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	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
2	The Role of Lipids in Allosteric Modulation of Dopamine D2 Receptorâ€"In Silico Study. Molecules, 2022, 27, 1335.	3.8	5
3	WaterMapâ€Guided Structureâ€Based Virtual Screening for Acetylcholinesterase Inhibitors. ChemMedChem, 2022, 17, .	3.2	5
4	Screening and Structureâ€"Activity Relationship of D2AAK1 Derivatives for Potential Application in the Treatment of Neurodegenerative Diseases. Molecules, 2022, 27, 2239.	3.8	1
5	In vitro and in vivo evaluation of antioxidant and neuroprotective properties of antipsychotic D2AAK1. Neurochemical Research, 2022, 47, 1778-1789.	3.3	2
6	Overcoming Depression with 5-HT2A Receptor Ligands. International Journal of Molecular Sciences, 2022, 23, 10.	4.1	19
7	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
8	What are the challenges with multi-targeted drug design for complex diseases?. Expert Opinion on Drug Discovery, 2022, 17, 673-683.	5.0	14
9	Multitarget Derivatives of D2AAK1 as Potential Antipsychotics: The Effect of Substitution in the Indole Moiety. ChemMedChem, 2022, 17, .	3.2	5
10	Multi-targeted drug design strategies for the treatment of schizophrenia. Expert Opinion on Drug Discovery, 2021, 16, 101-114.	5.0	10
11	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
12	Synthesis, docking studies, and pharmacological evaluation of 2â€hydroxypropylâ€4â€arylpiperazine derivatives as serotoninergic ligands. Archiv Der Pharmazie, 2021, 354, 2000414.	4.1	7
13	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
14	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
15	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
16	Current Approaches and Tools Used in Drug Development against Parkinsonâ€™s Disease. Biomolecules, 2021, 11, 897.	4.0	11
17	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
18	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

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19	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
20	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
21	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
22	2,4-Dichlorophenoxyacetic Thiosemicarbazides as a New Class of Compounds against Stomach Cancer Potentially Intercalating with DNA. Biomolecules, 2020, 10, 296.	4.0	13
23	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
24	In Vitro and In Vivo Models for the Investigation of Potential Drugs Against Schizophrenia. Biomolecules, 2020, 10, 160.	4.0	15
25	1,2,4-Triazolin-5-thione derivatives with anticancer activity as CK1Î³ kinase inhibitors. Bioorganic Chemistry, 2020, 99, 103806.	4.1	13
26	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
27	Thyroid Peroxidase Activity is Inhibited by Phenolic Compoundsâ€"Impact of Interaction. Molecules, 2019, 24, 2766.	3.8	18
28	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
29	The Universal 3D QSAR Model for Dopamine D2 Receptor Antagonists. International Journal of Molecular Sciences, 2019, 20, 4555.	4.1	6
30	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
31	Molecular mechanisms of allosteric probe dependence in Î¼ opioid receptor. Journal of Biomolecular Structure and Dynamics, 2019, 37, 36-47.	3.5	12
32	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
33	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
34	Proteinâ€"Protein Docking in Drug Design and Discovery. Methods in Molecular Biology, 2018, 1762, 285-305.	0.9	17
35	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
36	Opportunities and Challenges in the Discovery of Allosteric Modulators of GPCRs. Methods in Molecular Biology, 2018, 1705, 297-319.	0.9	16

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37	Challenges and Opportunities in Drug Discovery of Biased Ligands. Methods in Molecular Biology, 2018, 1705, 321-334.	0.9	6
38	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
39	Multi-Target Approach for Drug Discovery against Schizophrenia. International Journal of Molecular Sciences, 2018, 19, 3105.	4.1	66
40	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
41	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
42	Current Concepts and Treatments of Schizophrenia. Molecules, 2018, 23, 2087.	3.8	284
43	Synthesis, Experimental and Computational Studies of N-(4-amino-6-oxo-) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 502 Td (1,6-d	0.5	2
44	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
45	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
46	Recent Advances and Applications of Molecular Docking to G Protein-Coupled Receptors. Molecules, 2017, 22, 340.	3.8	51
47	Signaling within Allosteric Machines: Signal Transmission Pathways Inside G Protein-Coupled Receptors. Molecules, 2017, 22, 1188.	3.8	11
48	Novel Antibacterial Compounds and their Drug Targets - Successes and Challenges. Current Medicinal Chemistry, 2017, 24, 1948-1982.	2.4	31
49	Computational methods for studying G protein-coupled receptors (GPCRs). Methods in Cell Biology, 2016, 132, 359-399.	1.1	31
50	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
51	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
52	Structureâ€Based Virtual Screening for Dopamine D₂ Receptor Ligands as Potential Antipsychotics. ChemMedChem, 2016, 11, 718-729.	3.2	51
53	In silicoExploration of the Conformational Universe of GPCRs. Molecular Informatics, 2016, 35, 227-237.	2.5	7
54	The Pseudo-Michael Reaction of 2-Hydrazinylidene-1-Arylimidazolidines with Diethyl Ethoxymethylenemalonate. Journal of Heterocyclic Chemistry, 2016, 53, 571-578.	2.6	0

