Shengyong Yang

List of Publications by Year
in descending order

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		159585	102487
103	5,090	30	66
papers	citations	h-index	g-index

105	105	105	7403
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Targeting epigenetic regulators for cancer therapy: mechanisms and advances in clinical trials. Signal Transduction and Targeted Therapy, 2019, 4, 62.	17.1	618
2	Small molecules in targeted cancer therapy: advances, challenges, and future perspectives. Signal Transduction and Targeted Therapy, 2021, 6, 201.	17.1	607
3	Concepts of Artificial Intelligence for Computer-Assisted Drug Discovery. Chemical Reviews, 2019, 119, 10520-10594.	47.7	499
4	Dopamine-loaded blood exosomes targeted to brain for better treatment of Parkinson's disease. Journal of Controlled Release, 2018, 287, 156-166.	9.9	329
5	SARS-CoV-2 M ^{pro} inhibitors with antiviral activity in a transgenic mouse model. Science, 2021, 371, 1374-1378.	12.6	324
6	Cationic nanocarriers induce cell necrosis through impairment of Na+/K+-ATPase and cause subsequent inflammatory response. Cell Research, 2015, 25, 237-253.	12.0	218
7	Discovery of a small molecule targeting ULK1-modulated cell death of triple negative breast cancer in vitro and in vivo. Chemical Science, 2017, 8, 2687-2701.	7.4	120
8	Ligand recognition and allosteric regulation of DRD1-Gs signaling complexes. Cell, 2021, 184, 943-956.e18.	28.9	94
9	From Monoâ€Triazolium Salt to Bisâ€Triazolium Salt: Improvement of the Asymmetric Intermolecular Benzoin Condensation. Advanced Synthesis and Catalysis, 2008, 350, 2645-2651.	4.3	86
10	Site-Divergent Delivery of Terminal Propargyls to Carbohydrates by Synergistic Catalysis. CheM, 2017, 3, 834-845.	11.7	83
11	Ni-Catalyzed Suzukiâ€“Miyaura Cross-Coupling of Î±-Oxo-vinylsulfones To Prepare C-Aryl Glycals and Acyclic Vinyl Ethers. Journal of the American Chemical Society, 2019, 141, 7680-7686.	13.7	80
12	Crystal structure of SARS-CoV-2 nsp10/nsp16 2â€²-O-methylase and its implication on antiviral drug design. Signal Transduction and Targeted Therapy, 2020, 5, 131.	17.1	72
13	Discovery of N1-(4-((7-Cyclopentyl-6-(dimethylcarbamoyl)-7H-pyrrolo[2,3-d]pyrimidin-2-yl)amino)phenyl)-N8-hydroxyoct as a Novel Inhibitor Targeting Cyclin-dependent Kinase 4/9 (CDK4/9) and Histone Deacetlyase1 (HDAC1) against Malignant Cancer. Journal of Medicinal Chemistry, 2018, 61, 3166-3192.	6.4	63
14	An orally available Mpro inhibitor is effective against wild-type SARS-CoV-2 and variants including Omicron. Nature Microbiology, 2022, 7, 716-725.	13.3	62
15	Progress of small molecular inhibitors in the development of anti-influenza virus agents. Theranostics, 2017, 7, 826-845.	10.0	61
16	Porphyrins with intense absorptivity: highly efficient sensitizers with a photovoltaic efficiency of up to 10.7% without a cosensitizer and a coabsorbate. Journal of Materials Chemistry A, 2016, 4, 11829-11834.	10.3	56
17	Targeting Pin1 by inhibitor APIâ€1 regulates microRNA biogenesis and suppresses hepatocellular carcinoma development. Hepatology, 2018, 68, 547-560.	7.3	55
18	Structures of signaling complexes of lipid receptors S1PR1 and S1PR5 reveal mechanisms of activation and drug recognition. Cell Research, 2021, 31, 1263-1274.	12.0	51

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19	Structural and functional insights into the regulation of the lysisâ€“lysogeny decision in viral communities. Nature Microbiology, 2018, 3, 1285-1294.	13.3	49
20	Structural Analysis of Rabies Virus Glycoprotein Reveals pH-Dependent Conformational Changes and Interactions with a Neutralizing Antibody. Cell Host and Microbe, 2020, 27, 441-453.e7.	11.0	49
21	Novel hybrid molecule overcomes the limited response of solid tumours to HDAC inhibitors via suppressing JAK1-STAT3-BCL2 signalling. Theranostics, 2018, 8, 4995-5011.	10.0	48
