RafaÅ, Kurczab

List of Publications by Year
in descending order

74	1,284	304743	454955
papers	citations	22 h-index	30 g-index

75	75	75	1546
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hydrogen Bonds with Fluorine in Ligandâ€“Protein Complexes-the PDB Analysis and Energy Calculations. Molecules, 2022, 27, 1005.	3.8	15
2	Mining anionâ€“aromatic interactions in the Protein Data Bank. Chemical Science, 2022, 13, 3984-3998.	7.4	8
3	An exit beyond the pharmacophore model for 5-HT6R agents - a new strategy to gain dual 5-HT6/5-HT2A action for triazine derivatives with procognitive potential. Bioorganic Chemistry, 2022, 121, 105695.	4.1	8
4	Overcoming undesirable hERG affinity by incorporating fluorine atoms: A case of MAO-B inhibitors derived from 1ÂH-pyrrolo-[3,2-c]quinolines. European Journal of Medicinal Chemistry, 2022, 236, 114329.	5.5	8
5	Imidazopyridine-Based 5-HT₆ Receptor Neutral Antagonists: Impact of N¹-Benzyl and N¹-Phenylsulfonyl Fragments on Different Receptor Conformational States. Journal of Medicinal Chemistry, 2021, 64, 1180-1196.	6.4	14
6	2-Phenyl-1H-pyrrole-3-carboxamide as a New Scaffold for Developing 5-HT₆ Receptor Inverse Agonists with Cognition-Enhancing Activity. ACS Chemical Neuroscience, 2021, 12, 1228-1240.	3.5	9
7	Mutual Support of Ligand- and Structure-Based Approachesâ€”To What Extent We Can Optimize the Power of Predictive Model? Case Study of Opioid Receptors. Molecules, 2021, 26, 1607.	3.8	0
8	How can fluorine directly and indirectly affect the hydrogen bonding in molecular systems? â€“ A case study for monofluoroanilines. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 252, 119536.	3.9	5
9	Influence of fluorine substitution on nonbonding interactions in selected paraâ€‘halogeno anilines. ChemPhysChem, 2021, 22, 2115-2127.	2.1	3
10	N-Skatyltryptaminesâ€”Dual 5-HT6R/D2R Ligands with Antipsychotic and Procognitive Potential. Molecules, 2021, 26, 4605.	3.8	3
11	Tuning the activity of known drugs via the introduction of halogen atoms, a case study of SERT ligands â€“ Fluoxetine and fluvoxamine. European Journal of Medicinal Chemistry, 2021, 220, 113533.	5.5	16
12	Structure-Based Design and Optimization of FPPQ, a Dual-Acting 5-HT₃ and 5-HT₆ Receptor Antagonist with Antipsychotic and Procognitive Properties. Journal of Medicinal Chemistry, 2021, 64, 13279-13298.	6.4	14
13	Pharmacoprint: A Combination of a Pharmacophore Fingerprint and Artificial Intelligence as a Tool for Computer-Aided Drug Design. Journal of Chemical Information and Modeling, 2021, 61, 5054-5065.	5.4	11
14	Data-Driven Analysis of Fluorination of Ligands of Aminergic G Protein Coupled Receptors. Biomolecules, 2021, 11, 1647.	4.0	2
15	Virtual screening-driven discovery of dual 5-HT6/5-HT2A receptor ligands with pro-cognitive properties. European Journal of Medicinal Chemistry, 2020, 185, 111857.	5.5	26
16	A dual-acting 5-HT6 receptor inverse agonist/MAO-B inhibitor displays glioprotective and pro-cognitive properties. European Journal of Medicinal Chemistry, 2020, 208, 112765.	5.5	15
17	Theoretical Investigations on Interactions of Arylsulphonyl Indazole Derivatives as Potential Ligands of VEGFR2 Kinase. International Journal of Molecular Sciences, 2020, 21, 4793.	4.1	5
18	10-Methylthiocolchicine complexes with lithium, sodium, potassium, rubidium and cesium metal cations salts â€“ Cytotoxic, semi-empirical and molecular modelling studies. Polyhedron, 2020, 190, 114791.	2.2	1

