Chao-Yie Yang

List of Publications by Citations

99 papers	5,862 citations	44 h-index	75 g-index
112 ext. papers	6,952 ext. citations	7.2 avg, IF	5.66 L-index

#	Paper	IF	Citations
99	The PDBbind database: methodologies and updates. *Journal of Medicinal Chemistry*, **2005**, 48, 4111-9	8.3	462
98	Structure-based design of potent small-molecule inhibitors of anti-apoptotic Bcl-2 proteins. *Journal of Medicinal Chemistry*, **2006**, 49, 6139-42	8.3	257
97	A potent and orally active antagonist (SM-406/AT-406) of multiple inhibitor of apoptosis proteins (IAPs) in clinical development for cancer treatment. *Journal of Medicinal Chemistry*, **2011**, 54, 2714-26	8.3	207
96	Discovery of a Small-Molecule Degrader of Bromodomain and Extra-Terminal (BET) Proteins with Picomolar Cellular Potencies and Capable of Achieving Tumor Regression. *Journal of Medicinal Chemistry*, **2018**, 61, 462-481	8.3	197
95	Design of triazole-stapled BCL9 α-helical peptides to target the β-catenin/B-cell CLL/lymphoma 9 (BCL9) protein-protein interaction. *Journal of Medicinal Chemistry*, **2012**, 55, 1137-46	8.3	195
94	A Potent and Selective Small-Molecule Degrader of STAT3 Achieves Complete Tumor Regression In Vivo. *Cancer Cell*, **2019**, 36, 498-511.e17	24.3	181
93	Design, synthesis, and characterization of a potent, nonpeptide, cell-permeable, bivalent Smac mimetic that concurrently targets both the BIR2 and BIR3 domains in XIAP. *Journal of the American Chemical Society*, **2007**, 129, 15279-94	16.4	175
92	Discovery of ARD-69 as a Highly Potent Proteolysis Targeting Chimera (PROTAC) Degrader of Androgen Receptor (AR) for the Treatment of Prostate Cancer. *Journal of Medicinal Chemistry*, **2019**, 62, 941-964	8.3	157
91	Structure-based design of potent, conformationally constrained Smac mimetics. *Journal of the American Chemical Society*, **2004**, 126, 16686-7	16.4	143
90	Targeting the MDM2-p53 Protein-Protein Interaction for New Cancer Therapy: Progress and Challenges. *Cold Spring Harbor Perspectives in Medicine*, **2017**, 7,	5.4	137
89	Analysis of ligand-bound water molecules in high-resolution crystal structures of protein-ligand complexes. *Journal of Chemical Information and Modeling*, **2007**, 47, 668-75	6.1	134
88	Discovery of QCA570 as an Exceptionally Potent and Efficacious Proteolysis Targeting Chimera (PROTAC) Degrader of the Bromodomain and Extra-Terminal (BET) Proteins Capable of Inducing Complete and Durable Tumor Regression. *Journal of Medicinal Chemistry*, **2018**, 61, 6685-6704	8.3	133
87	Discovery of MD-224 as a First-in-Class, Highly Potent, and Efficacious Proteolysis Targeting Chimera Murine Double Minute 2 Degrader Capable of Achieving Complete and Durable Tumor Regression. *Journal of Medicinal Chemistry*, **2019**, 62, 448-466	8.3	132
86	Structure-based design, synthesis, and evaluation of conformationally constrained mimetics of the second mitochondria-derived activator of caspase that target the X-linked inhibitor of apoptosis protein/caspase-9 interaction site. *Journal of Medicinal Chemistry*, **2004**, 47, 4147-50	8.3	131
85	Design of small-molecule peptidic and nonpeptidic Smac mimetics. *Accounts of Chemical Research*, **2008**, 41, 1264-77	24.3	124
84	CSAR benchmark exercise of 2010: combined evaluation across all submitted scoring functions. *Journal of Chemical Information and Modeling*, **2011**, 51, 2115-31	6.1	117
83	Targeted Degradation of BET Proteins in Triple-Negative Breast Cancer. *Cancer Research*, **2017**, 77, 2476-2487	12.8	115

