Shengyong Yang

List of Publications by Citations

99 papers	2,412 citations	23 h-index	46 g-index
105 ext. papers	3,672 ext. citations	10.7 avg, IF	5.27 L-index

#	Paper	IF	Citations
99	Targeting epigenetic regulators for cancer therapy: mechanisms and advances in clinical trials. *Signal Transduction and Targeted Therapy*, **2019**, 4, 62	21	284
98	Concepts of Artificial Intelligence for Computer-Assisted Drug Discovery. *Chemical Reviews*, **2019**, 119, 10520-10594	68.1	243
97	Dopamine-loaded blood exosomes targeted to brain for better treatment of Parkinson's disease. *Journal of Controlled Release*, **2018**, 287, 156-166	11.7	168
96	Cationic nanocarriers induce cell necrosis through impairment of Na(+)/K(+)-ATPase and cause subsequent inflammatory response. *Cell Research*, **2015**, 25, 237-53	24.7	162
95	SARS-CoV-2 M inhibitors with antiviral activity in a transgenic mouse model. *Science*, **2021**, 371, 1374-1378	33.3	124
94	Small molecules in targeted cancer therapy: advances, challenges, and future perspectives. *Signal Transduction and Targeted Therapy*, **2021**, 6, 201	21	103
93	Discovery of a small molecule targeting ULK1-modulated cell death of triple negative breast cancer and. *Chemical Science*, **2017**, 8, 2687-2701	9.4	78
92	From Mono-Triazolium Salt to Bis-Triazolium Salt: Improvement of the Asymmetric Intermolecular Benzoin Condensation. *Advanced Synthesis and Catalysis*, **2008**, 350, 2645-2651	5.6	78
91	Site-Divergent Delivery of Terminal Propargyls to Carbohydrates by Synergistic Catalysis. *CheM*, **2017**, 3, 834-845	16.2	56
90	Discovery of N1-(4-((7-Cyclopentyl-6-(dimethylcarbamoyl)-7 H-pyrrolo[2,3-d]pyrimidin-2-yl)amino)phenyl)- N8-hydroxyoctanediamide 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	8.3	48
89	Crystal structure of SARS-CoV-2 nsp10/nsp16 2'-O-methylase and its implication on antiviral drug design. *Signal Transduction and Targeted Therapy*, **2020**, 5, 131	21	46
88	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	12	45
87	Progress of small molecular inhibitors in the development of anti-influenza virus agents. *Theranostics*, **2017**, 7, 826-845	12.1	41
86	Targeting Pin1 by inhibitor API-1 regulates microRNA biogenesis and suppresses hepatocellular carcinoma development. *Hepatology*, **2018**, 68, 547-560	11.2	41
85	Ni-Catalyzed Suzuki-Miyaura Cross-Coupling of β-Oxo-vinylsulfones To Prepare C-Aryl Glycals and Acyclic Vinyl Ethers. *Journal of the American Chemical Society*, **2019**, 141, 7680-7686	16.4	40
84	Novel hybrid molecule overcomes the limited response of solid tumours to HDAC inhibitors via suppressing JAK1-STAT3-BCL2 signalling. *Theranostics*, **2018**, 8, 4995-5011	12.1	32
83	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	15.6	30

