Agnieszka Anna Kaczor

List of Publications by Year
in descending order

111	1,785	331670 21	361022 35
papers	citations	h-index	g-index

113	113	113	2162
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Current Concepts and Treatments of Schizophrenia. Molecules, 2018, 23, 2087.	3.8	284
2	Multi-Target Approach for Drug Discovery against Schizophrenia. International Journal of Molecular Sciences, 2018, 19, 3105.	4.1	66
3	Chiral 1,3,4-Oxadiazol-2-ones as Highly Selective FAAH Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 8484-8496.	6.4	54
4	Oligomerization of G Protein-Coupled Receptors: Biochemical and Biophysical Methods. Current Medicinal Chemistry, 2011, 18, 4606-4634.	2.4	53
5	Structureâ€Based Virtual Screening for Dopamine D₂ Receptor Ligands as Potential Antipsychotics. ChemMedChem, 2016, 11, 718-729.	3.2	51
6	Recent Advances and Applications of Molecular Docking to G Protein-Coupled Receptors. Molecules, 2017, 22, 340.	3.8	51
7	Oligomerization of G Protein-Coupled Receptors: Computational Methods. Current Medicinal Chemistry, 2011, 18, 4588-4605.	2.4	35
8	Interplay between Two Allosteric Sites and Their Influence on Agonist Binding in Human Î¼ Opioid Receptor. Journal of Chemical Information and Modeling, 2016, 56, 563-570.	5.4	35
9	InÂvitro, molecular modeling and behavioral studies of 3-{[4-(5-methoxy-1H-indol-3-yl)-1,2,3,6-tetrahydropyridin-1-yl]methyl}-1,2-dihydroquinolin-2-one (D2AAK1) as a potential antipsychotic. Neurochemistry International, 2016, 96, 84-99.	3.8	35
10	Activation and Allosteric Modulation of Human Î¼ Opioid Receptor in Molecular Dynamics. Journal of Chemical Information and Modeling, 2015, 55, 2421-2434.	5.4	31
11	Computational methods for studying G protein-coupled receptors (GPCRs). Methods in Cell Biology, 2016, 132, 359-399.	1.1	31
12	Novel Antibacterial Compounds and their Drug Targets - Successes and Challenges. Current Medicinal Chemistry, 2017, 24, 1948-1982.	2.4	31
13	Non-peptide Opioid Receptor Ligands - Recent Advances. Part I - Agonists. Current Medicinal Chemistry, 2002, 9, 1567-1589.	2.4	30
14	Non-peptide Opioid Receptor Ligands - Recent Advances. Part II - Antagonists. Current Medicinal Chemistry, 2002, 9, 1591-1603.	2.4	29
15	Molecular Structure of Ionotropic Glutamate Receptors. Current Medicinal Chemistry, 2010, 17, 2608-2635.	2.4	29
16	Comparative molecular field analysis and molecular dynamics studies of Î±/Î² hydrolase domain containing 6 (ABHD6) inhibitors. Journal of Molecular Modeling, 2015, 21, 250.	1.8	29
17	Optimization of 1,2,5â€Thiadiazole Carbamates as Potent and Selective ABHD6 Inhibitors. ChemMedChem, 2015, 10, 253-265.	3.2	29
18	The dopamine D2 receptor dimer and its interaction with homobivalent antagonists: homology modeling, docking and molecular dynamics. Journal of Molecular Modeling, 2016, 22, 203.	1.8	28

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19	Modeling Complexes of Transmembrane Proteins: Systematic Analysis of Proteinï£¿Protein Docking Tools. Molecular Informatics, 2013, 32, 717-733.	2.5	27
20	Novel thiosemicarbazide derivatives with 4-nitrophenyl group as multi-target drugs: Î±-glucosidase inhibitors with antibacterial and antiproliferative activity. Biomedicine and Pharmacotherapy, 2017, 93, 1269-1276.	5.6	25