82	The FHA and BRCT domains recognize ADP-ribosylation during DNA damage response. *Genes and Development*, **2013**, 27, 1752-68	12.6	107
81	Discovery of ERD-308 as a Highly Potent Proteolysis Targeting Chimera (PROTAC) Degrader of Estrogen Receptor (ER). *Journal of Medicinal Chemistry*, **2019**, 62, 1420-1442	8.3	106
80	CSAR benchmark exercise of 2010: selection of the protein-ligand complexes. *Journal of Chemical Information and Modeling*, **2011**, 51, 2036-46	6.1	102
79	RNF111-dependent neddylation activates DNA damage-induced ubiquitination. *Molecular Cell*, **2013**, 49, 897-907	17.6	93
78	Design, synthesis, and evaluation of a potent, cell-permeable, conformationally constrained second mitochondria derived activator of caspase (Smac) mimetic. *Journal of Medicinal Chemistry*, **2006**, 49, 7916-20	8.3	93
77	Binding free energy contributions of interfacial waters in HIV-1 protease/inhibitor complexes. *Journal of the American Chemical Society*, **2006**, 128, 11830-9	16.4	80
76	MCL-1 inhibition in cancer treatment. *OncoTargets and Therapy*, **2018**, 11, 7301-7314	4.4	79
75	Structure-Based Discovery of SD-36 as a Potent, Selective, and Efficacious PROTAC Degrader of STAT3 Protein. *Journal of Medicinal Chemistry*, **2019**, 62, 11280-11300	8.3	75
74	Structure-based design, synthesis, evaluation, and crystallographic studies of conformationally constrained Smac mimetics as inhibitors of the X-linked inhibitor of apoptosis protein (XIAP). *Journal of Medicinal Chemistry*, **2008**, 51, 7169-80	8.3	72
73	Structural and Electronic Characterization of Chemical and Conformational Defects in Conjugated Polymers. *Journal of Physical Chemistry B*, **2001**, 105, 6103-6107	3.4	70
72	Acylpyrogallols as inhibitors of antiapoptotic Bcl-2 proteins. *Journal of Medicinal Chemistry*, **2008**, 51, 717-20	8.3	67
71	Structure-Based Design of □Carboline Analogues as Potent and Specific BET Bromodomain Inhibitors. *Journal of Medicinal Chemistry*, **2015**, 58, 4927-39	8.3	66
70	The making of I-BET762, a BET bromodomain inhibitor now in clinical development. *Journal of Medicinal Chemistry*, **2013**, 56, 7498-500	8.3	65
69	Accurate variational calculations and analysis of the HOCl vibrational energy spectrum. *Journal of Chemical Physics*, **1998**, 109, 10273-10283	3.9	64
68	M-score: a knowledge-based potential scoring function accounting for protein atom mobility. *Journal of Medicinal Chemistry*, **2006**, 49, 5903-11	8.3	62
67	Discovery of Highly Potent and Efficient PROTAC Degraders of Androgen Receptor (AR) by Employing Weak Binding Affinity VHL E3 Ligase Ligands. *Journal of Medicinal Chemistry*, **2019**, 62, 11218-11231	8.3	61
66	Small-molecule PROTAC degraders of the Bromodomain and Extra Terminal (BET) proteins - A review. *Drug Discovery Today: Technologies*, **2019**, 31, 43-51	7.1	59
65	Importance of ligand reorganization free energy in protein-ligand binding-affinity prediction. *Journal of the American Chemical Society*, **2009**, 131, 13709-21	16.4	59

