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	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
2	Skin whitening agents: medicinal chemistry perspective of tyrosinase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 403-425.	5.2	554
3	Inhibitors of Melanogenesis: An Updated Review. Journal of Medicinal Chemistry, 2018, 61, 7395-7418.	6.4	200
4	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
5	Overview of Recent Strategic Advances in Medicinal Chemistry. Journal of Medicinal Chemistry, 2019, 62, 9375-9414.	6.4	108
6	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
7	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
8	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
9	Characterization of P2X4 receptor agonists and antagonists by calcium influx and radioligand binding studies. Biochemical Pharmacology, 2017, 125, 41-54.	4.4	47
10	2,4,6-Substituted Quinazolines with Extraordinary Inhibitory Potency toward ABCG2. Journal of Medicinal Chemistry, 2018, 61, 7952-7976.	6.4	37
11	Agonists and Antagonists for Purinergic Receptors. Methods in Molecular Biology, 2020, 2041, 45-64.	0.9	37
12	The promiscuous ectonucleotidase NPP1: molecular insights into substrate binding and hydrolysis. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 603-614.	2.4	36
13	Substrate-Dependence of Competitive Nucleotide Pyrophosphatase/Phosphodiesterase1 (NPP1) Inhibitors. Frontiers in Pharmacology, 2017, 8, 54.	3.5	36
14	Development of Potent and Selective Antagonists for the UTP-Activated P2Y₄ Receptor. Journal of Medicinal Chemistry, 2017, 60, 3020-3038.	6.4	33
15	Thioesterase-mediated side chain transesterification generates potent Gq signaling inhibitor FR900359. Nature Communications, 2021, 12, 144.	12.8	32
16	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
17	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
18	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

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19	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
20	Role of extracellular cysteine residues in the adenosine A2A receptor. Purinergic Signalling, 2016, 12, 313-329.	2.2	23
21	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
22	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
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	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
25	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
26	Recommended tool compounds and drugs for blocking P2X and P2Y receptors. Purinergic Signalling, 2021, 17, 633-648.	2.2	21
27	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
28	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
29	C@PA: Computer-Aided Pattern Analysis to Predict Multitarget ABC Transporter Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 3350-3366.	6.4	18
30	Searching for Coordinated Activity Cliffs Using Particle Swarm Optimization. Journal of Chemical Information and Modeling, 2012, 52, 927-934.	5.4	17
31	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
32	A_{2B} Adenosine Receptor Antagonists with Picomolar Potency. Journal of Medicinal Chemistry, 2019, 62, 4032-4055.	6.4	17
33	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
34	Cancer cells adapt FAM134B/BiP mediated ER-phagy to survive hypoxic stress. Cell Death and Disease, 2022, 13, 357.	6.3	15
35	Design, Synthesis, and Characterization of Some Hybridized Pyrazolone Pharmacophore Analogs against Mycobacterium tuberculosis. Archiv Der Pharmazie, 2016, 349, 383-397.	4.1	14
36	Prediction of Individual Compounds Forming Activity Cliffs Using Emerging Chemical Patterns. Journal of Chemical Information and Modeling, 2013, 53, 3131-3139.	5.4	13

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37	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
38	Computational Investigations on the Binding Mode of Ligands for the Cannabinoid-Activated G Protein-Coupled Receptor GPR18. Biomolecules, 2020, 10, 686.	4.0	13
39	Structural feature-driven pattern analysis for multitarget modulator landscapes. Bioinformatics, 2022, 38, 1385-1392.	4.1	13
40	Development of a selective and highly sensitive fluorescence assay for nucleoside triphosphate diphosphohydrolase1 (NTPDase1, CD39). Analyst, The, 2018, 143, 5417-5430.	3.5	12
41	Medicinal Chemistry of A2B Adenosine Receptors. , 2018, , 137-168.		12
42	P2Y₁â€like nucleotide receptorsâ€”Structures, molecular modeling, mutagenesis, and oligomerization. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1464.	14.6	12
43	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
44	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
45	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
46	Chemistry and Analysis of Organic Compounds in Dinosaurs. Biology, 2022, 11, 670.	2.8	11
47	Exploring SAR Continuity in the Vicinity of Activity Cliffs. Chemical Biology and Drug Design, 2012, 79, 22-29.	3.2	10
48	Integrative approaches in HIV â€1 nonâ€nucleoside reverse transcriptase inhibitor design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1328.	14.6	10
49	Unraveling binding mechanism and kinetics of macrocyclic Gî±q protein inhibitors. Pharmacological Research, 2021, 173, 105880.	7.1	10
50	Macrocyclic Hepatitis C Virus NS3/4A Protease Inhibitors: An Overview of Medicinal Chemistry. Current Medicinal Chemistry, 2016, 23, 3404-3447.	2.4	10
51	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
52	Interaction of Approved Drugs with Synaptic Vesicle Protein 2A. Archiv Der Pharmazie, 2017, 350, 1700003.	4.1	9
53	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
54	Strategies to gain novel Alzheimer's disease diagnostics and therapeutics using modulators of ABCA transporters.. Free Neuropathology, 2021, 2, .	3.0	9

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55	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
56	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
57	An Overview of Spike Surface Glycoprotein in Severe Acute Respiratory Syndromeâ€“Coronavirus. Frontiers in Molecular Biosciences, 2021, 8, 637550.	3.5	8
58	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
59	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
60	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
61	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
62	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
63	Discovery of P2Y₂ Receptor Antagonist Scaffolds through Virtual High-Throughput Screening. Journal of Chemical Information and Modeling, 2022, 62, 1538-1549.	5.4	6
64	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
65	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
66	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
67	2â€Substituted thienotetrahydropyridine derivatives: Allosteric ectonucleotidase inhibitors. Archiv Der Pharmazie, 2021, 354, e2100300.	4.1	4
68	Die Hauptprotease von SARSâ€CoVâ€2 als Zielstruktur: Von der Etablierung eines Hochdurchsatzâ€Screenings zum Design maÃŸgeschneiderter Inhibitoren. Angewandte Chemie, 2021, 133, 10515-10521.	2.0	3
69	Repurposing drugs targeting epidemic viruses. Drug Discovery Today, 2022, , .	6.4	3
70	Cover Image, Volume 8, Issue 1. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1356.	14.6	0
71	Design and synthesis of sulfonamidophenylethylamides as novel cardiac myosin activator. Bioorganic and Medicinal Chemistry, 2019, 27, 4110-4123.	3.0	0