Irini Doytchinova

List of Publications by Year
in descending order

115	7,153	126858	64755
papers	citations	33 h-index	79 g-index

116	116	116	6014
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	VaxiJen: a server for prediction of protective antigens, tumour antigens and subunit vaccines. BMC Bioinformatics, 2007, 8, 4.	1.2	1,740
2	AllerTOP v.2â€"a server for in silico prediction of allergens. Journal of Molecular Modeling, 2014, 20, 2278.	0.8	663
3	AllergenFP: allergenicity prediction by descriptor fingerprints. Bioinformatics, 2014, 30, 846-851.	1.8	471
4	T-cell epitope vaccine design by immunoinformatics. Open Biology, 2013, 3, 120139.	1.5	324
5	AllerTOP - a server for in silico prediction of allergens. BMC Bioinformatics, 2013, 14, S4.	1.2	293
6	Hydrazones of 1,2-benzisothiazole hydrazides: synthesis, antimicrobial activity and QSAR investigations. European Journal of Medicinal Chemistry, 2002, 37, 553-564.	2.6	235
7	MHCPred: a server for quantitative prediction of peptide-MHC binding. Nucleic Acids Research, 2003, 31, 3621-3624.	6.5	228
8	Identifying candidate subunit vaccines using an alignment-independent method based on principal amino acid properties. Vaccine, 2007, 25, 856-866.	1.7	174
9	In Silico Identification of Supertypes for Class II MHCs. Journal of Immunology, 2005, 174, 7085-7095.	0.4	173
10	Synthesis andÂantiproliferative activity ofÂbenzo[d]isothiazole hydrazones. European Journal of Medicinal Chemistry, 2006, 41, 624-632.	2.6	149
11	EpiJen: a server for multistep T cell epitope prediction. BMC Bioinformatics, 2006, 7, 131.	1.2	144
12	JenPep: a database of quantitative functional peptide data for immunology. Bioinformatics, 2002, 18, 434-439.	1.8	137
13	Toward the Quantitative Prediction of T-Cell Epitopes:Â CoMFA and CoMSIA Studies of Peptides with Affinity for the Class I MHC Molecule HLA-A*0201. Journal of Medicinal Chemistry, 2001, 44, 3572-3581.	2.9	128
14	Identifiying Human MHC Supertypes Using Bioinformatic Methods. Journal of Immunology, 2004, 172, 4314-4323.	0.4	123
15	Synthesis of some new S-triazine based chalcones and their derivatives as potent antimicrobial agents. European Journal of Medicinal Chemistry, 2010, 45, 510-518.	2.6	92
16	Additive Method for the Prediction of Proteinâ^'Peptide Binding Affinity. Application to the MHC Class I Molecule HLA-A*0201. Journal of Proteome Research, 2002, 1, 263-272.	1.8	89
17	Towards the in silico identification of class II restricted T-cell epitopes: a partial least squares iterative self-consistent algorithm for affinity prediction. Bioinformatics, 2003, 19, 2263-2270.	1.8	78
18	JenPep:â€‰ A Novel Computational Information Resource for Immunobiology and Vaccinology. Journal of Chemical Information and Computer Sciences, 2003, 43, 1276-1287.	2.8	77