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19	Chlorine substituents and linker topology as factors of 5-HT6R activity for novel highly active 1,3,5-triazine derivatives with procognitive properties inÂvivo. European Journal of Medicinal Chemistry, 2020, 203, 112529.	5.5	14
20	The Significance of Halogen Bonding in Ligandâ€“Receptor Interactions: The Lesson Learned from Molecular Dynamic Simulations of the D4 Receptor. Molecules, 2020, 25, 91.	3.8	15
21	Antifungal, anticancer, and docking studies of colchiceine complexes with monovalent metal cation salts. Chemical Biology and Drug Design, 2019, 94, 1930-1943.	3.2	14
22	Role of Staple Molecules in the Formation of SÂ·Â·Â·S Contact in Thioamides: Experimental Charge Density and Theoretical Studies. Crystal Growth and Design, 2019, 19, 7324-7335.	3.0	5
23	Synthesis and computer-aided SAR studies for derivatives of phenoxyalkyl-1,3,5-triazine as the new potent ligands for serotonin receptors 5-HT6. European Journal of Medicinal Chemistry, 2019, 178, 740-751.	5.5	18
24	2-Aminoimidazole-based antagonists of the 5-HT6 receptor â€“ A new concept in aminergic GPCR ligand design. European Journal of Medicinal Chemistry, 2019, 179, 1-15.	5.5	20
25	Dual 5-HT₆ and D₃ Receptor Antagonists in a Group of 1H-Pyrrolo[3,2-c]quinolines with Neuroprotective and Procognitive Activity. ACS Chemical Neuroscience, 2019, 10, 3183-3196.	3.5	24
26	Fluorinated indole-imidazole conjugates: Selective orally bioavailable 5-HT7 receptor low-basicity agonists, potential neuropathic painkillers. European Journal of Medicinal Chemistry, 2019, 170, 261-275.	5.5	22
27	Recognition of repulsive and attractive regions of selected serotonin receptor binding site using FMO-EDA approach. Journal of Molecular Modeling, 2019, 25, 114.	1.8	11
28	Are the Hydantoin-1,3,5-triazine 5-HT6R Ligands a Hope to a Find New Procognitive and Anti-Obesity Drug? Considerations Based on Primary In Vivo Assays and ADME-Tox Profile In Vitro. Molecules, 2019, 24, 4472.	3.8	18
29	Synthesis and computer-aided analysis of the role of linker for novel ligands of the 5-HT6 serotonin receptor among substituted 1,3,5-triazinylpiperazines. Bioorganic Chemistry, 2019, 84, 319-325.	4.1	13
30	Polypharmacology â€“ a challenge for current drug design approaches. Science Technology and Innovation, 2019, 6, 19-23.	0.0	0
31	ONIOM and FMOâ€EDA study of metabotropic glutamate receptor 1: Quantum insights into the allosteric binding site. International Journal of Quantum Chemistry, 2018, 118, e25617.	2.0	6
32	Computer-aided insights into receptor-ligand interaction for novel 5-arylhydantoin derivatives as serotonin 5-HT 7 receptor agents with antidepressant activity. European Journal of Medicinal Chemistry, 2018, 147, 102-114.	5.5	16
33	Design, synthesis, and biological evaluation of novel combretastatin A-4 thio derivatives as microtubule targeting agents. European Journal of Medicinal Chemistry, 2018, 144, 797-816.	5.5	23
34	Computer-Aided Studies for Novel Arylhydantoin 1,3,5-Triazine Derivatives as 5-HT6 Serotonin Receptor Ligands with Antidepressive-Like, Anxiolytic and Antiobesity Action In Vivo. Molecules, 2018, 23, 2529.	3.8	18
35	Salt Bridge in Ligandâ€“Protein Complexesâ€”Systematic Theoretical and Statistical Investigations. Journal of Chemical Information and Modeling, 2018, 58, 2224-2238.	5.4	49
36	Amino Acid Hot Spots of Halogen Bonding: A Combined Theoretical and Experimental Case Study of the 5-HT₇ Receptor. Journal of Medicinal Chemistry, 2018, 61, 8717-8733.	6.4	28

