

Maria Natália Dias Soeiro Cordeiro

List of Publications by Year in descending order

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354
papers

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#	ARTICLE	IF	CITATIONS
1	Molecular simulations of interfacial systems: challenges, applications and future perspectives. <i>Molecular Simulation</i> , 2023, 49, 1229-1266.	0.9	14
2	An integrated protocol to study hydrogen abstraction reactions by atomic hydrogen in flexible molecules: application to butanol isomers. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3043-3058.	1.3	6
3	A simple electrochemical detection of atorvastatin based on disposable screen-printed carbon electrodes modified by molecularly imprinted polymer: Experiment and simulation. <i>Analytica Chimica Acta</i> , 2022, 1194, 339410.	2.6	14
4	N ₂ O Hydrogenation on Silver Doped Gold Catalysts, a DFT Study. <i>Nanomaterials</i> , 2022, 12, 394.	1.9	0
5	First multi-target QSAR model for predicting the cytotoxicity of acrylic acid-based dental monomers. <i>Dental Materials</i> , 2022, 38, 333-346.	1.6	9
6	Insights into the Mechanism of Methanol Steam Reforming for Hydrogen Production over Ni ²⁺ -Cu-Based Catalysts. <i>ACS Catalysis</i> , 2022, 12, 512-526.	5.5	31
7	Computational Modeling on Binding Interactions of Cyclodextrins with the Human Multidrug Resistance P-glycoprotein Toward Efficient Drug-Delivery System Applications.. <i>Current Topics in Medicinal Chemistry</i> , 2022, 22, .	1.0	3
8	Turning deep-eutectic solvents into value-added products for CO ₂ capture: A desirability-based virtual screening study. <i>Journal of CO₂ Utilization</i> , 2022, 58, 101926.	3.3	23
9	Moving Average-Based Multitasking In Silico Classification Modeling: Where Do We Stand and What Is Next?. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4937.	1.8	7
10	Computational Modelling and Sustainable Synthesis of a Highly Selective Electrochemical MIP-Based Sensor for Citalopram Detection. <i>Molecules</i> , 2022, 27, 3315.	1.7	5
11	Exploring the conformational binding mechanism of fibrinogen induced by interactions with penicillin β -lactam antibiotic drugs. <i>Journal of Molecular Liquids</i> , 2021, 324, 114667.	2.3	12
12	Rational development of molecular imprinted carbon paste electrode for Furazolidone detection: theoretical and experimental approach. <i>Sensors and Actuators B: Chemical</i> , 2021, 329, 129112.	4.0	43
13	Light alcohols reforming towards renewable hydrogen production on multicomponent catalysts. <i>Renewable and Sustainable Energy Reviews</i> , 2021, 138, 110523.	8.2	12
14	Insights into the catalytic activity of trimetallic Al/Zn/Cu surfaces for the water gas shift reaction. <i>Applied Surface Science</i> , 2021, 542, 148589.	3.1	12
15	Molecularly imprinted polymer-based electrochemical sensors for environmental analysis. <i>Biosensors and Bioelectronics</i> , 2021, 172, 112719.	5.3	149
16	Structure and noncovalent interactions in ionic liquids mixtures and deep eutectic solvents. , 2021, , 105-157.		3
17	First-principles-based kinetic Monte Carlo simulations of CO oxidation on catalytic Au(110) and Ag(110) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14037-14050.	1.3	7
18	New Mechanistic Insights on Carbon Nanotubes'™ Nanotoxicity Using Isolated Submitochondrial Particles, Molecular Docking, and Nano-QSTR Approaches. <i>Biology</i> , 2021, 10, 171.	1.3	4

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19	Nanomarker for Early Detection of Alzheimer's Disease Combining Ab initio DFT Simulations and Molecular Docking Approach. <i>Biophysica</i> , 2021, 1, 76-86.	0.6	4
