Maria NatÃ¡lia Dias Soeiro Cordeiro

List of Publications by Year
in descending order

354 papers	9,443 citations	43973 48 h-index	85405 71 g-index
367 all docs	367 docs citations	367 times ranked	8923 citing authors

#	Article	IF	Citations
1	Molecular simulations of interfacial systems: challenges, applications and future perspectives. Molecular Simulation, 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. Physical Chemistry Chemical Physics, 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. Analytica Chimica Acta, 2022, 1194, 339410.	2.6	14
4	N2O Hydrogenation on Silver Doped Gold Catalysts, a DFT Study. Nanomaterials, 2022, 12, 394.	1.9	0
5	First multi-target QSAR model for predicting the cytotoxicity of acrylic acid-based dental monomers. Dental Materials, 2022, 38, 333-346.	1.6	9
6	Insights into the Mechanism of Methanol Steam Reforming for Hydrogen Production over Niâ€“Cu-Based Catalysts. ACS Catalysis, 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.. Current Topics in Medicinal Chemistry, 2022, 22, .	1.0	3
8	Turning deep-eutectic solvents into value-added products for CO2 capture: A desirability-based virtual screening study. Journal of CO2 Utilization, 2022, 58, 101926.	3.3	23
9	Moving Average-Based Multitasking In Silico Classification Modeling: Where Do We Stand and What Is Next?. International Journal of Molecular Sciences, 2022, 23, 4937.	1.8	7
10	Computational Modelling and Sustainable Synthesis of a Highly Selective Electrochemical MIP-Based Sensor for Citalopram Detection. Molecules, 2022, 27, 3315.	1.7	5
11	Exploring the conformational binding mechanism of fibrinogen induced by interactions with penicillin Î²-lactam antibiotic drugs. Journal of Molecular Liquids, 2021, 324, 114667.	2.3	12
12	Rational development of molecular imprinted carbon paste electrode for Furazolidone detection: theoretical and experimental approach. Sensors and Actuators B: Chemical, 2021, 329, 129112.	4.0	43
13	Light alcohols reforming towards renewable hydrogen production on multicomponent catalysts. Renewable and Sustainable Energy Reviews, 2021, 138, 110523.	8.2	12
14	Insights into the catalytic activity of trimetallic Al/Zn/Cu surfaces for the water gas shift reaction. Applied Surface Science, 2021, 542, 148589.	3.1	12
15	Molecularly imprinted polymer-based electrochemical sensors for environmental analysis. Biosensors and Bioelectronics, 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. Physical Chemistry Chemical Physics, 2021, 23, 14037-14050.	1.3	7
18	New Mechanistic Insights on Carbon Nanotubesâ€™ Nanotoxicity Using Isolated Submitochondrial Particles, Molecular Docking, and Nano-QSTR Approaches. Biology, 2021, 10, 171.	1.3	4