21	Investigation of novel ropinirole analogues: synthesis, pharmacological evaluation and computational analysis of dopamine D2 receptor functionalized congeners and homobivalent ligands. MedChemComm, 2014, 5, 891-898.	3.4	23
22	The formation of a neutral manganese(III) complex containing a tetradentate Schiff base and a ketone â€“ synthesis and characterization. Journal of Coordination Chemistry, 2015, 68, 3701-3717.	2.2	23
23	Molecular structure and infrared spectra of the monomeric 3-(methoxy)-1,2-benzisothiazole 1,1-dioxide (methyl pseudosaccharyl ether). Journal of Molecular Structure, 2008, 876, 77-85.	3.6	22
24	Pharmacological and molecular studies on the interaction of varenicline with different nicotinic acetylcholine receptor subtypes. Potential mechanism underlying partial agonism at human Î±4Î²2 and Î±3Î²4 subtypes. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 731-741.	2.6	21
25	Synthesis, pharmacological and structural studies of 5-substituted-3-(1-arylmethyl-1,2,3,6-tetrahydropyridin-4-yl)-1H-indoles as multi-target ligands of aminergic GPCRs. European Journal of Medicinal Chemistry, 2019, 180, 673-689.	5.5	19
26	Application of BRET for Studying G Protein-Coupled Receptors. Mini-Reviews in Medicinal Chemistry, 2014, 14, 411-425.	2.4	19
27	Overcoming Depression with 5-HT2A Receptor Ligands. International Journal of Molecular Sciences, 2022, 23, 10.	4.1	19
28	Computational Analysis of Chlorophyll Structure and UV-Vis Spectra: A Student Research Project on the Spectroscopy of Natural Complexes. Spectroscopy Letters, 2014, 47, 147-152.	1.0	18
29	Potent and selective N-(4-sulfamoylphenyl)thiourea-based GPR55 agonists. European Journal of Medicinal Chemistry, 2016, 107, 119-132.	5.5	18
30	Thyroid Peroxidase Activity is Inhibited by Phenolic Compoundsâ€”Impact of Interaction. Molecules, 2019, 24, 2766.	3.8	18
31	Fractal dimension as a measure of surface roughness of G protein-coupled receptors: implications for structure and function. Journal of Molecular Modeling, 2012, 18, 4465-4475.	1.8	17
32	Proteinâ€“Protein Docking in Drug Design and Discovery. Methods in Molecular Biology, 2018, 1762, 285-305.	0.9	17
33	Opportunities and Challenges in the Discovery of Allosteric Modulators of GPCRs. Methods in Molecular Biology, 2018, 1705, 297-319.	0.9	16
34	Multiâ€Component Protein â€“ Protein Docking Based Protocol with External Scoring for Modeling Dimers of G Proteinâ€Coupled Receptors. Molecular Informatics, 2015, 34, 246-255.	2.5	15
35	In Vitro and In Vivo Models for the Investigation of Potential Drugs Against Schizophrenia. Biomolecules, 2020, 10, 160.	4.0	15
36	Modeling of Glutamate GluR6 Receptor and Its Interactions with Novel Noncompetitive Antagonists. Journal of Chemical Information and Modeling, 2009, 49, 1094-1104.	5.4	14

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37	Experimental and theoretical investigations on the ketoâ€“enol tautomerism of 4-substituted Structure, 2011, 994, 313-320.	3.6	14
38	Structural studies, homology modeling and molecular docking of novel non-competitive antagonists of GluK1/GluK2 receptors. Bioorganic and Medicinal Chemistry, 2014, 22, 787-795.	3.0	14
