Maria Natlia Dias Soeiro Cordeiro

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Insights into the Mechanism of Methanol Steam Reforming for Hydrogen Production over NiCu-Based Catalysts. *ACS Catalysis*, **2022**, 12, 512-526	13.1	2
338	An integrated protocol to study hydrogen abstraction reactions by atomic hydrogen in flexible molecules: application to butanol isomers.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	1
337	A simple electrochemical detection of atorvastatin based on disposable screen-printed carbon electrodes modified by molecularly imprinted polymer: Experiment and simulation.. *Analytica Chimica Acta*, **2022**, 1194, 339410	6.6	3
336	Turning deep-eutectic solvents into value-added products for CO2 capture: A desirability-based virtual screening study. *Journal of CO2 Utilization*, **2022**, 58, 101926	7.6	3
335	Computational Modelling and Sustainable Synthesis of a Highly Selective Electrochemical MIP-Based Sensor for Citalopram Detection. *Molecules*, **2022**, 27, 3315	4.8	
334	Chemometric Modeling of Daphnia Toxicity **2021**, 293-317		
333	Aiming High versus Aiming All **2021**, 167-179		
332	Multi-Target In Silico Prediction of Inhibitors for Mitogen-Activated Protein Kinase-Interacting Kinases. *Biomolecules*, **2021**, 11,	5.9	3
331	Nanomarker for Early Detection of Alzheimer Disease Combining Ab initio DFT Simulations and Molecular Docking Approach. *Biophysica*, **2021**, 1, 76-86		1
330	QSAR-Co-X: an open source toolkit for multitarget QSAR modelling. *Journal of Cheminformatics*, **2021**, 13, 29	8.6	6
329	AKT Inhibitors: The Road Ahead to Computational Modeling-Guided Discovery. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
328	Ionic liquid metal interface: The origins of capacitance peaks. *Electrochimica Acta*, **2021**, 379, 138148	6.7	6
327	Corrigendum to: Computational Modeling of Environmental Co-exposure on Oil-Derived Hydrocarbon Overload by Using Substrate-Specific Transport Protein (TodX) with Graphene Nanostructures. *Current Topics in Medicinal Chemistry*, **2021**, 21, 839	3	
326	Exploring the conformational binding mechanism of fibrinogen induced by interactions with penicillin lactam antibiotic drugs. *Journal of Molecular Liquids*, **2021**, 324, 114667	6	4
325	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
324	Light alcohols reforming towards renewable hydrogen production on multicomponent catalysts. *Renewable and Sustainable Energy Reviews*, **2021**, 138, 110523	16.2	7
323	Insights into the catalytic activity of trimetallic Al/Zn/Cu surfaces for the water gas shift reaction. *Applied Surface Science*, **2021**, 542, 148589	6.7	5

322	Molecularly imprinted polymer-based electrochemical sensors for environmental analysis. *Biosensors and Bioelectronics*, **2021**, 172, 112719	11.8	63
321	Structure and noncovalent interactions in ionic liquids mixtures and deep eutectic solvents **2021**, 105-157		2
320	First-principles-based kinetic Monte Carlo simulations of CO oxidation on catalytic Au(110) and Ag(110) surfaces. *Physical Chemistry Chemical Physics*, **2021**, 23, 14037-14050	3.6	1
319	Molecular dynamic study of alcohol-based deep eutectic solvents. *Journal of Chemical Physics*, **2021** , 155, 064506	3.9	4
318	Density of Deep Eutectic Solvents: The Path Forward Cheminformatics-Driven Reliable Predictions for Mixtures. *Molecules*, **2021**, 26,	4.8	5
317	Heavy metal ion separation from industrial wastewater using stacked graphene Membranes: A molecular dynamics simulation study. *Journal of Molecular Liquids*, **2021**, 338, 116688	6	5