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19	Coupling In Silico and In Vitro Analysis of Peptide-MHC Binding: A Bioinformatic Approach Enabling Prediction of Superbinding Peptides and Anchorless Epitopes. Journal of Immunology, 2004, 172, 7495-7502.	0.4	67
20	Galantamine derivatives with indole moiety: Docking, design, synthesis and acetylcholinesterase inhibitory activity. Bioorganic and Medicinal Chemistry, 2015, 23, 5382-5389.	1.4	67
21	MHCPred 2.0. Applied Bioinformatics, 2006, 5, 55-61.	1.7	65
22	Physicochemical explanation of peptide binding to HLA-A*0201 major histocompatibility complex: A three-dimensional quantitative structure-activity relationship study. Proteins: Structure, Function and Bioinformatics, 2002, 48, 505-518.	1.5	61
23	EpiTOPâ€"a proteochemometric tool for MHC class II binding prediction. Bioinformatics, 2010, 26, 2066-2068.	1.8	55
24	Quantitative online prediction of peptide binding to the major histocompatibility complex. Journal of Molecular Graphics and Modelling, 2004, 22, 195-207.	1.3	54
25	Peptide binding prediction for the human class II MHC allele HLA-DP2: a molecular docking approach. BMC Structural Biology, 2011, 11, 32.	2.3	52
26	Towards the chemometric dissection of peptide â€“ HLA-A*0201 binding affinity: comparison of local and global QSAR models. Journal of Computer-Aided Molecular Design, 2005, 19, 203-212.	1.3	51
27	EpiDOCK: a molecular docking-based tool for MHC class II binding prediction. Protein Engineering, Design and Selection, 2013, 26, 631-634.	1.0	51
28	Quantitative approaches to computational vaccinology. Immunology and Cell Biology, 2002, 80, 270-279.	1.0	46
29	Analysis of Peptideâ^'Protein Binding Using Amino Acid Descriptors:â€‰ Prediction and Experimental Verification for Human Histocompatibility Complex HLA-A*0201. Journal of Medicinal Chemistry, 2005, 48, 7418-7425.	2.9	46
30	Transporter Associated with Antigen Processing Preselection of Peptides Binding to the MHC: A Bioinformatic Evaluation. Journal of Immunology, 2004, 173, 6813-6819.	0.4	40
31	A comparative molecular similarity index analysis (CoMSIA) study identifies an HLA-A2 binding supermotif. Journal of Computer-Aided Molecular Design, 2002, 16, 535-544.	1.3	36
32	Curcumin Inhibits the Primary Nucleation of Amyloid-Beta Peptide: A Molecular Dynamics Study. Biomolecules, 2020, 10, 1323.	1.8	36
33	The HLA-A2-supermotif: a QSAR definitionElectronic supplementary information (ESI) available: matrices for A*6802, A*0206, A*0203, A*0202 and A*0201. See http://www.rsc.org/suppdata/ob/b3/b300707c/. Organic and Biomolecular Chemistry, 2003, 1, 2648.	1.5	34
34	Novel hits for acetylcholinesterase inhibition derived by docking-based screening on ZINC database. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 768-776.	2.5	32
35	Quantitative structureâ€"activity relationships and the prediction of MHC supermotifs. Methods, 2004, 34, 444-453.	1.9	31
36	Quantitative structureâ€"plasma protein binding relationships of acidic drugs. Journal of Pharmaceutical Sciences, 2012, 101, 4627-4641.	1.6	31

