Shaomeng Wang

List of Publications by Citations

354 papers	26,369 citations	87 h-index	147 g-index
529 ext. papers	29,365 ext. citations	7.5 avg, IF	6.87 L-index

#	Paper	IF	Citations
354	Further development and validation of empirical scoring functions for structure-based binding affinity prediction. *Journal of Computer-Aided Molecular Design*, **2002**, 16, 11-26	4.2	842
353	Comparative evaluation of 11 scoring functions for molecular docking. *Journal of Medicinal Chemistry*, **2003**, 46, 2287-303	8.3	749
352	Therapeutic targeting of BET bromodomain proteins in castration-resistant prostate cancer. *Nature* , **2014**, 510, 278-82	50.4	650
351	Structure-based design of spiro-oxindoles as potent, specific small-molecule inhibitors of the MDM2-p53 interaction. *Journal of Medicinal Chemistry*, **2006**, 49, 3432-5	8.3	581
350	The PDBbind database: collection of binding affinities for protein-ligand complexes with known three-dimensional structures. *Journal of Medicinal Chemistry*, **2004**, 47, 2977-80	8.3	577
349	Temporal activation of p53 by a specific MDM2 inhibitor is selectively toxic to tumors and leads to complete tumor growth inhibition. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 3933-8	11.5	574
348	Structure-based design of potent non-peptide MDM2 inhibitors. *Journal of the American Chemical Society*, **2005**, 127, 10130-1	16.4	543
347	Small-molecule inhibitors of the MDM2-p53 protein-protein interaction to reactivate p53 function: a novel approach for cancer therapy. *Annual Review of Pharmacology and Toxicology*, **2009**, 49, 223-41	17.9	477
346	The PDBbind database: methodologies and updates. *Journal of Medicinal Chemistry*, **2005**, 48, 4111-9	8.3	462
345	Endocrine-therapy-resistant ESR1 variants revealed by genomic characterization of breast-cancer-derived xenografts. *Cell Reports*, **2013**, 4, 1116-30	10.6	447
344	A low-molecular-weight compound discovered through virtual database screening inhibits Stat3 function in breast cancer cells. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 4700-5	11.5	412
343	Development and optimization of a binding assay for the XIAP BIR3 domain using fluorescence polarization. *Analytical Biochemistry*, **2004**, 332, 261-73	3.1	400
342	Small-molecule inhibitors of the MDM2-p53 protein-protein interaction (MDM2 Inhibitors) in clinical trials for cancer treatment. *Journal of Medicinal Chemistry*, **2015**, 58, 1038-52	8.3	314
341	Discovery of embelin as a cell-permeable, small-molecular weight inhibitor of XIAP through structure-based computational screening of a traditional herbal medicine three-dimensional structure database. *Journal of Medicinal Chemistry*, **2004**, 47, 2430-40	8.3	313
340	Discovery of small-molecule inhibitors of Bcl-2 through structure-based computer screening. *Journal of Medicinal Chemistry*, **2001**, 44, 4313-24	8.3	306
339	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
338	Coumarin-based inhibitors of HIV integrase. *Journal of Medicinal Chemistry*, **1997**, 40, 242-9	8.3	255

337	Targeting the MDM2-p53 interaction for cancer therapy. *Clinical Cancer Research*, **2008**, 14, 5318-24	12.9	248
336	How does consensus scoring work for virtual library screening? An idealized computer experiment. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1422-6		236
335	Computer Automated log P Calculations Based on an Extended Group Contribution Approach. *Journal of Chemical Information and Computer Sciences*, **1994**, 34, 752-781		230
334	An extensive test of 14 scoring functions using the PDBbind refined set of 800 protein-ligand complexes. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 2114-25		215
333	Conformational changes of small molecules binding to proteins. *Bioorganic and Medicinal Chemistry* , **1995**, 3, 411-28	3.4	215
332	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
331	SAR405838: an optimized inhibitor of MDM2-p53 interaction that induces complete and durable tumor regression. *Cancer Research*, **2014**, 74, 5855-65	10.1	205
330	Targeting MLL1 H3K4 methyltransferase activity in mixed-lineage leukemia. *Molecular Cell*, **2014**, 53, 247-61	17.6	203
329	Depsides and depsidones as inhibitors of HIV-1 integrase: discovery of novel inhibitors through 3D database searching. *Journal of Medicinal Chemistry*, **1997**, 40, 942-51	8.3	199
328	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
327	A potent small-molecule inhibitor of the MDM2-p53 interaction (MI-888) achieved complete and durable tumor regression in mice. *Journal of Medicinal Chemistry*, **2013**, 56, 5553-61	8.3	196
326	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
325	3-(Hydroxymethyl)-bearing phosphatidylinositol ether lipid analogues and carbonate surrogates block PI3-K, Akt, and cancer cell growth. *Journal of Medicinal Chemistry*, **2000**, 43, 3045-51	8.3	187
324	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
323	Comparison of the NCI open database with seven large chemical structural databases. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 702-12		179
322	Blockage of epidermal growth factor receptor-phosphatidylinositol 3-kinase-AKT signaling increases radiosensitivity of K-RAS mutated human tumor cells in vitro by affecting DNA repair. *Clinical Cancer Research*, **2006**, 12, 4119-26	12.9	177
321	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
320	Diastereomeric spirooxindoles as highly potent and efficacious MDM2 inhibitors. *Journal of the American Chemical Society*, **2013**, 135, 7223-34	16.4	165