20	QSAR-Co-X: an open source toolkit for multitarget QSAR modelling. <i>Journal of Cheminformatics</i> , 2021, 13, 29.	2.8	28
21	AKT Inhibitors: The Road Ahead to Computational Modeling-Guided Discovery. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3944.	1.8	12
22	Ionic liquid-metal interface: The origins of capacitance peaks. <i>Electrochimica Acta</i> , 2021, 379, 138148.	2.6	28
23	Corrigendum to: Computational Modeling of Environmental Co-exposure on Oil-Derived Hydrocarbon Overload by Using Substrate-Specific Transport Protein (TodX) with Graphene Nanostructures. <i>Current Topics in Medicinal Chemistry</i> , 2021, 21, 839-839.	1.0	0
24	Molecular dynamic study of alcohol-based deep eutectic solvents. <i>Journal of Chemical Physics</i> , 2021, 155, 064506.	1.2	15
25	Unravelling the Interactions of Magnetic Ionic Liquids by Energy Decomposition Schemes: Towards a Transferable Polarizable Force Field. <i>Molecules</i> , 2021, 26, 5526.	1.7	3
26	Density of Deep Eutectic Solvents: The Path Forward Cheminformatics-Driven Reliable Predictions for Mixtures. <i>Molecules</i> , 2021, 26, 5779.	1.7	23
27	Heavy metal ion separation from industrial wastewater using stacked graphene Membranes: A molecular dynamics simulation study. <i>Journal of Molecular Liquids</i> , 2021, 338, 116688.	2.3	26
28	Development of a molecular imprinted electrochemiluminescence sensor for amitriptyline detection: From MD simulations to experimental implementation. <i>Electrochimica Acta</i> , 2021, 397, 139273.	2.6	8
29	Structural behavior of monomer of SARS-CoV-2 spike protein during initial stage of adsorption on graphene. <i>Materials Today Chemistry</i> , 2021, 22, 100572.	1.7	11
30	Medical Social Networks, Epidemiology and Health Systems. <i>Advances in Information Quality and Management</i> , 2021, , 1827-1838.	0.3	0
31	Multi-Target In Silico Prediction of Inhibitors for Mitogen-Activated Protein Kinase-Interacting Kinases. <i>Biomolecules</i> , 2021, 11, 1670.	1.8	13
32	Computational and experimental study of propeline: A choline chloride based deep eutectic solvent. <i>Journal of Molecular Liquids</i> , 2020, 298, 111978.	2.3	25
33	Probing the efficiency of platinum nanotubes for the H ₂ production by water gas shift reaction: A DFT study. <i>Applied Catalysis B: Environmental</i> , 2020, 263, 118301.	10.8	19
34	A unified in silico model based on perturbation theory for assessing the genotoxicity of metal oxide nanoparticles. <i>Chemosphere</i> , 2020, 244, 125489.	4.2	16
35	Understanding the Binding Specificity of G-Protein Coupled Receptors toward G-Proteins and Arrestins: Application to the Dopamine Receptor Family. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3969-3984.	2.5	8
36	Mapping the underlying mechanisms of fibrinogen benzothiazole drug interactions using computational and experimental approaches. <i>International Journal of Biological Macromolecules</i> , 2020, 163, 730-744.	3.6	10

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37	Targeting Beta-Blocker Drug – Drug Interactions with Fibrinogen Blood Plasma Protein: A Computational and Experimental Study. <i>Molecules</i> , 2020, 25, 5425.	1.7	6
38	Covalent Functionalization of Graphene with PAMAM Dendrimer and Its Implications on Graphene's™s Dispersion and Cytotoxicity. <i>ACS Applied Polymer Materials</i> , 2020, 2, 3587-3600.	2.0	11
39	Interaction of Coumarin Phytoestrogens with ER α and ER β : A Molecular Dynamics Simulation Study. <i>Molecules</i> , 2020, 25, 1165.	1.7	11
40	Azithromycin electrochemical detection using a molecularly imprinted polymer prepared on a disposable screen-printed electrode. <i>Analytical Methods</i> , 2020, 12, 1486-1494.	1.3	43
