Sun Choi

List of Publications by Year in Descending Order

103 papers	2,261 citations	24 h-index	43 g-index
106 ext. papers	2,815 ext. citations	5.4 avg, IF	5.04 L-index

#	Paper	IF	Citations
103	Big data and artificial intelligence (AI) methodologies for computer-aided drug design (CADD).. *Biochemical Society Transactions*, **2022**,	5.1	3
102	Recent Applications of Deep Learning Methods on Evolution- and Contact-Based Protein Structure Prediction. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	3
101	Discovery and Biological Evaluation of -Methyl-pyrrolo[2,3-]pyridine-5-carboxamide Derivatives as JAK1-Selective Inhibitors. *Journal of Medicinal Chemistry*, **2021**, 64, 958-979	8.3	6
100	N-terminus-independent activation of c-Src via binding to a tetraspan(in) TM4SF5 in hepatocellular carcinoma is abolished by the TM4SF5 C-terminal peptide application. *Theranostics*, **2021**, 11, 8092-8111	12.1	1
99	Structural Characterization of Receptor-Receptor Interactions in the Allosteric Modulation of G Protein-Coupled Receptor (GPCR) Dimers. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
98	Subtle Chemical Changes Cross the Boundary between Agonist and Antagonist: New A Adenosine Receptor Homology Models and Structural Network Analysis Can Predict This Boundary. *Journal of Medicinal Chemistry*, **2021**, 64, 12525-12536	8.3	3
97	2-(Halogenated Phenyl) acetamides and propanamides as potent TRPV1 antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2021**, 48, 128266	2.9	0
96	Discovery of Benzopyridone-Based Transient Receptor Potential Vanilloid 1 Agonists and Antagonists and the Structural Elucidation of Their Activity Shift. *Journal of Medicinal Chemistry*, **2021**, 64, 370-384	8.3	3
95	Emerging computational approaches for the study of regio- and stereoselectivity in organic synthesis. *Organic Chemistry Frontiers*, **2021**, 8, 5165-5181	5.2	4
94	Asymmetric Total Syntheses of Kopsane Alkaloids via a PtCl -Catalyzed Intramolecular [3+2] Cycloaddition. *Angewandte Chemie - International Edition*, **2020**, 59, 12832-12836	16.4	15
93	Multiscale Molecular Modeling in G Protein-Coupled Receptor (GPCR)-Ligand Studies. *Biomolecules*, **2020**, 10,	5.9	3
92	Asymmetric Total Syntheses of Kopsane Alkaloids via a PtCl2-Catalyzed Intramolecular [3+2] Cycloaddition. *Angewandte Chemie*, **2020**, 132, 12932-12936	3.6	6
91	Advances in Molecular Dynamics Simulations and Enhanced Sampling Methods for the Study of Protein Systems. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	25
90	Importance of protein dynamics in the structure-based drug discovery of class A G protein-coupled receptors (GPCRs). *Current Opinion in Structural Biology*, **2019**, 55, 147-153	8.1	20
89	Transmembrane 4L Six Family Member 5 Senses Arginine for mTORC1 Signaling. *Cell Metabolism*, **2019**, 29, 1306-1319.e7	24.6	29
88	Discovery of Conformationally Restricted Human Glutaminyl Cyclase Inhibitors as Potent Anti-Alzheimer's Agents by Structure-Based Design. *Journal of Medicinal Chemistry*, **2019**, 62, 8011-8027	8.3	7
87	Total Synthesis of Hoiamide A Using an Evans-Tishchenko Reaction as a Key Step. *Organic Letters*, **2019**, 21, 5471-5474	6.2	12

86	Water-Soluble Phthalocyanines Selectively Bind to Albumin Dimers: A Green Approach Toward Enhancing Tumor-Targeted Photodynamic Therapy. *Theranostics*, **2019**, 9, 6412-6423	12.1	17
85	In Vivo Albumin Traps Photosensitizer Monomers from Self-Assembled Phthalocyanine Nanovesicles: A Facile and Switchable Theranostic Approach. *Journal of the American Chemical Society*, **2019**, 141, 1366-1372	16.4	105
84	Structure-activity relationship investigation of Phe-Arg mimetic region of human glutaminyl cyclase inhibitors. *Bioorganic and Medicinal Chemistry*, **2018**, 26, 3133-3144	3.4	7
