Bartosz Trzaskowski

List of Publications by Year
in descending order

111 papers	2,784 citations	236612 25 h-index	205818 48 g-index
112 all docs	112 docs citations	112 times ranked	3242 citing authors

#	Article	IF	Citations
1	Action of Molecular Switches in GPCRs - Theoretical and Experimental Studies. Current Medicinal Chemistry, 2012, 19, 1090-1109.	1.2	395
2	Status of GPCR Modeling and Docking as Reflected by Community-wide GPCR Dock 2010 Assessment. Structure, 2011, 19, 1108-1126.	1.6	269
3	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. Nature Reviews Drug Discovery, 2009, 8, 455-463.	21.5	260
4	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	1.6	149
5	Fullerene as an electron buffer: Charge transfer in Li@C60. Chemical Physics Letters, 2007, 442, 339-343.	1.2	73
6	Cyclic Alkyl Amino Ruthenium Complexesâ€"Efficient Catalysts for Macrocyclization and Acrylonitrile Cross Metathesis. ACS Catalysis, 2017, 7, 5443-5449.	5.5	72
7	3D Structure Prediction of TAS2R38 Bitter Receptors Bound to Agonists Phenylthiocarbamide (PTC) and 6-n-Propylthiouracil (PROP). Journal of Chemical Information and Modeling, 2012, 52, 1875-1885.	2.5	69
8	Genetically Encoded Photo-cross-linkers Map the Binding Site of an Allosteric Drug on a G Protein-Coupled Receptor. ACS Chemical Biology, 2012, 7, 967-972.	1.6	67
9	A theoretical study of zinc(II) interactions with amino acid models and peptide fragments. Journal of Biological Inorganic Chemistry, 2007, 13, 133-137.	1.1	65
10	Predicted 3D structures for adenosine receptors bound to ligands: Comparison to the crystal structure. Journal of Structural Biology, 2010, 170, 10-20.	1.3	58
11	Specialized Ruthenium Olefin Metathesis Catalysts Bearing Bulky Unsymmetrical NHC Ligands: Computations, Synthesis, and Application. ACS Catalysis, 2019, 9, 587-598.	5.5	50
12	Decomposition of Ruthenium Olefin Metathesis Catalyst. Catalysts, 2020, 10, 887.	1.6	45
13	Dialkylgallium Alkoxides Stabilized with N-Heterocyclic Carbenes: Opportunities and Limitations for the Controlled and Stereoselective Polymerization of rac-Lactide. Organometallics, 2015, 34, 3480-3496.	1.1	42
14	Ligand- and mutation-induced conformational selection in the CCR5 chemokine G protein-coupled receptor. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 13040-13045.	3.3	40
15	Structural and Mechanistic Basis of the Fast Metathesis Initiation by a Six-Coordinated Ruthenium Catalyst. Organometallics, 2013, 32, 3625-3630.	1.1	39
16	Molecular dynamics studies of protein-fragment models encapsulated into carbon nanotubes. Chemical Physics Letters, 2006, 430, 97-100.	1.2	38
17	Use of G-Protein-Coupled and -Uncoupled CCR5 Receptors by CCR5 Inhibitor-Resistant and -Sensitive Human Immunodeficiency Virus Type 1 Variants. Journal of Virology, 2013, 87, 6569-6581.	1.5	38
18	SuperBiHelix method for predicting the pleiotropic ensemble of G-proteinâ€"coupled receptor conformations. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E72-8.	3.3	38