41	Computational modeling on mitochondrial channel nanotoxicity. <i>Nano Today</i> , 2020, 34, 100913.	6.2	7
42	Theoretical insights on helix repacking as the origin of P-glycoprotein promiscuity. <i>Scientific Reports</i> , 2020, 10, 9823.	1.6	15
43	Importance of Data Curation in QSAR Studies Especially While Modeling Large-Size Datasets. <i>Methods in Pharmacology and Toxicology</i> , 2020, , 97-109.	0.1	6
44	On the Relevance of Feature Selection Algorithms While Developing Non-linear QSARs. <i>Methods in Pharmacology and Toxicology</i> , 2020, , 177-194.	0.1	3
45	Hysteresis in the MD Simulations of Differential Capacitance at the Ionic Liquid – Au Interface. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10408-10413.	2.1	14
46	Advanced in Silico Methods for the Development of Anti- Leishmaniasis and Anti-Trypanosomiasis Agents. <i>Current Medicinal Chemistry</i> , 2020, 27, 697-718.	1.2	12
47	Developing a Multi-target Model to Predict the Activity of Monoamine Oxidase A and B Drugs. <i>Current Topics in Medicinal Chemistry</i> , 2020, 20, 1593-1600.	1.0	8
48	PTML Multi-Label Algorithms: Models, Software, and Applications. <i>Current Topics in Medicinal Chemistry</i> , 2020, 20, 2326-2337.	1.0	8
49	Got to Write a Classic: Classical and Perturbation-Based QSAR Methods, Machine Learning, and the Monitoring of Nanoparticle Ecotoxicity. <i>Methods in Pharmacology and Toxicology</i> , 2020, , 195-213.	0.1	1
50	Supported Vanadium Catalysts: Heterogeneous Molecular Complexes, Electrocatalysis and Biomass Transformation. <i>RSC Catalysis Series</i> , 2020, , 241-284.	0.1	0
51	Computational Modeling of Environmental Co-exposure on Oil-Derived Hydrocarbon Overload by Using Substrate-Specific Transport Protein (TodX) with Graphene Nanostructures. <i>Current Topics in Medicinal Chemistry</i> , 2020, 20, 2308-2325.	1.0	3
52	Structural and energetic evolution of fibrinogen toward to the betablocker interactions. <i>International Journal of Biological Macromolecules</i> , 2019, 137, 405-419.	3.6	11
53	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. <i>Current Topics in Medicinal Chemistry</i> , 2019, 19, 957-969.	1.0	8
54	Influence of alcohols on the inter-ion interactions in ionic liquids: A molecular dynamics study. <i>Journal of Molecular Liquids</i> , 2019, 294, 111538.	2.3	12

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55	Alignment-Free Method to Predict Enzyme Classes and Subclasses. <i>International Journal of Molecular Sciences</i> , 2019, 20, 5389.	1.8	19
56	Multi-Target Chemometric Modelling, Fragment Analysis and Virtual Screening with ERK Inhibitors as Potential Anticancer Agents. <i>Molecules</i> , 2019, 24, 3909.	1.7	18
57	Dynamical Rearrangement of Human Epidermal Growth Factor Receptor 2 upon Antibody Binding: Effects on the Dimerization. <i>Biomolecules</i> , 2019, 9, 706.	1.8	6
58	Development of Multi-Target Chemometric Models for the Inhibition of Class I PI3K Enzyme Isoforms: A Case Study Using QSAR-Co Tool. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4191.	1.8	17
59	CompScore: Boosting Structure-Based Virtual Screening Performance by Incorporating Docking Scoring Function Components into Consensus Scoring. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3655-3666.	2.5	20
60	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. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4070-4076.	2.5	46
61	From biomedical to <i>in silico</i> models and back to therapeutics: a review on the advancement of peptidic modeling. <i>Future Medicinal Chemistry</i> , 2019, 11, 2313-2331.	1.1	3