39	N-(2-Hydroxyphenyl)-1-[3-(2-oxo-2,3-dihydro-1H- benzimidazol-1-yl)propyl]piperidine-4-Carboxamide (D2AAK4), a Multi-Target Ligand of Aminergic GPCRs, as a Potential Antipsychotic. Biomolecules, 2020, 10, 349.	4.0	14
40	Preferential Coupling of Dopamine D2S and D2L Receptor Isoforms with Gi1 and Gi2 Proteinsâ€”In Silico Study. International Journal of Molecular Sciences, 2020, 21, 436.	4.1	14
41	What are the challenges with multi-targeted drug design for complex diseases?. Expert Opinion on Drug Discovery, 2022, 17, 673-683.	5.0	14
42	Simulating G Protein-Coupled Receptors in Native-Like Membranes. Methods in Cell Biology, 2013, 117, 63-90.	1.1	13
43	Discovery of nitroaryl urea derivatives with antiproliferative properties. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 608-618.	5.2	13
44	2,4-Dichlorophenoxyacetic Thiosemicarbazides as a New Class of Compounds against Stomach Cancer Potentially Intercalating with DNA. Biomolecules, 2020, 10, 296.	4.0	13
45	1,2,4-Triazolin-5-thione derivatives with anticancer activity as CK1Î³ kinase inhibitors. Bioorganic Chemistry, 2020, 99, 103806.	4.1	13
46	Molecular mechanisms of allosteric probe dependence in Î¼ opioid receptor. Journal of Biomolecular Structure and Dynamics, 2019, 37, 36-47.	3.5	12
47	Molecular interactions of type I and type II positive allosteric modulators with the human Î±7 nicotinic acetylcholine receptor: an in silico study. Journal of Biomolecular Structure and Dynamics, 2019, 37, 411-439.	3.5	12
48	EMCA and DEEM as Michael Reagents Used in Organic Synthesis. Current Organic Chemistry, 2005, 9, 1237-1259.	1.6	11
49	Theoretical Studies on the Structure and Symmetry of the Transmembrane Region of Glutamatergic GluR5 Receptor. Journal of Medicinal Chemistry, 2008, 51, 3765-3776.	6.4	11
50	Experimental and computational studies on the tautomerism of N-substituted 3-amino-5-oxo-4-phenyl-1H-pyrazolo-1-carboxamides with antibacterial activity. Journal of Molecular Structure, 2013, 1051, 188-196.	3.6	11
51	Signaling within Allosteric Machines: Signal Transmission Pathways Inside G Protein-Coupled Receptors. Molecules, 2017, 22, 1188.	3.8	11
52	Synthesis, crystal structure, thermal, spectroscopic and theoretical studies of N3O2-donor Schiff base and its complex with CuII ions. Polyhedron, 2018, 139, 271-281.	2.2	11
53	Synthesis, Structural and Thermal Studies of 3-(1-Benzyl-1,2,3,6-tetrahydropyridin-4-yl)-5-ethoxy-1H-indole (D2AAK1_3) as Dopamine D2 Receptor Ligand. Molecules, 2018, 23, 2249.	3.8	11
54	Current Approaches and Tools Used in Drug Development against Parkinsonâ€™s Disease. Biomolecules, 2021, 11, 897.	4.0	11

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55	Structural and Molecular Docking Studies of 4-Benzyl-3-[(1-methylpyrrol-) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 747 Td (2-yl) 313-328.	1.5	11
56	Structure-Based Molecular Modeling Approaches to GPCR Oligomerization. Methods in Cell Biology, 2013, 117, 91-104.	1.1	10
57	Revisiting 1,3,4-Oxadiazol-2-ones: Utilization in the Development of ABHD6 Inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 6335-6345.	3.0	10
58	Positive allosteric modulators of Î±7 nicotinic acetylcholine receptors affect neither the function of other ligand- and voltage-gated ion channels and acetylcholinesterase, nor Î²-amyloid content. International Journal of Biochemistry and Cell Biology, 2016, 76, 19-30.	2.8	10