83	Potent human glutaminyl cyclase inhibitors as potential anti-Alzheimer's agents: Structure-activity relationship study of Arg-mimetic region. *Bioorganic and Medicinal Chemistry*, **2018**, 26, 1035-1049	3.4	11
82	Understanding G Protein-Coupled Receptor Allostery via Molecular Dynamics Simulations: Implications for Drug Discovery. *Methods in Molecular Biology*, **2018**, 1762, 455-472	1.4	4
81	Recent Advances in Structure-Based Drug Design Targeting Class A G Protein-Coupled Receptors Utilizing Crystal Structures and Computational Simulations. *Journal of Medicinal Chemistry*, **2018**, 61, 1-46	8.3	55
80	Inhibitory effect of tartrate against phosphate-induced DJ-1 aggregation. *International Journal of Biological Macromolecules*, **2018**, 107, 1650-1658	7.9	3
79	Exploring G Protein-Coupled Receptors (GPCRs) Ligand Space via Cheminformatics Approaches: Impact on Rational Drug Design. *Frontiers in Pharmacology*, **2018**, 9, 128	5.6	43
78	4-Aminophenyl acetamides and propanamides as potent transient receptor potential vanilloid 1 (TRPV1) ligands. *Bioorganic and Medicinal Chemistry*, **2018**, 26, 4509-4517	3.4	3
77	Evolution of In Silico Strategies for Protein-Protein Interaction Drug Discovery. *Molecules*, **2018**, 23,	4.8	50
76	Integrated Ligand and Structure-Based Investigation of Structural Requirements for Silent Information Regulator 1 (SIRT1) Activation. *Current Topics in Medicinal Chemistry*, **2018**, 18, 2313-2324	3	1
75	Structural and Biochemical Characterization of the Curcumin-Reducing Activity of CurA from Vibrio vulnificus. *Journal of Agricultural and Food Chemistry*, **2018**, 66, 10608-10616	5.7	7
74	Adaptable Small Ligand of CYP1 Enzymes for Use in Understanding the Structural Features Determining Isoform Selectivity. *ACS Medicinal Chemistry Letters*, **2018**, 9, 1247-1252	4.3	3
73	Discovery of Potent Human Glutaminyl Cyclase Inhibitors as Anti-Alzheimer's Agents Based on Rational Design. *Journal of Medicinal Chemistry*, **2017**, 60, 2573-2590	8.3	23
72	t-Butyl pyridine and phenyl C-region analogues of 2-(3-fluoro-4-methylsulfonylaminophenyl)propanamides as potent TRPV1 antagonists. *Bioorganic and Medicinal Chemistry*, **2017**, 25, 2451-2462	3.4	6
71	N-Substituted 5'N-Methylcarbamoyl-4'selenoadenosines as Potent and Selective A Adenosine Receptor Agonists with Unusual Sugar Puckering and Nucleobase Orientation. *Journal of Medicinal Chemistry*, **2017**, 60, 3422-3437	8.3	17
70	MLACP: machine-learning-based prediction of anticancer peptides. *Oncotarget*, **2017**, 8, 77121-77136	3.3	134
69	Expediting the Design, Discovery and Development of Anticancer Drugs using Computational Approaches. *Current Medicinal Chemistry*, **2017**, 24, 4753-4778	4.3	12

68	Pyrazole C-region analogues of 2-(3-fluoro-4-methylsulfonylaminophenyl)propanamides as potent TRPV1 antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2017**, 27, 4383-4388	2.9	8
67	In silico prediction of multiple-category classification model for cytochrome P450 inhibitors and non-inhibitors using machine-learning method. *SAR and QSAR in Environmental Research*, **2017**, 28, 863-874	3.5	12
66	A novel pyrazole derivative protects from ovariectomy-induced osteoporosis through the inhibition of NADPH oxidase. *Scientific Reports*, **2016**, 6, 22389	4.9	28
65	Discovery of N-(3-fluoro-4-methylsulfonamidomethylphenyl)urea as a potent TRPV1 antagonistic template. *Bioorganic and Medicinal Chemistry Letters*, **2016**, 26, 3603-7	2.9	10
64	2-Sulfonamidopyridine C-region analogs of 2-(3-fluoro-4-methylsulfonamidophenyl)propanamides as potent TRPV1 antagonists. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 1231-40	3.4	9
63	Polymodal Transient Receptor Potential Vanilloid Type 1 Nocisensor: Structure, Modulators, and Therapeutic Applications. *Advances in Protein Chemistry and Structural Biology*, **2016**, 104, 81-125	5.3	31