316	Development of a molecular imprinted electrochemiluminescence sensor for amitriptyline detection: From MD simulations to experimental implementation. *Electrochimica Acta*, **2021**, 397, 139273	6.7	2
315	Structural behavior of monomer of SARS-CoV-2 spike protein during initial stage of adsorption on graphene. *Materials Today Chemistry*, **2021**, 22, 100572	6.2	6
314	Medical Social Networks, Epidemiology and Health Systems. *Advances in Information Quality and Management*, **2021**, 1827-1838	0.1	
313	Interaction of Coumarin Phytoestrogens with ER and ER: A Molecular Dynamics Simulation Study. *Molecules*, **2020**, 25,	4.8	8
312	Azithromycin electrochemical detection using a molecularly imprinted polymer prepared on a disposable screen-printed electrode. *Analytical Methods*, **2020**, 12, 1486-1494	3.2	21
311	Computational modeling on mitochondrial channel nanotoxicity. *Nano Today*, **2020**, 34, 100913	17.9	3
310	Theoretical insights on helix repacking as the origin of P-glycoprotein promiscuity. *Scientific Reports* , **2020**, 10, 9823	4.9	9
309	Got to Write a Classic: Classical and Perturbation-Based QSAR Methods, Machine Learning, and the Monitoring of Nanoparticle Ecotoxicity. *Methods in Pharmacology and Toxicology*, **2020**, 195-213	1.1	1
308	Chapter 11:Supported Vanadium Catalysts: Heterogeneous Molecular Complexes, Electrocatalysis and Biomass Transformation. *RSC Catalysis Series*, **2020**, 241-284	0.3	
307	Computational Modeling of Environmental Co-exposure on Oil-Derived Hydrocarbon Overload by Using Substrate-Specific Transport Protein (TodX) with Graphene Nanostructures. *Current Topics in Medicinal Chemistry*, **2020**, 20, 2308-2325	3	1
306	Advanced in Silico Methods for the Development of Anti- Leishmaniasis and Anti-Trypanosomiasis Agents. *Current Medicinal Chemistry*, **2020**, 27, 697-718	4.3	6
305	Developing a Multi-target Model to Predict the Activity of Monoamine Oxidase A and B Drugs. *Current Topics in Medicinal Chemistry*, **2020**, 20, 1593-1600	3	3

304	PTML Multi-Label Algorithms: Models, Software, and Applications. *Current Topics in Medicinal Chemistry*, **2020**, 20, 2326-2337	3	3
303	Hysteresis in the MD Simulations of Differential Capacitance at the Ionic Liquid-Au Interface. *Journal of Physical Chemistry Letters*, **2020**, 11, 10408-10413	6.4	4
302	Probing the efficiency of platinum nanotubes for the H2 production by water gas shift reaction: A DFT study. *Applied Catalysis B: Environmental*, **2020**, 263, 118301	21.8	14
301	A unified in silico model based on perturbation theory for assessing the genotoxicity of metal oxide nanoparticles. *Chemosphere*, **2020**, 244, 125489	8.4	13
300	Understanding the Binding Specificity of G-Protein Coupled Receptors toward G-Proteins and Arrestins: Application to the Dopamine Receptor Family. *Journal of Chemical Information and Modeling*, **2020**, 60, 3969-3984	6.1	3
299	Mapping the underlying mechanisms of fibrinogen benzothiazole drug interactions using computational and experimental approaches. *International Journal of Biological Macromolecules*, **2020**, 163, 730-744	7.9	5
298	Targeting Beta-Blocker Drug-Drug Interactions with Fibrinogen Blood Plasma Protein: A Computational and Experimental Study. *Molecules*, **2020**, 25,	4.8	2
297	Covalent Functionalization of Graphene with PAMAM Dendrimer and Its Implications on Graphene Dispersion and Cytotoxicity. *ACS Applied Polymer Materials*, **2020**, 2, 3587-3600	4.3	6
296	Computational and experimental study of propeline: A choline chloride based deep eutectic solvent. *Journal of Molecular Liquids*, **2020**, 298, 111978	6	16
