Vigneshwaran Namasivayam

List of Publications by Year
in descending order

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71	2,808	331670	189892
papers	citations	21 h-index	50 g-index

72	72	72	4391
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Discovery of P2Y₂ Receptor Antagonist Scaffolds through Virtual High-Throughput Screening. Journal of Chemical Information and Modeling, 2022, 62, 1538-1549.	5.4	6
2	Structural feature-driven pattern analysis for multitarget modulator landscapes. Bioinformatics, 2022, 38, 1385-1392.	4.1	13
3	Cancer cells adapt FAM134B/BiP mediated ER-phagy to survive hypoxic stress. Cell Death and Disease, 2022, 13, 357.	6.3	15
4	Repurposing drugs targeting epidemic viruses. Drug Discovery Today, 2022, , .	6.4	3
5	Chemistry and Analysis of Organic Compounds in Dinosaurs. Biology, 2022, 11, 670.	2.8	11
6	Physicochemistry shapes bioactivity landscape of pan-ABC transporter modulators: Anchor point for innovative Alzheimer's disease therapeutics. International Journal of Biological Macromolecules, 2022, 217, 775-791.	7.5	12
7	Structural Insights to Human Immunodeficiency Virus (HIV-1) Targets and Their Inhibition. Advances in Experimental Medicine and Biology, 2021, 1322, 63-95.	1.6	4
8	Thioesterase-mediated side chain transesterification generates potent Gq signaling inhibitor FR900359. Nature Communications, 2021, 12, 144.	12.8	32
9	Scaffold fragmentation and substructure hopping reveal potential, robustness, and limits of computer-aided pattern analysis (C@PA). Computational and Structural Biotechnology Journal, 2021, 19, 3269-3283.	4.1	12
10	Rational drug design of 6-substituted 4-anilino-2-phenylpyrimidines for exploration of novel ABCG2 binding site. European Journal of Medicinal Chemistry, 2021, 212, 113045.	5.5	17
11	Targeting the Main Protease of SARSâ€CoVâ€2: From the Establishment of High Throughput Screening to the Design of Tailored Inhibitors. Angewandte Chemie - International Edition, 2021, 60, 10423-10429.	13.8	95
12	C@PA: Computer-Aided Pattern Analysis to Predict Multitarget ABC Transporter Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 3350-3366.	6.4	18
13	Die Hauptprotease von SARSâ€CoVâ€2 als Zielstruktur: Von der Etablierung eines Hochdurchsatzâ€Screenings zum Design maÄŸgeschneiderter Inhibitoren. Angewandte Chemie, 2021, 133, 10515-10521.	2.0	3
14	An Overview of Spike Surface Glycoprotein in Severe Acute Respiratory Syndromeâ€“Coronavirus. Frontiers in Molecular Biosciences, 2021, 8, 637550.	3.5	8
15	Adenosine A_{2A}R/A₁R Antagonists Enabling Additional H₃R Antagonism for the Treatment of Parkinsonâ€™s Disease. Journal of Medicinal Chemistry, 2021, 64, 8246-8262.	6.4	6
16	Feature-Based Molecular Networking for the Targeted Identification of G_q-Inhibiting FR900359 Derivatives. Journal of Natural Products, 2021, 84, 1941-1953.	3.0	7
17	Recommended tool compounds and drugs for blocking P2X and P2Y receptors. Purinergic Signalling, 2021, 17, 633-648.	2.2	21
18	Unraveling binding mechanism and kinetics of macrocyclic GÎ±q protein inhibitors. Pharmacological Research, 2021, 173, 105880.	7.1	10

