

# Shengyong Yang

## List of Publications by Year in descending order

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103  
papers

5,090  
citations

159358

30  
h-index

102304

66  
g-index

105  
all docs

105  
docs citations

105  
times ranked

7403  
citing authors

#	ARTICLE	IF	CITATIONS
1	Targeting epigenetic regulators for cancer therapy: mechanisms and advances in clinical trials. <i>Signal Transduction and Targeted Therapy</i> , 2019, 4, 62.	7.1	618
2	Small molecules in targeted cancer therapy: advances, challenges, and future perspectives. <i>Signal Transduction and Targeted Therapy</i> , 2021, 6, 201.	7.1	607
3	Concepts of Artificial Intelligence for Computer-Assisted Drug Discovery. <i>Chemical Reviews</i> , 2019, 119, 10520-10594.	23.0	499
4	Dopamine-loaded blood exosomes targeted to brain for better treatment of Parkinson's disease. <i>Journal of Controlled Release</i> , 2018, 287, 156-166.	4.8	329
5	SARS-CoV-2 M <sup>pro</sup> inhibitors with antiviral activity in a transgenic mouse model. <i>Science</i> , 2021, 371, 1374-1378.	6.0	324
6	Cationic nanocarriers induce cell necrosis through impairment of Na <sup>+</sup> /K <sup>+</sup> -ATPase and cause subsequent inflammatory response. <i>Cell Research</i> , 2015, 25, 237-253.	5.7	218
7	Discovery of a small molecule targeting ULK1-modulated cell death of triple negative breast cancer in vitro and in vivo. <i>Chemical Science</i> , 2017, 8, 2687-2701.	3.7	120
8	Ligand recognition and allosteric regulation of DRD1-Gs signaling complexes. <i>Cell</i> , 2021, 184, 943-956.e18.	13.5	94
9	From Mono- to Bis-Triazolium Salt to Bis-Triazolium Salt: Improvement of the Asymmetric Intermolecular Benzoin Condensation. <i>Advanced Synthesis and Catalysis</i> , 2008, 350, 2645-2651.	2.1	86
10	Site-Divergent Delivery of Terminal Propargyls to Carbohydrates by Synergistic Catalysis. <i>Chem</i> , 2017, 3, 834-845.	5.8	83
11	Ni-Catalyzed Suzuki-Miyaura Cross-Coupling of $\alpha$ -Oxo-vinylsulfones To Prepare $\alpha$ -Aryl Glycals and Acyclic Vinyl Ethers. <i>Journal of the American Chemical Society</i> , 2019, 141, 7680-7686.	6.6	80
12	Crystal structure of SARS-CoV-2 nsp10/nsp16 2'-O-methylase and its implication on antiviral drug design. <i>Signal Transduction and Targeted Therapy</i> , 2020, 5, 131.	7.1	72
13	Discovery of N-(4-((7-Cyclopentyl-6-(dimethylcarbamoyl)-7H-pyrrolo[2,3-d]pyrimidin-2-yl)amino)phenyl)-8-hydroxyoctanamide as a Novel Inhibitor Targeting Cyclin-dependent Kinase 4/9 (CDK4/9) and Histone Deacetylase1 (HDAC1) against Malignant Cancer. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 3166-3192.	2.9	63
14	An orally available Mpro inhibitor is effective against wild-type SARS-CoV-2 and variants including Omicron. <i>Nature Microbiology</i> , 2022, 7, 716-725.	5.9	62
15	Progress of small molecular inhibitors in the development of anti-influenza virus agents. <i>Theranostics</i> , 2017, 7, 826-845.	4.6	61
16	Porphyrins with intense absorptivity: highly efficient sensitizers with a photovoltaic efficiency of up to 10.7% without a cosensitizer and a coabsorbate. <i>Journal of Materials Chemistry A</i> , 2016, 4, 11829-11834.	5.2	56
17	Targeting Pin1 by inhibitor API-1 regulates microRNA biogenesis and suppresses hepatocellular carcinoma development. <i>Hepatology</i> , 2018, 68, 547-560.	3.6	55
18	Structures of signaling complexes of lipid receptors S1PR1 and S1PR5 reveal mechanisms of activation and drug recognition. <i>Cell Research</i> , 2021, 31, 1263-1274.	5.7	51