62	Probing the Environmental Toxicity of Deep Eutectic Solvents and Their Components: An In Silico Modeling Approach. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 10649-10660.	3.2	99
63	Distance Angle Descriptors of the Interionic and Ion-Solvent Interactions in Imidazolium-Based Ionic Liquid Mixtures with Aprotic Solvents: A Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6065-6075.	1.2	15
64	On the role of the surface charge plane position at Au(hkl)-BMImPF ₆ interfaces. <i>Electrochimica Acta</i> , 2019, 318, 76-82.	2.6	15
65	Local structure and hydrogen bonding in liquid γ -butyrolactone and propylene carbonate: A molecular dynamics simulation. <i>Journal of Molecular Liquids</i> , 2019, 287, 110912.	2.3	16
66	PTML Model of Enzyme Subclasses for Mining the Proteome of Biofuel Producing Microorganisms. <i>Journal of Proteome Research</i> , 2019, 18, 2735-2746.	1.8	29
67	QSAR-Co: An Open Source Software for Developing Robust Multitasking or Multitarget Classification-Based QSAR Models. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2538-2544.	2.5	73
68	Computational MitoTarget Scanning Based on Topological Vacancies of Single-Walled Carbon Nanotubes with the Human Mitochondrial Voltage-Dependent Anion Channel (hVDAC1). <i>Chemical Research in Toxicology</i> , 2019, 32, 566-577.	1.7	4
69	Salt separation from water using graphene oxide nanochannels: A molecular dynamics simulation study. <i>Desalination</i> , 2019, 460, 1-14.	4.0	60
70	Development of Predictive Linear and Non-linear QSTR Models for Aliivibrio Fischeri Toxicity of Deep Eutectic Solvents. <i>International Journal of Quantitative Structure-Property Relationships</i> , 2019, 4, 50-69.	1.1	4
71	MitoTarget Modeling Using ANN-Classification Models Based on Fractal SEM Nano-Descriptors: Carbon Nanotubes as Mitochondrial FOF1-ATPase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 86-97.	2.5	11
72	Improving Vibrational Mode Interpretation Using Bayesian Regression. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 456-470.	2.3	37

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73	Enhancement of differential double layer capacitance and charge accumulation by tuning the composition of ionic liquids mixtures. <i>Electrochimica Acta</i> , 2018, 261, 214-220.	2.6	23
74	On the thickness of the double layer in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10275-10285.	1.3	40
75	A further development of the QNAR model to predict the cellular uptake of nanoparticles by pancreatic cancer cells. <i>Food and Chemical Toxicology</i> , 2018, 112, 571-580.	1.8	13
76	Computer-Aided Drug Design Approaches to Study Key Therapeutic Targets in Alzheimer's Disease. <i>Neuromethods</i> , 2018, , 61-106.	0.2	2
77	A DFT and QTAIM study of the adsorption of organic molecules over the copper-doped coronene and circumcoronene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 95, 59-70.	1.3	15
78	Mixed Self-Assembled Monolayers on Gold Nanoparticles: Synthesis, Properties, and Applications. , 2018, , 769-776.		0
79	Prediction of the Toxicity of Binary Mixtures by QSAR Approach Using the Hypothetical Descriptors. <i>International Journal of Molecular Sciences</i> , 2018, 19, 3423.	1.8	28
80	Mr. Silva and Patient Zero: A Medical Social Network and Data Visualization Information System. <i>Lecture Notes in Computer Science</i> , 2018, , 111-117.	1.0	2
81	Estimation of the Toxicity of Different Substituted Aromatic Compounds to the Aquatic Ciliate <i>Tetrahymena pyriformis</i> by QSAR Approach. <i>Molecules</i> , 2018, 23, 1002.	1.7	5