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19	G protein-coupled receptors--recent advances. Acta Biochimica Polonica, 2012, 59, 515-29.	0.3	36
20	The Effect of Gas Adsorption on Carbon Nanotubes Properties. Journal of Computational and Theoretical Nanoscience, 2006, 3, 664-669.	0.4	35
21	Lipid Receptor S1P1 Activation Scheme Concluded from Microsecond All-Atom Molecular Dynamics Simulations. PLoS Computational Biology, 2013, 9, e1003261.	1.5	31
22	Synthesis and antiâ€“tumour, immunomodulating activity of diosgenin and tigogenin conjugates. Journal of Steroid Biochemistry and Molecular Biology, 2020, 198, 105573.	1.2	29
23	Structures, stabilities and tautomerizations of uracil and diphosphouracil tautomers. Chemical Physics, 2007, 332, 152-161.	0.9	26
24	3-Bromopyridine As a Sixth Ligand in Sulfoxide-Based Hoveyda Complexes: A Study on Catalytic Properties. Organometallics, 2013, 32, 2192-2198.	1.1	26
25	Superseding Î²â€Diketiminato Ligands: An Amido Imidazolineâ€2â€Imine Ligand Stabilizes the Exhaustive Series of B=X Boranes (X=O, S, Se, Te). Angewandte Chemie - International Edition, 2021, 60, 4633-4639.	7.2	25
26	Conformational Flexibility of Hoveyda-Type and Grubbs-Type Complexes Bearing Acyclic Carbenes and Its Impact on Their Catalytic Properties. Organometallics, 2015, 34, 563-570.	1.1	23
27	Performance of electrochemical immunoassays for clinical diagnostics of SARS-CoV-2 based on selective nucleocapsid N protein detection: Boron-doped diamond, gold and glassy carbon evaluation. Biosensors and Bioelectronics, 2022, 209, 114222.	5.3	23
28	The Role of Water in Activation Mechanism of Human N-Formyl Peptide Receptor 1 (FPR1) Based on Molecular Dynamics Simulations. PLoS ONE, 2012, 7, e47114.	1.1	22
29	Study of the structural and electronic properties of 1-(4, 5 and 6-selenenyl) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 347 Td (der 1039-1047.	0.8	21
30	Impact of Local Curvature and Structural Defects on Grapheneâ€“C₆₀ Fullerene Fusion Reaction Barriers. Journal of Physical Chemistry C, 2013, 117, 19664-19671.	1.5	20
31	Functionalization of carbon nanocones by free radicals: A theoretical study. Chemical Physics Letters, 2007, 444, 314-318.	1.2	19
32	Molecular effects of encapsulation of glucose oxidase dimer by graphene. RSC Advances, 2015, 5, 13570-13578.	1.7	19
33	Modelling of Octahedral Manganese II Complexes with Inorganic Ligands: A Problem with Spin-States. International Journal of Molecular Sciences, 2003, 4, 503-511.	1.8	18
34	Theoretical investigation of the electronic structure of 1-(3,4; 3,5 and 3,6-bis-selenocyanato-phenyl) pyrrolidinofullerenes. Journal of Organometallic Chemistry, 2006, 691, 4589-4594.	0.8	18
35	Controlling the charge transfer flow at the graphene/pyreneâ€“nitrilotriacetic acid interface. Journal of Materials Chemistry C, 2018, 6, 5046-5054.	2.7	18
36	5-HT1A and 5-HT2A receptors affinity, docking studies and pharmacological evaluation of a series of 8-acetyl-7-hydroxy-4-methylcoumarin derivatives. Bioorganic and Medicinal Chemistry, 2018, 26, 527-535.	1.4	18

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37	Ruthenium-Catalysed Olefin Metathesis in Environmentally Friendly Solvents: 2-Methyltetrahydrofuran Revisited. European Journal of Organic Chemistry, 2019, 2019, 640-646.	1.2	18
38	Selective NaNO2 recognition by a simple heteroditopic salt receptor based on l-ornithine molecular scaffold. Dalton Transactions, 2013, 42, 15271.	1.6	17
39	Hoveydaâ€“Grubbs catalyst analogues bearing the derivatives of N-phenylpyrrol in the carbene ligand â€“ structure, stability, activity and unique rutheniumâ€“phenyl interactions. Dalton Transactions, 2017, 46, 11790-11799.	1.6	17
40	Sterically Tuned N-Heterocyclic Carbene Ligands for the Efficient Formation of Hindered Products in Ru-Catalyzed Olefin Metathesis. ACS Catalysis, 2020, 10, 11394-11404.	5.5	17
41	Azoliniums, Adducts, NHCs and Azomethine Ylides: Divergence in Wanzlick Equilibrium and Olefin Metathesis Catalyst Formation. Chemistry - A European Journal, 2018, 24, 4785-4789.	1.7	16
42	Chloromethane and dichloromethane decompositions inside nanotubes as models of reactions in confined space. Theoretical Chemistry Accounts, 2009, 124, 95-103.	0.5	15
43	Conformational Ensemble View of G Protein-Coupled Receptors and the Effect of Mutations and Ligand Binding. Methods in Enzymology, 2013, 520, 31-48.	0.4	15
44	Nitrenium ions and trivalent boron ligands as analogues of N-heterocyclic carbenes in olefin metathesis: a computational study. Dalton Transactions, 2015, 44, 20021-20026.	1.6	15
45	Molecular Modeling of Mechanisms of Decomposition of Ruthenium Metathesis Catalysts by Acrylonitrile. Organometallics, 2020, 39, 239-246.	1.1	15
46	The influence of the cationic carbenes on the initiation kinetics of ruthenium-based metathesis catalysts; a DFT study. Beilstein Journal of Organic Chemistry, 2018, 14, 2872-2880.	1.3	13
47	The anti-inflammatory potential of cefazolin as common gamma chain cytokine inhibitor. Scientific Reports, 2020, 10, 2886.	1.6	13
48	â€œGive me fiveâ€•â€“ an amino imidazoline-2-imine ligand stabilises the first neutral five-membered cyclic triel(<scp>i</scp>) carbenoides. Chemical Communications, 2021, 57, 2816-2819.	2.2	13
49	Computational study of molecular properties of aggregates of C60 and (16,0) zigzag nanotube. Chemical Physics Letters, 2007, 446, 87-91.	1.2	12
50	Altering the Orientation of Proteins on Self-Assembled Monolayers: A Computational Study. Biomacromolecules, 2008, 9, 3239-3245.	2.6	12
51	Binding affinity of fluorochromes and fluorescent proteins to Taxolâ„¢ crystals. Materials Science and Engineering C, 2009, 29, 1609-1615.	3.8	12
52	Hoveyda-Grubbs complexes with boryl anions are predicted to be fast metathesis catalysts. Catalysis Communications, 2016, 86, 133-138.	1.6	12
53	Ruthenium Olefin Metathesis Catalysts Systematically Modified in Chelating Benzylidene Ether Fragment: Experiment and Computations. European Journal of Inorganic Chemistry, 2018, 2018, 3675-3685.	1.0	12
54	2-Methyltetrahydrofuran as a Solvent of Choice for Spontaneous Metathesis/Isomerization Sequence. ACS Omega, 2019, 4, 1831-1837.	1.6	12

