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List of Publications by Year
in descending order

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41	2,021	236925	265206
papers	citations	25 h-index	42 g-index

42	42	42	1483
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	3D proteochemometrics: using three-dimensional information of proteins and ligands to address aspects of the selectivity of serine proteases. MedChemComm, 2017, 8, 1037-1045.	3.4	7
2	Predictive proteochemometric models for kinases derived from 3D protein field-based descriptors. MedChemComm, 2016, 7, 1007-1015.	3.4	12
3	Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. MedChemComm, 2015, 6, 24-50.	3.4	109
4	Design and evaluation of substrate-based octapeptide and non substrate-based tetrapeptide inhibitors of dengue virus NS2Bâ€“NS3 proteases. Biochemical and Biophysical Research Communications, 2013, 434, 767-772.	2.1	34
5	Visually Interpretable Models of Kinase Selectivity Related Features Derived from Field-Based Proteochemometrics. Journal of Chemical Information and Modeling, 2013, 53, 3021-3030.	5.4	30
6	Proteochemometrics analysis of substrate interactions with dengue virus NS3 proteases. Bioorganic and Medicinal Chemistry, 2008, 16, 9369-9377.	3.0	47
7	Proteochemometric modeling of HIV protease susceptibility. BMC Bioinformatics, 2008, 9, 181.	2.6	70
8	A Look Inside HIV Resistance through Retroviral Protease Interaction Maps. PLoS Computational Biology, 2007, 3, e48.	3.2	23
9	Proteochemometric modelling of antibody-antigen interactions using SPOT synthesised peptide arrays. Protein Engineering, Design and Selection, 2007, 20, 301-307.	2.1	17
10	QSAR of multiple mutated antibodies. Journal of Molecular Recognition, 2007, 20, 97-102.	2.1	6
11	Proteochemometric modeling reveals the interaction site for Trp9 modified Î±-MSH peptides in melanocortin receptors. Proteins: Structure, Function and Bioinformatics, 2007, 67, 653-660.	2.6	16
12	Proteochemometric analysis of small cyclic peptides' interaction with wild-type and chimeric melanocortin receptors. Proteins: Structure, Function and Bioinformatics, 2007, 69, 83-96.	2.6	15
13	Probing the substrate specificity of the dengue virus type 2 NS3 serine protease by using internally quenched fluorescent peptides. Biochemical Journal, 2006, 397, 203-211.	3.7	52
14	Rough set-based proteochemometrics modeling of G-protein-coupled receptor-ligand interactions. Proteins: Structure, Function and Bioinformatics, 2006, 63, 24-34.	2.6	26
15	Generalized modeling of enzyme-ligand interactions using proteochemometrics and local protein substructures. Proteins: Structure, Function and Bioinformatics, 2006, 65, 568-579.	2.6	38
16	Prediction of indirect interactions in proteins. BMC Bioinformatics, 2006, 7, 167.	2.6	38
17	Unbiased descriptor and parameter selection confirms the potential of proteochemometric modelling. BMC Bioinformatics, 2005, 6, 50.	2.6	32
18	Proteochemometric Mapping of the Interaction of Organic Compounds with Melanocortin Receptor Subtypes. Molecular Pharmacology, 2005, 67, 50-59.	2.3	38

