Maria NatÃ¡lia Dias Soeiro Cordeiro

List of Publications by Year
in descending order

354 papers	9,443 citations	44042 48 h-index	85498 71 g-index
367 all docs	367 docs citations	367 times ranked	8923 citing authors

#	Article	IF	Citations
1	Quinoxaline, its derivatives and applications: A State of the Art review. European Journal of Medicinal Chemistry, 2015, 97, 664-672.	2.6	328
2	Phenolic acid derivatives with potential anticancer propertiesâ€“â€“a structureâ€“activity relationship study. Part 1: Methyl, propyl and octyl esters of caffeic and gallic acids. Bioorganic and Medicinal Chemistry, 2004, 12, 3581-3589.	1.4	285
3	Applications of 2D Descriptors in Drug Design: A DRAGON Tale. Current Topics in Medicinal Chemistry, 2008, 8, 1628-1655.	1.0	173
4	Molecularly imprinted polymer-based electrochemical sensors for environmental analysis. Biosensors and Bioelectronics, 2021, 172, 112719.	5.3	149
5	Activity cliffs in drug discovery: Dr Jekyll or Mr Hyde?. Drug Discovery Today, 2014, 19, 1069-1080.	3.2	140
6	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, 14686-14694.	4.6	124
7	Computer-aided nanotoxicology: assessing cytotoxicity of nanoparticles under diverse experimental conditions by using a novel QSTR-perturbation approach. Nanoscale, 2014, 6, 10623.	2.8	118
8	Intrinsic Structure and Dynamics of the Water/Nitrobenzene Interface. Journal of Physical Chemistry C, 2007, 111, 17612-17626.	1.5	113
9	Density Functional Theory Study of the Water Dissociation on Platinum Surfaces: General Trends. Journal of Physical Chemistry A, 2014, 118, 5832-5840.	1.1	106
10	Computational ecotoxicology: Simultaneous prediction of ecotoxic effects of nanoparticles under different experimental conditions. Environment International, 2014, 73, 288-294.	4.8	102
11	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
12	Influence of step sites in the molecular mechanism of the water gas shift reaction catalyzed by copper. Journal of Catalysis, 2009, 268, 131-141.	3.1	96
13	Probing the toxicity of nanoparticles: a unified in silico machine learning model based on perturbation theory. Nanotoxicology, 2017, 11, 891-906.	1.6	90
14	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.	1.5	89
15	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, 4848-4855.	1.4	87
16	Descriptors controlling the catalytic activity of metallic surfaces toward water splitting. Journal of Catalysis, 2010, 276, 92-100.	3.1	86
17	Long-Term Follow-Up of Breast Capsule Contracture Rates in Cosmetic and Reconstructive Cases. Plastic and Reconstructive Surgery, 2010, 126, 769-778.	0.7	83
18	Molecular Dynamics Simulation of the Water/2-Heptanone Liquid-Liquid Interface. Journal of Physical Chemistry B, 1999, 103, 6290-6299.	1.2	74

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19	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, 273-279.	1.9	74
20	Î²-Nitrostyrene derivatives as potential antibacterial agents: A structureâ€“propertyâ€“activity relationship study. Bioorganic and Medicinal Chemistry, 2006, 14, 4078-4088.	1.4	73
21	On the theoretical understanding of the unexpected O₂activation by nanoporous gold. Chemical Communications, 2011, 47, 8403-8405.	2.2	73
22	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
23	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
24	Adsorption of Atomic and Molecular Oxygen on the Au(321) Surface:â€‰ DFT Study. Journal of Physical Chemistry C, 2007, 111, 17311-17321.	1.5	65
25	DFT Study of the CO Oxidation on the Au(321) Surface. Journal of Physical Chemistry C, 2008, 112, 17291-17302.	1.5	65
26	A Critical Assessment of Methods for the Intrinsic Analysis of Liquid Interfaces: 2. Density Profiles. Journal of Physical Chemistry C, 2010, 114, 18656-18663.	1.5	64
27	A systematic molecular simulation study of ionic liquid surfaces using intrinsic analysis methods. Physical Chemistry Chemical Physics, 2012, 14, 5200.	1.3	64
28	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
29	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.	1.8	61
30	Synthesis and QSAR study of the anticancer activity of some novel indane carbocyclic nucleosides. Bioorganic and Medicinal Chemistry, 2003, 11, 4999-5006.	1.4	60
31	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, 6239-6244.	1.4	60
32	Salt separation from water using graphene oxide nanochannels: A molecular dynamics simulation study. Desalination, 2019, 460, 1-14.	4.0	60
33	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, 236-243.	1.1	59
34	Quantitative structure carcinogenicity relationship for detecting structural alerts in nitroso-compounds. Toxicology and Applied Pharmacology, 2007, 221, 189-202.	1.3	59
35	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
36	Predicting multiple ecotoxicological profiles in agrochemical fungicides: A multi-species chemoinformatic approach. Ecotoxicology and Environmental Safety, 2012, 80, 308-313.	2.9	58