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19	Structural and functional insights into the regulation of the lysis–lysogeny decision in viral communities. <i>Nature Microbiology</i> , 2018, 3, 1285-1294.	5.9	49
20	Structural Analysis of Rabies Virus Glycoprotein Reveals pH-Dependent Conformational Changes and Interactions with a Neutralizing Antibody. <i>Cell Host and Microbe</i> , 2020, 27, 441-453.e7.	5.1	49
21	Novel hybrid molecule overcomes the limited response of solid tumours to HDAC inhibitors via suppressing JAK1-STAT3-BCL2 signalling. <i>Theranostics</i> , 2018, 8, 4995-5011.	4.6	48
22	KMT2C deficiency promotes small cell lung cancer metastasis through DNMT3A-mediated epigenetic reprogramming. <i>Nature Cancer</i> , 2022, 3, 753-767.	5.7	41
23	Discovery of Potent and Selective Inhibitors of Cdc2-Like Kinase 1 (CLK1) as a New Class of Autophagy Inducers. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 6337-6352.	2.9	40
24	Liposomal honokiol induced lysosomal degradation of Hsp90 client proteins and protective autophagy in both gefitinib-sensitive and gefitinib-resistant NSCLC cells. <i>Biomaterials</i> , 2017, 141, 188-198.	5.7	39
25	Jumonji domain-containing 6 (JMJD6) identified as a potential therapeutic target in ovarian cancer. <i>Signal Transduction and Targeted Therapy</i> , 2019, 4, 24.	7.1	39
26	Molecular mechanism of allosteric modulation for the cannabinoid receptor CB1. <i>Nature Chemical Biology</i> , 2022, 18, 831-840.	3.9	38
27	Discovery of a highly selective JAK3 inhibitor for the treatment of rheumatoid arthritis. <i>Scientific Reports</i> , 2018, 8, 5273.	1.6	36
28	ZY0511, a novel, potent and selective LSD1 inhibitor, exhibits anticancer activity against solid tumors via the DDIT4/mTOR pathway. <i>Cancer Letters</i> , 2019, 454, 179-190.	3.2	35
29	TIFA suppresses hepatocellular carcinoma progression via MALT1-dependent and -independent signaling pathways. <i>Signal Transduction and Targeted Therapy</i> , 2016, 1, 16013.	7.1	34
30	Novel cyclin-dependent kinase 9 (CDK9) inhibitor with suppression of cancer stemness activity against non-small-cell lung cancer. <i>European Journal of Medicinal Chemistry</i> , 2019, 181, 111535.	2.6	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. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 6389-6409.	2.9	33
32	Discovery of New SIRT2 Inhibitors by Utilizing a Consensus Docking/Scoring Strategy and Structure–Activity Relationship Analysis. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 669-679.	2.5	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. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 11398-11414.	2.9	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. <i>European Journal of Medicinal Chemistry</i> , 2021, 209, 112842.	2.6	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. <i>European Journal of Medicinal Chemistry</i> , 2018, 144, 517-528.	2.6	31
36	Discovery of Novel Dual Histone Deacetylase and Mammalian Target of Rapamycin Target Inhibitors as a Promising Strategy for Cancer Therapy. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 1577-1592.	2.9	31

