Csaba Hetenyi

List of Publications by Year
in descending order

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75 papers	3,514 citations	172457 29 h-index	144013 57 g-index
76 all docs	76 docs citations	76 times ranked	5157 citing authors

#	Article	IF	Citations
1	Mechanism of Blebbistatin Inhibition of Myosin II. Journal of Biological Chemistry, 2004, 279, 35557-35563.	3.4	839
2	Efficient docking of peptides to proteins without prior knowledge of the binding site. Protein Science, 2009, 11, 1729-1737.	7.6	370
3	Blind docking of drug-sized compounds to proteins with up to a thousand residues. FEBS Letters, 2006, 580, 1447-1450.	2.8	253
4	The autoimmune regulator PHD finger binds to nonâ€methylated histone H3K4 to activate gene expression. EMBO Reports, 2008, 9, 370-376.	4.5	210
5	The autoimmune regulator PHD finger binds to non-methylated histone H3K4 to activate gene expression. EMBO Reports, 2008, 9, 370-376.	4.5	131
6	A new easy-to-prepare homogeneous continuous electrochromatographic bed for enantiomer recognition. Electrophoresis, 2000, 21, 3116-3125.	2.4	91
7	Some studies of the chromatographic properties of gels (â€˜Artificial antibodies/receptorsâ€™) for selective adsorption of proteins. Chromatographia, 2001, 54, 7-14.	1.3	79
8	In vitro model of neurotoxicity of A? 1?42 and neuroprotection by a pentapeptide: irreversible events during the first hour. Neurobiology of Disease, 2004, 17, 507-515.	4.4	65
9	Pentapeptide Amides Interfere with the Aggregation of Î²-Amyloid Peptide of Alzheimer's Disease. Biochemical and Biophysical Research Communications, 2002, 292, 931-936.	2.1	64
10	Toward prediction of functional protein pockets using blind docking and pocket search algorithms. Protein Science, 2011, 20, 880-893.	7.6	59
11	Drug Effect Prediction by Polypharmacology-Based Interaction Profiling. Journal of Chemical Information and Modeling, 2012, 52, 134-145.	5.4	57
12	Drug efficiency indices for improvement of molecular docking scoring functions. Journal of Computational Chemistry, 2010, 31, 174-184.	3.3	53
13	Alternatively Spliced Exon B of Myosin Va Is Essential for Binding the Tail-Associated Light Chain Shared by Dynein. Biochemistry, 2006, 45, 12582-12595.	2.5	50
14	Interaction of mycotoxin zearalenone with human serum albumin. Journal of Photochemistry and Photobiology B: Biology, 2017, 170, 16-24.	3.8	47
15	Mapping of Possible Binding Sequences of Two Beta-Sheet Breaker Peptides on Beta Amyloid Peptide of Alzheimer's Disease. Bioorganic and Medicinal Chemistry, 2002, 10, 1587-1593.	3.0	46
16	The Structure of an NDR/LATS Kinaseâ€“Mob Complex Reveals a Novel Kinaseâ€“Coactivator System and Substrate Docking Mechanism. PLoS Biology, 2015, 13, e1002146.	5.6	45
17	Extended Intermolecular Interactions in a Serine Proteaseâ€“Canonical Inhibitor Complex Account for Strong and Highly Specific Inhibition. Journal of Molecular Biology, 2005, 350, 156-169.	4.2	43
18	Ribosomal Intersubunit Bridge B2a Is Involved in Factor-Dependent Translation Initiation and Translational Processivity. Journal of Molecular Biology, 2009, 385, 405-422.	4.2	43