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19	Discovery of potent nucleotide pyrophosphatase/phosphodiesterase3 (NPP3) inhibitors with ancillary carbonic anhydrase inhibition for cancer (immuno)therapy. RSC Medicinal Chemistry, 2021, 12, 1187-1206.	3.9	5
20	2â€Substituted thienotetrahydropyridine derivatives: Allosteric ectonucleotidase inhibitors. Archiv Der Pharmazie, 2021, 354, e2100300.	4.1	4
21	Binding mode analysis of ABCA7 for the prediction of novel Alzheimer's disease therapeutics. Computational and Structural Biotechnology Journal, 2021, 19, 6490-6504.	4.1	10
22	Strategies to gain novel Alzheimer's disease diagnostics and therapeutics using modulators of ABCA transporters.. Free Neuropathology, 2021, 2, .	3.0	9
23	An Agonist Radioligand for the Proinflammatory Lipid-Activated G Protein-Coupled Receptor GPR84 Providing Structural Insights. Journal of Medicinal Chemistry, 2020, 63, 2391-2410.	6.4	21
24	Substituted 4-phenylthiazoles: Development of potent and selective A1, A3 and dual A1/A3 adenosine receptor antagonists. European Journal of Medicinal Chemistry, 2020, 186, 111879.	5.5	9
25	Ligand binding and activation of UTP-activated G protein-coupled P2Y2 and P2Y4 receptors elucidated by mutagenesis, pharmacological and computational studies. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129501.	2.4	6
26	Cellâ€permeable highâ€affinity tracers for G_q proteins provide structural insights, reveal distinct binding kinetics and identify small molecule inhibitors. British Journal of Pharmacology, 2020, 177, 1898-1916.	5.4	21
27	Non-nucleoside reverse transcriptase inhibitors (NNRTIs): a brief overview of clinically approved drugs and combination regimens. Current Opinion in Pharmacology, 2020, 54, 179-187.	3.5	23
28	Nucleotide Analog ARL67156 as a Lead Structure for the Development of CD39 and Dual CD39/CD73 Ectonucleotidase Inhibitors. Frontiers in Pharmacology, 2020, 11, 1294.	3.5	23
29	Superior Pyrimidine Derivatives as Selective ABCG2 Inhibitors and Broad-Spectrum ABCB1, ABCC1, and ABCG2 Antagonists. Journal of Medicinal Chemistry, 2020, 63, 10412-10432.	6.4	21
30	P2Y₁â€like nucleotide receptorsâ€”Structures, molecular modeling, mutagenesis, and oligomerization. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1464.	14.6	12
31	Computational Investigations on the Binding Mode of Ligands for the Cannabinoid-Activated G Protein-Coupled Receptor GPR18. Biomolecules, 2020, 10, 686.	4.0	13
32	Agonists and Antagonists for Purinergic Receptors. Methods in Molecular Biology, 2020, 2041, 45-64.	0.9	37
33	Vesicular ATP-binding cassette transporters in human disease: relevant aspects of their organization for future drug development. Future Drug Discovery, 2020, 2, .	2.1	8
34	Design and synthesis of sulfonamidophenylethylamides as novel cardiac myosin activator. Bioorganic and Medicinal Chemistry, 2019, 27, 4110-4123.	3.0	0
35	Overview of Recent Strategic Advances in Medicinal Chemistry. Journal of Medicinal Chemistry, 2019, 62, 9375-9414.	6.4	108
36	Structureâ€“Activity Relationship of Purine and Pyrimidine Nucleotides as Ecto-5â€²-Nucleotidase (CD73) Inhibitors. Journal of Medicinal Chemistry, 2019, 62, 3677-3695.	6.4	53

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37	A_{2B} Adenosine Receptor Antagonists with Picomolar Potency. Journal of Medicinal Chemistry, 2019, 62, 4032-4055.	6.4	17
38	Identification of Thienopyrimidine Scaffold as an Inhibitor of the ABC Transport Protein ABCC1 (MRP1) and Related Transporters Using a Combined Virtual Screening Approach. Journal of Medicinal Chemistry, 2019, 62, 4383-4400.	6.4	24
39	The Journey of HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors (NNRTIs) from Lab to Clinic. Journal of Medicinal Chemistry, 2019, 62, 4851-4883.	6.4	124
40	Fluorescent-Labeled Selective Adenosine A_{2B} Receptor Antagonist Enables Competition Binding Assay by Flow Cytometry. Journal of Medicinal Chemistry, 2018, 61, 4301-4316.	6.4	24
41	6-(Ar)Alkylamino-Substituted Uracil Derivatives: Lipid Mimetics with Potent Activity at the Orphan G Protein-Coupled Receptor 84 (GPR84). ACS Omega, 2018, 3, 3365-3383.	3.5	30
42	Integrative approaches in HIV â€1 nonâ€nucleoside reverse transcriptase inhibitor design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1328.	14.6	10
43	Cover Image, Volume 8, Issue 1. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1356.	14.6	0
44	Development of a selective and highly sensitive fluorescence assay for nucleoside triphosphate diphosphohydrolase1 (NTPDase1, CD39). Analyst, The, 2018, 143, 5417-5430.	3.5	12
45	Inhibitors of Melanogenesis: An Updated Review. Journal of Medicinal Chemistry, 2018, 61, 7395-7418.	6.4	200
46	Medicinal Chemistry of A2B Adenosine Receptors. , 2018, , 137-168.		12
47	3-(2-Carboxyethyl)indole-2-carboxylic Acid Derivatives: Structural Requirements and Properties of Potent Agonists of the Orphan G Protein-Coupled Receptor GPR17. Journal of Medicinal Chemistry, 2018, 61, 8136-8154.	6.4	19
48	2,4,6-Substituted Quinazolines with Extraordinary Inhibitory Potency toward ABCG2. Journal of Medicinal Chemistry, 2018, 61, 7952-7976.	6.4	37
49	Probing Substituents in the 1- and 3-Position: Tetrahydropyrazino-Annelated Water-Soluble Xanthine Derivatives as Multi-Target Drugs With Potent Adenosine Receptor Antagonistic Activity. Frontiers in Chemistry, 2018, 6, 206.	3.6	8
50	Radiosynthesis and in vivo evaluation of a fluorine-18 labeled pyrazine based radioligand for PET imaging of the adenosine A2B receptor. Bioorganic and Medicinal Chemistry, 2018, 26, 4650-4663.	3.0	17
51	Skin whitening agents: medicinal chemistry perspective of tyrosinase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 403-425.	5.2	554
52	Interaction of Approved Drugs with Synaptic Vesicle Protein 2A. Archiv Der Pharmazie, 2017, 350, 1700003.	4.1	9
53	Development of Potent and Selective Antagonists for the UTP-Activated P2Y₄ Receptor. Journal of Medicinal Chemistry, 2017, 60, 3020-3038.	6.4	33
54	The promiscuous ectonucleotidase NPP1: molecular insights into substrate binding and hydrolysis. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 603-614.	2.4	36