82	Influence of the anion on the properties of ionic liquid mixtures: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 14899-14918.	1.3	40
83	Exploring rare chemical phenomena using fractional nuclear charges: The <i>cis</i> effect in N_2F_2 . <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25662.	1.0	2
84	Detection of simple inorganic and organic molecules over Cu-decorated circumcoronene: a combined DFT and QTAIM study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16021-16032.	1.3	10
85	Structure and kinetics of water in highly confined conditions: A molecular dynamics simulation study. <i>Journal of Molecular Liquids</i> , 2018, 268, 625-636.	2.3	32
86	QSAR modelling: a therapeutic patent review 2010-present. <i>Expert Opinion on Therapeutic Patents</i> , 2018, 28, 467-476.	2.4	29
87	Q2DTor: A program to treat torsional anharmonicity through coupled pair torsions in flexible molecules. <i>Computer Physics Communications</i> , 2018, 232, 190-205.	3.0	23
88	Advanced Chemometric Modeling Approaches for the Design of Multitarget Drugs Against Neurodegenerative Diseases. <i>Methods in Pharmacology and Toxicology</i> , 2018, , 155-186.	0.1	3
89	A desirability-based multi objective approach for the virtual screening discovery of broad-spectrum anti-gastric cancer agents. <i>PLoS ONE</i> , 2018, 13, e0192176.	1.1	15
90	Cetuximab and the Head and Neck Squamous Cell Cancer. <i>Current Topics in Medicinal Chemistry</i> , 2018, 18, 192-198.	1.0	23

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91	Looking for New Inhibitors for the Epidermal Growth Factor Receptor. <i>Current Topics in Medicinal Chemistry</i> , 2018, 18, 219-232.	1.0	12
92	In Silico Studies Targeting G-protein Coupled Receptors for Drug Research Against Parkinson's Disease. <i>Current Neuropharmacology</i> , 2018, 16, 786-848.	1.4	18
93	Driving Forces in the Sharpless Epoxidation Reaction: A Coupled AIMD/QTAIM Study. <i>Inorganic Chemistry</i> , 2017, 56, 2124-2134.	1.9	9
94	Janus Gold Nanoparticles from Nanodroplets of Alkyl Thiols: A Molecular Dynamics Study. <i>Langmuir</i> , 2017, 33, 3056-3067.	1.6	10
95	Molecular Simulations of the Synthesis of Periodic Mesoporous Silica Phases at High Surfactant Concentrations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 4564-4575.	1.5	29
96	Fragment-based in silico modeling of multi-target inhibitors against breast cancer-related proteins. <i>Molecular Diversity</i> , 2017, 21, 511-523.	2.1	53
97	Speeding up Early Drug Discovery in Antiviral Research: A Fragment-Based in Silico Approach for the Design of Virtual Anti-Hepatitis C Leads. <i>ACS Combinatorial Science</i> , 2017, 19, 501-512.	3.8	59
98	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. <i>Drug Discovery Today</i> , 2017, 22, 1489-1502.	3.2	28
99	Probing the toxicity of nanoparticles: a unified in silico machine learning model based on perturbation theory. <i>Nanotoxicology</i> , 2017, 11, 891-906.	1.6	90
100	Structure-function relationships in ABCG2: insights from molecular dynamics simulations and molecular docking studies. <i>Scientific Reports</i> , 2017, 7, 15534.	1.6	48
101	Removal of Pb(II) Ion Using PAMAM Dendrimer Grafted Graphene and Graphene Oxide Surfaces: A Molecular Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9320-9329.	1.1	16
102	New Force Field Model for Propylene Glycol: Insight to Local Structure and Dynamics. <i>Journal of Physical Chemistry B</i> , 2017, 121, 10906-10921.	1.2	24
103	De novo computational design of compounds virtually displaying potent antibacterial activity and desirable in vitro ADMET profiles. <i>Medicinal Chemistry Research</i> , 2017, 26, 2345-2356.	1.1	46