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19	Regulation of the Equilibrium between Closed and Open Conformations of Annexin A2 by N-Terminal Phosphorylation and S100A4-Binding. Structure, 2017, 25, 1195-1207.e5.	3.3	42
20	DrugLogit: Logistic Discrimination between Drugs and Nondrugs Including Disease-Specificity by Assigning Probabilities Based on Molecular Properties. Journal of Chemical Information and Modeling, 2012, 52, 2165-2180.	5.4	38
21	Quantification of Solvent Contribution to the Stability of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2013, 9, 4542-4551.	5.3	37
22	Molecular Property Filters Describing Pharmacokinetics and Drug Binding. Current Medicinal Chemistry, 2012, 19, 1646-1662.	2.4	36
23	Cooperative Binding of Cyclodextrin Dimers to Isoflavone Analogues Elucidated by Free Energy Calculations. Journal of Physical Chemistry C, 2014, 118, 7163-7173.	3.1	35
24	Interaction of Citrinin with Human Serum Albumin. Toxins, 2015, 7, 5155-5166.	3.4	35
25	Inhibitory Effects of Quercetin and Its Human and Microbial Metabolites on Xanthine Oxidase Enzyme. International Journal of Molecular Sciences, 2019, 20, 2681.	4.1	35
26	Hydrogen bonding interactions of benzylidene type Schiff bases studied by vibrational spectroscopic and computational methods. Physical Chemistry Chemical Physics, 2003, 5, 2009-2014.	2.8	33
27	Effects of Chrysin and Its Major Conjugated Metabolites Chrysin-7-Sulfate and Chrysin-7-Glucuronide on Cytochrome P450 Enzymes and on OATP, P-gp, BCRP, and MRP2 Transporters. Drug Metabolism and Disposition, 2020, 48, 1064-1073.	3.3	33
28	Combination of a Modified Scoring Function with Two-Dimensional Descriptors for Calculation of Binding Affinities of Bulky, Flexible Ligands to Proteins. Journal of the American Chemical Society, 2006, 128, 1233-1239.	13.7	31
29	Structural assembly of the signaling competent ERK2â€“RSK1 heterodimeric protein kinase complex. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2711-2716.	7.1	31
30	Mobility-based prediction of hydration structures of protein surfaces. Bioinformatics, 2015, 31, 1959-1965.	4.1	30
31	Exploration of Interfacial Hydration Networks of Targetâ€“Ligand Complexes. Journal of Chemical Information and Modeling, 2016, 56, 148-158.	5.4	30
32	Investigation of Non-Covalent Interactions of Aflatoxins (B1, B2, G1, G2, and M1) with Serum Albumin. Toxins, 2017, 9, 339.	3.4	30
33	Interactions of zearalenone and its reduced metabolites Î±-zearalenol and Î²-zearalenol with serum albumins: species differences, binding sites, and thermodynamics. Mycotoxin Research, 2018, 34, 269-278.	2.3	30
34	The role of water in ligand binding. Current Opinion in Structural Biology, 2021, 67, 1-8.	5.7	30
35	Selective Perturbation of the Myosin Recovery Stroke by Point Mutations at the Base of the Lever Arm Affects ATP Hydrolysis and Phosphate Release. Journal of Biological Chemistry, 2007, 282, 17658-17664.	3.4	28
36	Pharmacokinetic interaction of diosmetin and silibinin with other drugs: Inhibition of CYP2C9-mediated biotransformation and displacement from serum albumin. Biomedicine and Pharmacotherapy, 2018, 102, 912-921.	5.6	27

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37	Interaction of Chrysin and Its Main Conjugated Metabolites Chrysin-7-Sulfate and Chrysin-7-Glucuronide with Serum Albumin. International Journal of Molecular Sciences, 2018, 19, 4073.	4.1	27
38	Structure-based calculation of drug efficiency indices. Bioinformatics, 2007, 23, 2678-2685.	4.1	26
39	Structural Evidence for Non-canonical Binding of Ca2+ to a Canonical EF-hand of a Conventional Myosin. Journal of Biological Chemistry, 2005, 280, 41458-41464.	3.4	20
40	Systematic exploration of multiple drug binding sites. Journal of Cheminformatics, 2017, 9, 65.	6.1	20
41	Testing the Pharmacokinetic Interactions of 24 Colonic Flavonoid Metabolites with Human Serum Albumin and Cytochrome P450 Enzymes. Biomolecules, 2020, 10, 409.	4.0	20
42	Myosin cleft closure determines the energetics of the actomyosin interaction. FASEB Journal, 2011, 25, 111-121.	0.5	19
43	Novel Drug-Like Somatostatin Receptor 4 Agonists are Potential Analgesics for Neuropathic Pain. International Journal of Molecular Sciences, 2019, 20, 6245.	4.1	19
44	Contribution of 2D and 3D Structural Features of Drug Molecules in the Prediction of Drug Profile Matching. Journal of Chemical Information and Modeling, 2012, 52, 1733-1744.	5.4	16
45	DYNLL2 Dynein Light Chain Binds to an Extended Linear Motif of Myosin 5a Tail That Has Structural Plasticity. Biochemistry, 2014, 53, 7107-7122.	2.5	15
46	Synthesis of Spin-Labelled Bergamottin: A Potent CYP3A4 Inhibitor with Antiproliferative Activity. International Journal of Molecular Sciences, 2020, 21, 508.	4.1	15
47	A Comprehensive Docking Study on the Selectivity of Binding of Aromatic Compounds to Proteins. Journal of Chemical Information and Computer Sciences, 2003, 43, 1576-1583.	2.8	13
48	Pseudouridylation of 23S rRNA helix 69 promotes peptide release by release factor RF2 but not by release factor RF1. Biochimie, 2011, 93, 834-844.	2.6	13
49	Conformational Dynamics of Titin PEVK Explored with FRET Spectroscopy. Biophysical Journal, 2012, 103, 1480-1489.	0.5	12
50	Comparative investigation of thein vitroinhibitory potencies of 13-epimeric estrones and D-secoestrones towards 17Î²-hydroxysteroid dehydrogenase type 1. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 61-69.	5.2	12
51	Diseaseâ€Specific Differentiation Between Drugs and Nonâ€Drugs Using Principal Component Analysis of Their Molecular Descriptor Space. Molecular Informatics, 2012, 31, 369-383.	2.5	11
52	A Fragmenting Protocol with Explicit Hydration for Calculation of Binding Enthalpies of Target-Ligand Complexes at a Quantum Mechanical Level. International Journal of Molecular Sciences, 2019, 20, 4384.	4.1	11
53	Interaction of 2â€²R-ochratoxin A with Serum Albumins: Binding Site, Effects of Site Markers, Thermodynamics, Species Differences of Albumin-binding, and Influence of Albumin on Its Toxicity in MDCK Cells. Toxins, 2018, 10, 353.	3.4	10
54	Determination of Ligand Binding Modes in Hydrated Viral Ion Channels to Foster Drug Design and Repositioning. Journal of Chemical Information and Modeling, 2021, 61, 4011-4022.	5.4	10