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37	Jumonji domain-containing protein 6 protein and its role in cancer. <i>Cell Proliferation</i> , 2020, 53, e12747.	2.4	31
38	Capsule Networks Showed Excellent Performance in the Classification of hERG Blockers/Nonblockers. <i>Frontiers in Pharmacology</i> , 2019, 10, 1631.	1.6	31
39	Cul4 E3 ubiquitin ligase regulates ovarian cancer drug resistance by targeting the antiapoptotic protein BIRC3. <i>Cell Death and Disease</i> , 2019, 10, 104.	2.7	30
40	SKLB060 Reversibly Binds to Colchicine Site of Tubulin and Possesses Efficacy in Multidrug-Resistant Cell Lines. <i>Cellular Physiology and Biochemistry</i> , 2018, 47, 489-504.	1.1	29
41	Arginine Methyltransferase 1 in the Nucleus Accumbens Regulates Behavioral Effects of Cocaine. <i>Journal of Neuroscience</i> , 2015, 35, 12890-12902.	1.7	28
42	IFPTarget: A Customized Virtual Target Identification Method Based on Protein-Ligand Interaction Fingerprinting Analyses. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1640-1651.	2.5	28
43	ICAM3 mediates inflammatory signaling to promote cancer cell stemness. <i>Cancer Letters</i> , 2018, 422, 29-43.	3.2	28
44	Identification of Pyrrolo[2,3- <i>d</i> ]pyrimidine-Based Derivatives as Potent and Orally Effective Fms-like Tyrosine Receptor Kinase 3 (FLT3) Inhibitors for Treating Acute Myelogenous Leukemia. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 4158-4173.	2.9	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. <i>Journal of Biological Chemistry</i> , 2016, 291, 26750-26761.	1.6	26
46	Metal-Free Aerobic Oxidative Selective C-C Bond Cleavage in Heteroaryl-Containing Primary and Secondary Alcohols. <i>Organic Letters</i> , 2019, 21, 3028-3033.	2.4	26
47	Discovery of a highly potent, selective and novel CDK9 inhibitor as an anticancer drug candidate. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017, 27, 3231-3237.	1.0	25
48	Structural insights into sphingosine-1-phosphate recognition and ligand selectivity of S1PR3-Gi signaling complexes. <i>Cell Research</i> , 2022, 32, 218-221.	5.7	25
49	Structure of the human gonadotropin-releasing hormone receptor GnRH1R reveals an unusual ligand binding mode. <i>Nature Communications</i> , 2020, 11, 5287.	5.8	24
50	Overexpression of Oct4 suppresses the metastatic potential of breast cancer cells via Rnd1 downregulation. <i>Biochimica Et Biophysica Acta - Molecular Basis of Disease</i> , 2014, 1842, 2087-2095.	1.8	23
51	Discovery of Potent Small-Molecule SIRT6 Activators: Structure-Activity Relationship and Anti-Pancreatic Ductal Adenocarcinoma Activity. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 10474-10495.	2.9	22
52	Discovery and structure-activity relationship studies of 1-aryl-1H-naphtho[2,3- <i>d</i> ][1,2,3]triazole-4,9-dione derivatives as potent dual inhibitors of indoleamine 2,3-dioxygenase 1 (IDO1) and tryptophan 2,3-dioxygenase (TDO). <i>European Journal of Medicinal Chemistry</i> , 2020, 207, 112703.	2.6	22
53	Loss of PRMT7 reprograms glycine metabolism to selectively eradicate leukemia stem cells in CML. <i>Cell Metabolism</i> , 2022, 34, 818-835.e7.	7.2	22
54	Tmem30a Plays Critical Roles in Ensuring the Survival of Hematopoietic Cells and Leukemia Cells in Mice. <i>American Journal of Pathology</i> , 2018, 188, 1457-1468.	1.9	20