62	Harnessing the Therapeutic Potential of Capsaicin and Its Analogues in Pain and Other Diseases. *Molecules*, **2016**, 21,	4.8	73
61	Synthesis and biological evaluation of 3-substituted 5-benzylidene-1-methyl-2-thiohydantoins as potent NADPH oxidase (NOX) inhibitors. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4144-4151	3.4	11
60	Design, synthesis, and anticancer activity of C8-substituted-4Sthionucleosides as potential HSP90 inhibitors. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 3418-28	3.4	11
59	Ultraslow Water-Mediated Transmembrane Interactions Regulate the Activation of A2A Adenosine Receptor. *Biophysical Journal*, **2016**, 111, 1180-1191	2.9	22
58	The discovery of 2,5-isomers of triazole-pyrrolopyrimidine as selective Janus kinase 2 (JAK2) inhibitors versus JAK1 and JAK3. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 5036-5046	3.4	10
57	Role of computer-aided drug design in modern drug discovery. *Archives of Pharmacal Research*, **2015**, 38, 1686-701	6.1	272
56	Substituted 2-(3-fluoro-4-methylsulfonamidophenyl)acetamides as potent TRPV1 antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 2326-30	2.9	10
55	Communication over the network of binary switches regulates the activation of A2A adenosine receptor. *PLoS Computational Biology*, **2015**, 11, e1004044	5	24
54	Anti-angiogenic activity of thienopyridine derivative LCB03-0110 by targeting VEGFR-2 and JAK/STAT3 Signalling. *Experimental Dermatology*, **2015**, 24, 503-9	4	10
53	5-Lipoxygenase inhibitors suppress RANKL-induced osteoclast formation via NFATc1 expression. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 7069-78	3.4	13
52	Structure activity relationships of benzyl C-region analogs of 2-(3-fluoro-4-methylsulfonamidophenyl)propanamides as potent TRPV1 antagonists. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 6844-54	3.4	7
51	Total synthesis of the putative structure of the proposed Banyasin A. *Frontiers in Chemistry*, **2015**, 3, 19	5	

50	Structure-Activity Relationships of Neplanocin A Analogues as S-Adenosylhomocysteine Hydrolase Inhibitors and Their Antiviral and Antitumor Activities. *Journal of Medicinal Chemistry*, **2015**, 58, 5108-20	8.3	24
49	The Cell Shape-determining Csd6 Protein from Helicobacter pylori Constitutes a New Family of L,D-Carboxypeptidase. *Journal of Biological Chemistry*, **2015**, 290, 25103-17	5.4	19
48	6,6-Fused heterocyclic ureas as highly potent TRPV1 antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 803-6	2.9	3
47	Transient receptor potential vanilloid type 1 antagonists: a patent review (2011 - 2014). *Expert Opinion on Therapeutic Patents*, **2015**, 25, 291-318	6.8	58
46	Promiscuous gating modifiers target the voltage sensor of K(v)7.2, TRPV1, and H(v)1 cation channels. *FASEB Journal*, **2014**, 28, 2591-602	0.9	9
45	Asymmetric synthesis and receptor activity of chiral simplified resiniferatoxin (sRTX) analogues as transient receptor potential vanilloid 1 (TRPV1) ligands. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 382-5	2.9	8
44	Synthesis and anti-renal fibrosis activity of conformationally locked truncated 2-hexynyl-N(6)-substituted-(N)-methanocarba-nucleosides as A3 adenosine receptor antagonists and partial agonists. *Journal of Medicinal Chemistry*, **2014**, 57, 1344-54	8.3	19
43	2-Alkyl/alkenyl substituted pyridine C-region analogues of 2-(3-fluoro-4-methylsulfonylaminophenyl)propanamides as highly potent TRPV1 antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 4039-43	2.9	13
42	2-Aryl substituted pyridine C-region analogues of 2-(3-fluoro-4-methylsulfonylaminophenyl)propanamides as highly potent TRPV1 antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 4044-7	2.9	15
41	Structural basis of the phosphorylation dependent complex formation of neurodegenerative disease protein Ataxin-1 and RBM17. *Biochemical and Biophysical Research Communications*, **2014**, 449, 399-404	3.4	6