64	Design of Bcl-2 and Bcl-xL inhibitors with subnanomolar binding affinities based upon a new scaffold. *Journal of Medicinal Chemistry*, **2012**, 55, 4664-82	8.3	55
63	Simple Structural Modifications Converting a Bona fide MDM2 PROTAC Degrader into a Molecular Glue Molecule: A Cautionary Tale in the Design of PROTAC Degraders. *Journal of Medicinal Chemistry*, **2019**, 62, 9471-9487	8.3	54
62	Design and synthesis of a new, conformationally constrained, macrocyclic small-molecule inhibitor of STAT3 via Sclick chemistryS *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 3939-42	2.9	50
61	Recent Advances of SHP2 Inhibitors in Cancer Therapy: Current Development and Clinical Application. *Journal of Medicinal Chemistry*, **2020**, 63, 11368-11396	8.3	49
60	A potent small-molecule inhibitor of the DCN1-UBC12 interaction that selectively blocks cullin 3 neddylation. *Nature Communications*, **2017**, 8, 1150	17.4	48
59	Interaction of a cyclic, bivalent smac mimetic with the x-linked inhibitor of apoptosis protein. *Biochemistry*, **2008**, 47, 9811-24	3.2	48
58	Structure-based design, synthesis and biochemical testing of novel and potent Smac peptido-mimetics. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 793-7	2.9	48
57	Hydrophobic Binding Hot Spots of Bcl-xL Protein-Protein Interfaces by Cosolvent Molecular Dynamics Simulation. *ACS Medicinal Chemistry Letters*, **2011**, 2, 280-4	4.3	45
56	Potent, orally bioavailable diazabicyclic small-molecule mimetics of second mitochondria-derived activator of caspases. *Journal of Medicinal Chemistry*, **2008**, 51, 8158-62	8.3	45
55	Structure-based discovery of BM-957 as a potent small-molecule inhibitor of Bcl-2 and Bcl-xL capable of achieving complete tumor regression. *Journal of Medicinal Chemistry*, **2012**, 55, 8502-14	8.3	44
54	Structure-based design of potent Bcl-2/Bcl-xL inhibitors with strong in vivo antitumor activity. *Journal of Medicinal Chemistry*, **2012**, 55, 6149-61	8.3	43
53	Pyrogallol-based molecules as potent inhibitors of the antiapoptotic Bcl-2 proteins. *Journal of Medicinal Chemistry*, **2007**, 50, 1723-6	8.3	40
52	Nonpeptidic and potent small-molecule inhibitors of cIAP-1/2 and XIAP proteins. *Journal of Medicinal Chemistry*, **2010**, 53, 6361-7	8.3	39
51	Discovery of SHP2-D26 as a First, Potent, and Effective PROTAC Degrader of SHP2 Protein. *Journal of Medicinal Chemistry*, **2020**, 63, 7510-7528	8.3	38
50	Potent bivalent Smac mimetics: effect of the linker on binding to inhibitor of apoptosis proteins (IAPs) and anticancer activity. *Journal of Medicinal Chemistry*, **2011**, 54, 3306-18	8.3	38
49	Design, synthesis, and evaluation of potent, nonpeptidic mimetics of second mitochondria-derived activator of caspases. *Journal of Medicinal Chemistry*, **2009**, 52, 593-6	8.3	38
48	Instantaneous normal mode analysis of hydrated electron solvation dynamics. *Journal of Chemical Physics*, **2001**, 114, 3598-3611	3.9	37
47	Structure-based design of flavonoid compounds as a new class of small-molecule inhibitors of the anti-apoptotic Bcl-2 proteins. *Journal of Medicinal Chemistry*, **2007**, 50, 3163-6	8.3	36