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37	Class I T-cell epitope prediction: Improvements using a combination of proteasome cleavage, TAP affinity, and MHC binding. Molecular Immunology, 2006, 43, 2037-2044.	1.0	30
38	Novel camphane-based anti-tuberculosis agents with nanomolar activity. European Journal of Medicinal Chemistry, 2013, 70, 372-379.	2.6	30
39	Proteomics in Vaccinology and Immunobiology: An Informatics Perspective of the Immunone. Journal of Biomedicine and Biotechnology, 2003, 2003, 267-290.	3.0	29
40	Peptide binding to the HLA-DRB1 supertype: A proteochemometrics analysis. European Journal of Medicinal Chemistry, 2010, 45, 236-243.	2.6	27
41	Aminothiazole derivatives with antidegenerative activity on cartilage. Bioorganic and Medicinal Chemistry, 2003, 11, 2983-2989.	1.4	26
42	Immunogenicity Prediction by VaxiJen: A Ten Year Overview. Journal of Proteomics and Bioinformatics, 2017, 10, .	0.4	26
43	Toward Prediction of Class II Mouse Major Histocompatibility Complex Peptide Binding Affinity:Â in Silico Bioinformatic Evaluation Using Partial Least Squares, a Robust Multivariate Statistical Technique. Journal of Chemical Information and Modeling, 2006, 46, 1491-1502.	2.5	25
44	VaxiJen Dataset of Bacterial Immunogens: An Update. Current Computer-Aided Drug Design, 2019, 15, 398-400.	0.8	25
45	Molecular Docking Study on Galantamine Derivatives as Cholinesterase Inhibitors. Molecular Informatics, 2015, 34, 394-403.	1.4	24
46	Drug Designâ€"Past, Present, Future. Molecules, 2022, 27, 1496.	1.7	24
47	Dockingâ€based design and synthesis of galantamineâ€“camphane hybrids as inhibitors of acetylcholinesterase. Chemical Biology and Drug Design, 2017, 90, 709-718.	1.5	23
48	Reversed-phase high-performance liquid chromatography for evaluating the distribution of pharmaceutical substances in suppository baseâ€“phosphate buffer system. Journal of Pharmaceutical and Biomedical Analysis, 2000, 23, 955-964.	1.4	22
49	Predicting Class I Major Histocompatibility Complex (MHC) Binders Using Multivariate Statistics:â€‰ Comparison of Discriminant Analysis and Multiple Linear Regression. Journal of Chemical Information and Modeling, 2007, 47, 234-238.	2.5	22
50	A comparative molecular similarity indices (CoMSIA) study of peptide binding to the HLA-A3 superfamily. Bioorganic and Medicinal Chemistry, 2003, 11, 2307-2311.	1.4	21
51	Prediction of Steady-State Volume of Distribution of Acidic Drugs by Quantitative Structureâ€“Pharmacokinetics Relationships. Journal of Pharmaceutical Sciences, 2012, 101, 1253-1266.	1.6	21
52	Using databases and data mining in vaccinology. Expert Opinion on Drug Discovery, 2007, 2, 19-35.	2.5	20
53	MHC Class II Binding Predictionâ€"A Little Help from a Friend. Journal of Biomedicine and Biotechnology, 2010, 2010, 1-8.	3.0	20
54	Synthetic piperine amide analogs with antimycobacterial activity. Chemical Biology and Drug Design, 2018, 91, 763-768.	1.5	20

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55	Modeling the Peptideâ^'T Cell Receptor Interaction by the Comparative Molecular Similarity Indices Analysisâ^'Soft Independent Modeling of Class Analogy Technique. Journal of Medicinal Chemistry, 2006, 49, 2193-2199.	2.9	19
56	Galantamine-Curcumin Hybrids as Dual-Site Binding Acetylcholinesterase Inhibitors. Molecules, 2020, 25, 3341.	1.7	19
57	A Novel Galantamine-Curcumin Hybrid as a Potential Multi-Target Agent against Neurodegenerative Disorders. Molecules, 2021, 26, 1865.	1.7	19
58	In Silico Prediction of Peptide Binding Affinity to Class I Mouse Major Histocompatibility Complexes:â€‰ A Comparative Molecular Similarity Index Analysis (CoMSIA) Study. Journal of Chemical Information and Modeling, 2005, 45, 1415-1423.	2.5	18
59	Topical anal fissure treatment: placebo-controlled study of mononitrate and trinitrate therapies. International Journal of Colorectal Disease, 2009, 24, 461-464.	1.0	18
60	Associations between Milk and Egg Allergens and the HLA-DRB1/DQ Polymorphism: A Bioinformatics Approach. International Archives of Allergy and Immunology, 2016, 169, 33-39.	0.9	18
61	Peptide binding to HLA-DP proteins at pH 5.0 and pH 7.0: a quantitative molecular docking study. BMC Structural Biology, 2012, 12, 20.	2.3	17
62	Phenolic derivatives in raspberry (Rubus L.) germplasm collection in Bulgaria. Biochemical Systematics and Ecology, 2013, 50, 419-427.	0.6	17
63	New horizons in mouse immunoinformatics: reliable in silico prediction of mouse class I histocompatibility major complex peptide binding affinity. Organic and Biomolecular Chemistry, 2004, 2, 3274.	1.5	16
64	HLAâ€ÐP2 binding prediction by molecular dynamics simulations. Protein Science, 2011, 20, 1918-1928.	3.1	16
65	MHC Class II Binding Prediction by Molecular Docking. Molecular Informatics, 2011, 30, 368-375.	1.4	16
66	Antimycobacterial activity of chiral aminoalcohols with camphane scaffold. European Journal of Medicinal Chemistry, 2014, 81, 150-157.	2.6	16
67	Quantitative Structure â€“ Pharmacokinetics Relationships Analysis of Basic Drugs: Volume of Distribution. Journal of Pharmacy and Pharmaceutical Sciences, 2015, 18, 515.	0.9	16
68	Docking-based Design of Galantamine Derivatives with Dual-site Binding to Acetylcholinesterase. Molecular Informatics, 2016, 35, 278-285.	1.4	16
69	Integrating In Silico and In Vitro Analysis of Peptide Binding Affinity to HLA-Cw*0102: A Bioinformatic Approach to the Prediction of New Epitopes. PLoS ONE, 2009, 4, e8095.	1.1	15
70	Quantitative Structure â€“ Clearance Relationships of Acidic Drugs. Molecular Pharmaceutics, 2013, 10, 3758-3768.	2.3	14
71	Predicting Immunogenicity Risk in Biopharmaceuticals. Symmetry, 2021, 13, 388.	1.1	14
72	Quantitative Structure â€“ Activity Relationship Study on Saponins as Cytotoxicity Enhancers. Letters in Drug Design and Discovery, 2014, 12, 166-171.	0.4	14