40	Mapping the intramolecular signal transduction of G-protein coupled receptors. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 727-43	4.2	35
39	TRPV1 antagonist with high analgesic efficacy: 2-Thio pyridine C-region analogues of 2-(3-fluoro-4-methylsulfonylaminophenyl)propanamides. *Bioorganic and Medicinal Chemistry*, **2013**, 21, 6657-64	3.4	17
38	The carbonate analogues of 5Shalogenated resiniferatoxin as TRPV1 ligands. *European Journal of Medicinal Chemistry*, **2013**, 68, 233-43	6.8	5
37	Identification of active Plasmodium falciparum calpain to establish screening system for Pf-calpain-based drug development. *Malaria Journal*, **2013**, 12, 47	3.6	10
36	2-(3-Fluoro-4-methylsulfonylaminophenyl)propanamides as potent TRPV1 antagonists: structure activity relationships of the 2-oxy pyridine C-region. *European Journal of Medicinal Chemistry*, **2013**, 64, 589-602	6.8	21
35	Heterocycle-linked phenylbenzyl amides as novel TRPV1 antagonists and their TRPV1 binding modes: constraint-induced enhancement of in vitro and in vivo activities. *Chemistry - an Asian Journal*, **2013**, 8, 400-9	4.5	4
34	Molecular modeling studies of the novel inhibitors of DNA methyltransferases SGI-1027 and CBC12: implications for the mechanism of inhibition of DNMTs. *PLoS ONE*, **2013**, 8, e62152	3.7	44
33	N-4-t-Butylbenzyl 2-(4-methylsulfonylaminophenyl) propanamide TRPV1 antagonists: Structure-activity relationships in the A-region. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 215-24	3.4	12

32	Structure-activity relationships and molecular modeling of the N-(3-pivaloyloxy-2-benzylpropyl)-NS[4-(methylsulfonylamino)benzyl] thiourea template for TRPV1 antagonism. *Bioorganic and Medicinal Chemistry Letters*, **2012**, 22, 3656-60	2.9	5
31	2-(3-fluoro-4-methylsulfonylaminophenyl)propanamides as potent transient receptor potential vanilloid 1 (TRPV1) antagonists: structure-activity relationships of 2-amino derivatives in the N-(6-trifluoromethylpyridin-3-ylmethyl) C-region. *Journal of Medicinal Chemistry*, **2012**, 55, 8392-408	8.3	31
30	Structural origins for the loss of catalytic activities of bifunctional human LTA4H revealed through molecular dynamics simulations. *PLoS ONE*, **2012**, 7, e41063	3.7	4
29	Structure-activity relationships of truncated C2- or C8-substituted adenosine derivatives as dual acting A□A and A□adenosine receptor ligands. *Journal of Medicinal Chemistry*, **2012**, 55, 342-56	8.3	31
28	Selectivity enhancement arising from interactions at the PI3K unique pocket. *ChemMedChem*, **2012**, 7, 1379-83	3.7	4
27	8-Hydroxy-2-deoxyguanosine prevents plaque formation and inhibits vascular smooth muscle cell activation through Rac1 inactivation. *Free Radical Biology and Medicine*, **2012**, 53, 109-21	7.8	21
26	Link between allosteric signal transduction and functional dynamics in a multisubunit enzyme: S-adenosylhomocysteine hydrolase. *Journal of the American Chemical Society*, **2011**, 133, 19807-15	16.4	17
25	trans-Stilbenoids: potent and selective inhibitors for human cytochrome P450 1B1. *MedChemComm* , **2011**, 2, 402	5	14
24	Novel oxidative modifications in redox-active cysteine residues. *Molecular and Cellular Proteomics*, **2011**, 10, M110.000513	7.6	65
23	Structural insights into transient receptor potential vanilloid type 1 (TRPV1) from homology modeling, flexible docking, and mutational studies. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 317-27	4.2	56
22	X-ray crystal structure and binding mode analysis of human S-adenosylhomocysteine hydrolase complexed with novel mechanism-based inhibitors, haloneplanocin A analogues. *Journal of Medicinal Chemistry*, **2011**, 54, 930-8	8.3	27
21	Receptor activity and conformational analysis of 5Shalogenated resiniferatoxin analogs as TRPV1 ligands. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 299-302	2.9	5