59	Multi-targeted drug design strategies for the treatment of schizophrenia. Expert Opinion on Drug Discovery, 2021, 16, 101-114.	5.0	10
60	N-(3-{4-[3-(trifluoromethyl)phenyl]piperazin-1-yl}propyl)-1H-indazole-3-carboxamide (D2AAK3) as a potential antipsychotic: In vitro, in silico and in vivo evaluation of a multi-target ligand. Neurochemistry International, 2021, 146, 105016.	3.8	10
61	Structure-based virtual screening for novel inhibitors of Japanese encephalitis virus NS3 helicase/nucleoside triphosphatase. FEMS Immunology and Medical Microbiology, 2010, 58, 91-101.	2.7	9
62	Synthesis, Structural Studies and Molecular Modelling of a Novel Imidazoline Derivative with Antifungal Activity. Molecules, 2015, 20, 14761-14776.	3.8	9
63	Thermal and spectroscopic studies of 2,3,5-trisubstituted and 1,2,3,5-tetrasubstituted indoles as non-competitive antagonists of GluK1/GluK2 receptors. Journal of Thermal Analysis and Calorimetry, 2018, 133, 935-944.	3.6	9
64	Novel Positive Allosteric Modulators of Âμ Opioid Receptorâ€"Insight from In Silico and In Vivo Studies. International Journal of Molecular Sciences, 2020, 21, 8463.	4.1	9
65	Docking-Based 3D-QSAR Studies for 1,3,4-oxadiazol-2-one Derivatives as FAAH Inhibitors. International Journal of Molecular Sciences, 2021, 22, 6108.	4.1	9
66	Rational design of the survivin/CDK4 complex by combining proteinâ€"protein docking and molecular dynamics simulations. Journal of Molecular Modeling, 2013, 19, 1507-1514.	1.8	8
67	Synthesis, central nervous system activity and structureâ€"activity relationship of N-substituted derivatives of 1-arylimidazolidyn-2-ylideneurea and products of their cyclization. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 746-760.	5.2	8
68	Some Dietary Phenolic Compounds Can Activate Thyroid Peroxidase and Inhibit Lipoxygenase-Preliminary Study in the Model Systems. International Journal of Molecular Sciences, 2021, 22, 5108.	4.1	8
69	Synthesis, Pharmacological Activity and Molecular Modeling of 1-Aryl-7-hydroxy-2,3-dihydroimidazo[1,2-a]pyrimidine-5(1H)-ones and their 6-Substituted Derivatives. Medicinal Chemistry, 2014, 10, 460-475.	1.5	8
70	Synthesis, central nervous system activity, and structureâ€"activity relationship of 1-aryl-6-benzyl-7-hydroxy-2,3-dihydroimidazo[1,2-a]pyrimidine-5(1H)-ones. Medicinal Chemistry Research, 2014, 23, 4221-4237.	2.4	7
71	In silicoExploration of the Conformational Universe of GPCRs. Molecular Informatics, 2016, 35, 227-237.	2.5	7
72	Comparative molecular field analysis and molecular dynamics studies of the dopamine D2 receptor antagonists without a protonatable nitrogen atom. Medicinal Chemistry Research, 2018, 27, 1149-1166.	2.4	7

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73	Synthesis, docking studies, and pharmacological evaluation of 5HT_{2C} ligands containing the Nâ€²â€cyanoisonicotinamidine or Nâ€²â€cyanopicolinamidine nucleus. Archiv Der Pharmazie, 2019, 352, e1800373.	4.1	7
74	Role of N-terminus in function and dynamics of sirtuin 7: an in silico study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1283-1291.	3.5	7