319	Chimeric (alpha/beta + alpha)-peptide ligands for the BH3-recognition cleft of Bcl-XL: critical role of the molecular scaffold in protein surface recognition. *Journal of the American Chemical Society*, **2005**, 127, 11966-8	16.4	161
318	Targeting of AKT1 enhances radiation toxicity of human tumor cells by inhibiting DNA-PKcs-dependent DNA double-strand break repair. *Molecular Cancer Therapeutics*, **2008**, 7, 1772-81	6.1	160
317	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
316	(alpha/beta+alpha)-peptide antagonists of BH3 domain/Bcl-x(L) recognition: toward general strategies for foldamer-based inhibition of protein-protein interactions. *Journal of the American Chemical Society*, **2007**, 129, 139-54	16.4	156
315	SM-164: a novel, bivalent Smac mimetic that induces apoptosis and tumor regression by concurrent removal of the blockade of cIAP-1/2 and XIAP. *Cancer Research*, **2008**, 68, 9384-93	10.1	155
314	Potent and orally active small-molecule inhibitors of the MDM2-p53 interaction. *Journal of Medicinal Chemistry*, **2009**, 52, 7970-3	8.3	150
313	Targeting Bcl-2 and Bcl-XL with nonpeptidic small-molecule antagonists. *Seminars in Oncology*, **2003**, 30, 133-42	5.5	150
312	Antiretroviral agents as inhibitors of both human immunodeficiency virus type 1 integrase and protease. *Journal of Medicinal Chemistry*, **1996**, 39, 2472-81	8.3	146
311	Structure-based design of potent, conformationally constrained Smac mimetics. *Journal of the American Chemical Society*, **2004**, 126, 16686-7	16.4	143
310	Molecular mechanism of gossypol-induced cell growth inhibition and cell death of HT-29 human colon carcinoma cells. *Biochemical Pharmacology*, **2003**, 66, 93-103	6	140
309	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
308	Preclinical studies of TW-37, a new nonpeptidic small-molecule inhibitor of Bcl-2, in diffuse large cell lymphoma xenograft model reveal drug action on both Bcl-2 and Mcl-1. *Clinical Cancer Research* , **2007**, 13, 2226-35	12.9	135
307	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
306	Molecular modeling of the three-dimensional structure of dopamine 3 (D3) subtype receptor: discovery of novel and potent D3 ligands through a hybrid pharmacophore- and structure-based database searching approach. *Journal of Medicinal Chemistry*, **2003**, 46, 4377-92	8.3	134
305	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
304	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
303	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
302	A novel BH3 mimetic reveals a mitogen-activated protein kinase-dependent mechanism of melanoma cell death controlled by p53 and reactive oxygen species. *Cancer Research*, **2006**, 66, 11348-59	10.1	130