82	Structural and functional insights into the regulation of the lysis-lysogeny decision in viral communities. *Nature Microbiology*, **2018**, 3, 1285-1294	26.6	30
81	Discovery of New SIRT2 Inhibitors by Utilizing a Consensus Docking/Scoring Strategy and Structure-Activity Relationship Analysis. *Journal of Chemical Information and Modeling*, **2017**, 57, 669-679	6.1	27
80	TIFA suppresses hepatocellular carcinoma progression via MALT1-dependent and -independent signaling pathways. *Signal Transduction and Targeted Therapy*, **2016**, 1, 16013	21	26
79	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	8.3	26
78	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	8.3	24
77	Ligand recognition and allosteric regulation of DRD1-Gs signaling complexes. *Cell*, **2021**, 184, 943-956.e18	36.2	24
76	Discovery of a highly selective JAK3 inhibitor for the treatment of rheumatoid arthritis. *Scientific Reports*, **2018**, 8, 5273	4.9	23
75	IFPTarget: A Customized Virtual Target Identification Method Based on Protein-Ligand Interaction Fingerprinting Analyses. *Journal of Chemical Information and Modeling*, **2017**, 57, 1640-1651	6.1	23
74	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	6.8	23
73	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	9.9	21
72	Arginine Methyltransferase 1 in the Nucleus Accumbens Regulates Behavioral Effects of Cocaine. *Journal of Neuroscience*, **2015**, 35, 12890-902	6.6	21
71	Overexpression of Oct4 suppresses the metastatic potential of breast cancer cells via Rnd1 downregulation. *Biochimica Et Biophysica Acta - Molecular Basis of Disease*, **2014**, 1842, 2087-95	6.9	21
70	Identification of 5-(2,3-Dihydro-1 H-indol-5-yl)-7 H-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	8.3	21
69	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, 6389-409	8.3	20
68	Jumonji domain-containing 6 (JMJD6) identified as a potential therapeutic target in ovarian cancer. *Signal Transduction and Targeted Therapy*, **2019**, 4, 24	21	20
67	SKLB060 Reversibly Binds to Colchicine Site of Tubulin and Possesses Efficacy in Multidrug-Resistant Cell Lines. *Cellular Physiology and Biochemistry*, **2018**, 47, 489-504	3.9	19
66	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	23.4	18
65	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	5.4	18

64	Metal-Free Aerobic Oxidative Selective C-C Bond Cleavage in Heteroaryl-Containing Primary and Secondary Alcohols. *Organic Letters*, **2019**, 21, 3028-3033	6.2	17
63	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	8.3	17
62	Discovery of a highly potent, selective and novel CDK9 inhibitor as an anticancer drug candidate. *Bioorganic and Medicinal Chemistry Letters*, **2017**, 27, 3231-3237	2.9	16
61	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	6.8	16
60	Jumonji domain-containing protein 6 protein and its role in cancer. *Cell Proliferation*, **2020**, 53, e12747	7.9	15
59	SKLB-23bb, A HDAC6-Selective Inhibitor, Exhibits Superior and Broad-Spectrum Antitumor Activity via Additionally Targeting Microtubules. *Molecular Cancer Therapeutics*, **2018**, 17, 763-775	6.1	15
58	ICAM3 mediates inflammatory signaling to promote cancer cell stemness. *Cancer Letters*, **2018**, 422, 29-43	9.9	14
57	Cul4 E3 ubiquitin ligase regulates ovarian cancer drug resistance by targeting the antiapoptotic protein BIRC3. *Cell Death and Disease*, **2019**, 10, 104	9.8	13
56	Highly Selective, Potent, and Oral mTOR Inhibitor for Treatment of Cancer as Autophagy Inducer. *Journal of Medicinal Chemistry*, **2018**, 61, 881-904	8.3	13
55	Synthesis and biological evaluation of novel naphthalene compounds as potential antidepressant agents. *European Journal of Medicinal Chemistry*, **2014**, 82, 263-73	6.8	13
54	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	6.8	13
53	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	5.6	12
52	Tmem30a Plays Critical Roles in Ensuring the Survival of Hematopoietic Cells and Leukemia Cells in Mice. *American Journal of Pathology*, **2018**, 188, 1457-1468	5.8	11
51	The bromodomain protein BRD4 positively regulates necroptosis via modulating MLKL expression. *Cell Death and Differentiation*, **2019**, 26, 1929-1941	12.7	11
50	Capsule Networks Showed Excellent Performance in the Classification of hERG Blockers/Nonblockers. *Frontiers in Pharmacology*, **2019**, 10, 1631	5.6	10
49	Novel dual inhibitors targeting CDK4 and VEGFR2 synergistically suppressed cancer progression and angiogenesis. *European Journal of Medicinal Chemistry*, **2019**, 181, 111541	6.8	10
48	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	6.8	9
47	Structures of signaling complexes of lipid receptors S1PR1 and S1PR5 reveal mechanisms of activation and drug recognition. *Cell Research*, **2021**, 31, 1263-1274	24.7	9