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37	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
38	Density functional theory model study of size and structure effects on water dissociation by platinum nanoparticles. Journal of Chemical Physics, 2012, 137, 034701.	1.2	56
39	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, 2746-2759.	2.5	55
40	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
41	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, 848-861.	1.2	53
42	Fragment-based in silico modeling of multi-target inhibitors against breast cancer-related proteins. Molecular Diversity, 2017, 21, 511-523.	2.1	53
43	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.	3.8	51
44	Molecular Dynamics Study of the Transfer of Iodide across Two Liquid/Liquid Interfaces. Journal of Physical Chemistry B, 1999, 103, 8930-8939.	1.2	50
45	Computational chemistry approach for the early detection of drugâ€induced idiosyncratic liver toxicity. Journal of Computational Chemistry, 2008, 29, 533-549.	1.5	50
46	What does an ionic liquid surface really look like? Unprecedented details from molecular simulations. Physical Chemistry Chemical Physics, 2011, 13, 21230.	1.3	50
47	DFT Study of the Adsorption of <scp>d</scp>-(<scp>l</scp>-)Cysteine on Flat and Chiral Stepped Gold Surfaces. Langmuir, 2013, 29, 8856-8864.	1.6	50
48	Model for High-Throughput Screening of Multitarget Drugs in Chemical Neurosciences: Synthesis, Assay, and Theoretic Study of Rasagiline Carbamates. ACS Chemical Neuroscience, 2013, 4, 1393-1403.	1.7	50
49	Combining QSAR classification models for predictive modeling of human monoamine oxidase inhibitors. European Journal of Medicinal Chemistry, 2013, 59, 75-90.	2.6	50
50	Rutheniumâ€“Platinum Catalysts and Direct Methanol Fuel Cells (DMFC): A Review of Theoretical and Experimental Breakthroughs. Catalysts, 2017, 7, 47.	1.6	50
51	Desirabilityâ€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, 2445-2459.	1.5	49
52	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, 1870-1879.	1.4	48
53	New insights toward the discovery of antibacterial agents: Multi-tasking QSBER model for the simultaneous prediction of anti-tuberculosis activity and toxicological profiles of drugs. European Journal of Pharmaceutical Sciences, 2013, 48, 812-818.	1.9	48
54	Dermic diffusion and stratum corneum: A state of the art review of mathematical models. Journal of Controlled Release, 2014, 177, 74-83.	4.8	48

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55	Structure-function relationships in ABCG2: insights from molecular dynamics simulations and molecular docking studies. Scientific Reports, 2017, 7, 15534.	1.6	48
56	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.	3.3	46
57	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
58	A Machine Learning Approach for Hot-Spot Detection at Protein-Protein Interfaces. International Journal of Molecular Sciences, 2016, 17, 1215.	1.8	46
59	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
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	Simultaneous Modeling of Antimycobacterial Activities and ADMET Profiles: A Chemoinformatic Approach to Medicinal Chemistry. Current Topics in Medicinal Chemistry, 2013, 13, 1656-1665.	1.0	45
62	Molecular Dynamics Study of the Interface between Water and 2-Nitrophenyl Octyl Ether. Journal of Physical Chemistry B, 2008, 112, 2415-2429.	1.2	44
63	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
64	Fragment-based QSAR model toward the selection of versatile anti-sarcoma leads. European Journal of Medicinal Chemistry, 2011, 46, 5910-5916.	2.6	43
65	Azithromycin electrochemical detection using a molecularly imprinted polymer prepared on a disposable screen-printed electrode. Analytical Methods, 2020, 12, 1486-1494.	1.3	43
66	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
67	Quantitative Structureâ^'Carcinogenicity Relationship for Detecting Structural Alerts in Nitroso Compounds: Species, Rat; Sex, Female; Route of Administration, Gavage. Chemical Research in Toxicology, 2008, 21, 633-642.	1.7	42
68	3D-MEDNEs: An Alternative â€œin Silicoâ€•Technique for Chemical Research in Toxicology. 2. Quantitative Proteomeâ^'Toxicity Relationships (QPTR) based on Mass Spectrum Spiral Entropy. Chemical Research in Toxicology, 2008, 21, 619-632.	1.7	42
69	Generalized BrÃ¸nstedâ€“Evansâ€“Polanyi relationships and descriptors for Oâ€“H bond cleavage of organic molecules on transition metal surfaces. Journal of Catalysis, 2014, 313, 24-33.	3.1	42
70	Molecular Simulation of Silica/Surfactant Self-Assembly in the Synthesis of Periodic Mesoporous Silicas. Journal of the American Chemical Society, 2007, 129, 15414-15415.	6.6	41
71	Molecular Dynamics Simulation of the Early Stages of the Synthesis of Periodic Mesoporous Silica. Journal of Physical Chemistry B, 2009, 113, 708-718.	1.2	41
72	Chemoinformatics in Multi-target Drug Discovery for Anti-cancer Therapy: In Silico Design of Potent and Versatile Anti-brain Tumor Agents. Anti-Cancer Agents in Medicinal Chemistry, 2012, 12, 678-685.	0.9	41