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19	Nanomarker for Early Detection of Alzheimerâ€™s Disease Combining Ab initio DFT Simulations and Molecular Docking Approach. Biophysica, 2021, 1, 76-86.	0.6	4
20	QSAR-Co-X: an open source toolkit for multitarget QSAR modelling. Journal of Cheminformatics, 2021, 13, 29.	2.8	28
21	AKT Inhibitors: The Road Ahead to Computational Modeling-Guided Discovery. International Journal of Molecular Sciences, 2021, 22, 3944.	1.8	12
22	Ionic liquidâ€“metal interface: The origins of capacitance peaks. Electrochimica Acta, 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. Current Topics in Medicinal Chemistry, 2021, 21, 839-839.	1.0	0
24	Molecular dynamic study of alcohol-based deep eutectic solvents. Journal of Chemical Physics, 2021, 155, 064506.	1.2	15
25	Unravelling the Interactions of Magnetic Ionic Liquids by Energy Decomposition Schemes: Towards a Transferable Polarizable Force Field. Molecules, 2021, 26, 5526.	1.7	3
26	Density of Deep Eutectic Solvents: The Path Forward Cheminformatics-Driven Reliable Predictions for Mixtures. Molecules, 2021, 26, 5779.	1.7	23
27	Heavy metal ion separation from industrial wastewater using stacked graphene Membranes: A molecular dynamics simulation study. Journal of Molecular Liquids, 2021, 338, 116688.	2.3	26
28	Development of a molecular imprinted electrochemiluminescence sensor for amitriptyline detection: From MD simulations to experimental implementation. Electrochimica Acta, 2021, 397, 139273.	2.6	8
29	Structural behavior of monomer of SARS-CoV-2 spike protein during initial stage of adsorption on graphene. Materials Today Chemistry, 2021, 22, 100572.	1.7	11
30	Medical Social Networks, Epidemiology and Health Systems. Advances in Information Quality and Management, 2021, , 1827-1838.	0.3	0
31	Multi-Target In Silico Prediction of Inhibitors for Mitogen-Activated Protein Kinase-Interacting Kinases. Biomolecules, 2021, 11, 1670.	1.8	13
32	Computational and experimental study of propeline: A choline chloride based deep eutectic solvent. Journal of Molecular Liquids, 2020, 298, 111978.	2.3	25
33	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.	10.8	19
34	A unified in silico model based on perturbation theory for assessing the genotoxicity of metal oxide nanoparticles. Chemosphere, 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. Journal of Chemical Information and Modeling, 2020, 60, 3969-3984.	2.5	8
36	Mapping the underlying mechanisms of fibrinogen benzothiazole drug interactions using computational and experimental approaches. International Journal of Biological Macromolecules, 2020, 163, 730-744.	3.6	10

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37	Targeting Beta-Blocker Drugâ€“Drug Interactions with Fibrinogen Blood Plasma Protein: A Computational and Experimental Study. Molecules, 2020, 25, 5425.	1.7	6
38	Covalent Functionalization of Graphene with PAMAM Dendrimer and Its Implications on Grapheneâ€™s Dispersion and Cytotoxicity. ACS Applied Polymer Materials, 2020, 2, 3587-3600.	2.0	11
39	Interaction of Coumarin Phytoestrogens with ERÎ± and ERÎ²: A Molecular Dynamics Simulation Study. Molecules, 2020, 25, 1165.	1.7	11
40	Azithromycin electrochemical detection using a molecularly imprinted polymer prepared on a disposable screen-printed electrode. Analytical Methods, 2020, 12, 1486-1494.	1.3	43
41	Computational modeling on mitochondrial channel nanotoxicity. Nano Today, 2020, 34, 100913.	6.2	7
42	Theoretical insights on helix repacking as the origin of P-glycoprotein promiscuity. Scientific Reports, 2020, 10, 9823.	1.6	15
43	Importance of Data Curation in QSAR Studies Especially While Modeling Large-Size Datasets. Methods in Pharmacology and Toxicology, 2020, , 97-109.	0.1	6
44	On the Relevance of Feature Selection Algorithms While Developing Non-linear QSARs. Methods in Pharmacology and Toxicology, 2020, , 177-194.	0.1	3
45	Hysteresis in the MD Simulations of Differential Capacitance at the Ionic Liquidâ€“Au Interface. Journal of Physical Chemistry Letters, 2020, 11, 10408-10413.	2.1	14
46	Advanced in Silico Methods for the Development of Anti- Leishmaniasis and Anti-Trypanosomiasis Agents. Current Medicinal Chemistry, 2020, 27, 697-718.	1.2	12
47	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.	1.0	8
48	PTML Multi-Label Algorithms: Models, Software, and Applications. Current Topics in Medicinal Chemistry, 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. Methods in Pharmacology and Toxicology, 2020, , 195-213.	0.1	1
50	Supported Vanadium Catalysts: Heterogeneous Molecular Complexes, Electrocatalysis and Biomass Transformation. RSC Catalysis Series, 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. Current Topics in Medicinal Chemistry, 2020, 20, 2308-2325.	1.0	3
52	Structural and energetic evolution of fibrinogen toward to the betablocker interactions. International Journal of Biological Macromolecules, 2019, 137, 405-419.	3.6	11
53	Ensemble-Based Modeling of Chemical Compounds with Antimalarial Activity. Current Topics in Medicinal Chemistry, 2019, 19, 957-969.	1.0	8
54	Influence of alcohols on the inter-ion interactions in ionic liquids: A molecular dynamics study. Journal of Molecular Liquids, 2019, 294, 111538.	2.3	12