295	Importance of Data Curation in QSAR Studies Especially While Modeling Large-Size Datasets. *Methods in Pharmacology and Toxicology*, **2020**, 97-109	1.1	4
294	On the Relevance of Feature Selection Algorithms While Developing Non-linear QSARs. *Methods in Pharmacology and Toxicology*, **2020**, 177-194	1.1	1
293	Development of Multi-Target Chemometric Models for the Inhibition of Class I PI3K Enzyme Isoforms: A Case Study Using QSAR-Co Tool. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	12
292	CompScore: Boosting Structure-Based Virtual Screening Performance by Incorporating Docking Scoring Function Components into Consensus Scoring. *Journal of Chemical Information and Modeling*, **2019**, 59, 3655-3666	6.1	14
291	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
290	From biomedicinal to models and back to therapeutics: a review on the advancement of peptidic modeling. *Future Medicinal Chemistry*, **2019**, 11, 2313-2331	4.1	1
289	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
288	Distance Angle Descriptors of the Interionic and Ion-Solvent Interactions in Imidazolium-Based Ionic Liquid Mixtures with Aprotic Solvents: A Molecular Dynamics Simulation Study. *Journal of Physical Chemistry B*, **2019**, 123, 6065-6075	3.4	11
287	On the role of the surface charge plane position at Au(hkl)BMImPF6 interfaces. *Electrochimica Acta*, **2019**, 318, 76-82	6.7	5

286	Local structure and hydrogen bonding in liquid γ-butyrolactone and propylene carbonate: A molecular dynamics simulation. *Journal of Molecular Liquids*, **2019**, 287, 110912	6	12
285	PTML Model of Enzyme Subclasses for Mining the Proteome of Biofuel Producing Microorganisms. *Journal of Proteome Research*, **2019**, 18, 2735-2746	5.6	18
284	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
283	Computational MitoTarget Scanning Based on Topological Vacancies of Single-Walled Carbon Nanotubes with the Human Mitochondrial Voltage-Dependent Anion Channel (hVDAC1). *Chemical Research in Toxicology*, **2019**, 32, 566-577	4	4
282	Salt separation from water using graphene oxide nanochannels: A molecular dynamics simulation study. *Desalination*, **2019**, 460, 1-14	10.3	29
281	Structural and energetic evolution of fibrinogen toward to the betablocker interactions. *International Journal of Biological Macromolecules*, **2019**, 137, 405-419	7.9	8
280	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. *Current Topics in Medicinal Chemistry*, **2019**, 19, 957-969	3	6
279	Influence of alcohols on the inter-ion interactions in ionic liquids: A molecular dynamics study. *Journal of Molecular Liquids*, **2019**, 294, 111538	6	8
278	Alignment-Free Method to Predict Enzyme Classes and Subclasses. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	8
277	Multi-Target Chemometric Modelling, Fragment Analysis and Virtual Screening with ERK Inhibitors as Potential Anticancer Agents. *Molecules*, **2019**, 24,	4.8	11
276	Dynamical Rearrangement of Human Epidermal Growth Factor Receptor 2 upon Antibody Binding: Effects on the Dimerization. *Biomolecules*, **2019**, 9,	5.9	1
275	Development of Predictive Linear and Non-linear QSTR Models for Aliivibrio Fischeri Toxicity of Deep Eutectic Solvents. *International Journal of Quantitative Structure-Property Relationships*, **2019**, 4, 50-69	1.2	2
274	MitoTarget Modeling Using ANN-Classification Models Based on Fractal SEM Nano-Descriptors: Carbon Nanotubes as Mitochondrial F0F1-ATPase Inhibitors. *Journal of Chemical Information and Modeling*, **2019**, 59, 86-97	6.1	8
273	Improving Vibrational Mode Interpretation Using Bayesian Regression. *Journal of Chemical Theory and Computation*, **2019**, 15, 456-470	6.4	16