104	Water dissociation on multimetallic catalysts. <i>Applied Catalysis B: Environmental</i> , 2017, 218, 199-207.	10.8	14
105	Prediction of metallic nanotube reactivity for H ₂ O activation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19188-19195.	1.3	1
106	Predictors of satisfaction in patient with silicone breast implants and its association with drug intake habits. <i>Acta Chirurgica Belgica</i> , 2017, 117, 89-98.	0.2	1
107	Strengths, Weaknesses, Opportunities and Threats: Computational Studies of Mn- and Fe-Catalyzed Epoxidations. <i>Catalysts</i> , 2017, 7, 2.	1.6	15
108	Ruthenium-Platinum Catalysts and Direct Methanol Fuel Cells (DMFC): A Review of Theoretical and Experimental Breakthroughs. <i>Catalysts</i> , 2017, 7, 47.	1.6	50

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109	Consensus strategy in genes prioritization and combined bioinformatics analysis for preeclampsia pathogenesis. <i>BMC Medical Genomics</i> , 2017, 10, 50.	0.7	18
110	Machine Learning Approach to Predict Enzyme Subclasses. , 2017, , 37-53.		0
111	Speeding Up the Virtual Design and Screening of Therapeutic Peptides. , 2017, , 127-147.		11
112	Advanced In Silico Approaches for Drug Discovery: Mining Information from Multiple Biological and Chemical Data Through mtk- QSBER and pt-QSPR Strategies. <i>Current Medicinal Chemistry</i> , 2017, 24, 1687-1704.	1.2	16
113	Rational Design of Multi-Target Estrogen Receptors ER α and ER β by QSAR Approaches. <i>Current Drug Targets</i> , 2017, 18, 576-591.	1.0	8
114	Fusing Docking Scoring Functions Improves the Virtual Screening Performance for Discovering Parkinson's Disease Dual Target Ligands. <i>Current Neuropharmacology</i> , 2017, 15, 1107-1116.	1.4	11
115	Cheminformatics Profiling of the Chromone Nucleus as a MAO-B/A2AAR Dual Binding Scaffold. <i>Current Neuropharmacology</i> , 2017, 15, 1117-1135.	1.4	5
116	QSAR-Based Studies of Nanomaterials in the Environment. , 2017, , 1504-1532.		2
117	QSAR-Based Studies of Nanomaterials in the Environment. , 2017, , 1339-1366.		1
118	A Machine Learning Approach for Hot-Spot Detection at Protein-Protein Interfaces. <i>International Journal of Molecular Sciences</i> , 2016, 17, 1215.	1.8	46
119	Molecular Dynamics Simulation Study of the Selectivity of a Silica Polymer for Ibuprofen. <i>International Journal of Molecular Sciences</i> , 2016, 17, 1083.	1.8	7
120	Striped gold nanoparticles: New insights from molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2016, 144, 244710.	1.2	12
121	Multiscale Model for the Templated Synthesis of Mesoporous Silica: The Essential Role of Silica Oligomers. <i>Chemistry of Materials</i> , 2016, 28, 2715-2727.	3.2	32
122	A computational study of the interaction of graphene structures with biomolecular units. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15312-15321.	1.3	18
123	Effect of the Exchange-Correlation Potential on the Transferability of Brønsted-Evans-Polanyi Relationships in Heterogeneous Catalysis. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2121-2126.	2.3	20
124	Improved Force Field Model for the Deep Eutectic Solvent Ethaline: Reliable Physicochemical Properties. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10124-10137.	1.2	63
125	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. <i>RSC Advances</i> , 2016, 6, 110642-110655.	1.7	2
126	Enabling the Discovery and Virtual Screening of Potent and Safe Antimicrobial Peptides. Simultaneous Prediction of Antibacterial Activity and Cytotoxicity. <i>ACS Combinatorial Science</i> , 2016, 18, 490-498.	3.8	73