46	Design, synthesis, and evaluation of tricyclic, conformationally constrained small-molecule mimetics of second mitochondria-derived activator of caspases. *Journal of Medicinal Chemistry*, **2008**, 51, 7352-5	8.3	34
45	Targeting inhibitors of apoptosis proteins (IAPs) for new breast cancer therapeutics. *Journal of Mammary Gland Biology and Neoplasia*, **2012**, 17, 217-28	2.4	33
44	High-Affinity Peptidomimetic Inhibitors of the DCN1-UBC12 Protein-Protein Interaction. *Journal of Medicinal Chemistry*, **2018**, 61, 1934-1950	8.3	31
43	A potent and highly efficacious Bcl-2/Bcl-xL inhibitor. *Journal of Medicinal Chemistry*, **2013**, 56, 3048-3067	8.3	31
42	LRIG1 modulates cancer cell sensitivity to Smac mimetics by regulating TNF□expression and receptor tyrosine kinase signaling. *Cancer Research*, **2012**, 72, 1229-38	10.1	31
41	Cyclopeptide Smac mimetics as antagonists of IAP proteins. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 3043-6	2.9	31
40	Structure-based discovery of nonpeptidic small organic compounds to block the T cell response to myelin basic protein. *Journal of Medicinal Chemistry*, **2004**, 47, 4989-97	8.3	31
39	Analysis of Flexibility and Hotspots in Bcl-xL and Mcl-1 Proteins for the Design of Selective Small-Molecule Inhibitors. *ACS Medicinal Chemistry Letters*, **2012**, 3, 308-12	4.3	30
38	Bivalent Smac mimetics with a diazabicyclic core as highly potent antagonists of XIAP and cIAP1/2 and novel anticancer agents. *Journal of Medicinal Chemistry*, **2012**, 55, 106-14	8.3	29
37	Design, synthesis, and evaluation of potent and selective ligands for the dopamine 3 (D3) receptor with a novel in vivo behavioral profile. *Journal of Medicinal Chemistry*, **2008**, 51, 5905-8	8.3	27
36	Potent and selective small-molecule inhibitors of cIAP1/2 proteins reveal that the binding of Smac mimetics to XIAP BIR3 is not required for their effective induction of cell death in tumor cells. *ACS Chemical Biology*, **2014**, 9, 994-1002	4.9	26
35	Pyrimido[4,5-d]pyrimidin-4(1H)-one derivatives as selective inhibitors of EGFR threonine790 to methionine790 (T790M) mutants. *Angewandte Chemie - International Edition*, **2013**, 52, 8387-90	16.4	25
34	Computational analysis of protein hotspots. *ACS Medicinal Chemistry Letters*, **2010**, 1, 125-9	4.3	24
33	The effect of angular momentum on the unimolecular dissociation HCO-þH+CO. *Journal of Chemical Physics*, **1997**, 107, 7773-7786	3.9	24
32	Enantiomerically pure hexahydropyrazinoquinolines as potent and selective dopamine 3 subtype receptor ligands. *Journal of Medicinal Chemistry*, **2005**, 48, 3171-81	8.3	24
31	Structure-Based Discovery of 4-(6-Methoxy-2-methyl-4-(quinolin-4-yl)-9H-pyrimido[4,5-b]indol-7-yl)-3,5-dimethylisoxazole (CD161) as a Potent and Orally Bioavailable BET Bromodomain Inhibitor. *Journal of Medicinal Chemistry*, **2017**, 60, 3887-3901	8.3	23
30	Identification of potential small molecule allosteric modulator sites on IL-1R1 ectodomain using accelerated conformational sampling method. *PLoS ONE*, **2015**, 10, e0118671	3.7	22
29	From proteomics to discovery of first-in-class ST2 inhibitors active in vivo. *JCI Insight*, **2018**, 3,	9.9	20