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73	In Silico Discovery and Virtual Screening of Multi-Target Inhibitors for Proteins in Mycobacterium tuberculosis. Combinatorial Chemistry and High Throughput Screening, 2012, 15, 666-673.	0.6	41
74	Multi-Target Inhibitors for Proteins Associated with Alzheimer: In Silico Discovery using Fragment-Based Descriptors. Current Alzheimer Research, 2013, 10, 117-124.	0.7	41
75	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.	0.9	41
76	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, 2727-2732.	1.4	40
77	On the thickness of the double layer in ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 10275-10285.	1.3	40
78	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
79	Quantum and simulation studies of Xâ˜'(H2O)n systems. Electrochimica Acta, 1999, 45, 659-673.	2.6	39
80	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.	1.5	39
81	Influence of Ion Size and Charge in Ion Transfer Processes Across a Liquid|Liquid Interface. Journal of Physical Chemistry B, 2000, 104, 2278-2286.	1.2	38
82	Probing the Anticancer Activity of Nucleoside Analogues:Â A QSAR Model Approach Using an Internally Consistent Training Set. Journal of Medicinal Chemistry, 2007, 50, 1537-1545.	2.9	38
83	Gas-phase molecular structure and energetics of anionic silicates. Geochimica Et Cosmochimica Acta, 2008, 72, 4421-4439.	1.6	38
84	A ligand-based approach for the in silico discovery of multi-target inhibitors for proteins associated with HIV infection. Molecular BioSystems, 2012, 8, 2188.	2.9	38
85	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
86	Physical Properties at the Base for the Development of an All-Atom Force Field for Ethylene Glycol. Journal of Physical Chemistry B, 2011, 115, 3013-3019.	1.2	37
87	Role of Ligand-Based Drug Design Methodologies toward the Discovery of New Anti- Alzheimer Agents: Futures Perspectives in Fragment-Based Ligand Design. Current Medicinal Chemistry, 2012, 19, 1635-1645.	1.2	37
88	Improving Vibrational Mode Interpretation Using Bayesian Regression. Journal of Chemical Theory and Computation, 2019, 15, 456-470.	2.3	37
89	A Comparative Study of the Anion Transfer Kinetics Across a Water/Nitrobenzene Interface by Means of Electrochemical Impedance Spectroscopy and Square-Wave Voltammetry at Thin Organic Film-Modified Electrodes. Langmuir, 2006, 22, 3404-3412.	1.6	36
90	Unraveling the mechanism of the NO reduction by CO on gold based catalysts. Journal of Catalysis, 2012, 289, 11-20.	3.1	36