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127	Efficient and biologically relevant consensus strategy for Parkinson's disease gene prioritization. BMC Medical Genomics, 2016, 9, 12.	0.7	29
128	Interactions in the ionic liquid [EMIM][FAP]: a coupled experimental and computational analysis. Physical Chemistry Chemical Physics, 2016, 18, 2617-2628.	1.3	25
129	Molecular dynamics study of wetting behavior of grafted thermo-responsive PNIPAAm brushes. Soft Matter, 2016, 12, 3093-3102.	1.2	18
130	Methanol dissociation on bimetallic surfaces: validity of the general Brønsted-Evans-Polanyi relationship for O-H bond cleavage. RSC Advances, 2016, 6, 18695-18702.	1.7	10
131	Roots of Acetate-Vanadium Linkage Isomerism: A QAIM Study. Inorganic Chemistry, 2016, 55, 3653-3662.	1.9	9
132	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, 588-598.	2.5	57
133	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, 661-668.	2.0	13
134	Ligand-Based Virtual Screening Using Tailored Ensembles: A Prioritization Tool for Dual Adenosine Receptor Antagonists / Monoamine Oxidase B Inhibitors. Current Pharmaceutical Design, 2016, 22, 3082-3096.	0.9	13
135	Probing the Hypothesis of SAR Continuity Restoration by the Removal of Activity Cliffs Generators in QSAR. Current Pharmaceutical Design, 2016, 22, 5043-5056.	0.9	7
136	Editorial (Thematic Issue: Multi-Target Drug Discovery in Medicinal Chemistry: Current Status and Tj ETQq0 0 0 rgBT./Overlock 10 Tf 50	1.1	1
137	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.	0.7	9
138	Effect of van der Waals interactions in the DFT description of self-assembled monolayers of thiols on gold. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	17
139	Fischer-Tropsch Synthesis on Multicomponent Catalysts: What Can We Learn from Computer Simulations?. Catalysts, 2015, 5, 3-17.	1.6	20
140	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, 245-256.	2.5	46
141	Structure of Mixed Self-Assembled Monolayers on Gold Nanoparticles at Three Different Arrangements. Journal of Physical Chemistry C, 2015, 119, 3199-3209.	1.5	28
142	Computational modeling in nanomedicine: prediction of multiple antibacterial profiles of nanoparticles using a quantitative structure-activity relationship perturbation model. Nanomedicine, 2015, 10, 193-204.	1.7	55
143	Effect of replacing [NTf ₂] by [PF ₆] anion on the [BMIm][NTf ₂] ionic liquid confined by gold. Molecular Simulation, 2015, 41, 455-462.	0.9	17
144	Molecular Dynamics Study of the Gold/Ionic Liquids Interface. Journal of Physical Chemistry B, 2015, 119, 9883-9892.	1.2	35

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145	Mechanistic Study of Carbon Monoxide Methanation over Pure and Rhodium- or Ruthenium-Doped Nickel Catalysts. <i>Journal of Physical Chemistry C</i> , 2015, 119, 16537-16551.	1.5	44
146	Simple descriptors for assessing the outcome of aza-Diels-Alder reactions. <i>RSC Advances</i> , 2015, 5, 50729-50740.	1.7	3
147	Solvent Accessible Surface Area-Based Hot-Spot Detection Methods for Protein-Protein and Protein-Nucleic Acid Interfaces. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1077-1086.	2.5	33
148	Molecular Dynamics Simulations of Poly(ethylene oxide) Grafted onto Silica Immersed in Melt of Homopolymers. <i>Langmuir</i> , 2015, 31, 10254-10264.	1.6	16
149	Harmonization of QSAR Best Practices and Molecular Docking Provides an Efficient Virtual Screening Tool for Discovering New G-Quadruplex Ligands. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2094-2110.	2.5	20
150	Competitive Paths for Methanol Decomposition on Ruthenium: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27382-27391.	1.5	25
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