Hwangseo Park

List of Publications by Year
in descending order

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98 papers	2,206 citations	201674 27 h-index	254184 43 g-index
99 all docs	99 docs citations	99 times ranked	3612 citing authors

#	Article	IF	Citations
1	Resveratrol induces autophagy by directly inhibiting mTOR through ATP competition. Scientific Reports, 2016, 6, 21772.	3.3	200
2	Critical assessment of the automated AutoDock as a new docking tool for virtual screening. Proteins: Structure, Function and Bioinformatics, 2006, 65, 549-554.	2.6	160
3	Discovery of novel Î±-glucosidase inhibitors based on the virtual screening with the homology-modeled protein structure. Bioorganic and Medicinal Chemistry, 2008, 16, 284-292.	3.0	120
4	Thiazolidinedione derivatives as PTP1B inhibitors with antihyperglycemic and antiobesity effects. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6161-6165.	2.2	82
5	Structural and Dynamical Basis of Broad Substrate Specificity, Catalytic Mechanism, and Inhibition of Cytochrome P450 3A4. Journal of the American Chemical Society, 2005, 127, 13634-13642.	13.7	80
6	Discovery and biological evaluation of novel Î±-glucosidase inhibitors with in vivo antidiabetic effect. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 3711-3715.	2.2	79
7	Discovery of EGF Receptor Inhibitors That Are Selective for the d746<b>â€<b>750/T790M/C797S Mutant through Structureâ€Based de Novo Design. Angewandte Chemie - International Edition, 2017, 56, 7634-7638.	13.8	58
8	Prediction of Molecular Solvation Free Energy Based on the Optimization of Atomic Solvation Parameters with Genetic Algorithm. Journal of Chemical Information and Modeling, 2007, 47, 509-514.	5.4	51
9	NPCARE: database of natural products and fractional extracts for cancer regulation. Journal of Cheminformatics, 2017, 9, 2.	6.1	48
10	Binding Mechanism and Synergetic Effects of Xanthone Derivatives as Noncompetitive Î±-Glucosidase Inhibitors: A Theoretical and Experimental Study. Journal of Physical Chemistry B, 2013, 117, 13464-13471.	2.6	45
11	Structural basis for recognition of the tumor suppressor protein PTPN14 by the oncoprotein E7 of human papillomavirus. PLoS Biology, 2019, 17, e3000367.	5.6	45
12	A Structureâ€Based Virtual Screening Approach toward the Discovery of Histone Deacetylase Inhibitors: Identification of Promising Zincâ€Chelating Groups. ChemMedChem, 2010, 5, 591-597.	3.2	44
13	A novel class of Hsp90 inhibitors isolated by structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 6345-6349.	2.2	43
14	Rapid and simple detection of Tamiflu-resistant influenza virus: Development of oseltamivir derivative-based lateral flow biosensor for point-of-care (POC) diagnostics. Scientific Reports, 2018, 8, 12999.	3.3	42
15	Discovery of novel PRL-3 inhibitors based on the structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 2250-2255.	2.2	39
16	Structure-based virtual screening approach to identify novel classes of PTP1B inhibitors. European Journal of Medicinal Chemistry, 2009, 44, 3280-3284.	5.5	39
17	Discovery of Novel Cdc25 Phosphatase Inhibitors with Micromolar Activity Based on the Structure-Based Virtual Screening. Journal of Medicinal Chemistry, 2008, 51, 5533-5541.	6.4	38
18	Fluorinated NSC as a Cdc25 inhibitor. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 2351-2354.	2.2	36