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55	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
56	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
57	Potent and selective N-(4-sulfamoylphenyl)thiourea-based GPR55 agonists. European Journal of Medicinal Chemistry, 2016, 107, 119-132.	5.5	18
58	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
59	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
60	Discovery of nitroaryl urea derivatives with antiproliferative properties. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 608-618.	5.2	13
61	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
62	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
63	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
64	Synthesis, Structural Studies and Molecular Modelling of a Novel Imidazoline Derivative with Antifungal Activity. Molecules, 2015, 20, 14761-14776.	3.8	9
65	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
66	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
67	Synthesis and molecular docking of novel non-competitive antagonists of GluK2 receptor. Medicinal Chemistry Research, 2015, 24, 810-817.	2.4	2
68	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
69	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
70	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
71	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
72	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

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73	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
74	Optimization of 1,2,5â€Thiadiazole Carbamates as Potent and Selective ABHD6 Inhibitors. ChemMedChem, 2015, 10, 253-265.	3.2	29
75	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
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	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
79	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
80	Synthesis and molecular docking of indole and carbazole derivatives with potential pharmacological activity. Heterocyclic Communications, 2014, 20, 103-109.	1.2	2
81	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
82	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
83	Application of BRET for Studying G Protein-Coupled Receptors. Mini-Reviews in Medicinal Chemistry, 2014, 14, 411-425.	2.4	19
84	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
85	Modeling the Active Conformation of Human µ Opioid Receptor. Letters in Drug Design and Discovery, 2014, 11, 1053-1061.	0.7	3
86	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
87	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
88	Modeling Complexes of Transmembrane Proteins: Systematic Analysis of Proteinï£¿Protein Docking Tools. Molecular Informatics, 2013, 32, 717-733.	2.5	27
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	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

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91	Chiral 1,3,4-Oxadiazol-2-ones as Highly Selective FAAH Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 8484-8496.	6.4	54
92	Structure-Based Molecular Modeling Approaches to GPCR Oligomerization. Methods in Cell Biology, 2013, 117, 91-104.	1.1	10
93	Simulating G Protein-Coupled Receptors in Native-Like Membranes. Methods in Cell Biology, 2013, 117, 63-90.	1.1	13
94	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
95	Structural and Molecular Docking Studies of 4-Benzyl-3-[(1-methylpyrrol-) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 587 Td (2-yl) 313-328.	1.5	11
96	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
97	Novel Non-Competitive Antagonists of Kainate GluK1/GluK2 Receptors. Letters in Drug Design and Discovery, 2012, 9, 891-898.	0.7	4
98	Novel Non-Competitive Antagonists of Kainate GluK1/GluK2 Receptors. Letters in Drug Design and Discovery, 2012, 9, 891-898.	0.7	3
99	Experimental and theoretical investigations on the ketoâ€“enol tautomerism of 4-substituted Structure, 2011, 994, 313-320.	3.6	14
100	Oligomerization of G Protein-Coupled Receptors: Computational Methods. Current Medicinal Chemistry, 2011, 18, 4588-4605.	2.4	35
101	Oligomerization of G Protein-Coupled Receptors: Biochemical and Biophysical Methods. Current Medicinal Chemistry, 2011, 18, 4606-4634.	2.4	53
102	Molecular Structure of Ionotropic Glutamate Receptors. Current Medicinal Chemistry, 2010, 17, 2608-2635.	2.4	29
103	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
104	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
105	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
106	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
107	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
108	EMCA and DEEM as Michael Reagents Used in Organic Synthesis. Current Organic Chemistry, 2005, 9, 1237-1259.	1.6	11

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109	Non-peptide Opioid Receptor Ligands - Recent Advances. Part I - Agonists. Frontiers in Drug Design and Discovery, 2004, 1, 477-500.	0.3	1
110	Non-peptide Opioid Receptor Ligands - Recent Advances. Part I - Agonists. Current Medicinal Chemistry, 2002, 9, 1567-1589.	2.4	30
111	Non-peptide Opioid Receptor Ligands - Recent Advances. Part II - Antagonists. Current Medicinal Chemistry, 2002, 9, 1591-1603.	2.4	29