272	Enhancement of differential double layer capacitance and charge accumulation by tuning the composition of ionic liquids mixtures. *Electrochimica Acta*, **2018**, 261, 214-220	6.7	16
271	On the thickness of the double layer in ionic liquids. *Physical Chemistry Chemical Physics*, **2018**, 20, 10275-10285	3.6	27
270	A further development of the QNAR model to predict the cellular uptake of nanoparticles by pancreatic cancer cells. *Food and Chemical Toxicology*, **2018**, 112, 571-580	4.7	9
269	Computer-Aided Drug Design Approaches to Study Key Therapeutic Targets in Alzheimer's Disease. *Neuromethods*, **2018**, 61-106	0.4	1

268	A DFT and QTAIM study of the adsorption of organic molecules over the copper-doped coronene and circumcoronene. *Physica E: Low-Dimensional Systems and Nanostructures*, **2018**, 95, 59-70	3	12
267	Structure and kinetics of water in highly confined conditions: A molecular dynamics simulation study. *Journal of Molecular Liquids*, **2018**, 268, 625-636	6	19
266	QSAR modelling: a therapeutic patent review 2010-present. *Expert Opinion on Therapeutic Patents*, **2018**, 28, 467-476	6.8	21
265	Q2DTor: A program to treat torsional anharmonicity through coupled pair torsions in flexible molecules. *Computer Physics Communications*, **2018**, 232, 190-205	4.2	15
264	Advanced Chemometric Modeling Approaches for the Design of Multitarget Drugs Against Neurodegenerative Diseases. *Methods in Pharmacology and Toxicology*, **2018**, 155-186	1.1	2
263	A desirability-based multi objective approach for the virtual screening discovery of broad-spectrum anti-gastric cancer agents. *PLoS ONE*, **2018**, 13, e0192176	3.7	11
262	Cetuximab and the Head and Neck Squamous Cell Cancer. *Current Topics in Medicinal Chemistry*, **2018**, 18, 192-198	3	15
261	Looking for New Inhibitors for the Epidermal Growth Factor Receptor. *Current Topics in Medicinal Chemistry*, **2018**, 18, 219-232	3	7
260	In Silico Studies Targeting G-protein Coupled Receptors for Drug Research Against Parkinson's Disease. *Current Neuropharmacology*, **2018**, 16, 786-848	7.6	10
259	Mixed Self-Assembled Monolayers on Gold Nanoparticles: Synthesis, Properties, and Applications **2018**, 769-776		
258	Prediction of the Toxicity of Binary Mixtures by QSAR Approach Using the Hypothetical Descriptors. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	15
257	Mr. Silva and Patient Zero: A Medical Social Network and Data Visualization Information System. *Lecture Notes in Computer Science*, **2018**, 111-117	0.9	1
256	Estimation of the Toxicity of Different Substituted Aromatic Compounds to the Aquatic Ciliate by QSAR Approach. *Molecules*, **2018**, 23,	4.8	5
255	Influence of the anion on the properties of ionic liquid mixtures: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2018**, 20, 14899-14918	3.6	27
254	Exploring rare chemical phenomena using fractional nuclear charges: The cis-effect in N2F2. *International Journal of Quantum Chemistry*, **2018**, 118, e25662	2.1	2
253	Detection of simple inorganic and organic molecules over Cu-decorated circumcoronene: a combined DFT and QTAIM study. *Physical Chemistry Chemical Physics*, **2018**, 20, 16021-16032	3.6	10
252	Driving Forces in the Sharpless Epoxidation Reaction: A Coupled AIMD/QTAIM Study. *Inorganic Chemistry*, **2017**, 56, 2124-2134	5.1	7
251	Janus Gold Nanoparticles from Nanodroplets of Alkyl Thiols: A Molecular Dynamics Study. *Langmuir* , **2017**, 33, 3056-3067	4	9

250	Molecular Simulations of the Synthesis of Periodic Mesoporous Silica Phases at High Surfactant Concentrations. *Journal of Physical Chemistry C*, **2017**, 121, 4564-4575	3.8	17