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55	Disentangling the role of solvent polarity and protein solvation in folding and self-assembly of Î±-lactalbumin. Journal of Colloid and Interface Science, 2020, 561, 749-761.	5.0	12
56	Superseding Î²â€Diketiminato Ligands: An Amido Imidazolineâ€2â€Imine Ligand Stabilizes the Exhaustive Series of B=X Boranes (X=O, S, Se, Te). Angewandte Chemie, 2021, 133, 4683-4689.	1.6	12
57	Heterogeneous and homogeneous nucleation of Taxolâ„¢ crystals in aqueous solutions and gels: Effect of tubulin proteins. Colloids and Surfaces B: Biointerfaces, 2010, 76, 199-206.	2.5	11
58	Role of Metal Centers in Tuning the Electronic Properties of Graphene-Based Conductive Interfaces. Journal of Physical Chemistry C, 2019, 123, 8623-8632.	1.5	11
59	Structural analogues of Hoveydaâ€“Grubbs catalysts bearing the 1-benzofuran moiety or isopropoxy-1-benzofuran derivatives as olefin metathesis catalysts. RSC Advances, 2016, 6, 21423-21429.	1.7	10
60	Faster initiating olefin metathesis catalysts from introducing double bonds into cyclopropyl, cyclobutyl and cyclopentyl derivatives of Hoveyda-Grubbs precatalysts. Molecular Catalysis, 2017, 433, 313-320.	1.0	10
61	A computational study of structures and catalytic activities of Hoveyda-Grubbs analogues bearing coumarin or isopropoxycoumarin moiety. Catalysis Communications, 2017, 91, 43-47.	1.6	10
62	Probing the Mâ€“C_{NHC} Bond and Its Effect on the Synthesis, Structure, and Reactivity of R₂MOR(NHC) (M = Al, Ga, In) Complexes. Organometallics, 2018, 37, 4585-4598.	1.1	10
63	Synthesis of new spiroâ€[isothiochromeneâ€3,5â€²â€isoxazolidin]â€4(1H)â€ones. Journal of Heterocyclic Chemistry, 2007, 44, 711-716.	1.4	9
64	Pharmacophore guided discovery of small-molecule interleukin 15 inhibitors. European Journal of Medicinal Chemistry, 2017, 136, 543-547.	2.6	9
65	Assessing the Charge Transfer at the Cytochrome c₅₅₃/Graphene Interface: A Multiscale Investigation. Journal of Physical Chemistry C, 2018, 122, 29405-29413.	1.5	9
66	Impact of the olefin structure on the catalytic cycle and decomposition rates of Hoveydaâ€“Grubbs metathesis catalysts. Physical Chemistry Chemical Physics, 2020, 22, 13062-13069.	1.3	9
67	Impact of the Carbene Derivative Charge on the Decomposition Rates of Hoveydaâ€“Grubbs-like Metathesis Catalysts. Journal of Physical Chemistry A, 2020, 124, 6158-6167.	1.1	9
68	Reactions of a Fourâ€Membered Borete with Carbon, Silicon, and Gallium Donor Ligands: Fused and Spiroâ€Type Boracycles. Chemistry - A European Journal, 2022, 28, .	1.7	9
69	Formation of glyoxal in hydroxyacetaldehyde and glycine nonenzymatic browning Maillard reaction: A computational study. Food Chemistry, 2007, 103, 359-368.	4.2	8
70	Development of selective agents targeting serotonin 5HT1A receptors with subnanomolar activities based on a coumarin core. MedChemComm, 2017, 8, 1690-1696.	3.5	8
71	6-Acetyl-5-hydroxy-4,7-dimethylcoumarin derivatives: Design, synthesis, modeling studies, 5-HT1A, 5-HT2A and D2 receptors affinity. Bioorganic Chemistry, 2020, 100, 103912.	2.0	8
72	Structural and Electronic Properties of Boranes Containing Boronâ€Chalcogen Multiple Bonds and Stabilized by Amido Imidazolineâ€2â€imine Ligands. Chemistry - A European Journal, 2022, 28, .	1.7	8