22	KMT2C deficiency promotes small cell lung cancer metastasis through DNMT3A-mediated epigenetic reprogramming. Nature Cancer, 2022, 3, 753-767.	13.2	41
23	Discovery of Potent and Selective Inhibitors of Cdc2-Like Kinase 1 (CLK1) as a New Class of Autophagy Inducers. Journal of Medicinal Chemistry, 2017, 60, 6337-6352.	6.4	40
24	Liposomal honokiol induced lysosomal degradation of Hsp90 client proteins and protective autophagy in both gefitinib-sensitive and gefitinib-resistant NSCLC cells. Biomaterials, 2017, 141, 188-198.	11.4	39
25	Jumonji domain-containing 6 (JMJD6) identified as a potential therapeutic target in ovarian cancer. Signal Transduction and Targeted Therapy, 2019, 4, 24.	17.1	39
26	Molecular mechanism of allosteric modulation for the cannabinoid receptor CB1. Nature Chemical Biology, 2022, 18, 831-840.	8.0	38
27	Discovery of a highly selective JAK3 inhibitor for the treatment of rheumatoid arthritis. Scientific Reports, 2018, 8, 5273.	3.3	36
28	ZY0511, a novel, potent and selective LSD1 inhibitor, exhibits anticancer activity against solid tumors via the DDIT4/mTOR pathway. Cancer Letters, 2019, 454, 179-190.	7.2	35
29	TIFA suppresses hepatocellular carcinoma progression via MALT1-dependent and -independent signaling pathways. Signal Transduction and Targeted Therapy, 2016, 1, 16013.	17.1	34
30	Novel cyclin-dependent kinase 9 (CDK9) inhibitor with suppression of cancer stemness activity against non-small-cell lung cancer. European Journal of Medicinal Chemistry, 2019, 181, 111535.	5.5	34
31	Discovery of a Teraryl Oxazolidinone Compound (S)-N-((3-(3-Fluoro-4-(4-(pyridin-2-yl)-1H-pyrazol-1-yl)phenyl)-2-oxooxazolidin-5-yl)methyl)acetamide Phosphate as a Novel Antimicrobial Agent with Enhanced Safety Profile and Efficacies. Journal of Medicinal Chemistry, 2015, 58, 6389-6409.	6.4	33
32	Discovery of New SIRT2 Inhibitors by Utilizing a Consensus Docking/Scoring Strategy and Structureâ€“Activity Relationship Analysis. Journal of Chemical Information and Modeling, 2017, 57, 669-679.	5.4	33
33	Identification of 5-(2,3-Dihydro-1H-indol-5-yl)-7H-pyrrolo[2,3-d]pyrimidin-4-amine Derivatives as a New Class of Receptor-Interacting Protein Kinase 1 (RIPK1) Inhibitors, Which Showed Potent Activity in a Tumor Metastasis Model. Journal of Medicinal Chemistry, 2018, 61, 11398-11414.	6.4	33
34	Structure-activity relationship studies of phenothiazine derivatives as a new class of ferroptosis inhibitors together with the therapeutic effect in an ischemic stroke model. European Journal of Medicinal Chemistry, 2021, 209, 112842.	5.5	33
35	Design, synthesis, and biological evaluation of polo-like kinase 1/eukaryotic elongation factor 2 kinase (PLK1/EEF2K) dual inhibitors for regulating breast cancer cells apoptosis and autophagy. European Journal of Medicinal Chemistry, 2018, 144, 517-528.	5.5	31
36	Discovery of Novel Dual Histone Deacetylase and Mammalian Target of Rapamycin Target Inhibitors as a Promising Strategy for Cancer Therapy. Journal of Medicinal Chemistry, 2019, 62, 1577-1592.	6.4	31

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37	Jumonji domainâ€containing protein 6 protein and its role in cancer. Cell Proliferation, 2020, 53, e12747.	5.3	31
38	Capsule Networks Showed Excellent Performance in the Classification of hERG Blockers/Nonblockers. Frontiers in Pharmacology, 2019, 10, 1631.	3.5	31
39	Cul4 E3 ubiquitin ligase regulates ovarian cancer drug resistance by targeting the antiapoptotic protein BIRC3. Cell Death and Disease, 2019, 10, 104.	6.3	30
40	SKLB060 Reversibly Binds to Colchicine Site of Tubulin and Possesses Efficacy in Multidrug-Resistant Cell Lines. Cellular Physiology and Biochemistry, 2018, 47, 489-504.	1.6	29
41	Arginine Methyltransferase 1 in the Nucleus Accumbens Regulates Behavioral Effects of Cocaine. Journal of Neuroscience, 2015, 35, 12890-12902.	3.6	28