249	Fragment-based in silico modeling of multi-target inhibitors against breast cancer-related proteins. *Molecular Diversity*, **2017**, 21, 511-523	3.1	41
248	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
247	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. *Drug Discovery Today*, **2017**, 22, 1489-1502	8.8	17
246	Consensus strategy in genes prioritization and combined bioinformatics analysis for preeclampsia pathogenesis. *BMC Medical Genomics*, **2017**, 10, 50	3.7	14
245	Machine Learning Approach to Predict Enzyme Subclasses **2017**, 37-53		
244	Speeding Up the Virtual Design and Screening of Therapeutic Peptides: Simultaneous Prediction of Anticancer Activity and Cytotoxicity **2017**, 127-147		7
243	Probing the toxicity of nanoparticles: a unified in silico machine learning model based on perturbation theory. *Nanotoxicology*, **2017**, 11, 891-906	5.3	64
242	Structure-function relationships in ABCG2: insights from molecular dynamics simulations and molecular docking studies. *Scientific Reports*, **2017**, 7, 15534	4.9	39
241	Removal of Pb(II) Ion Using PAMAM Dendrimer Grafted Graphene and Graphene Oxide Surfaces: A Molecular Dynamics Study. *Journal of Physical Chemistry A*, **2017**, 121, 9320-9329	2.8	14
240	New Force Field Model for Propylene Glycol: Insight to Local Structure and Dynamics. *Journal of Physical Chemistry B*, **2017**, 121, 10906-10921	3.4	19
239	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
238	Water dissociation on multimetallic catalysts. *Applied Catalysis B: Environmental*, **2017**, 218, 199-207	21.8	11
237	Prediction of metallic nanotube reactivity for HO activation. *Physical Chemistry Chemical Physics*, **2017**, 19, 19188-19195	3.6	1
236	Predictors of satisfaction in patient with silicone breast implants and its association with drug intake habits. *Acta Chirurgica Belgica*, **2017**, 117, 89-98	0.9	
235	Strengths, Weaknesses, Opportunities and Threats: Computational Studies of Mn- and Fe-Catalyzed Epoxidations. *Catalysts*, **2017**, 7, 2	4	13
234	RutheniumPlatinum Catalysts and Direct Methanol Fuel Cells (DMFC): A Review of Theoretical and Experimental Breakthroughs. *Catalysts*, **2017**, 7, 47	4	36
233	Advanced In Silico Approaches for Drug Discovery: Mining Information from Multiple Biological and Chemical Data Through mtk- QSBER and pt-QSPR Strategies. *Current Medicinal Chemistry*, **2017**, 24, 1687-1704	4.3	13

232	Rational Design of Multi-Target Estrogen Receptors ERα and ERβ by QSAR Approaches. *Current Drug Targets*, **2017**, 18, 576-591	3	7
231	Fusing Docking Scoring Functions Improves the Virtual Screening Performance for Discovering Parkinson's Disease Dual Target Ligands. *Current Neuropharmacology*, **2017**, 15, 1107-1116	7.6	6
230	Chemoinformatics Profiling of the Chromone Nucleus as a MAO-B/A2AAR Dual Binding Scaffold. *Current Neuropharmacology*, **2017**, 15, 1117-1135	7.6	3
229	QSAR-Based Studies of Nanomaterials in the Environment **2017**, 1504-1532		1
228	QSAR-Based Studies of Nanomaterials in the Environment **2017**, 1339-1366		1
227	Measurement artifacts identified in the UV-vis spectroscopic study of adduct formation within the context of molecular imprinting of naproxen. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2016**, 153, 661-8	4.4	9
226	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
225	On the effects of the basis set superposition error on the change of QTAIM charges in adduct formation. Application to complexes between morphine and cocaine and their main metabolites. *RSC Advances*, **2016**, 6, 110642-110655	3.7	2
224	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