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91	Molecular Dynamics Study of the Gold/Ionic Liquids Interface. Journal of Physical Chemistry B, 2015, 119, 9883-9892.	1.2	35
92	Towards the Discovery of a Novel Class of Monoamine Oxidase Inhibitors: Structureâ€“Propertyâ€“Activity and Docking Studies on Chromone Amides. ChemMedChem, 2011, 6, 628-632.	1.6	34
93	Discovery of MAO-B Inhibitors - Present Status and Future Directions Part I: Oxygen Heterocycles and Analogs. Mini-Reviews in Medicinal Chemistry, 2012, 12, 907-919.	1.1	34
94	Quantitative structure carcinogenicity relationship for detecting structural alerts in nitroso-compoundsâ˜†Species: Rat; Sex: Male; Route of administration: Water. Toxicology and Applied Pharmacology, 2008, 231, 197-207.	1.3	33
95	Application of Bioinformatics for the Search of Novel Anti-Viral Therapies: Rational Design of Anti-Herpes Agents. Current Bioinformatics, 2011, 6, 81-93.	0.7	33
96	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
97	Calibration sets and the accuracy of vibrational scaling factors: A case study with the X3LYP hybrid functional. Journal of Chemical Physics, 2010, 133, 114109.	1.2	32
98	Ionic and radical adsorption on the Au(hkl) surfaces: A DFT study. Surface Science, 2012, 606, 69-77.	0.8	32
99	Water Dissociation on Bimetallic Surfaces: General Trends. Journal of Physical Chemistry C, 2012, 116, 10120-10128.	1.5	32
100	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
101	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
102	Ab initiocopper-water interaction potential for the simulation of aqueous solutions. Journal of Computational Chemistry, 1993, 14, 629-638.	1.5	31
103	Application of the replacement method as novel variable selection in QSPR. 2. Soil sorption coefficients. Chemometrics and Intelligent Laboratory Systems, 2007, 88, 197-203.	1.8	31
104	Calculation of the Intrinsic Solvation Free Energy Profile of an Ionic Penetrant Across a Liquidâ€“Liquid Interface with Computer Simulations. Journal of Physical Chemistry B, 2013, 117, 16148-16156.	1.2	31
105	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
106	Surface Chemistry and Atomic-Scale Reconstruction of Kerogenâ€“Silica Composites. Journal of Physical Chemistry C, 2014, 118, 2429-2438.	1.5	29
107	Efficient and biologically relevant consensus strategy for Parkinsonâ€™s disease gene prioritization. BMC Medical Genomics, 2016, 9, 12.	0.7	29
108	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

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109	QSAR modelling: a therapeutic patent review 2010-present. Expert Opinion on Therapeutic Patents, 2018, 28, 467-476.	2.4	29
110	PTML Model of Enzyme Subclasses for Mining the Proteome of Biofuel Producing Microorganisms. Journal of Proteome Research, 2019, 18, 2735-2746.	1.8	29
111	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
112	Cluster and periodic DFT calculations of adsorption of hydroxyl on the Au(hkl) surfaces. Computational and Theoretical Chemistry, 2010, 946, 43-50.	1.5	28
113	DFT study on the reaction of NO oxidation on a stepped gold surface. Applied Catalysis A: General, 2010, 379, 111-120.	2.2	28
114	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
115	From flamingo dance to (desirable) drug discovery: a nature-inspired approach. Drug Discovery Today, 2017, 22, 1489-1502.	3.2	28
116	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
117	QSAR-Co-X: an open source toolkit for multitarget QSAR modelling. Journal of Cheminformatics, 2021, 13, 29.	2.8	28
118	Ionic liquidâ€“metal interface: The origins of capacitance peaks. Electrochimica Acta, 2021, 379, 138148.	2.6	28
119	Stochastic molecular descriptors for polymers. 4. Study of complex mixtures with topological indices of mass spectra spiral and star networks: The blood proteome case. Polymer, 2008, 49, 5575-5587.	1.8	27
120	Quantitative structure-activity relationship modelling of the carcinogenic risk of nitroso compounds using regression analysis and the TOPS-MODE approach. SAR and QSAR in Environmental Research, 2010, 21, 277-304.	1.0	26
121	The Impact of Triamcinolone Acetonide in Early Breast Capsule Formation in a Rabbit Model. Aesthetic Plastic Surgery, 2012, 36, 986-994.	0.5	26
122	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
123	Matrix Trace Operators: From Spectral Moments of Molecular Graphs and Complex Networks to Perturbations in Synthetic Reactions, Micelle Nanoparticles, and Drug ADME Processes. Current Drug Metabolism, 2014, 15, 470-488.	0.7	26
124	Experimental and DFT study of the aza-Dielsâ€“Alder reaction between cyclopentadiene and protonated benzylimine derivated from glyoxylates. Tetrahedron, 2005, 61, 10951-10957.	1.0	25
125	A topological substructural molecular design approach for predicting mutagenesis end-points of Î±, Î²-unsaturated carbonyl compounds. Toxicology, 2010, 268, 64-77.	2.0	25
126	Competitive Paths for Methanol Decomposition on Ruthenium: A DFT Study. Journal of Physical Chemistry C, 2015, 119, 27382-27391.	1.5	25