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73	Boronâ€“boron, carbonâ€“carbon and nitrogenâ€“nitrogen bonding in N-heterocyclic carbenes and their diazaboryl and triazole analogues: Wanzlick equilibrium revisited. New Journal of Chemistry, 2018, 42, 6183-6190.	1.4	7
74	Cross metathesis with acrylates: N â€heterocyclic carbene (NHC)â€•versus cyclic alkyl amino carbene (CAAC)â€bbased ruthenium catalysts, an unanticipated influence of the carbene type on efficiency and selectivity of the reaction. ChemCatChem, 2020, 12, 6366-6374.	1.8	7
75	Rate-Limiting Steps in the Intramolecular Câ€“H Activation of Ruthenium N-Heterocyclic Carbene Complexes. Journal of Physical Chemistry A, 2020, 124, 3609-3617.	1.1	7
76	Enhancement of direct electron transfer in graphene bioelectrodes containing novel cytochrome c variants with optimized heme orientation. Bioelectrochemistry, 2021, 140, 107818.	2.4	7
77	Development of a universal conductive platform for anchoring photo- and electroactive proteins using organometallic terpyridine molecular wires. Nanoscale, 2021, 13, 9773-9787.	2.8	7
78	Ruthenium Olefin Metathesis Catalysts Bearing a Macrocyclic Nâ€Heterocyclic Carbene Ligand: Improved Stability and Activity. Angewandte Chemie - International Edition, 2022, 61, .	7.2	7
79	Theoretical study of molecular and electronic structure of 2-Se-(2-methyl-2-propenyl)-1-benzoic acid. International Journal of Quantum Chemistry, 2007, 107, 152-158.	1.0	6
80	Predicted Ligands for the Human Urotensinâ€II Gâ€...Proteinâ€Coupled Receptor with Some Experimental Validation. ChemMedChem, 2014, 9, 1732-1743.	1.6	6
81	Modeling Tubulin at Interfaces. Immobilization of Microtubules on Self-Assembled Monolayers. Journal of Physical Chemistry B, 2005, 109, 17734-17742.	1.2	5
82	Metallization of nanobiostructures: a theoretical study of copper nanowires growth in microtubules. Journal of Materials Chemistry, 2006, 16, 4649.	6.7	5
83	THEORETICAL, EMPIRICAL AND EXPERIMENTAL ELECTRON AFFINITIES OF SF₆: SOLVING THE DENSITY FUNCTIONAL ENIGMA. Journal of Theoretical and Computational Chemistry, 2007, 06, 747-759.	1.8	5
84	Computational note on thermochemical stability of the HO2â€“CHClO complex. Computational and Theoretical Chemistry, 2007, 816, 1-3.	1.5	5
85	Electron affinities, gas phase acidities, and potential energy curves: Benzene. International Journal of Quantum Chemistry, 2007, 107, 1115-1125.	1.0	5
86	The Predicted 3D Structure of Bitter Taste Receptors, TAS2R38 Based on a BiHelix and SuperBiHelix Methodologies. Procedia Environmental Sciences, 2011, 8, 543-548.	1.3	5
87	Olefin Metathesis Catalyzed by a Hoveydaâ€“Grubbs-like Complex Chelated to Bis(2-mercaptoimidazolyl) Methane: A Predictive DFT Study. Journal of Physical Chemistry A, 2022, 126, 720-732.	1.1	5
88	Synthesis and Physical Characterization of 2-((E)-1-(3-((E)-1-(2-hydroxyphenyl)ethylideneamino)-2-methylphenylimino)ethyl)phenol. MolBank, 2006, 2006, M455.	0.2	4
89	Exploring structures and properties of new geodesic polyarenes. Chemical Physics Letters, 2014, 595-596, 6-12.	1.2	3
90	Molecular mechanism of direct electron transfer in the robust cytochrome-functionalised graphene nanosystem. RSC Advances, 2021, 11, 18860-18869.	1.7	3