46	SKLB188 inhibits the growth of head and neck squamous cell carcinoma by suppressing EGFR signalling. *British Journal of Cancer*, **2017**, 117, 1154-1163	8.7	8
45	Synergistic antitumor effect of 5-fluorouracil with the novel LSD1 inhibitor ZY0511 in colorectal cancer. *Therapeutic Advances in Medical Oncology*, **2020**, 12, 1758835920937428	5.4	8
44	An Epigenetic Mechanism Underlying Chromosome 17p Deletion-Driven Tumorigenesis. *Cancer Discovery*, **2021**, 11, 194-207	24.4	8
43	Deciphering the regulatory and catalytic mechanisms of an unusual SAM-dependent enzyme. *Signal Transduction and Targeted Therapy*, **2019**, 4, 17	21	6
42	Preclinical pharmacodynamic evaluation of a new Src/FOSL1 inhibitor, LY-1816, in pancreatic ductal adenocarcinoma. *Cancer Science*, **2019**, 110, 1408-1419	6.9	6
41	Transition-Metal-Catalyzed Transformation of Sulfonates via S-O Bond Cleavage: Synthesis of Alkyl Aryl Ether and Diaryl Ether. *Organic Letters*, **2019**, 21, 8879-8883	6.2	6
40	Studies of Interaction between Ergosta-4,6,8(14),22-tetraen-3-one (Ergone) and Human Serum Albumin by Molecular Spectroscopy and Modeling. *Journal of the Chinese Chemical Society*, **2011**, 58, 602-610	1.5	6
39	Discovery of Potent Small-Molecule SIRT6 Activators: Structure-Activity Relationship and Anti-Pancreatic Ductal Adenocarcinoma Activity. *Journal of Medicinal Chemistry*, **2020**, 63, 10474-10495	8.3	6
38	Antimicrobial peptide DP7 with potential activity against SARS coronavirus infections. *Signal Transduction and Targeted Therapy*, **2021**, 6, 140	21	6
37	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	8.3	5
36	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	5.6	5
35	Discovery of 4-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	8.3	5
34	Structural insights into sphingosine-1-phosphate recognition and ligand selectivity of S1PR3-Gi signaling complexes. *Cell Research*, **2021**,	24.7	5
33	An orally available M inhibitor is effective against wild-type SARS-CoV-2 and variants including Omicron.. *Nature Microbiology*, **2022**, 7, 716-725	26.6	5
32	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	4.8	4
31	Structure-Guided Discovery of a Potent and Selective Cell-Active Inhibitor of SETDB1 Tudor Domain. *Angewandte Chemie - International Edition*, **2021**, 60, 8760-8765	16.4	4
30	Discovery of a new class of JMJD6 inhibitors and structure-activity relationship study. *Bioorganic and Medicinal Chemistry Letters*, **2021**, 44, 128109	2.9	4
29	Novel mitochondria-targeted and fluorescent DNA alkylation agents with highly selective activity against cancer cells. *Dyes and Pigments*, **2019**, 170, 107610	4.6	3