223	Efficient and biologically relevant consensus strategy for Parkinson's disease gene prioritization. *BMC Medical Genomics*, **2016**, 9, 12	3.7	15
222	Interactions in the ionic liquid [EMIM][FAP]: a coupled experimental and computational analysis. *Physical Chemistry Chemical Physics*, **2016**, 18, 2617-28	3.6	16
221	Molecular dynamics study of wetting behavior of grafted thermo-responsive PNIPAAm brushes. *Soft Matter*, **2016**, 12, 3093-102	3.6	13
220	Methanol dissociation on bimetallic surfaces: validity of the general Brønsted–Evans–Polanyi relationship for O–H bond cleavage. *RSC Advances*, **2016**, 6, 18695-18702	3.7	10
219	Roots of Acetate-Vanadium Linkage Isomerism: A QTAIM Study. *Inorganic Chemistry*, **2016**, 55, 3653-62	5.1	7
218	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
217	Ligand-Based Virtual Screening Using Tailored Ensembles: A Prioritization Tool for Dual A2AAdenosine Receptor Antagonists / Monoamine Oxidase B Inhibitors. *Current Pharmaceutical Design*, **2016**, 22, 3082-96	3.3	10
216	Probing the Hypothesis of SAR Continuity Restoration by the Removal of Activity Cliffs Generators in QSAR. *Current Pharmaceutical Design*, **2016**, 22, 5043-5056	3.3	5
215	A Machine Learning Approach for Hot-Spot Detection at Protein-Protein Interfaces. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	33

214	Molecular Dynamics Simulation Study of the Selectivity of a Silica Polymer for Ibuprofen. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	5
213	Striped gold nanoparticles: New insights from molecular dynamics simulations. *Journal of Chemical Physics*, **2016**, 144, 244710	3.9	10
212	Multiscale Model for the Templated Synthesis of Mesoporous Silica: The Essential Role of Silica Oligomers. *Chemistry of Materials*, **2016**, 28, 2715-2727	9.6	22
211	A computational study of the interaction of graphene structures with biomolecular units. *Physical Chemistry Chemical Physics*, **2016**, 18, 15312-21	3.6	14
210	Effect of the Exchange-Correlation Potential on the Transferability of Brønsted-Evans-Polanyi Relationships in Heterogeneous Catalysis. *Journal of Chemical Theory and Computation*, **2016**, 12, 2121-6	6.4	15
209	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
208	Effect of replacing [NTf2] by [PF6] anion on the [BMIm][NTf2] ionic liquid confined by gold. *Molecular Simulation*, **2015**, 41, 455-462	2	14
207	Molecular Dynamics Study of the Gold/Ionic Liquids Interface. *Journal of Physical Chemistry B*, **2015**, 119, 9883-92	3.4	26
206	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
205	Simple descriptors for assessing the outcome of aza-Diels–Alder reactions. *RSC Advances*, **2015**, 5, 50729-50740	3.7	2
204	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
203	Molecular Dynamics Simulations of Poly(ethylene oxide) Grafted onto Silica Immersed in Melt of Homopolymers. *Langmuir*, **2015**, 31, 10254-64	4	15
202	Harmonization of QSAR Best Practices and Molecular Docking Provides an Efficient Virtual Screening Tool for Discovering New G-Quadruplex Ligands. *Journal of Chemical Information and Modeling*, **2015**, 55, 2094-110	6.1	14
201	Competitive Paths for Methanol Decomposition on Ruthenium: A DFT Study. *Journal of Physical Chemistry C*, **2015**, 119, 27382-27391	3.8	17
200	Quinoxaline, its derivatives and applications: A State of the Art review. *European Journal of Medicinal Chemistry*, **2015**, 97, 664-72	6.8	221
199	Review of Structures Containing Fullerene-C60 for Delivery of Antibacterial Agents. Multitasking model for Computational Assessment of Safety Profiles. *Current Bioinformatics*, **2015**, 10, 565-578	4.7	5