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91	Multilevel Quantum Chemistry Approach to the Development of a Database of the SAM-Ligand-Metal Ion-Protein Interactions. Journal of Computational and Theoretical Nanoscience, 2005, 2, 456-468.	0.4	3
92	Iminodiacetate as a Chelating Agent for Histidine: A Theoretical Study. Journal of Computational and Theoretical Nanoscience, 2006, 3, 775-784.	0.4	3
93	Cyclododecane and cyclotridecane complexes with cobalt as potent histidine chelators: A theoretical study. Polyhedron, 2007, 26, 2477-2481.	1.0	2
94	1-(<I>para</I>-substituted phenyl diazenyl) Pyrrolidinofullerenes. A Theoretical Study. Journal of Computational and Theoretical Nanoscience, 2008, 5, 2210-2215.	0.4	2
95	Design, Synthesis, and Biological Evaluation of a Series of 5- and 7-Hydroxycoumarin Derivatives as 5-HT1A Serotonin Receptor Antagonists. Pharmaceuticals, 2021, 14, 179.	1.7	2
96	Architecture and Function of Biohybrid Solar Cell and Solar-to-Fuel Nanodevices. Springer Series in Materials Science, 2020, , 227-274.	0.4	2
97	Diazonium-Based Covalent Molecular Wiring of Single-Layer Graphene Leads to Enhanced Unidirectional Photocurrent Generation through the p-doping Effect. Chemistry of Materials, 2022, 34, 3744-3758.	3.2	2
98	Experimental and theoretical investigation of the IR spectra and thermochemistry of four isomers of 2-N,N-dimethylaminecyclohexyl 1-N',N'-dimethylcarbamate. Ecletica Quimica, 2006, 31, 53-62.	0.2	1
99	Synthesis, Physical Characterization, Antibacterial and Antifungal activities of a novel bis(3-((E)-1-(2-hydroxyphenyl)ethylideneamino)phenyl)methanone. MolBank, 2006, 2006, M484.	0.2	1
100	New 1-(4-nitrophenyl)-5,5â€™-diisopropyl-3,3â€™-bipyrazole. MolBank, 2006, 2006, M490.	0.2	1
101	Theoretical modeling of the nonenzymatic solvolysis of CMP-NeuAc in an acidic environment. Computational and Theoretical Chemistry, 2007, 820, 90-97.	1.5	1
102	Nano-Encapsulation of Glucose Oxidase Dimer by Graphene. Materials Research Society Symposia Proceedings, 2015, 1725, 1.	0.1	1
103	Correction: â€œGive me fiveâ€•â€“ an amino imidazoline-2-imine ligand stabilises the first neutral five-membered cyclic triel(i) carbenoids. Chemical Communications, 2021, 57, 3824-3824.	2.2	1
104	The Interplay of Conjugation and Metal Coordination in Tuning the Electron Transfer Abilities of NTA-Graphene Based Interfaces. International Journal of Molecular Sciences, 2022, 23, 543.	1.8	1
105	Synthesis, Physical Characterization, Antibacterial and Antifungal Activities of 2-((E)-1-(2-((E)-1-(2-Hydroxyphenyl)ethylideneamino) phenylamino) ethyl) phenol. MolBank, 2006, 2006, M489.	0.2	0
106	New 1-(ethyl-ethanoate-yl)-5,5â€™-diisopropyl-3,3â€™-bipyrazole. MolBank, 2006, 2006, M491.	0.2	0
107	Erratum to â€œStructures, stabilities and tautomerizations of uracil and diphosphouracil tautomersâ€• [Chem. Phys. 332 (2007) 152â€“161]. Chemical Physics, 2008, 348, 254.	0.9	0
108	Geodesic Arenes. , 2016, , 115-139.		0

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109	Efficient glycosylation of natural Danshensu and its enantiomer by sugar and 2-deoxy sugar donors. Carbohydrate Research, 2018, 460, 19-28.	1.1	0
110	Structure and Properties of a Series of Arylselenium [60]Fulleropyrrolidine Derivatives. Journal of Computational and Theoretical Nanoscience, 2008, 5, 554-562.	0.4	0
111	Ruthenium Olefin Metathesis Catalysts Bearing Macrocyclic Nâ€Heterocyclic Carbene Ligand: Improved Stability and Activity. Angewandte Chemie, 0, , .	1.6	0