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55	Interaction of SZV 1287, a novel oxime analgesic drug candidate, and its metabolites with serum albumin. Journal of Molecular Liquids, 2021, 333, 115945.	4.9	10
56	Small molecule somatostatin receptor subtype 4 (sst4) agonists are novel anti-inflammatory and analgesic drug candidates. Neuropharmacology, 2020, 178, 108198.	4.1	9
57	Molecular Structure, Binding Affinity, and Biological Activity in the Epigenome. International Journal of Molecular Sciences, 2020, 21, 4134.	4.1	9
58	Towards Unraveling the Histone Code by Fragment Blind Docking. International Journal of Molecular Sciences, 2019, 20, 422.	4.1	8
59	Interaction of the mycotoxin metabolite dihydrocitrinone with serum albumin. Mycotoxin Research, 2019, 35, 129-139.	2.3	8
60	Computational studies on the binding of Î²-sheet breaker (BSB) peptides on amyloid Î²A(1â€“42). Computational and Theoretical Chemistry, 2001, 542, 25-31.	1.5	7
61	In Silico, In Vitro and In Vivo Pharmacodynamic Characterization of Novel Analgesic Drug Candidate Somatostatin SST4 Receptor Agonists. Frontiers in Pharmacology, 2020, 11, 601887.	3.5	7
62	Molecular pathomechanisms of Alzheimer's disease. Computational and Theoretical Chemistry, 2003, 666-667, 507-513.	1.5	5
63	Structure-Based Calculation of Binding Affinities of Î±2A-Adrenoceptor Agonists. ChemMedChem, 2007, 2, 801-805.	3.2	4
64	Ndr/Lats Kinases Bind Specific Mob-Family Coactivators through a Conserved and Modular Interface. Biochemistry, 2020, 59, 1688-1700.	2.5	4
65	Incorporation of Oxidized Phenylalanine Derivatives into Insulin Signaling Relevant Proteins May Link Oxidative Stress to Signaling Conditions Underlying Chronic Insulin Resistance. Biomedicines, 2022, 10, 975.	3.2	4
66	Exploration of Somatostatin Binding Mechanism to Somatostatin Receptor Subtype 4. International Journal of Molecular Sciences, 2022, 23, 6878.	4.1	4
67	Dynamic changes in binding interaction networks of sex steroids establish their non-classical effects. Scientific Reports, 2017, 7, 14847.	3.3	3
68	Analysis of the influence of simulation parameters on biomolecule-linked water networks. Journal of Molecular Graphics and Modelling, 2018, 82, 117-128.	2.4	2
69	Prerequisite Binding Modes Determine the Dynamics of Action of Covalent Agonists of Ion Channel TRPA1. Pharmaceuticals, 2021, 14, 988.	3.8	2
70	Systematic Exploration of Binding Modes of Ligands on Drug Targets. Methods in Molecular Biology, 2020, 2112, 107-121.	0.9	1
71	A new easy-to-prepare homogeneous continuous electrochromatographic bed for enantiomer recognition. Electrophoresis, 2000, 21, 3116-3125.	2.4	1
72	A Comprehensive Docking Study on the Selectivity of Binding of Aromatic Compounds to Proteins.. ChemInform, 2003, 34, no.	0.0	0

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73	Structure of Titin PEVK Explored with FRET Spectroscopy. Biophysical Journal, 2012, 102, 361a.	0.5	0
74	Somatostatin receptor subtype 4 is a promising drug target for the treatment of neuropathic pain, neurogenic inflammation, anxiety and depression. Proceedings for Annual Meeting of the Japanese Pharmacological Society, 2018, WCP2018, PO2-2-39.	0.0	0
75	Binding Networks Identify Targetable Protein Pockets for Mechanism-Based Drug Design. International Journal of Molecular Sciences, 2022, 23, 7313.	4.1	0