75	Synthesis, docking studies, and pharmacological evaluation of 2â€hydroxypropylâ€4â€arylpiperazine derivatives as serotoninergic ligands. Archiv Der Pharmazie, 2021, 354, 2000414.	4.1	7
76	Structural Studies on N-(1-naphthyl)-3-amino-5-oxo-4-phenyl-1Hpyrazole- 1-carboxamide with Antibacterial Activity. Letters in Organic Chemistry, 2014, 11, 40-48.	0.5	6
77	Synthesis, in vitro and in vivo studies, and molecular modeling of N-alkylated dextromethorphan derivatives as non-competitive inhibitors of Î±3Î²4 nicotinic acetylcholine receptor. Bioorganic and Medicinal Chemistry, 2014, 22, 6846-6856.	3.0	6
78	Synthesis, Central Nervous System Activity and Structure-Activity Relationships of Novel 1-(1-Alkyl-4-aryl-4,5-dihydro-1H-imidazo)-3-substituted Urea Derivatives. Molecules, 2015, 20, 3821-3840.	3.8	6
79	Synthesis and structure of new 1-cyanoacetyl-4-arylsemicarbazide derivatives with potential anticancer activity. Journal of Molecular Structure, 2016, 1104, 24-32.	3.6	6
80	Challenges and Opportunities in Drug Discovery of Biased Ligands. Methods in Molecular Biology, 2018, 1705, 321-334.	0.9	6
81	The Universal 3D QSAR Model for Dopamine D2 Receptor Antagonists. International Journal of Molecular Sciences, 2019, 20, 4555.	4.1	6
82	Tuning Down the Pain â€“ An Overview of Allosteric Modulation of Opioid Receptors: Mechanisms of Modulation, Allosteric Sites, Modulator Syntheses. Current Topics in Medicinal Chemistry, 2020, 20, 2852-2865.	2.1	5
83	Allosteric modulation of dopamine D2L receptor in complex with Gi1 and Gi2 proteins: the effect of subtle structural and stereochemical ligand modifications. Pharmacological Reports, 2022, 74, 406-424.	3.3	5
84	The Role of Lipids in Allosteric Modulation of Dopamine D2 Receptorâ€”In Silico Study. Molecules, 2022, 27, 1335.	3.8	5
85	WaterMapâ€Guided Structureâ€Based Virtual Screening for Acetylcholinesterase Inhibitors. ChemMedChem, 2022, 17, .	3.2	5
86	Multitarget Derivatives of D2AAK1 as Potential Antipsychotics: The Effect of Substitution in the Indole Moiety. ChemMedChem, 2022, 17, .	3.2	5
87	The Antipsychotic D2AAK1 as a Memory Enhancer for Treatment of Mental and Neurodegenerative Diseases. International Journal of Molecular Sciences, 2020, 21, 8849.	4.1	4
88	Novel Non-Competitive Antagonists of Kainate GluK1/GluK2 Receptors. Letters in Drug Design and Discovery, 2012, 9, 891-898.	0.7	4
89	The pseudo-Michael reaction of 1-aryl-4,5-dihydro-1H-imidazol-2-amines with ethyl ethoxymethylenecyanoacetate. Monatshefte FÃ¼r Chemie, 2013, 144, 1171-1182.	1.8	3
90	Novel Non-Competitive Antagonists of Kainate GluK1/GluK2 Receptors. Letters in Drug Design and Discovery, 2012, 9, 891-898.	0.7	3

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91	Modeling the Active Conformation of Human µ Opioid Receptor. Letters in Drug Design and Discovery, 2014, 11, 1053-1061.	0.7	3
92	Experimental and Computational Structural Studies of 2,3,5-Trisubstituted and 1,2,3,5-Tetrasubstituted Indoles as Non-Competitive Antagonists of GluK1/GluK2 Receptors. Molecules, 2022, 27, 2479.	3.8	3
93	Synthesis and molecular docking of indole and carbazole derivatives with potential pharmacological activity. Heterocyclic Communications, 2014, 20, 103-109.	1.2	2
94	Synthesis and molecular docking of novel non-competitive antagonists of GluK2 receptor. Medicinal Chemistry Research, 2015, 24, 810-817.	2.4	2