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37	Pyrroloquinoline scaffold-based 5-HT6R ligands: Synthesis, quantum chemical and molecular dynamic studies, and influence of nitrogen atom position in the scaffold on affinity. Bioorganic and Medicinal Chemistry, 2018, 26, 3588-3595.	3.0	15
38	The role of aryl-topology in balancing between selective and dual 5-HT₇R/5-HT_{1A}actions of 3,5-substituted hydantoins. MedChemComm, 2018, 9, 1033-1044.	3.4	7
39	Structural determinants influencing halogen bonding: a case study on azinesulfonamide analogs of aripiprazole as 5-HT1A, 5-HT7, and D2 receptor ligands. Chemistry Central Journal, 2018, 12, 55.	2.6	8
40	7-Deacetyl-10-alkylthiocolchicine derivatives â€“ new compounds with potent anticancer and fungicidal activity. MedChemComm, 2018, 9, 1708-1714.	3.4	11
41	Novel 5-HT 7 R antagonists, arylsulfonamide derivatives of (aryloxy)propyl piperidines: Add-on effect to the antidepressant activity of SSRI and DRI, and pro-cognitive profile. Bioorganic and Medicinal Chemistry, 2017, 25, 2789-2799.	3.0	18
42	The computer-aided discovery of novel family of the 5-HT6 serotonin receptor ligands among derivatives of 4-benzyl-1,3,5-triazine. European Journal of Medicinal Chemistry, 2017, 135, 117-124.	5.5	33
43	The impact of the halogen bonding on D 2 and 5-HT 1A /5-HT 7 receptor activity of azinesulfonamides of 4-[(2-ethyl)piperidinyl-1-yl]phenylpiperazines with antipsychotic and antidepressant properties. Bioorganic and Medicinal Chemistry, 2017, 25, 3638-3648.	3.0	24
44	Low-basicity 5-HT7 Receptor Agonists Synthesized Using the van Leusen Multicomponent Protocol. Scientific Reports, 2017, 7, 1444.	3.3	18
45	Synthesis and anticancer activity evaluation of a quinoline-based 1,2,3-triazoles. Medicinal Chemistry Research, 2017, 26, 2432-2442.	2.4	8
46	The evaluation of QM/MM-driven molecular docking combined with MM/GBSA calculations as a halogen-bond scoring strategy. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 188-194.	1.1	24
47	New N- and O-arylpiperazinylalkyl pyrimidines and 2-methylquinazolines derivatives as 5-HT7 and 5-HT1A receptor ligands: Synthesis, structure-activity relationships, and molecular modeling studies. Bioorganic and Medicinal Chemistry, 2017, 25, 1250-1259.	3.0	21
48	The Effect of Carboxamide/Sulfonamide Replacement in Arylpiperazinylalkyl Derivatives on Activity to Serotonin and Dopamine Receptors. Archiv Der Pharmazie, 2017, 350, 1700090.	4.1	5
49	The influence of the negative-positive ratio and screening database size on the performance of machine learning-based virtual screening. PLoS ONE, 2017, 12, e0175410.	2.5	11
50	Halogen bonding enhances activity in a series of dual 5-HT₆/D₂ ligands designed in a hybrid bioisostere generation/virtual screening protocol. RSC Advances, 2016, 6, 54918-54925.	3.6	6
51	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1
52	Towards new 5-HT 7 antagonists among arylsulfonamide derivatives of (aryloxy)ethyl-alkyl amines: Multiobjective based design, synthesis, and antidepressant and anxiolytic properties. European Journal of Medicinal Chemistry, 2016, 108, 334-346.	5.5	28
53	N-Alkylated arylsulfonamides of (aryloxy)ethyl piperidines: 5-HT7 receptor selectivity versus multireceptor profile. Bioorganic and Medicinal Chemistry, 2016, 24, 130-139.	3.0	16
54	An Algorithm to Identify Target-Selective Ligands â€“ A Case Study of 5-HT7/5-HT1A Receptor Selectivity. PLoS ONE, 2016, 11, e0156986.	2.5	12

