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	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
2	The influence of negative training set size on machine learning-based virtual screening. Journal of Cheminformatics, 2014, 6, 32.	6.1	62
3	Salt Bridge in Ligandâ€“Protein Complexesâ€”Systematic Theoretical and Statistical Investigations. Journal of Chemical Information and Modeling, 2018, 58, 2224-2238.	5.4	49
4	The influence of the inactives subset generation on the performance of machine learning methods. Journal of Cheminformatics, 2013, 5, 17.	6.1	37
5	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
6	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
7	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
8	Identification of Novel Serotonin Transporter Compounds by Virtual Screening. Journal of Chemical Information and Modeling, 2014, 54, 933-943.	5.4	32
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

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19	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
20	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
21	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
22	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
23	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
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	Evaluation of different machine learning methods for ligand-based virtual screening. Journal of Cheminformatics, 2011, 3, .	6.1	19
26	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
27	Low-basicity 5-HT7 Receptor Agonists Synthesized Using the van Leusen Multicomponent Protocol. Scientific Reports, 2017, 7, 1444.	3.3	18
28	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
29	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
30	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
31	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
32	Fingerprint-based consensus virtual screening towards structurally new 5-HT6R ligands. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1827-1830.	2.2	16
33	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
34	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
35	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
36	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

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37	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
38	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
39	Hydrogen Bonds with Fluorine in Ligandâ€“Protein Complexes-the PDB Analysis and Energy Calculations. Molecules, 2022, 27, 1005.	3.8	15
40	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
41	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
42	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
43	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
44	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
45	Arylsulfonamide derivatives of (aryloxy)ethylpiperidines as selective 5-HT₇ receptor antagonists and their psychotropic properties. MedChemComm, 2015, 6, 1272-1277.	3.4	13
46	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
47	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
48	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
49	7-Deacetyl-10-alkylthiocolchicine derivatives â€“ new compounds with potent anticancer and fungicidal activity. MedChemComm, 2018, 9, 1708-1714.	3.4	11
50	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
51	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
52	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
53	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
54	Synthesis and anticancer activity evaluation of a quinoline-based 1,2,3-triazoles. Medicinal Chemistry Research, 2017, 26, 2432-2442.	2.4	8

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55	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
56	Mining anionâ€“aromatic interactions in the Protein Data Bank. Chemical Science, 2022, 13, 3984-3998.	7.4	8
57	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
58	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
59	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
60	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
61	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
62	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
63	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
64	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
65	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
66	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
67	Influence of fluorine substitution on nonbonding interactions in selected paraâ€halogeno anilines. ChemPhysChem, 2021, 22, 2115-2127.	2.1	3
68	N-Skatyltryptaminesâ€”Dual 5-HT6R/D2R Ligands with Antipsychotic and Procognitive Potential. Molecules, 2021, 26, 4605.	3.8	3
69	The influence of training actives/inactives ratio on machine learning performance. Journal of Cheminformatics, 2013, 5, .	6.1	2
70	Data-Driven Analysis of Fluorination of Ligands of Aminergic G Protein Coupled Receptors. Biomolecules, 2021, 11, 1647.	4.0	2
71	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1
72	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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73	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
74	Polypharmacology â€“ a challenge for current drug design approaches. Science Technology and Innovation, 2019, 6, 19-23.	0.0	0