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55	Alignment-Free Method to Predict Enzyme Classes and Subclasses. International Journal of Molecular Sciences, 2019, 20, 5389.	1.8	19
56	Multi-Target Chemometric Modelling, Fragment Analysis and Virtual Screening with ERK Inhibitors as Potential Anticancer Agents. Molecules, 2019, 24, 3909.	1.7	18
57	Dynamical Rearrangement of Human Epidermal Growth Factor Receptor 2 upon Antibody Binding: Effects on the Dimerization. Biomolecules, 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. International Journal of Molecular Sciences, 2019, 20, 4191.	1.8	17
59	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.	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. Journal of Chemical Information and Modeling, 2019, 59, 4070-4076.	2.5	46
61	From biomedicinal to in silico models and back to therapeutics: a review on the advancement of peptidic modeling. Future Medicinal Chemistry, 2019, 11, 2313-2331.	1.1	3
62	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.	3.2	99
63	Distance Angle Descriptors of the Interionic and Ionâ€“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.	1.2	15
64	On the role of the surface charge plane position at Au(hkl)â€“BMImPF6 interfaces. Electrochimica Acta, 2019, 318, 76-82.	2.6	15
65	Local structure and hydrogen bonding in liquid Î³-butyrolactone and propylene carbonate: A molecular dynamics simulation. Journal of Molecular Liquids, 2019, 287, 110912.	2.3	16
66	PTML Model of Enzyme Subclasses for Mining the Proteome of Biofuel Producing Microorganisms. Journal of Proteome Research, 2019, 18, 2735-2746.	1.8	29
67	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.	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). Chemical Research in Toxicology, 2019, 32, 566-577.	1.7	4
69	Salt separation from water using graphene oxide nanochannels: A molecular dynamics simulation study. Desalination, 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. International Journal of Quantitative Structure-Property Relationships, 2019, 4, 50-69.	1.1	4
71	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.	2.5	11
72	Improving Vibrational Mode Interpretation Using Bayesian Regression. Journal of Chemical Theory and Computation, 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. Electrochimica Acta, 2018, 261, 214-220.	2.6	23
74	On the thickness of the double layer in ionic liquids. Physical Chemistry Chemical Physics, 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. Food and Chemical Toxicology, 2018, 112, 571-580.	1.8	13
76	Computer-Aided Drug Design Approaches to Study Key Therapeutic Targets in Alzheimerâ€™s Disease. Neuromethods, 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. Physica E: Low-Dimensional Systems and Nanostructures, 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. International Journal of Molecular Sciences, 2018, 19, 3423.	1.8	28
80	Mr. Silva and Patient Zero: A Medical Social Network and Data Visualization Information System. Lecture Notes in Computer Science, 2018, , 111-117.	1.0	2
81	Estimation of the Toxicity of Different Substituted Aromatic Compounds to the Aquatic Ciliate Tetrahymena pyriformis by QSAR Approach. Molecules, 2018, 23, 1002.	1.7	5
82	Influence of the anion on the properties of ionic liquid mixtures: a molecular dynamics study. Physical Chemistry Chemical Physics, 2018, 20, 14899-14918.	1.3	40
83	Exploring rare chemical phenomena using fractional nuclear charges: The cisâ€‹effect in N₂F₂. International Journal of Quantum Chemistry, 2018, 118, e25662.	1.0	2
84	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.	1.3	10
85	Structure and kinetics of water in highly confined conditions: A molecular dynamics simulation study. Journal of Molecular Liquids, 2018, 268, 625-636.	2.3	32
86	QSAR modelling: a therapeutic patent review 2010-present. Expert Opinion on Therapeutic Patents, 2018, 28, 467-476.	2.4	29
87	Q2DTor: A program to treat torsional anharmonicity through coupled pair torsions in flexible molecules. Computer Physics Communications, 2018, 232, 190-205.	3.0	23
88	Advanced Chemometric Modeling Approaches for the Design of Multitarget Drugs Against Neurodegenerative Diseases. Methods in Pharmacology and Toxicology, 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. PLoS ONE, 2018, 13, e0192176.	1.1	15
90	Cetuximab and the Head and Neck Squamous Cell Cancer. Current Topics in Medicinal Chemistry, 2018, 18, 192-198.	1.0	23