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19	Discovery of the inhibitors of tumor necrosis factor alpha with structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 6195-6198.	2.2	35
20	Computational Design and Discovery of Nanomolar Inhibitors of Ĩ¹B Kinase Î². Journal of the American Chemical Society, 2015, 137, 337-348.	13.7	35
21	Discovery of Picomolar ABL Kinase Inhibitors Equipotent for Wild Type and T315I Mutant via Structure-Based de Novo Design. Journal of the American Chemical Society, 2013, 135, 8227-8237.	13.7	34
22	The family-wide structure and function of human dual-specificity protein phosphatases. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 421-435.	2.5	34
23	Consensus Scoring Approach To Identify the Inhibitors of AMP-Activated Protein Kinase Î±2 with Virtual Screening. Journal of Chemical Information and Modeling, 2014, 54, 2139-2146.	5.4	34
24	Anticancer activity of a novel small molecule tubulin inhibitor STK899704. PLoS ONE, 2017, 12, e0173311.	2.5	32
25	Cubic equation governing the outer-region dielectric constant of globular proteins. Physical Review E, 2007, 75, 021916.	2.1	30
26	Identification of Novel Inhibitors of Tropomyosin-Related Kinase A through the Structure-Based Virtual Screening with Homology-Modeled Protein Structure. Journal of Chemical Information and Modeling, 2011, 51, 2986-2993.	5.4	30
27	Nocodazole is a Highâ€Affinity Ligand for the Cancerâ€Related Kinases ABL, câ€KIT, BRAF, and MEK. ChemMedChem, 2012, 7, 53-56.	3.2	29
28	Structure-based de novo design and biochemical evaluation of novel Cdc25 phosphatase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 4330-4334.	2.2	28
29	New solvation free energy function comprising intermolecular solvation and intramolecular self-solvation terms. Journal of Cheminformatics, 2013, 5, 8.	6.1	26
30	Investigations on recyclisation and hydrolysis in avibactam mediated serine Î²-lactamase inhibition. Organic and Biomolecular Chemistry, 2016, 14, 4116-4128.	2.8	23
31	Role of Solvent Dynamics in Stabilizing the Transition State of RNA Hydrolysis by Hairpin Ribozyme. Journal of Chemical Theory and Computation, 2006, 2, 858-862.	5.3	22
32	Systematic Computational Design and Identification of Low Picomolar Inhibitors of Aurora Kinase A. Journal of Chemical Information and Modeling, 2018, 58, 700-709.	5.4	20
33	Extended solvent-contact model approach to SAMPL4 blind prediction challenge for hydration free energies. Journal of Computer-Aided Molecular Design, 2014, 28, 175-186.	2.9	19
34	Application of Fragment-Based de Novo Design to the Discovery of Selective Picomolar Inhibitors of Glycogen Synthase Kinase-3 Beta. Journal of Medicinal Chemistry, 2016, 59, 9018-9034.	6.4	19
35	Structure-based virtual screening approach to the discovery of novel PTPMT1 phosphatase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 1271-1275.	2.2	18
36	Structureâ€Based Virtual Screening Approach to the Discovery of Novel Inhibitors of Eyes Absent 2 Phosphatase with Various Metal Chelating Moieties. Chemical Biology and Drug Design, 2011, 78, 642-650.	3.2	17

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37	Identification of small molecules that inhibit the histone chaperone Asf1 and its chromatin function. BMB Reports, 2015, 48, 685-690.	2.4	17
38	Computational prediction of octanolâ€“water partition coefficient based on the extended solvent-contact model. Journal of Molecular Graphics and Modelling, 2015, 60, 108-117.	2.4	16
39	The anti-ALS drug riluzole attenuates pericyte loss in the diabetic retinopathy of streptozotocin-treated mice. Toxicology and Applied Pharmacology, 2017, 315, 80-89.	2.8	16
40	Development of 6E3 antibody-mediated SERS immunoassay for drug-resistant influenza virus. Biosensors and Bioelectronics, 2021, 187, 113324.	10.1	16
41	Discovery of potent inhibitors of receptor protein tyrosine phosphatase sigma through the structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 6333-6337.	2.2	15
42	Identification of new Hsp90 inhibitors by structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 4839-4842.	2.2	14
43	Structure-based de novo design and biochemical evaluation of novel BRAF kinase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 1027-1030.	2.2	14
44	Structure-based virtual screening approach to identify novel classes of Cdc25B phosphatase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 4372-4375.	2.2	13
45	Discovery of Dual Inhibitors for Wild Type and D816V Mutant of c-KIT Kinase through Virtual and Biochemical Screening of Natural Products. Journal of Natural Products, 2016, 79, 293-299.	3.0	13
46	Structure-Based Virtual Screening and De Novo Design of PIM1 Inhibitors with Anticancer Activity from Natural Products. Pharmaceuticals, 2021, 14, 275.	3.8	13
47	Discovery of VHR Phosphatase Inhibitors with Micromolar Activity based on Structureâ€Based Virtual Screening. ChemMedChem, 2008, 3, 877-880.	3.2	11
48	Identification of novel inhibitors of mitogen-activated protein kinase phosphatase-1 with structure-based virtual screening. Journal of Computer-Aided Molecular Design, 2011, 25, 469-475.	2.9	11
49	Exploring binding sites other than the catalytic core in the crystal structure of the catalytic domain of MKP-4. Acta Crystallographica Section D: Biological Crystallography, 2011, 67, 25-31.	2.5	11
50	Discovery of Novel DUSP16 Phosphatase Inhibitors through Virtual Screening with Homology Modeled Protein Structure. Journal of Biomolecular Screening, 2014, 19, 1383-1390.	2.6	10
51	Accuracy enhancement in the estimation of molecular hydration free energies by implementing the intramolecular hydrogen bond effects. Journal of Cheminformatics, 2015, 7, 57.	6.1	10
52	Computational Prediction of Molecular Hydration Entropy with Hybrid Scaled Particle Theory and Free-Energy Perturbation Method. Journal of Chemical Theory and Computation, 2015, 11, 4933-4942.	5.3	10
53	Development and application of a comprehensive machine learning program for predicting molecular biochemical and pharmacological properties. Physical Chemistry Chemical Physics, 2019, 21, 5189-5199.	2.8	10
54	Development of A4 antibody for detection of neuraminidase I223R/H275Y-associated antiviral multidrug-resistant influenza virus. Nature Communications, 2020, 11, 3418.	12.8	10