301	Targeting apoptosis pathways for new cancer therapeutics. *Annual Review of Medicine*, **2014**, 65, 139-55	17.4	129
300	Residues in the second cysteine-rich region of protein kinase C delta relevant to phorbol ester binding as revealed by site-directed mutagenesis. *Journal of Biological Chemistry*, **1995**, 270, 21852-9	5.4	128
299	National Cancer Institute Drug Information System 3D database. *Journal of Chemical Information and Computer Sciences*, **1994**, 34, 1219-24		128
298	Estimation of aqueous solubility of organic molecules by the group contribution approach. Application to the study of biodegradation. *Journal of Chemical Information and Modeling*, **1992**, 32, 474-82	6.1	125
297	Design of small-molecule peptidic and nonpeptidic Smac mimetics. *Accounts of Chemical Research*, **2008**, 41, 1264-77	24.3	124
296	BET Bromodomain Inhibitors Enhance Efficacy and Disrupt Resistance to AR Antagonists in the Treatment of Prostate Cancer. *Molecular Cancer Research*, **2016**, 14, 324-31	6.6	120
295	Small molecule inhibitors of the MDM2-p53 interaction discovered by ensemble-based receptor models. *Journal of the American Chemical Society*, **2007**, 129, 12809-14	16.4	119
294	Discovery of novel, non-peptide HIV-1 protease inhibitors by pharmacophore searching. *Journal of Medicinal Chemistry*, **1996**, 39, 2047-54	8.3	119
293	Small-molecule SMAC mimetics as new cancer therapeutics. *Pharmacology & Therapeutics*, **2014**, 144, 82-95	13.9	118
292	High-affinity, small-molecule peptidomimetic inhibitors of MLL1/WDR5 protein-protein interaction. *Journal of the American Chemical Society*, **2013**, 135, 669-82	16.4	117
291	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
290	Discovery of HIV-1 integrase inhibitors by pharmacophore searching. *Journal of Medicinal Chemistry* , **1997**, 40, 930-6	8.3	117
289	Discovery of a nanomolar inhibitor of the human murine double minute 2 (MDM2)-p53 interaction through an integrated, virtual database screening strategy. *Journal of Medicinal Chemistry*, **2006**, 49, 3759-62	8.3	117
288	MCDOCK: a Monte Carlo simulation approach to the molecular docking problem. *Journal of Computer-Aided Molecular Design*, **1999**, 13, 435-51	4.2	117
287	Targeted Degradation of BET Proteins in Triple-Negative Breast Cancer. *Cancer Research*, **2017**, 77, 2476-2487	12.8	115
286	Superparamagnetic iron oxide nanotheranostics for targeted cancer cell imaging and pH-dependent intracellular drug release. *Molecular Pharmaceutics*, **2010**, 7, 1974-84	5.6	110
285	Reversal of cisplatin resistance with a BH3 mimetic, (-)-gossypol, in head and neck cancer cells: role of wild-type p53 and Bcl-xL. *Molecular Cancer Therapeutics*, **2005**, 4, 1096-104	6.1	109
284	In vitro effects of the BH3 mimetic, (-)-gossypol, on head and neck squamous cell carcinoma cells. *Clinical Cancer Research*, **2004**, 10, 7757-63	12.9	109