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91	Looking for New Inhibitors for the Epidermal Growth Factor Receptor. Current Topics in Medicinal Chemistry, 2018, 18, 219-232.	1.0	12
92	In Silico Studies Targeting G-protein Coupled Receptors for Drug Research Against Parkinsonâ€™s Disease. Current Neuropharmacology, 2018, 16, 786-848.	1.4	18
93	Driving Forces in the Sharpless Epoxidation Reaction: A Coupled AIMD/QTAIM Study. Inorganic Chemistry, 2017, 56, 2124-2134.	1.9	9
94	Janus Gold Nanoparticles from Nanodroplets of Alkyl Thiols: A Molecular Dynamics Study. Langmuir, 2017, 33, 3056-3067.	1.6	10
95	Molecular Simulations of the Synthesis of Periodic Mesoporous Silica Phases at High Surfactant Concentrations. Journal of Physical Chemistry C, 2017, 121, 4564-4575.	1.5	29
96	Fragment-based in silico modeling of multi-target inhibitors against breast cancer-related proteins. Molecular Diversity, 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. ACS Combinatorial Science, 2017, 19, 501-512.	3.8	59
98	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. Drug Discovery Today, 2017, 22, 1489-1502.	3.2	28
99	Probing the toxicity of nanoparticles: a unified in silico machine learning model based on perturbation theory. Nanotoxicology, 2017, 11, 891-906.	1.6	90
100	Structure-function relationships in ABCG2: insights from molecular dynamics simulations and molecular docking studies. Scientific Reports, 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. Journal of Physical Chemistry A, 2017, 121, 9320-9329.	1.1	16
102	New Force Field Model for Propylene Glycol: Insight to Local Structure and Dynamics. Journal of Physical Chemistry B, 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. Medicinal Chemistry Research, 2017, 26, 2345-2356.	1.1	46
104	Water dissociation on multimetallic catalysts. Applied Catalysis B: Environmental, 2017, 218, 199-207.	10.8	14
105	Prediction of metallic nanotube reactivity for H2O activation. Physical Chemistry Chemical Physics, 2017, 19, 19188-19195.	1.3	1
106	Predictors of satisfaction in patient with silicone breast implants and its association with drug intake habits. Acta Chirurgica Belgica, 2017, 117, 89-98.	0.2	1
107	Strengths, Weaknesses, Opportunities and Threats: Computational Studies of Mn- and Fe-Catalyzed Epoxidations. Catalysts, 2017, 7, 2.	1.6	15
108	Rutheniumâ€“Platinum Catalysts and Direct Methanol Fuel Cells (DMFC): A Review of Theoretical and Experimental Breakthroughs. Catalysts, 2017, 7, 47.	1.6	50

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109	Consensus strategy in genes prioritization and combined bioinformatics analysis for preeclampsia pathogenesis. BMC Medical Genomics, 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. Current Medicinal Chemistry, 2017, 24, 1687-1704.	1.2	16
113	Rational Design of Multi-Target Estrogen Receptors ERÎ± and ERÎ² by QSAR Approaches. Current Drug Targets, 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. Current Neuropharmacology, 2017, 15, 1107-1116.	1.4	11
115	Chemoinformatics Profiling of the Chromone Nucleus as a MAO-B/A2AAR Dual Binding Scaffold. Current Neuropharmacology, 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. International Journal of Molecular Sciences, 2016, 17, 1215.	1.8	46
119	Molecular Dynamics Simulation Study of the Selectivity of a Silica Polymer for Ibuprofen. International Journal of Molecular Sciences, 2016, 17, 1083.	1.8	7
120	Striped gold nanoparticles: New insights from molecular dynamics simulations. Journal of Chemical Physics, 2016, 144, 244710.	1.2	12
121	Multiscale Model for the Templated Synthesis of Mesoporous Silica: The Essential Role of Silica Oligomers. Chemistry of Materials, 2016, 28, 2715-2727.	3.2	32
122	A computational study of the interaction of graphene structures with biomolecular units. Physical Chemistry Chemical Physics, 2016, 18, 15312-15321.	1.3	18
123	Effect of the Exchange-Correlation Potential on the Transferability of BrÃ¸nstedâ€“Evansâ€“Polanyi Relationships in Heterogeneous Catalysis. Journal of Chemical Theory and Computation, 2016, 12, 2121-2126.	2.3	20
124	Improved Force Field Model for the Deep Eutectic Solvent Ethaline: Reliable Physicochemical Properties. Journal of Physical Chemistry B, 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. RSC Advances, 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. ACS Combinatorial Science, 2016, 18, 490-498.	3.8	73