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55	Free energy perturbation approach for the rational engineering of the antibody for human hepatitis B virus. Journal of Molecular Graphics and Modelling, 2011, 29, 643-649.	2.4	9
56	Discovery of MEK/PI3K dual inhibitor via structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 4946-4950.	2.2	9
57	Virtual screening and biochemical evaluation to identify new inhibitors of mammalian target of rapamycin (mTOR). Bioorganic and Medicinal Chemistry Letters, 2014, 24, 835-838.	2.2	9
58	Discovery of Low Micromolar Dual Inhibitors for Wild Type and L1196M Mutant of Anaplastic Lymphoma Kinase through Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 802-810.	5.4	9
59	Identification of novel inhibitors of extracellular signal-regulated kinase 2 based on the structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 5372-5376.	2.2	8
60	Structure-based virtual screening approach to the discovery of p38 MAP kinase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 2195-2199.	2.2	8
61	Structural basis for the dephosphorylating activity of PTPRQ towards phosphatidylinositide substrates. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 1522-1529.	2.5	8
62	Structure-based de novo design and identification of D816V mutant-selective c-KIT inhibitors. Organic and Biomolecular Chemistry, 2014, 12, 4644-4655.	2.8	8
63	Predicting the Electrochemical Properties of Lithium-Ion Battery Electrode Materials with the Quantum Neural Network Algorithm. Journal of Physical Chemistry C, 2019, 123, 4682-4690.	3.1	8
64	Quantum Artificial Neural Network Approach to Derive a Highly Predictive 3D-QSAR Model for Bloodâ€“Brain Barrier Passage. International Journal of Molecular Sciences, 2021, 22, 10995.	4.1	8
65	New angleâ€dependent potential energy function for backboneâ€“backbone hydrogen bond in proteinâ€“protein interactions. Journal of Computational Chemistry, 2010, 31, 897-903.	3.3	7
66	Identification of novel BRAF kinase inhibitors with structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5753-5756.	2.2	7
67	Identification of common inhibitors of wild-type and T315I mutant of BCR-ABL through the parallel structure-based virtual screening. Journal of Computer-Aided Molecular Design, 2012, 26, 983-992.	2.9	7
68	Identification of novel PTPRQ phosphatase inhibitors based on the virtual screening with docking simulations. Theoretical Biology and Medical Modelling, 2013, 10, 49.	2.1	7
69	Structure-based de novo design and synthesis of aminothiazole-based p38 MAP kinase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 3784-3787.	2.2	7
70	Discovery of EGF Receptor Inhibitors That Are Selective for the d746â€750/T790M/C797S Mutant through Structureâ€Based de Novo Design. Angewandte Chemie, 2017, 129, 7742-7746.	2.0	7
71	Identifying New AMP-Activated Protein Kinase Inhibitors That Protect against Ischemic Brain Injury. ACS Chemical Neuroscience, 2019, 10, 2345-2354.	3.5	7
72	Development of antibody against drug-resistant respiratory syncytial virus: Rapid detection of mutant virus using split superfolder green fluorescent protein-antibody system. Biosensors and Bioelectronics, 2021, 194, 113593.	10.1	7