20	Discovery of New Human A(2A) Adenosine Receptor Agonists: Design, Synthesis, and Binding Mode of Truncated 2-Hexynyl-4Sthioadenosine. *ACS Medicinal Chemistry Letters*, **2010**, 2010, 516-520	4.3	13
19	Herbal compound farnesiferol C exerts antiangiogenic and antitumor activity and targets multiple aspects of VEGFR1 (Flt1) or VEGFR2 (Flk1) signaling cascades. *Molecular Cancer Therapeutics*, **2010**, 9, 389-99	6.1	48
18	Design, synthesis, and binding of homologated truncated 4Sthioadenosine derivatives at the human A3 adenosine receptors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 7015-21	3.4	12
17	In silico classification of adenosine receptor antagonists using Laplacian-modified na□e Bayesian, support vector machine, and recursive partitioning. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 883-90	2.8	10
16	Identification of a potent and noncytotoxic inhibitor of melanin production. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5602-9	3.4	21
15	Oxidative modifications of glyceraldehyde-3-phosphate dehydrogenase play a key role in its multiple cellular functions. *Biochemical Journal*, **2009**, 423, 253-64	3.8	121

14	3D-QSAR studies of cytotoxic heterocyclic quinones using calculated reduction potential. *Drug Development Research*, **2009**, 70, 438-444	5.1	1
13	Non-vanillyl resiniferatoxin analogues as potent and metabolically stable transient receptor potential vanilloid 1 agonists. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 690-8	3.4	8
12	Discovery of a new template for anticancer agents: 2Sdeoxy-2Sfluoro-4Sselenoarabinofuranosyl-cytosine (2SF-4Sseleno-ara-C). *Journal of Medicinal Chemistry*, **2009**, 52, 5303-6	8.3	36
11	Stereoselective synthesis and conformational study of novel 2Ş3SDidehydro-2Ş3Sdideoxy-4Sselenonucleosides. *Journal of Organic Chemistry*, **2008**, 73, 4259-62	4.2	19
10	Capsiate, a nonpungent capsaicin-like compound, inhibits angiogenesis and vascular permeability via a direct inhibition of Src kinase activity. *Cancer Research*, **2008**, 68, 227-35	10.1	74
9	3D-QSAR studies of heterocyclic quinones with inhibitory activity on vascular smooth muscle cell proliferation using pharmacophore-based alignment. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 9772-9	3.4	13
8	Alpha-substituted N-(4-tert-butylbenzyl)-NS[4-(methylsulfonylamino)benzyl]thiourea analogues as potent and stereospecific TRPV1 antagonists. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 6043-53	3.4	24
7	Design, synthesis, and molecular modeling studies of 5Sdeoxy-5Sureidoadenosine: 5Sureido group as multiple hydrogen bonding donor in the active site of S-adenosylhomocysteine hydrolase. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 4456-9	2.9	9
6	Binding mode analysis of topoisomerase inhibitors, 6-arylamino-7-chloro-quinazoline-5,8-diones, within the cleavable complex of human topoisomerase I and DNA. *Archives of Pharmacal Research*, **2007**, 30, 1526-35	6.1	3
5	Efficient synthesis of 2-substituted 2,3-dihydro-4-quinolones as potential intermediates for 2-substituted 1,2,3,4-tetrahydro-4-quinolone antitumor agents. *Archives of Pharmacal Research*, **2006**, 29, 369-74	6.1	9
4	Stereoselective functionalization of the 1Sposition of 4Sthionucleosides. *Organic Letters*, **2006**, 8, 4267-70	6.2	9
3	The effects of biasing torsional mutations in a conformational GA. *Journal of Chemical Information and Modeling*, **2006**, 46, 1862-70	6.1	5
2	Balancing focused combinatorial libraries based on multiple GPCR ligands. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 529-38	4.2	8
1	The design, synthesis and activity of pentapeptide pp60c-src inhibitors containing L-phosphotyrosine mimics. *Chemical Biology and Drug Design*, **1998**, 51, 271-81		12