42	IFPTarget: A Customized Virtual Target Identification Method Based on Proteinâ€“Ligand Interaction Fingerprinting Analyses. Journal of Chemical Information and Modeling, 2017, 57, 1640-1651.	5.4	28
43	ICAM3 mediates inflammatory signaling to promote cancer cell stemness. Cancer Letters, 2018, 422, 29-43.	7.2	28
44	Identification of Pyrrolo[2,3-d]pyrimidine-Based Derivatives as Potent and Orally Effective Fms-like Tyrosine Receptor Kinase 3 (FLT3) Inhibitors for Treating Acute Myelogenous Leukemia. Journal of Medicinal Chemistry, 2019, 62, 4158-4173.	6.4	28
45	Malignant Pleural Effusion and ascites Induce Epithelial-Mesenchymal Transition and Cancer Stem-like Cell Properties via the Vascular Endothelial Growth Factor (VEGF)/Phosphatidylinositol 3-Kinase (PI3K)/Akt/Mechanistic Target of Rapamycin (mTOR) Pathway. Journal of Biological Chemistry, 2016, 291, 26750-26761.	3.4	26
46	Metal-Free Aerobic Oxidative Selective Câ€“C Bond Cleavage in Heteroaryl-Containing Primary and Secondary Alcohols. Organic Letters, 2019, 21, 3028-3033.	4.6	26
47	Discovery of a highly potent, selective and novel CDK9 inhibitor as an anticancer drug candidate. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3231-3237.	2.2	25
48	Structural insights into sphingosine-1-phosphate recognition and ligand selectivity of S1PR3â€“Gi signaling complexes. Cell Research, 2022, 32, 218-221.	12.0	25
49	Structure of the human gonadotropin-releasing hormone receptor GnRH1R reveals an unusual ligand binding mode. Nature Communications, 2020, 11, 5287.	12.8	24
50	Overexpression of Oct4 suppresses the metastatic potential of breast cancer cells via Rnd1 downregulation. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2014, 1842, 2087-2095.	3.8	23
51	Discovery of Potent Small-Molecule SIRT6 Activators: Structureâ€“Activity Relationship and Anti-Pancreatic Ductal Adenocarcinoma Activity. Journal of Medicinal Chemistry, 2020, 63, 10474-10495.	6.4	22
52	Discovery and structure-activity relationship studies of 1-aryl-1H-naphtho[2,3-d][1,2,3]triazole-4,9-dione derivatives as potent dual inhibitors of indoleamine 2,3-dioxygenase 1 (IDO1) and trytophan 2,3-dioxygenase (TDO). European Journal of Medicinal Chemistry, 2020, 207, 112703.	5.5	22
53	Loss of PRMT7 reprograms glycine metabolism to selectively eradicate leukemia stem cells in CML. Cell Metabolism, 2022, 34, 818-835.e7.	16.2	22
54	Tmem30a Plays Critical Roles in Ensuring the Survival of Hematopoietic Cells and Leukemia Cells in Mice. American Journal of Pathology, 2018, 188, 1457-1468.	3.8	20

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55	The bromodomain protein BRD4 positively regulates necroptosis via modulating MLKL expression. Cell Death and Differentiation, 2019, 26, 1929-1941.	11.2	20
56	Synergistic antitumor effect of 5-fluorouracil with the novel LSD1 inhibitor ZY0511 in colorectal cancer. Therapeutic Advances in Medical Oncology, 2020, 12, 175883592093742.	3.2	20
57	Structureâ€Guided Discovery of a Potent and Selective Cellâ€Active Inhibitor of SETDB1 Tudor Domain. Angewandte Chemie - International Edition, 2021, 60, 8760-8765.	13.8	20
58	SKLB-23bb, A HDAC6-Selective Inhibitor, Exhibits Superior and Broad-Spectrum Antitumor Activity via Additionally Targeting Microtubules. Molecular Cancer Therapeutics, 2018, 17, 763-775.	4.1	19
59	Novel dual inhibitors targeting CDK4 and VEGFR2 synergistically suppressed cancer progression and angiogenesis. European Journal of Medicinal Chemistry, 2019, 181, 111541.	5.5	19
60	Novel CDKs inhibitors for the treatment of solid tumour by simultaneously regulating the cell cycle and transcription control. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 414-423.	5.2	19
61	Discovery of a novel and potent inhibitor with differential species-specific effects against NLRP3 and AIM2 inflammasome-dependent pyroptosis. European Journal of Medicinal Chemistry, 2022, 232, 114194.	5.5	19