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55	Arylsulfonamide derivatives of (aryloxy)ethylpiperidines as selective 5-HT₇ receptor antagonists and their psychotropic properties. MedChemComm, 2015, 6, 1272-1277.	3.4	13
56	Towards novel 5-HT7 versus 5-HT1A receptor ligands among LCAPs with cyclic amino acid amide fragments: Design, synthesis, and antidepressant properties. Part II. European Journal of Medicinal Chemistry, 2015, 92, 202-211.	5.5	16
57	Fingerprint-based consensus virtual screening towards structurally new 5-HT6R ligands. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1827-1830.	2.2	16
58	Synthesis, molecular docking study, and evaluation of the antiproliferative action of a new group of propargylthio- and propargylselenoquinolines. Medicinal Chemistry Research, 2014, 23, 3468-3477.	2.4	12
59	Solid-supported synthesis, molecular modeling, and biological activity of long-chain arylpiperazine derivatives with cyclic amino acid amide fragments as 5-HT7 and 5-HT1A receptor ligands. European Journal of Medicinal Chemistry, 2014, 78, 10-22.	5.5	23
60	Structureâ€“activity relationships and molecular modeling studies of novel arylpiperazinylalkyl 2-benzoxazolones and 2-benzothiazolones as 5-HT7 and 5-HT1A receptor ligands. European Journal of Medicinal Chemistry, 2014, 85, 716-726.	5.5	33
61	Identification of Novel Serotonin Transporter Compounds by Virtual Screening. Journal of Chemical Information and Modeling, 2014, 54, 933-943.	5.4	32
62	The influence of negative training set size on machine learning-based virtual screening. Journal of Cheminformatics, 2014, 6, 32.	6.1	62
63	The influence of the inactives subset generation on the performance of machine learning methods. Journal of Cheminformatics, 2013, 5, 17.	6.1	37
64	The influence of training actives/inactives ratio on machine learning performance. Journal of Cheminformatics, 2013, 5, .	6.1	2
65	A multidimensional analysis of machine learning methods performance in the classification of bioactive compounds. Chemometrics and Intelligent Laboratory Systems, 2013, 128, 89-100.	3.5	29
66	New Strategy for Receptor-Based Pharmacophore Query Construction: A Case Study for 5-HT₇ Receptor Ligands. Journal of Chemical Information and Modeling, 2013, 53, 3233-3243.	5.4	23
67	The multiobjective based design, synthesis and evaluation of the arylsulfonamide/amide derivatives of aryloxyethyl- and arylthioethyl- piperidines and pyrrolidines as a novel class of potent 5-HT7 receptor antagonists. European Journal of Medicinal Chemistry, 2012, 56, 348-360.	5.5	35
68	Molecular mechanism of serotonin transporter inhibition elucidated by a new flexible docking protocol. European Journal of Medicinal Chemistry, 2012, 47, 24-37.	5.5	26
69	Synthesis, 15N NMR spectra and GIAO calculated data of the seven positional isomers of 15N-labeled N,N-dimethylsulfamoylquinoline. Journal of Molecular Structure, 2012, 1015, 46-50.	3.6	4
70	Evaluation of different machine learning methods for ligand-based virtual screening. Journal of Cheminformatics, 2011, 3, .	6.1	19
71	Theoretical description of hydrogen bonding in oxalic acid dimer and trimer based on the combined extended-transition-state energy decomposition analysis and natural orbitals for chemical valence (ETS-NOCV). Journal of Molecular Modeling, 2010, 16, 1789-1795.	1.8	24
72	The development and validation of a novel virtual screening cascade protocol to identify potential serotonin 5-HT7R antagonists. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 2465-2468.	2.2	27

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73	Theoretical and spectroscopic studies of vibrational spectra of hydrogen bonds in molecular crystal of Î²-oxalic acid. Vibrational Spectroscopy, 2010, 52, 39-47.	2.2	14
74	Theoretical Analysis of the Resonance Assisted Hydrogen Bond Based on the Combined Extended Transition State Method and Natural Orbitals for Chemical Valence Scheme^{â€}. Journal of Physical Chemistry A, 2010, 114, 8581-8590.	2.5	94