28	Discovery of human TyrRS inhibitors by structure-based virtual screening, structural optimization, and bioassays.. *RSC Advances*, **2019**, 9, 9323-9330	3.7	3
27	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	2.9	3
26	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	2.9	3
25	Multispecific drugs: the fourth wave of biopharmaceutical innovation. *Signal Transduction and Targeted Therapy*, **2020**, 5, 86	21	3
24	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	2.9	3
23	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	3.9	3
22	Design and optimization of orally spleen tyrosine kinase (SYK) inhibitors for treatment of solid tumor. *Bioorganic Chemistry*, **2020**, 95, 103547	5.1	3
21	Structure of the human gonadotropin-releasing hormone receptor GnRH1R reveals an unusual ligand binding mode. *Nature Communications*, **2020**, 11, 5287	17.4	3
20	Role of Water in the Reaction Mechanism and endo/exo Selectivity of 1,3-Dipolar Cycloadditions Elucidated by Quantum Chemistry and Machine Learning. *Chemistry - A European Journal*, **2019**, 25, 8289-8303	4.8	2
19	Selective and novel cyclin-dependent kinases 4 inhibitor: synthesis and biological evaluation. *Medicinal Chemistry Research*, **2018**, 27, 1666-1678	2.2	2
18	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	6.8	2
17	Structural and Functional Insights into an Archaeal Lipid Synthase. *Cell Reports*, **2020**, 33, 108294	10.6	2
16	Discovery of 12O-A Novel Oral Multi-Kinase Inhibitor for the Treatment of Solid Tumor. *Molecules*, **2020**, 25,	4.8	2
15	Discovery of selective BPTF bromodomain inhibitors by screening and structure-based optimization. *Biochemical and Biophysical Research Communications*, **2021**, 545, 125-131	3.4	2
14	The novel LSD1 inhibitor ZY0511 suppresses diffuse large B-cell lymphoma proliferation by inducing apoptosis and autophagy. *Medical Oncology*, **2021**, 38, 124	3.7	2
13	Discovery of a potent and selective inhibitor of histone lysine demethylase KDM4D. *European Journal of Medicinal Chemistry*, **2021**, 223, 113662	6.8	2
12	KMT2C deficiency promotes small cell lung cancer metastasis through DNMT3A-mediated epigenetic reprogramming.. *Nature Cancer*, **2022**,	15.4	2
11	Discovery of 3,4-Dihydrobenzo[][1,4]oxazepin-5(2)-one Derivatives as a New Class of Selective TNIK Inhibitors and Evaluation of Their Anti-Colorectal Cancer Effects.. *Journal of Medicinal Chemistry*, **2022**,	8.3	1

10	Structural Optimization and Structure-Activity Relationship Studies of 6,6-Dimethyl-4-(phenylamino)-6-pyrimido[5,4-][1,4]oxazin-7(8)-one Derivatives as A New Class of Potent Inhibitors of Pan-Trk and Their Drug-Resistant Mutants.. *Journal of Medicinal Chemistry*, **2022**,	8.3	1
9	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	6.8	1
8	Preclinical pharmacodynamic evaluation of drug candidate SKLB-178 in the treatment of non-small cell lung cancer. *Oncotarget*, **2017**, 8, 12843-12854	3.3	1
7	Targeting glutaminase1 and synergizing with clinical drugs achieved more promising antitumor activity on multiple myeloma. *Oncotarget*, **2019**, 10, 5993-6005	3.3	1
6	Discovery of a potent and highly selective inhibitor of ataxia telangiectasia mutated and Rad3-Related (ATR) kinase: Structural activity relationship and antitumor activity both in‐vitro and in‐vivo.. *European Journal of Medicinal Chemistry*, **2022**, 232, 114187	6.8	0
5	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	2.9	0
4	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	6.8	0
3	Discovery of a potent, selective and cell active inhibitor of m6A demethylase ALKBH5. *European Journal of Medicinal Chemistry*, **2022**, 114446	6.8	0
2	Discovery of small molecule FLT3 inhibitors that are able to overcome drug-resistant mutations. *Bioorganic and Medicinal Chemistry Letters*, **2020**, 30, 127532	2.9	
1	Structure-Guided Discovery of a Potent and Selective Cell-Active Inhibitor of SETDB1 Tudor Domain. *Angewandte Chemie*, **2021**, 133, 8842-8847	3.6	