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55	The bromodomain protein BRD4 positively regulates necroptosis via modulating MLKL expression. <i>Cell Death and Differentiation</i> , 2019, 26, 1929-1941.	5.0	20
56	Synergistic antitumor effect of 5-fluorouracil with the novel LSD1 inhibitor ZY0511 in colorectal cancer. <i>Therapeutic Advances in Medical Oncology</i> , 2020, 12, 175883592093742.	1.4	20
57	Structure-Guided Discovery of a Potent and Selective Cell-Active Inhibitor of SETDB1 Tudor Domain. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 8760-8765.	7.2	20
58	SKLB-23bb, A HDAC6-Selective Inhibitor, Exhibits Superior and Broad-Spectrum Antitumor Activity via Additionally Targeting Microtubules. <i>Molecular Cancer Therapeutics</i> , 2018, 17, 763-775.	1.9	19
59	Novel dual inhibitors targeting CDK4 and VEGFR2 synergistically suppressed cancer progression and angiogenesis. <i>European Journal of Medicinal Chemistry</i> , 2019, 181, 111541.	2.6	19
60	Novel CDKs inhibitors for the treatment of solid tumour by simultaneously regulating the cell cycle and transcription control. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2020, 35, 414-423.	2.5	19
61	Discovery of a novel and potent inhibitor with differential species-specific effects against NLRP3 and AIM2 inflammasome-dependent pyroptosis. <i>European Journal of Medicinal Chemistry</i> , 2022, 232, 114194.	2.6	19
62	Structural Optimization and Structure-Activity Relationship Studies of 6,6-Dimethyl-4-(phenylamino)-6 <i>H</i> -pyrimido[5,4- <i>b</i> ][1,4]oxazin-7(8 <i>H</i> )-one Derivatives as A New Class of Potent Inhibitors of Pan-Trk and Their Drug-Resistant Mutants. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 2035-2058.	2.9	18
63	Highly Selective, Potent, and Oral mTOR Inhibitor for Treatment of Cancer as Autophagy Inducer. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 881-904.	2.9	17
64	Synthesis and biological evaluation of novel naphthalene compounds as potential antidepressant agents. <i>European Journal of Medicinal Chemistry</i> , 2014, 82, 263-273.	2.6	16
65	An epigenetic mechanism underlying chromosome 17p deletion-driven tumorigenesis. <i>Cancer Discovery</i> , 2020, 11, CD-20-0336.	7.7	15
66	Discovery of a potent, selective and cell active inhibitor of m6A demethylase ALKBH5. <i>European Journal of Medicinal Chemistry</i> , 2022, 238, 114446.	2.6	15
67	Antimicrobial peptide DP7 with potential activity against SARS coronavirus infections. <i>Signal Transduction and Targeted Therapy</i> , 2021, 6, 140.	7.1	14
68	SKLB188 inhibits the growth of head and neck squamous cell carcinoma by suppressing EGFR signalling. <i>British Journal of Cancer</i> , 2017, 117, 1154-1163.	2.9	13
69	Identification of triazolopyridine derivatives as a new class of AhR agonists and evaluation of anti-psoriasis effect in a mouse model. <i>European Journal of Medicinal Chemistry</i> , 2022, 231, 114122.	2.6	12
70	Deciphering the regulatory and catalytic mechanisms of an unusual SAM-dependent enzyme. <i>Signal Transduction and Targeted Therapy</i> , 2019, 4, 17.	7.1	11
71	Discovery of Pyrrolo[3,2- <i>d</i> ]pyrimidin-4-one Derivatives as a New Class of Potent and Cell-Active Inhibitors of P300/CBP-Associated Factor Bromodomain. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 4526-4542.	2.9	11
72	Preclinical pharmacodynamic evaluation of a new Src/FOSL1 inhibitor, LY-1816, in pancreatic ductal adenocarcinoma. <i>Cancer Science</i> , 2019, 110, 1408-1419.	1.7	11

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73	Structural and Functional Insights into an Archaeal Lipid Synthase. <i>Cell Reports</i> , 2020, 33, 108294.	2.9	11
74	Discovery of 5-(4-methylpiperazin-1-yl)-2-nitroaniline derivatives as a new class of SIRT6 inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 127215.	1.0	10
75	Discovery of a new class of JMJD6 inhibitors and structure-activity relationship study. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2021, 44, 128109.	1.0	10
76	Discovery of 3,4-Dihydrobenzo[1,4]oxazepin-5(2H)-one Derivatives as a New Class of Selective TNIK Inhibitors and Evaluation of Their Anti-Colorectal Cancer Effects. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 1786-1807.	2.9	10
77	Design and optimization of orally spleen tyrosine kinase (SYK) inhibitors for treatment of solid tumor. <i>Bioorganic Chemistry</i> , 2020, 95, 103547.	2.0	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. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 10691-10710.	2.9	8
79	Enhancement of Histone Deacetylase Inhibitor Sensitivity in Combination with Cyclin-Dependent Kinase Inhibition for the Treatment of Oral Squamous Cell Carcinoma. <i>Cellular Physiology and Biochemistry</i> , 2019, 53, 141-156.	1.1	8
80	Studies of Interaction between Ergosta-4,6,8(14),22-tetraen-3-one (Ergone) and Human Serum Albumin by Molecular Spectroscopy and Modeling. <i>Journal of the Chinese Chemical Society</i> , 2011, 58, 602-610.	0.8	7
81	A highly potent and selective inhibitor Roxyl-WL targeting IDO1 promotes immune response against melanoma. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2018, 33, 1089-1094.	2.5	7
82	Transition-Metal-Catalyzed Transformation of Sulfonates via S=O Bond Cleavage: Synthesis of Alkyl Aryl Ether and Diaryl Ether. <i>Organic Letters</i> , 2019, 21, 8879-8883.	2.4	7
83	Novel mitochondria-targeted and fluorescent DNA alkylation agents with highly selective activity against cancer cells. <i>Dyes and Pigments</i> , 2019, 170, 107610.	2.0	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2019, 29, 1609-1613.	1.0	7
85	Multispecific drugs: the fourth wave of biopharmaceutical innovation. <i>Signal Transduction and Targeted Therapy</i> , 2020, 5, 86.	7.1	7
86	Discovery of a potent and selective inhibitor of histone lysine demethylase KDM4D. <i>European Journal of Medicinal Chemistry</i> , 2021, 223, 113662.	2.6	7
87	The novel LSD1 inhibitor ZY0511 suppresses diffuse large B-cell lymphoma proliferation by inducing apoptosis and autophagy. <i>Medical Oncology</i> , 2021, 38, 124.	1.2	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 in vitro and in vivo. <i>European Journal of Medicinal Chemistry</i> , 2022, 232, 114187.	2.6	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. <i>BMC Cancer</i> , 2015, 15, 525.	1.1	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2019, 29, 2595-2603.	1.0	5