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127	Efficient and biologically relevant consensus strategy for Parkinsonâ€™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 BrÃ¸nstedâ€“Evansâ€“Polanyi relationship for Oâ€“H bond cleavage. RSC Advances, 2016, 6, 18695-18702.	1.7	10
131	Roots of Acetate-Vanadium Linkage Isomerism: A QTAIM 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 UVâ€“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 A_{2A} 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 structureâ€“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 structureâ€“activity relationship perturbation model. Nanomedicine, 2015, 10, 193-204.	1.7	55
143	Effect of replacing [NTf₂] by [PF₆] anion on the [BMIm][NTf₂] 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. Journal of Physical Chemistry C, 2015, 119, 16537-16551.	1.5	44
146	Simple descriptors for assessing the outcome of aza-Dielsâ€“Alder reactions. RSC Advances, 2015, 5, 50729-50740.	1.7	3
147	Solvent Accessible Surface Area-Based Hot-Spot Detection Methods for Proteinâ€“Protein and Proteinâ€“Nucleic Acid Interfaces. Journal of Chemical Information and Modeling, 2015, 55, 1077-1086.	2.5	33
148	Molecular Dynamics Simulations of Poly(ethylene oxide) Grafted onto Silica Immersed in Melt of Homopolymers. Langmuir, 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. Journal of Chemical Information and Modeling, 2015, 55, 2094-2110.	2.5	20
150	Competitive Paths for Methanol Decomposition on Ruthenium: A DFT Study. Journal of Physical Chemistry C, 2015, 119, 27382-27391.	1.5	25
151	Quinoxaline, its derivatives and applications: A State of the Art review. European Journal of Medicinal Chemistry, 2015, 97, 664-672.	2.6	328
152	A General ANN-Based Multitasking Model for the Discovery of Potent and Safer Antibacterial Agents. Methods in Molecular Biology, 2015, 1260, 45-64.	0.4	5
153	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, 305-314.	0.6	23
154	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.	1.1	19
155	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, 677-686.	1.1	29
156	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, 1801-1813.	1.0	24
157	Virtual Screening of Alkaloids from Apocynaceae with Potential Antitrypanosomal Activity. Current Bioinformatics, 2015, 10, 509-519.	0.7	10
158	QSAR-Based Studies of Nanomaterials in the Environment. Advances in Chemical and Materials Engineering Book Series, 2015, , 506-534.	0.2	1
159	Classification of natural estrogen-like isoflavonoids and diphenolics by QSAR tools. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 712-722.	0.6	0
160	Editorial (Thematic Issue: Chemoinformatics in Metabolomics, From Molecular Mechanics, Dynamics,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.7	1
161	Editorial (Thematic Issue: Chemoinformatics in Metabolomics, Modeling Chemical Reactivity and) Tj ETQq1 1 0.784314 rgBT /Overloc	0.7	0
162	How reliable is the ReaxFF Potential for Describing the Structure of Alkanethiols on Gold? A Molecular Dynamics Study. Journal of Physics: Conference Series, 2014, 490, 012006.	0.3	1

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163	Chemoinformatics for medicinal chemistry: in silico model to enable the discovery of potent and safer anti-cocci agents. Future Medicinal Chemistry, 2014, 6, 2013-2028.	1.1	38
164	How reliable is the ReaxFF potential for describing the structure of alkanethiols on gold? A molecular dynamics study. International Journal of Modeling, Simulation, and Scientific Computing, 2014, 05, 1441011.	0.9	1
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