95	Synthesis and antiviral activity of 1-(1,3-disubstitutedimidazolidyn-2-ylidene)-3-ethoxycarbonylmethylurea derivatives. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 31, 1-8.	5.2	2
96	Synthesis, antiviral activity and structureâ€“activity relationship of 1-(1-aryl-4,5-dihydro-1H-imidazoline)-3-chlorosulfonylureas and products of their cyclization. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 787-795.	5.2	2
97	Experimental and computational structural studies of 5-substituted-3-(1-arylmethyl-1,2,3,6-tetrahydropyridin-4-yl)-1H-indoles. Journal of Molecular Structure, 2021, 1245, 130998.	3.6	2
98	Synthesis, Experimental and Computational Studies of N-(4-amino-6-oxo-) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 462 Td (1,6-dihydropyri	0.5	2
99	In Vitro Screening of Some Heterocyclic Compounds Against Human ABHD6 and ABHD12 Hydrolases. Letters in Drug Design and Discovery, 2014, 11, 944-952.	0.7	2
100	In vitro and in vivo evaluation of antioxidant and neuroprotective properties of antipsychotic D2AAK1. Neurochemical Research, 2022, 47, 1778-1789.	3.3	2
101	Non-peptide Opioid Receptor Ligands - Recent Advances. Part I - Agonists. Frontiers in Drug Design and Discovery, 2004, 1, 477-500.	0.3	1
102	Fragmental Method KowWIN as the Powerful Tool for Prediction of Chromatographic Behavior of Novel Bioactive Urea Derivatives. Journal of the Brazilian Chemical Society, 2016, , .	0.6	1
103	Synthesis and Pharmacological Evaluation of Novel 1-(1,4-Alkylaryldisubstituted-4,5-dihydro-1H-imidazo)-3-substituted Urea Derivatives. Molecules, 2016, 21, 582.	3.8	1
104	Do new N-substituted 3-amino-4-phenyl-5-oxo-pyrazolinecarboxamide derivatives exhibit antitubercular potential?. European Journal of Pharmaceutical Sciences, 2018, 121, 155-165.	4.0	1
105	From Synthesis and Spectral Analysis to Molecular Modeling â€“ Multidimensional Teaching of Medicinal Chemistry: Aspirin as an Example. Indian Journal of Pharmaceutical Education and Research, 2015, 49, 82-87.	0.6	1
106	Inhibitory Effects of 1,4-disubstituted Thiosemicarbazide Derivatives on Streptococcus mutans and Streptococcus sanguinis Mono-species Biofilms. Letters in Drug Design and Discovery, 2018, 15, 843-850.	0.7	1
107	Screening and Structureâ€“Activity Relationship of D2AAK1 Derivatives for Potential Application in the Treatment of Neurodegenerative Diseases. Molecules, 2022, 27, 2239.	3.8	1
108	Crystal Structure of 1-(4-Chlorophenyl)-5(1H)-oxo-2,3-dihydroimidazo[1,2-a]-pyrimidine-6-carbonitrile. Analytical Sciences: X-ray Structure Analysis Online, 2008, 24, X119-X120.	0.1	0

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109	The Pseudo-Michael Reaction of 2-Hydrazinylidene-1-Arylimidazolidines with Diethyl Ethoxymethylenemalonate. Journal of Heterocyclic Chemistry, 2016, 53, 571-578.	2.6	0
110	5-Methoxy-1-methyl-2-{[4-(2-hydroxyphenyl)piperazin-1-yl]methyl}-1Hindole (KAD22) with Antioxidant Activity. Letters in Organic Chemistry, 2021, 18, .	0.5	0
111	Synthesis, Experimental and Computational Spectroscopic Studies, and Formation Thermodynamics of Diethyl [[2-(1-Aryl-4,5-dihydro-1H-imidazol- 2-yl)hydrazinyl]methylene]propanedioates. Letters in Organic Chemistry, 2014, 11, 493-497.	0.5	0