62	Structural Optimization and Structureâ€“Activity Relationship Studies of 6,6-Dimethyl-4-(phenylamino)-6H-pyrimido[5,4-b][1,4]oxazin-7(8H)-one Derivatives as A New Class of Potent Inhibitors of Pan-Trk and Their Drug-Resistant Mutants. Journal of Medicinal Chemistry, 2022, 65, 2035-2058.	6.4	18
63	Highly Selective, Potent, and Oral mTOR Inhibitor for Treatment of Cancer as Autophagy Inducer. Journal of Medicinal Chemistry, 2018, 61, 881-904.	6.4	17
64	Synthesis and biological evaluation of novel naphthalene compounds as potential antidepressant agents. European Journal of Medicinal Chemistry, 2014, 82, 263-273.	5.5	16
65	An epigenetic mechanism underlying chromosome 17p deletion-driven tumorigenesis. Cancer Discovery, 2020, 11, CD-20-0336.	9.4	15
66	Discovery of a potent, selective and cell active inhibitor of m6A demethylase ALKBH5. European Journal of Medicinal Chemistry, 2022, 238, 114446.	5.5	15
67	Antimicrobial peptide DP7 with potential activity against SARS coronavirus infections. Signal Transduction and Targeted Therapy, 2021, 6, 140.	17.1	14
68	SKLB188 inhibits the growth of head and neck squamous cell carcinoma by suppressing EGFR signalling. British Journal of Cancer, 2017, 117, 1154-1163.	6.4	13
69	Identification of triazolopyridine derivatives as a new class of AhR agonists and evaluation of anti-psoriasis effect in a mouse model. European Journal of Medicinal Chemistry, 2022, 231, 114122.	5.5	12
70	Deciphering the regulatory and catalytic mechanisms of an unusual SAM-dependent enzyme. Signal Transduction and Targeted Therapy, 2019, 4, 17.	17.1	11
71	Discovery of Pyrrolo[3,2-d]pyrimidin-4-one Derivatives as a New Class of Potent and Cell-Active Inhibitors of P300/CBP-Associated Factor Bromodomain. Journal of Medicinal Chemistry, 2019, 62, 4526-4542.	6.4	11
72	Preclinical pharmacodynamic evaluation of a new Src/<scp>FOSL</scp>1 inhibitor, <scp>LY</scp>â€1816, in pancreatic ductal adenocarcinoma. Cancer Science, 2019, 110, 1408-1419.	3.9	11

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73	Structural and Functional Insights into an Archaeal Lipid Synthase. Cell Reports, 2020, 33, 108294.	6.4	11
74	Discovery of 5-(4-methylpiperazin-1-yl)-2-nitroaniline derivatives as a new class of SIRT6 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127215.	2.2	10
75	Discovery of a new class of JMJD6 inhibitors and structureâ€“activity relationship study. Bioorganic and Medicinal Chemistry Letters, 2021, 44, 128109.	2.2	10
76	Discovery of 3,4-Dihydrobenzo[f][1,4]oxazepin-5(2H)-one Derivatives as a New Class of Selective TNIK Inhibitors and Evaluation of Their Anti-Colorectal Cancer Effects. Journal of Medicinal Chemistry, 2022, 65, 1786-1807.	6.4	10
77	Design and optimization of orally spleen tyrosine kinase (SYK) inhibitors for treatment of solid tumor. Bioorganic Chemistry, 2020, 95, 103547.	4.1	9
78	Discovery of 4H-Chromen-4-one Derivatives as a New Class of Selective Rho Kinase (ROCK) Inhibitors, which Showed Potent Activity in ex Vivo Diabetic Retinopathy Models. Journal of Medicinal Chemistry, 2019, 62, 10691-10710.	6.4	8
79	Enhancement of Histone Deacetylase Inhibitor Sensitivity in Combination with Cyclin-Dependent Kinase Inhibition for the Treatment of Oral Squamous Cell Carcinoma. Cellular Physiology and Biochemistry, 2019, 53, 141-156.	1.6	8
80	Studies of Interaction between Ergostaâ€4,6,8(14),22â€tetraenâ€3â€one (Ergone) and Human Serum Albumin by Molecular Spectroscopy and Modeling. Journal of the Chinese Chemical Society, 2011, 58, 602-610.	1.4	7
81	A highly potent and selective inhibitor Roxyl-WL targeting IDO1 promotes immune response against melanoma. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 1089-1094.	5.2	7