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73	Discovery of Novel DUSP4 Inhibitors through the Virtual Screening with Docking Simulations. Bulletin of the Korean Chemical Society, 2014, 35, 2655-2659.	1.9	7
74	Nanosecond molecular dynamics simulations of Cdc25B and its complex with a 1,4-naphthoquinone inhibitor: Implications for rational inhibitor design. Journal of Molecular Graphics and Modelling, 2008, 27, 13-19.	2.4	6
75	Identification of Potent VHZ Phosphatase Inhibitors with Structure-Based Virtual Screening. Journal of Biomolecular Screening, 2013, 18, 226-231.	2.6	6
76	Extended solvent-contact model approach to blind SAMPL5 prediction challenge for the distribution coefficients of drug-like molecules. Journal of Computer-Aided Molecular Design, 2016, 30, 1019-1033.	2.9	6
77	Identification of novel protein tyrosine phosphatase sigma inhibitors promoting neurite extension. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 87-93.	2.2	6
78	Rational Computational Design of Fourth-Generation EGFR Inhibitors to Combat Drug-Resistant Non-Small Cell Lung Cancer. International Journal of Molecular Sciences, 2020, 21, 9323.	4.1	6
79	A human protein hydroxylase that accepts D-residues. Communications Chemistry, 2020, 3, .	4.5	6
80	Toward the virtual screening of Cdc25A phosphatase inhibitors with the homology modeled protein structure. Journal of Molecular Modeling, 2008, 14, 833-841.	1.8	5
81	Structure-based de novo design of Eya2 phosphatase inhibitors. Journal of Molecular Graphics and Modelling, 2012, 38, 382-388.	2.4	5
82	Two-track virtual screening approach to identify both competitive and allosteric inhibitors of human small C-terminal domain phosphatase 1. Journal of Computer-Aided Molecular Design, 2017, 31, 743-753.	2.9	5
83	Structure-based virtual screening approach to the discovery of novel inhibitors of factor-inhibiting HIF-1: Identification of new chelating groups for the active-site ferrous ion. Bioorganic and Medicinal Chemistry, 2009, 17, 7769-7774.	3.0	4
84	Structure-based virtual screening approach to the discovery of phosphoinositide 3-kinase alpha inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 2021-2024.	2.2	4
85	Virtual screening and biochemical evaluation of the inhibitors of dual-specificity phosphatase 26. Medicinal Chemistry Research, 2013, 22, 3905-3910.	2.4	4
86	Homology modeling and virtual screening approaches to identify potent inhibitors of slingshot phosphatase 1. Journal of Molecular Graphics and Modelling, 2013, 39, 65-70.	2.4	4
87	Virtual Screening with Docking Simulations and Biochemical Evaluation of VHY Phosphatase Inhibitors. Chemical and Pharmaceutical Bulletin, 2015, 63, 807-811.	1.3	4
88	Kinase and GPCR polypharmacological approach for the identification of efficient anticancer medicines. Organic and Biomolecular Chemistry, 2020, 18, 8402-8413.	2.8	4
89	Force field design and molecular dynamics simulations of factor-inhibiting HIF-1 and its complex with known inhibitors: Implications for rational inhibitor design. Journal of Molecular Graphics and Modelling, 2010, 29, 221-228.	2.4	3
90	Extended solvent-contact model for protein solvation: Test cases for dipeptides. Journal of Molecular Graphics and Modelling, 2013, 42, 50-59.	2.4	3

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91	A Dynamic Substrate Pool Revealed by cryo-EM of a Lipid-Preserved Respiratory Supercomplex. Antioxidants and Redox Signaling, 2022, 36, 1101-1118.	5.4	3
92	Discovery of novel protein tyrosine phosphatase sigma inhibitors through the virtual screening with modified scoring function. Medicinal Chemistry Research, 2014, 23, 1016-1022.	2.4	2
93	Discovery of Novel Striatalâ€enriched Protein Tyrosine Phosphatase Inhibitors Through Structureâ€based Virtual Screening. Bulletin of the Korean Chemical Society, 2016, 37, 1783-1788.	1.9	2
94	Identification of N-(5-(phenoxymethyl)-1,3,4-thiadiazol-2-yl)acetamide derivatives as novel protein tyrosine phosphatase epsilon inhibitors exhibiting anti-osteoclastic activity. Bioorganic and Medicinal Chemistry, 2018, 26, 5204-5211.	3.0	2
95	Synthesis and biological evaluation of acylthiourea against DUSP1 inhibition. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 1746-1748.	2.2	2
96	Identification of Potent Leukocyte Common Antigen-Related Phosphatase Inhibitors via Structure-Based Virtual Screening. Bulletin of the Korean Chemical Society, 2013, 34, 2006-2010.	1.9	2
97	Molecular Characterization of Two Monoclonal Antibodies against the Same Epitope on B-Cell Receptor Associated Protein 31. PLoS ONE, 2016, 11, e0167527.	2.5	1
98	Virtual Screening and Biochemical Evaluation to Identify the Allosteric Inhibitors of Dual Specificity Phosphatase 1. Bulletin of the Korean Chemical Society, 2019, 40, 236-242.	1.9	0