283	The FHA and BRCT domains recognize ADP-ribosylation during DNA damage response. *Genes and Development*, **2013**, 27, 1752-68	12.6	107
282	Yawning and hypothermia in rats: effects of dopamine D3 and D2 agonists and antagonists. *Psychopharmacology*, **2007**, 193, 159-70	4.7	107
281	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
280	cIAP1 and cIAP2 limit macrophage necroptosis by inhibiting Rip1 and Rip3 activation. *Cell Death and Differentiation*, **2012**, 19, 1791-801	12.7	105
279	Comprehensive biomarker and genomic analysis identifies p53 status as the major determinant of response to MDM2 inhibitors in chronic lymphocytic leukemia. *Blood*, **2008**, 111, 1584-93	2.2	103
278	CSAR benchmark exercise of 2010: selection of the protein-ligand complexes. *Journal of Chemical Information and Modeling*, **2011**, 51, 2036-46	6.1	102
277	Hydrazide-containing inhibitors of HIV-1 integrase. *Journal of Medicinal Chemistry*, **1997**, 40, 937-41	8.3	97
276	Self-Guided Molecular Dynamics Simulation for Efficient Conformational Search. *Journal of Physical Chemistry B*, **1998**, 102, 7238-7250	3.4	96
275	Discovery of 4-((3R,4S,5R)-6?-Chloro-4R(3-chloro-2-fluorophenyl)-1Rethyl-2?-oxodispiro[cyclohexane-1,2Rpyrrolidine-3R3?-indoline]-5 Acid (AA-115/APG-115): A Potent and Orally Active Murine Double Minute 2 (MDM2) Inhibitor in Clinical Development. *Journal of Medicinal Chemistry*, **2017**, 60, 2819-2839	8.3	93
274	RNF111-dependent neddylation activates DNA damage-induced ubiquitination. *Molecular Cell*, **2013**, 49, 897-907	17.6	93
273	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
272	Identification of a More Potent Analogue of the Naturally Occurring Alkaloid Huperzine A. Predictive Molecular Modeling of Its Interaction with AChE. *Journal of the American Chemical Society*, **1996**, 118, 11357-11362	16.4	93
271	Bcl-2 acts in a proangiogenic signaling pathway through nuclear factor-kappaB and CXC chemokines. *Cancer Research*, **2005**, 65, 5063-9	10.1	91
270	Nonphosphorylated peptide ligands for the Grb2 Src homology 2 domain. *Journal of Biological Chemistry*, **1997**, 272, 29046-52	5.4	89
269	beta2-chimaerin is a novel target for diacylglycerol: binding properties and changes in subcellular localization mediated by ligand binding to its C1 domain. *Proceedings of the National Academy of Sciences of the United States of America*, **1999**, 96, 11854-9	11.5	89
268	Activating STAT6 mutations in follicular lymphoma. *Blood*, **2015**, 125, 668-79	2.2	87
267	(-)-Gossypol enhances response to radiation therapy and results in tumor regression of human prostate cancer. *Molecular Cancer Therapeutics*, **2005**, 4, 197-205	6.1	87
266	(-)-gossypol inhibits growth and promotes apoptosis of human head and neck squamous cell carcinoma in vivo. *Neoplasia*, **2006**, 8, 163-72	6.4	84

265	Cardiac glycosides inhibit p53 synthesis by a mechanism relieved by Src or MAPK inhibition. *Cancer Research*, **2009**, 69, 6556-64	10.1	80
264	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
263	Breast cancer cells can evade apoptosis-mediated selective killing by a novel small molecule inhibitor of Bcl-2. *Cancer Research*, **2004**, 64, 7947-53	10.1	79
262	Synthesis and evaluation of the sunflower derived trypsin inhibitor as a potent inhibitor of the type II transmembrane serine protease, matriptase. *Bioorganic and Medicinal Chemistry Letters*, **2001**, 11, 2515-9	2.9	77
261	Multiple distinct molecular mechanisms influence sensitivity and resistance to MDM2 inhibitors in adult acute myelogenous leukemia. *Blood*, **2010**, 116, 71-80	2.2	75
260	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
259	Structure-Based Design of Conformationally Constrained, Cell-Permeable STAT3 Inhibitors. *ACS Medicinal Chemistry Letters*, **2010**, 1, 85-89	4.3	74
258	Targeting transcriptional regulation of SARS-CoV-2 entry factors and. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**,	11.5	74
257	Antiangiogenic effect of TW37, a small-molecule inhibitor of Bcl-2. *Cancer Research*, **2006**, 66, 8698-706	10.1	73
256	Structure-based approach for the discovery of bis-benzamidines as novel inhibitors of matriptase. *Journal of Medicinal Chemistry*, **2001**, 44, 1349-55	8.3	73
255	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
254	Pharmacophore-based discovery of substituted pyridines as novel dopamine transporter inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2003**, 13, 513-7	2.9	72
253	Structure-based design of high-affinity macrocyclic peptidomimetics to block the menin-mixed lineage leukemia 1 (MLL1) protein-protein interaction. *Journal of Medicinal Chemistry*, **2013**, 56, 1113-23	8.3	71
252	TW-37, a small-molecule inhibitor of Bcl-2, inhibits cell growth and induces apoptosis in pancreatic cancer: involvement of Notch-1 signaling pathway. *Cancer Research*, **2009**, 69, 2757-65	10.1	71
251	The discovery of novel, structurally diverse protein kinase C agonists through computer 3D-database pharmacophore search. Molecular modeling studies. *Journal of Medicinal Chemistry*, **1994**, 37, 4479-89	8.3	71
250	Reactivation of p53 by a specific MDM2 antagonist (MI-43) leads to p21-mediated cell cycle arrest and selective cell death in colon cancer. *Molecular Cancer Therapeutics*, **2008**, 7, 1533-42	6.1	69
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248	A computer automated structure evaluation (CASE) approach to calculation of partition coefficient. *Journal of Computational Chemistry*, **1991**, 12, 1025-1032	3.5	67