82	Transition-Metal-Catalyzed Transformation of Sulfonates via Sâ€“O Bond Cleavage: Synthesis of Alkyl Aryl Ether and Diaryl Ether. Organic Letters, 2019, 21, 8879-8883.	4.6	7
83	Novel mitochondria-targeted and fluorescent DNA alkylation agents with highly selective activity against cancer cells. Dyes and Pigments, 2019, 170, 107610.	3.7	7
84	Discovery of 5-(5-fluoro-1H-pyrrolo[2,3-b]pyridin-3-yl)pyrazin-2(1H)-one derivatives as new potent PB2 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 1609-1613.	2.2	7
85	Multispecific drugs: the fourth wave of biopharmaceutical innovation. Signal Transduction and Targeted Therapy, 2020, 5, 86.	17.1	7
86	Discovery of a potent and selective inhibitor of histone lysine demethylase KDM4D. European Journal of Medicinal Chemistry, 2021, 223, 113662.	5.5	7
87	The novel LSD1 inhibitor ZY0511 suppresses diffuse large B-cell lymphoma proliferation by inducing apoptosis and autophagy. Medical Oncology, 2021, 38, 124.	2.5	6
88	Discovery of a potent and highly selective inhibitor of ataxia telangiectasia mutated and Rad3-Related (ATR) kinase: Structural activity relationship and antitumor activity both inÂvitro and inÂvivo. European Journal of Medicinal Chemistry, 2022, 232, 114187.	5.5	6
89	A small molecular agent YL529 inhibits VEGF-D-induced lymphangiogenesis and metastasis in preclinical tumor models in addition to its known antitumor activities. BMC Cancer, 2015, 15, 525.	2.6	5
90	Discovery of 1,8-disubstituted-[1,2,3]triazolo[4,5-c]quinoline derivatives as a new class of Hippo signaling pathway inhibitors. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 2595-2603.	2.2	5

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91	Discovery of selective BPTF bromodomain inhibitors by screening and structure-based optimization. Biochemical and Biophysical Research Communications, 2021, 545, 125-131.	2.1	5
92	Selective and novel cyclin-dependent kinases 4 inhibitor: synthesis and biological evaluation. Medicinal Chemistry Research, 2018, 27, 1666-1678.	2.4	4
93	Dihydroartemisinin Inhibits mTORC1 Signaling by Activating the AMPK Pathway in Rhabdomyosarcoma Tumor Cells. Cells, 2021, 10, 1363.	4.1	4
94	Preclinical pharmacodynamic evaluation of drug candidate SKLB-178 in the treatment of non-small cell lung cancer. Oncotarget, 2017, 8, 12843-12854.	1.8	4
95	Discovery and structural optimization of potent epidermal growth factor receptor (EGFR) inhibitors against L858R/T790M/C797S resistance mutation for lung cancer treatment. European Journal of Medicinal Chemistry, 2022, 237, 114381.	5.5	4
96	Discovery of human TyrRS inhibitors by structure-based virtual screening, structural optimization, and bioassays. RSC Advances, 2019, 9, 9323-9330.	3.6	3
97	Role of Water in the Reaction Mechanism and endo / exo Selectivity of 1,3â€Dipolar Cycloadditions Elucidated by Quantum Chemistry and Machine Learning. Chemistry - A European Journal, 2019, 25, 8289-8303.	3.3	3
98	Discovery of 12Oâ€”A Novel Oral Multi-Kinase Inhibitor for the Treatment of Solid Tumor. Molecules, 2020, 25, 5199.	3.8	3
99	Targeting glutaminase1 and synergizing with clinical drugs achieved more promising antitumor activity on multiple myeloma. Oncotarget, 2019, 10, 5993-6005.	1.8	3
100	Discovery of benzo[d]oxazol-2(3H)-one derivatives as a new class of TNIK inhibitors for the treatment of colorectal cancer. Bioorganic and Medicinal Chemistry Letters, 2022, 67, 128745.	2.2	3
101	Lipidomic profiling reveals lipid regulation by a novel LSD1 inhibitor treatment. Oncology Reports, 2021, 46, .	2.6	2
102	Structureâ€Guided Discovery of a Potent and Selective Cellâ€Active Inhibitor of SETDB1 Tudor Domain. Angewandte Chemie, 2021, 133, 8842-8847.	2.0	1
103	Discovery of small molecule FLT3 inhibitors that are able to overcome drug-resistant mutations. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127532.	2.2	0