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55	Molecular Recognition of Agonists and Antagonists by the Nucleotide-Activated G Protein-Coupled P2Y₂ Receptor. Journal of Medicinal Chemistry, 2017, 60, 8425-8440.	6.4	27
56	Characterization of P2X4 receptor agonists and antagonists by calcium influx and radioligand binding studies. Biochemical Pharmacology, 2017, 125, 41-54.	4.4	47
57	Probing the binding mechanism of mercaptoguanine derivatives as inhibitors of HPPK by docking and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2017, 35, 3507-3521.	3.5	11
58	Substrate-Dependence of Competitive Nucleotide Pyrophosphatase/Phosphodiesterase1 (NPP1) Inhibitors. Frontiers in Pharmacology, 2017, 8, 54.	3.5	36
59	HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors: SAR and Lead Optimization Using CoMFA and CoMSIA Studies (1995-2016). Current Medicinal Chemistry, 2017, 24, 3774-3812.	2.4	13
60	Design, Synthesis, and Characterization of Some Hybridized Pyrazolone Pharmacophore Analogs against Mycobacterium tuberculosis. Archiv Der Pharmazie, 2016, 349, 383-397.	4.1	14
61	Role of extracellular cysteine residues in the adenosine A2A receptor. Purinergic Signalling, 2016, 12, 313-329.	2.2	23
62	An Overview of Severe Acute Respiratory Syndromeâ€“Coronavirus (SARS-CoV) 3CL Protease Inhibitors: Peptidomimetics and Small Molecule Chemotherapy. Journal of Medicinal Chemistry, 2016, 59, 6595-6628.	6.4	602
63	Macrocyclic Hepatitis C Virus NS3/4A Protease Inhibitors: An Overview of Medicinal Chemistry. Current Medicinal Chemistry, 2016, 23, 3404-3447.	2.4	10
64	Prediction of Compounds in Different Local Structureâ€“Activity Relationship Environments Using Emerging Chemical Patterns. Journal of Chemical Information and Modeling, 2014, 54, 1301-1310.	5.4	6
65	Prediction of Individual Compounds Forming Activity Cliffs Using Emerging Chemical Patterns. Journal of Chemical Information and Modeling, 2013, 53, 3131-3139.	5.4	13
66	Classification of Compounds with Distinct or Overlapping Multi-Target Activities and Diverse Molecular Mechanisms Using Emerging Chemical Patterns. Journal of Chemical Information and Modeling, 2013, 53, 1272-1281.	5.4	20
67	Searching for Coordinated Activity Cliffs Using Particle Swarm Optimization. Journal of Chemical Information and Modeling, 2012, 52, 927-934.	5.4	17
68	Multiobjective Particle Swarm Optimization: Automated Identification of Structureâ€“Activity Relationship-Informative Compounds with Favorable Physicochemical Property Distributions. Journal of Chemical Information and Modeling, 2012, 52, 2848-2855.	5.4	8
69	Exploring SAR Continuity in the Vicinity of Activity Cliffs. Chemical Biology and Drug Design, 2012, 79, 22-29.	3.2	10
70	Extraction of Discontinuous Structureâ€“Activity Relationships from Compound Data Sets through Particle Swarm Optimization. Journal of Chemical Information and Modeling, 2011, 51, 1545-1551.	5.4	4
71	Research Article: <scp>pso</scp>@<scp>autodock</scp>: A Fast Flexible Molecular Docking Program Based on Swarm Intelligence. Chemical Biology and Drug Design, 2007, 70, 475-484.	3.2	105