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19	Improved approach for proteochemometrics modeling: application to organic compound--amine G protein-coupled receptor interactions. Bioinformatics, 2005, 21, 4289-4296.	4.1	76
20	Synthesis and Quantitative Structureâ^'Activity Relationship of Hydrazones ofN-Amino-Nâ€˜-hydroxyguanidine as Electron Acceptors for Xanthine Oxidase. Journal of Medicinal Chemistry, 2004, 47, 3105-3110.	6.4	22
21	QSAR and Proteo-chemometric Analysis of the Interaction of a Series of Organic Compounds with Melanocortin Receptor Subtypes. Journal of Medicinal Chemistry, 2003, 46, 2572-2579.	6.4	48
22	Proteo-chemometrics analysis of MSH peptide binding to melanocortin receptors. Protein Engineering, Design and Selection, 2002, 15, 305-311.	2.1	28
23	Proteochemometrics Modeling of the Interaction of Amine G-Protein Coupled Receptors with a Diverse Set of Ligands. Molecular Pharmacology, 2002, 61, 1465-1475.	2.3	85
24	Classification of G-protein coupled receptors by alignment-independent extraction of principal chemical properties of primary amino acid sequences. Protein Science, 2002, 11, 795-805.	7.6	124
25	Development of proteo-chemometrics: a novel technology for the analysis of drug-receptor interactions. Biochimica Et Biophysica Acta - General Subjects, 2001, 1525, 180-190.	2.4	118
26	Design of new small cyclic melanocortin receptor-binding peptides using molecular modelling: Role of the His residue in the melanocortin peptide core. European Journal of Medicinal Chemistry, 2001, 36, 137-146.	5.5	22
27	Detection of regions in the MC1 receptor of importance for the selectivity of the MC1 receptor super-selective MS04/MS05 peptides. BBA - Proteins and Proteomics, 2001, 1544, 278-282.	2.1	6
28	PLS modeling of chimeric MS04/MSH-peptide and MC1/MC3-receptor interactions reveals a novel method for the analysis of ligandâ€“receptor interactions. BBA - Proteins and Proteomics, 2001, 1544, 350-357.	2.1	42
29	Identification of the binding pocket for the TRH peptide in the melanocortin 1 receptor. International Journal of Peptide Research and Therapeutics, 2000, 7, 225-228.	0.1	2
30	New aspects on the melanocortins and their receptors. Pharmacological Research, 2000, 42, 393-420.	7.1	313
31	Long term orexigenic effect of a novel melanocortin 4 receptor selective antagonist. British Journal of Pharmacology, 1999, 126, 27-34.	5.4	70
32	Thyrotropin releasing hormone (TRH) selectively binds and activates the melanocortin 1 receptor. Peptides, 1999, 20, 395-400.	2.4	21
33	Discovery of novel melanocortin4 receptor selective MSH analogues. British Journal of Pharmacology, 1998, 124, 75-82.	5.4	129
34	Characterization of the enzymatic activity for biphasic competition by guanoxabenz (1-(2,6-dichlorobenzylidene-amino)-3-hydroxyguanidine) at Î±2-adrenoceptors. Biochemical Pharmacology, 1998, 56, 1121-1128.	4.4	5
35	Conditions for biphasic competition curves in radioligand binding for ligands subjected to metabolic transformation. Biochemical Pharmacology, 1998, 56, 1129-1137.	4.4	3
36	Selective properties of C- and N-terminals and core residues of the melanocyte-stimulating hormone on binding to the human melanocortin receptor subtypes. European Journal of Pharmacology, 1998, 349, 359-366.	3.5	32

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37	Binding of cyclic and linear MSH core peptides to the melanocortin receptor subtypes. European Journal of Pharmacology, 1997, 319, 369-373.	3.5	47
38	Characterisation of D117A and H260A mutations in the melanocortin 1 receptor. Molecular and Cellular Endocrinology, 1997, 126, 213-219.	3.2	23
39	Selectivity of Cyclic [d-Nal7] and [d-Phe7] Substituted MSH Analogues for the Melanocortin Receptor Subtypes. Peptides, 1997, 18, 1009-1013.	2.4	84
40	Modeling of the three-dimensional structure of the human melanocortin 1 receptor, using an automated method and docking of a rigid cyclic melanocyte-stimulating hormone core peptide. Journal of Molecular Graphics and Modelling, 1997, 15, 307-317.	2.4	64
41	Evidence Indicating That the TM4, EL2, and TM5 of the Melanocortin 3 Receptor Do Not Participate in Ligand Binding. Biochemical and Biophysical Research Communications, 1996, 229, 687-692.	2.1	18