247	Structure-Based Design of β-Carboline Analogues as Potent and Specific BET Bromodomain Inhibitors. *Journal of Medicinal Chemistry*, **2015**, 58, 4927-39	8.3	66
246	The making of I-BET762, a BET bromodomain inhibitor now in clinical development. *Journal of Medicinal Chemistry*, **2013**, 56, 7498-500	8.3	65
245	Modeling, chemistry, and biology of the benzolactam analogues of indolactam V (ILV). 2. Identification of the binding site of the benzolactams in the CRD2 activator-binding domain of PKCdelta and discovery of an ILV analogue of improved isozyme selectivity. *Journal of Medicinal Chemistry*, **1997**, 40, 1316-26	8.3	65
244	Discovery of a novel dopamine transporter inhibitor, 4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidyl 4-methylphenyl ketone, as a potential cocaine antagonist through 3D-database pharmacophore searching. Molecular modeling, structure-activity relationships, and behavioral pharmacological studies. *Journal of Medicinal Chemistry*, **2000**, 43, 351-60	8.3	65
243	Preclinical studies of a nonpeptidic small-molecule inhibitor of Bcl-2 and Bcl-X(L) [(-)-gossypol] against diffuse large cell lymphoma. *Molecular Cancer Therapeutics*, **2005**, 4, 13-21	6.1	65
242	M-score: a knowledge-based potential scoring function accounting for protein atom mobility. *Journal of Medicinal Chemistry*, **2006**, 49, 5903-11	8.3	62
241	Direct observation of the folding and unfolding of a beta-hairpin in explicit water through computer simulation. *Journal of the American Chemical Society*, **2002**, 124, 5282-3	16.4	62
240	Synthesis and biology of the conformationally restricted ACPD analogue, 2-aminobicyclo[2.1.1]hexane-2,5-dicarboxylic acid-I, a potent mGluR agonist. *Journal of Medicinal Chemistry*, **1998**, 41, 1641-50	8.3	62
239	Combined targeting of epidermal growth factor receptor, signal transducer and activator of transcription-3, and Bcl-X(L) enhances antitumor effects in squamous cell carcinoma of the head and neck. *Molecular Pharmacology*, **2008**, 73, 1632-42	4.3	61
238	BM-1197: a novel and specific Bcl-2/Bcl-xL inhibitor inducing complete and long-lasting tumor regression in vivo. *PLoS ONE*, **2014**, 9, e99404	3.7	61
237	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
236	Preclinical studies of Apogossypolone: a new nonpeptidic pan small-molecule inhibitor of Bcl-2, Bcl-XL and Mcl-1 proteins in Follicular Small Cleaved Cell Lymphoma model. *Molecular Cancer*, **2008**, 7, 20	42.1	60
235	Design, synthesis, and characterization of new embelin derivatives as potent inhibitors of X-linked inhibitor of apoptosis protein. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 5805-8	2.9	60
234	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
233	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
232	Therapeutic potential and molecular mechanism of a novel, potent, nonpeptide, Smac mimetic SM-164 in combination with TRAIL for cancer treatment. *Molecular Cancer Therapeutics*, **2011**, 10, 902-14	6.1	59
231	Phorbol esters and related analogs regulate the subcellular localization of beta 2-chimaerin, a non-protein kinase C phorbol ester receptor. *Journal of Biological Chemistry*, **2001**, 276, 18303-12	5.4	59
230	Enhancing systematic motion in molecular dynamics simulation. *Journal of Chemical Physics*, **1999**, 110, 9401-9410	3.9	59

