of structurally diverse compounds with beta-cyclodextrins. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 896-904	3.4	23
235	Application of Bioinformatics for the Search of Novel Anti-Viral Therapies: Rational Design of Anti-Herpes Agents. *Current Bioinformatics*, **2011**, 6, 81-93	4.7	23
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230	Solvent accessible surface area-based hot-spot detection methods for protein-protein and protein-nucleic acid interfaces. *Journal of Chemical Information and Modeling*, **2015**, 55, 1077-86	6.1	21
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228	QSAR modelling: a therapeutic patent review 2010-present. *Expert Opinion on Therapeutic Patents*, **2018**, 28, 467-476	6.8	21
227	The impact of triamcinolone acetonide in early breast capsule formation in a rabbit model. *Aesthetic Plastic Surgery*, **2012**, 36, 986-94	2	21
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225	A topological substructural molecular design approach for predicting mutagenesis end-points of alpha, beta-unsaturated carbonyl compounds. *Toxicology*, **2010**, 268, 64-77	4.4	21
224	DFT study of the Au(321) surface reconstruction by consecutive deposition of oxygen atoms. *Surface Science*, **2008**, 602, 424-435	1.8	21
223	Molecular dynamics study of 2-nitrophenyl octyl ether and nitrobenzene. *Journal of Physical Chemistry B*, **2006**, 110, 12530-8	3.4	21
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206	Competitive Paths for Methanol Decomposition on Ruthenium: A DFT Study. *Journal of Physical Chemistry C*, **2015**, 119, 27382-27391	3.8	17
205	QSPR modelling with the topological substructural molecular design approach: beta-cyclodextrin complexation. *Journal of Pharmaceutical Sciences*, **2009**, 98, 4557-76	3.9	17
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190	Cetuximab and the Head and Neck Squamous Cell Cancer. *Current Topics in Medicinal Chemistry*, **2018**, 18, 192-198	3	15
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188	Rational development of molecular imprinted carbon paste electrode for Furazolidone detection: theoretical and experimental approach. *Sensors and Actuators B: Chemical*, **2021**, 329, 129112	8.5	15
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185	Effect of replacing [NTf2] by [PF6] anion on the [BMIm][NTf2] ionic liquid confined by gold. *Molecular Simulation*, **2015**, 41, 455-462	2	14
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