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127	Interactions in the ionic liquid [EMIM][FAP]: a coupled experimental and computational analysis. Physical Chemistry Chemical Physics, 2016, 18, 2617-2628.	1.3	25
128	Computational and experimental study of propeline: A choline chloride based deep eutectic solvent. Journal of Molecular Liquids, 2020, 298, 111978.	2.3	25
129	Molecular Dynamics Study of 2-Nitrophenyl Octyl Ether and Nitrobenzene. Journal of Physical Chemistry B, 2006, 110, 12530-12538.	1.2	24
130	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
131	QSPR and Flow Cytometry Analysis (QSPR-FCA): Review and New Findings on Parallel Study of Multiple Interactions of Chemical Compounds with Immune Cellular and Molecular Targets. Current Drug Metabolism, 2014, 15, 414-428.	0.7	24
132	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
133	The role of many-body interactions in the stability of hydrated Cu2+ clusters. Chemical Physics, 1990, 141, 379-392.	0.9	23
134	Interfacial Tension Behaviour of Water/Hydrocarbon Liquidâ€“Liquid Interfaces: A Molecular Dynamics Simulation. Molecular Simulation, 2003, 29, 817-827.	0.9	23
135	Convenient QSAR model for predicting the complexation of structurally diverse compounds with Î²-cyclodextrins. Bioorganic and Medicinal Chemistry, 2009, 17, 896-904.	1.4	23
136	QSAR models to predict mutagenicity of acrylates, methacrylates and Î±,Î²-unsaturated carbonyl compounds. Dental Materials, 2010, 26, 397-415.	1.6	23
137	DFT study on the reaction of O2 dissociation catalyzed by gold surfaces doped with transition metal atoms. Applied Catalysis A: General, 2013, 458, 90-102.	2.2	23
138	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
139	Q2DTor: A program to treat torsional anharmonicity through coupled pair torsions in flexible molecules. Computer Physics Communications, 2018, 232, 190-205.	3.0	23
140	Density of Deep Eutectic Solvents: The Path Forward Cheminformatics-Driven Reliable Predictions for Mixtures. Molecules, 2021, 26, 5779.	1.7	23
141	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
142	Cetuximab and the Head and Neck Squamous Cell Cancer. Current Topics in Medicinal Chemistry, 2018, 18, 192-198.	1.0	23
143	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
144	QSAR modeling of the rodent carcinogenicity of nitrocompounds. Bioorganic and Medicinal Chemistry, 2008, 16, 3395-3407.	1.4	22

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145	DFT study of the Au(321) surface reconstruction by consecutive deposition of oxygen atoms. Surface Science, 2008, 602, 424-435.	0.8	22
146	Prediction of the baseline toxicity of non-polar narcotic chemical mixtures by QSAR approach. Chemosphere, 2013, 90, 1980-1986.	4.2	22
147	Jointly Handling Potency and Toxicity of Antimicrobial Peptidomimetics by Simple Rules from Desirability Theory and Chemoinformatics. Journal of Chemical Information and Modeling, 2011, 51, 3060-3077.	2.5	21
148	On the Need for Spin Polarization in Heterogeneously Catalyzed Reactions on Nonmagnetic Metallic Surfaces. Journal of Chemical Theory and Computation, 2012, 8, 1737-1743.	2.3	21
149	Coupling of Cyclic Voltammetry and Electrochemical Impedance Spectroscopy for Probing the Thermodynamics of Facilitated Ion Transfer Reactions Exhibiting Chemical Kinetic Hindrances. Journal of Physical Chemistry C, 2008, 112, 153-161.	1.5	20
150	QSPR modelling with the topological substructural molecular design approach: Î²-cyclodextrin complexation. Journal of Pharmaceutical Sciences, 2009, 98, 4557-4576.	1.6	20
151	Molecular Dynamics Study of Hydrated Poly(ethylene oxide) Chains Grafted on Siloxane Surface. Macromolecules, 2011, 44, 3639-3648.	2.2	20
152	Effects of Coagulase-Negative Staphylococci and Fibrin on Breast Capsule Formation in a Rabbit Model. Aesthetic Surgery Journal, 2011, 31, 420-428.	0.9	20
153	Computer-Aided Drug Design Methodologies Toward the Design of Anti-Hepatitis C Agents. Current Topics in Medicinal Chemistry, 2012, 12, 802-813.	1.0	20
154	Fischer-Tropsch Synthesis on Multicomponent Catalysts: What Can We Learn from Computer Simulations?. Catalysts, 2015, 5, 3-17.	1.6	20
155	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
156	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
157	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
158	Molecular Simulation of the Interface between Two Immiscible Electrolyte Solutions. Journal of Physical Chemistry B, 2001, 105, 981-993.	1.2	19
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