28	Significant Differences in the Development of Acquired Resistance to the MDM2 Inhibitor SAR405838 between In Vitro and In Vivo Drug Treatment. *PLoS ONE*, **2015**, 10, e0128807	3.7	19
27	Enrichment of druggable conformations from apo protein structures using cosolvent-accelerated molecular dynamics. *Biology*, **2015**, 4, 344-66	4.9	16
26	Design of High-Affinity Stapled Peptides To Target the Repressor Activator Protein 1 (RAP1)/Telomeric Repeat-Binding Factor 2 (TRF2) Protein-Protein Interaction in the Shelterin Complex. *Journal of Medicinal Chemistry*, **2016**, 59, 328-34	8.3	15
25	Structure-Based Discovery of CF53 as a Potent and Orally Bioavailable Bromodomain and Extra-Terminal (BET) Bromodomain Inhibitor. *Journal of Medicinal Chemistry*, **2018**, 61, 6110-6120	8.3	15
24	Computational modeling toward understanding agonist binding on dopamine 3. *Journal of Chemical Information and Modeling*, **2010**, 50, 1633-43	6.1	15
23	A systematic analysis of the effect of small-molecule binding on protein flexibility of the ligand-binding sites. *Journal of Medicinal Chemistry*, **2005**, 48, 5648-50	8.3	15
22	EEDi-5285: An Exceptionally Potent, Efficacious, and Orally Active Small-Molecule Inhibitor of Embryonic Ectoderm Development. *Journal of Medicinal Chemistry*, **2020**, 63, 7252-7267	8.3	14
21	A novel Bcl-2 small molecule inhibitor 4-(3-methoxy-phenylsulfannyl)-7-nitro-benzofurazan-3-oxide (MNB)-induced apoptosis in leukemia cells. *Annals of Hematology*, **2007**, 86, 471-81	3	13
20	Buried Hydrogen Bond Interactions Contribute to the High Potency of Complement Factor D Inhibitors. *ACS Medicinal Chemistry Letters*, **2016**, 7, 1092-1096	4.3	9
19	Allosteric Inactivation of Polycomb Repressive Complex 2 (PRC2) by Inhibiting Its Adapter Protein: Embryonic Ectodomain Development (EED). *Journal of Medicinal Chemistry*, **2017**, 60, 2212-2214	8.3	8
18	Conformational Sampling and Binding Site Assessment of Suppression of Tumorigenicity 2 Ectodomain. *PLoS ONE*, **2016**, 11, e0146522	3.7	7
17	Discovery of EEDi-5273 as an Exceptionally Potent and Orally Efficacious EED Inhibitor Capable of Achieving Complete and Persistent Tumor Regression. *Journal of Medicinal Chemistry*, **2021**, 64, 14540-14556	8.3	7
16	Discovery of CJ-2360 as a Potent and Orally Active Inhibitor of Anaplastic Lymphoma Kinase Capable of Achieving Complete Tumor Regression. *Journal of Medicinal Chemistry*, **2020**, 63, 13994-14016	8.3	7
15	Solution Conformations of Wild-Type and Mutated Bak BH3 Peptides via Dynamical Conformational Sampling and Implication to Their Binding to Antiapoptotic Bcl-2 Proteins. *Journal of Physical Chemistry B*, **2004**, 108, 1467-1477	3.4	6
14	Cyclic Peptidic Mimetics of Apollo Peptides Targeting Telomeric Repeat Binding Factor 2 (TRF2) and Apollo Interaction. *ACS Medicinal Chemistry Letters*, **2018**, 9, 507-511	4.3	5
13	Comparative Analyses of the Conformational Dynamics Between the Soluble and Membrane-Bound Cytokine Receptors. *Scientific Reports*, **2020**, 10, 7399	4.9	4
12	Correction to CSAR Benchmark Exercise of 2010: Selection of the Protein□igand Complexes. *Journal of Chemical Information and Modeling*, **2011**, 51, 2146-2146	6.1	4
11	Targeting DCN1-UBC12 Protein-Protein Interaction for Regulation of Neddylation Pathway. *Advances in Experimental Medicine and Biology*, **2020**, 1217, 349-362	3.6	3

List of Publications

10	SD-91 as A Potent and Selective STAT3 Degrader Capable of Achieving Complete and Long-Lasting Tumor Regression. *ACS Medicinal Chemistry Letters*, **2021**, 12, 996-1004	4.3	3
9	Design and synthesis of a potent biotinylated Smac mimetic. *Tetrahedron Letters*, **2005**, 46, 7015-7018	2	2
8	The Similarity of Class II HLA Genotypes Defines Patterns of Autoreactivity in Idiopathic Bone Marrow Failure Disorders. *Blood*, **2021**,	2.2	2
7	Chapter 11 Recent Advances in Design of Small-Molecule Ligands to Target Protein□Protein Interactions. *Annual Reports in Computational Chemistry*, **2006**, 197-219	1.8	1
6	Selective inhibition of cullin 3 neddylation through covalent targeting DCN1 protects mice from acetaminophen-induced liver toxicity. *Nature Communications*, **2021**, 12, 2621	17.4	1
5	Design, Synthesis, and Biological Evaluation of Apcin-Based CDC20 Inhibitors.. *ACS Medicinal Chemistry Letters*, **2022**, 13, 188-195	4.3	0
4	N-terminal modified cyclopeptidic mimetics of Apollo as inhibitors of TRF2. *Bioorganic and Medicinal Chemistry Letters*, **2020**, 30, 127401	2.9	0
3	Basic Principles and Practices of Computer-Aided Drug Design259-278		
2	Electron propagation along a nanowire: a study in chattering. *Nanotechnology*, **1998**, 9, 365-368	3.4	
1	Small Molecule ST2 Inhibitors Cause Reduction of Soluble ST2 and Improve Gvhd and Survival In Vivo. *Blood*, **2016**, 128, 528-528	2.2	