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91	Discovery of selective BPTF bromodomain inhibitors by screening and structure-based optimization. <i>Biochemical and Biophysical Research Communications</i> , 2021, 545, 125-131.	1.0	5
92	Selective and novel cyclin-dependent kinases 4 inhibitor: synthesis and biological evaluation. <i>Medicinal Chemistry Research</i> , 2018, 27, 1666-1678.	1.1	4
93	Dihydroartemisinin Inhibits mTORC1 Signaling by Activating the AMPK Pathway in Rhabdomyosarcoma Tumor Cells. <i>Cells</i> , 2021, 10, 1363.	1.8	4
94	Preclinical pharmacodynamic evaluation of drug candidate SKLB-178 in the treatment of non-small cell lung cancer. <i>Oncotarget</i> , 2017, 8, 12843-12854.	0.8	4
95	Discovery and structural optimization of potent epidermal growth factor receptor (EGFR) inhibitors against L858R/T790M/C797S resistance mutation for lung cancer treatment. <i>European Journal of Medicinal Chemistry</i> , 2022, 237, 114381.	2.6	4
96	Discovery of human TyrRS inhibitors by structure-based virtual screening, structural optimization, and bioassays. <i>RSC Advances</i> , 2019, 9, 9323-9330.	1.7	3
97	Role of Water in the Reaction Mechanism and endo / exo Selectivity of 1,3- $\Delta^2$ -Dipolar Cycloadditions Elucidated by Quantum Chemistry and Machine Learning. <i>Chemistry - A European Journal</i> , 2019, 25, 8289-8303.	1.7	3
98	Discovery of 12O- $\beta$ -A Novel Oral Multi-Kinase Inhibitor for the Treatment of Solid Tumor. <i>Molecules</i> , 2020, 25, 5199.	1.7	3
99	Targeting glutaminase 1 and synergizing with clinical drugs achieved more promising antitumor activity on multiple myeloma. <i>Oncotarget</i> , 2019, 10, 5993-6005.	0.8	3
100	Discovery of benzo[d]oxazol-2(3H)-one derivatives as a new class of TNIK inhibitors for the treatment of colorectal cancer. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2022, 67, 128745.	1.0	3
101	Lipidomic profiling reveals lipid regulation by a novel LSD1 inhibitor treatment. <i>Oncology Reports</i> , 2021, 46, .	1.2	2
102	Structure-Guided Discovery of a Potent and Selective Cell-Active Inhibitor of SETDB1 Tudor Domain. <i>Angewandte Chemie</i> , 2021, 133, 8842-8847.	1.6	1
103	Discovery of small molecule FLT3 inhibitors that are able to overcome drug-resistant mutations. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 127532.	1.0	0