229	Androgen receptor degraders overcome common resistance mechanisms developed during prostate cancer treatment. *Neoplasia*, **2020**, 22, 111-119	6.4	58
228	Development of Peptidomimetic Inhibitors of the ERG Gene Fusion Product in Prostate Cancer. *Cancer Cell*, **2017**, 31, 532-548.e7	24.3	57
227	An MDM2 antagonist (MI-319) restores p53 functions and increases the life span of orally treated follicular lymphoma bearing animals. *Molecular Cancer*, **2009**, 8, 115	42.1	57
226	Application of a Molecular Dynamics Simulation Method with a Generalized Effective Potential to the Flexible Molecular Docking Problems. *Journal of Physical Chemistry B*, **2000**, 104, 354-359	3.4	57
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224	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
223	MDM2 inhibitor MI-319 in combination with cisplatin is an effective treatment for pancreatic cancer independent of p53 function. *European Journal of Cancer*, **2010**, 46, 1122-31	7.5	54
222	(-)-Gossypol acts directly on the mitochondria to overcome Bcl-2- and Bcl-X(L)-mediated apoptosis resistance. *Molecular Cancer Therapeutics*, **2005**, 4, 23-31	6.1	54
221	Nonpeptidic small-molecule inhibitor of Bcl-2 and Bcl-XL, (-)-Gossypol, enhances biological effect of genistein against BxPC-3 human pancreatic cancer cell line. *Pancreas*, **2005**, 31, 317-24	2.6	53
220	Targeting the MDM2-p53 Protein-Protein Interaction for New Cancer Therapeutics. *Topics in Medicinal Chemistry*, **2012**, 57-79	0.4	51
219	Synthesis of spirooxindoles via asymmetric 1,3-dipolar cycloaddition. *Tetrahedron Letters*, **2005**, 46, 5949-5951	2	51
218	Resistance to BET Inhibitor Leads to Alternative Therapeutic Vulnerabilities in Castration-Resistant Prostate Cancer. *Cell Reports*, **2018**, 22, 2236-2245	10.6	50
217	Analysis of the binding of mixed lineage leukemia 1 (MLL1) and histone 3 peptides to WD repeat domain 5 (WDR5) for the design of inhibitors of the MLL1-WDR5 interaction. *Journal of Medicinal Chemistry*, **2010**, 53, 5179-85	8.3	50
216	Design and synthesis of a new, conformationally constrained, macrocyclic small-molecule inhibitor of STAT3 via R‐click chemistryR *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 3939-42	2.9	50
215	Discovery of a Highly Potent, Cell-Permeable Macrocyclic Peptidomimetic (MM-589) Targeting the WD Repeat Domain 5 Protein (WDR5)-Mixed Lineage Leukemia (MLL) Protein-Protein Interaction. *Journal of Medicinal Chemistry*, **2017**, 60, 4818-4839	8.3	49
214	Synthesis, molecular modeling, and biology of the 1-benzyl derivative of APDC-an apparent mGluR6 selective ligand. *Bioorganic and Medicinal Chemistry Letters*, **1997**, 7, 601-606	2.9	49
213	Structure-based design and synthesis of small molecule protein-tyrosine phosphatase 1B inhibitors. *Bioorganic and Medicinal Chemistry*, **1998**, 6, 1799-810	3.4	49
212	Helix Folding of an Alanine-Based Peptide in Explicit Water. *Journal of Physical Chemistry B*, **2001**, 105, 2227-2235	3.4	49

211	A potent small-molecule inhibitor of the DCN1-UBC12 interaction that selectively blocks cullin 3 neddylation. *Nature Communications*, **2017**, 8, 1150	17.4	48
210	Interaction of a cyclic, bivalent smac mimetic with the x-linked inhibitor of apoptosis protein. *Biochemistry*, **2008**, 47, 9811-24	3.2	48
209	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
208	Design of chemically stable, potent, and efficacious MDM2 inhibitors that exploit the retro-mannich ring-opening-cyclization reaction mechanism in spiro-oxindoles. *Journal of Medicinal Chemistry*, **2014**, 57, 10486-98	8.3	47
207	Design of small-molecule Smac mimetics as IAP antagonists. *Current Topics in Microbiology and Immunology*, **2011**, 348, 89-113	3.3	47
206	TW-37, a small-molecule inhibitor of Bcl-2, inhibits cell growth and invasion in pancreatic cancer. *International Journal of Cancer*, **2008**, 123, 958-66	7.5	47
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204	Molecular modeling studies of the Akt PH domain and its interaction with phosphoinositides. *Journal of Medicinal Chemistry*, **2001**, 44, 898-908	8.3	46
203	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
202	TW-37, a small-molecule inhibitor of Bcl-2, mediates S-phase cell cycle arrest and suppresses head and neck tumor angiogenesis. *Molecular Cancer Therapeutics*, **2009**, 8, 893-903	6.1	45
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