198	Effect of van der Waals interactions in the DFT description of self-assembled monolayers of thiols on gold. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	15
197	Fischer-Tropsch Synthesis on Multicomponent Catalysts: What Can We Learn from Computer Simulations?. *Catalysts*, **2015**, 5, 3-17	4	18

196	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
195	Structure of Mixed Self-Assembled Monolayers on Gold Nanoparticles at Three Different Arrangements. *Journal of Physical Chemistry C*, **2015**, 119, 3199-3209	3.8	25
194	Computer-aided discovery in antimicrobial research: In silico model for virtual screening of potent and safe anti-pseudomonas agents. *Combinatorial Chemistry and High Throughput Screening*, **2015**, 18, 305-14	1.3	16
193	Enabling virtual screening of potent and safer antimicrobial agents against noma: mtk-QSBER model for simultaneous prediction of antibacterial activities and ADMET properties. *Mini-Reviews in Medicinal Chemistry*, **2015**, 15, 194-202	3.2	13
192	In silico assessment of the acute toxicity of chemicals: recent advances and new model for multitasking prediction of toxic effect. *Mini-Reviews in Medicinal Chemistry*, **2015**, 15, 677-86	3.2	22
191	Multi-Target QSAR Approaches for Modeling Protein Inhibitors. Simultaneous Prediction of Activities Against Biomacromolecules Present in Gram-Negative Bacteria. *Current Topics in Medicinal Chemistry*, **2015**, 15, 1801-13	3	20
190	Virtual Screening of Alkaloids from Apocynaceae with Potential Antitrypanosomal Activity. *Current Bioinformatics*, **2015**, 10, 509-519	4.7	6
189	A general ANN-based multitasking model for the discovery of potent and safer antibacterial agents. *Methods in Molecular Biology*, **2015**, 1260, 45-64	1.4	5
188	QSAR-Based Studies of Nanomaterials in the Environment. *Advances in Chemical and Materials Engineering Book Series*, **2015**, 506-534	0.2	
187	Classification of natural estrogen-like isoflavonoids and diphenolics by QSAR tools. *Combinatorial Chemistry and High Throughput Screening*, **2015**, 18, 712-22	1.3	
186	Charge distribution in Mn(salen) complexes. *International Journal of Quantum Chemistry*, **2014**, 114, 525-533	2.1	11
185	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
184	Surface Chemistry and Atomic-Scale Reconstruction of Kerogen–Silica Composites. *Journal of Physical Chemistry C*, **2014**, 118, 2429-2438	3.8	19
183	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
182	Effects of axial coordination on immobilized Mn(salen) catalysts. *Journal of Physical Chemistry A*, **2014**, 118, 10788-96	2.8	9
181	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
180	Molecular dynamics simulations of complex mixtures aimed at the preparation of naproxen-imprinted xerogels. *Journal of Chemical Information and Modeling*, **2014**, 54, 3330-43	6.1	5
179	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

178	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
177	Dynamic structure of NGF and proNGF complexed with p75NTR: pro-peptide effect. *Journal of Chemical Information and Modeling*, **2014**, 54, 2051-67	6.1	4
176	Principal component analysis of Mn(salen) catalysts. *Physical Chemistry Chemical Physics*, **2014**, 16, 25364-76	3.66	11
175	Molecular dynamics study of mixed alkanethiols covering a gold surface at three different arrangements. *Chemical Physics Letters*, **2014**, 600, 79-86	2.5	13
174	Computational ecotoxicology: simultaneous prediction of ecotoxic effects of nanoparticles under different experimental conditions. *Environment International*, **2014**, 73, 288-94	12.9	84
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