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73	Proteochemometrics-Based Prediction of Peptide Binding to HLA-DP Proteins. Journal of Chemical Information and Modeling, 2018, 58, 297-304.	2.5	13
74	Thiazolyl-N-substituted amides: A group of effective anti-inflammatory agents with potential for local anesthetic properties. Synthesis, biological evaluation, and a QSAR approach. Drug Development Research, 1999, 48, 53-60.	1.4	12
75	Bacterial Immunogenicity Prediction by Machine Learning Methods. Vaccines, 2020, 8, 709.	2.1	12
76	Allergenicity prediction by artificial neural networks. Journal of Chemometrics, 2014, 28, 282-286.	0.7	11
77	Design, Synthesis, and Antimycobacterial Activity of Novel Theophyllineâ€7âEAcetic Acid Derivatives With Amino Acid Moieties. Chemical Biology and Drug Design, 2016, 87, 335-341.	1.5	11
78	Bone protective effects of purified extract from Ruscus aculeatus on ovariectomy-induced osteoporosis in rats. Food and Chemical Toxicology, 2019, 132, 110668.	1.8	11
79	2D and 3D QSAR analysis of some valproic acid metabolites and analogues as anticonvulsant agents. Pharmaceutical Research, 2000, 17, 727-732.	1.7	10
80	Platinum Complexes with 5â€Methylâ€5(4â€pyridyl)hydantoin and Its 3â€Methyl Derivatives: Synthesis and Cytotoxic Activity â€“ Quantitative Structureâ€Activity Relationships. Archiv Der Pharmazie, 2011, 344, 209-216.	2.1	10
81	Effects of Curcumin and Ferulic Acid on the Folding of Amyloid-Î² Peptide. Molecules, 2021, 26, 2815.	1.7	10
82	Virtual Screening and Hit Selection of Natural Compounds as Acetylcholinesterase Inhibitors. Molecules, 2022, 27, 3139.	1.7	10
83	CoMFA Study on Adenosine A2A Receptor Agonists. QSAR and Combinatorial Science, 2001, 20, 124-129.	1.4	9
84	Discovery of a Novel Acetylcholinesterase Inhibitor by Fragment-Based Design and Virtual Screening. Molecules, 2021, 26, 2058.	1.7	9
85	Histidine Hydrogen Bonding in MHC at pH 5 and pH 7 Modeled by Molecular Docking and Molecular Dynamics Simulations. Current Computer-Aided Drug Design, 2014, 10, 41-49.	0.8	9
86	In silico prediction of cancer immunogens: current state of the art. BMC Immunology, 2018, 19, 11.	0.9	8
87	Preparation and Evaluation of Isosorbide Mononitrate Hydrogels for Topical Fissure Treatment. Current Drug Delivery, 2012, 9, 452-458.	0.8	7
88	In-depth characterization of the GOTCAB saponins in seven cultivated Gypsophila L. species (Caryophyllaceae) by liquid chromatography coupled with quadrupole-Orbitrap mass spectrometer. Biochemical Systematics and Ecology, 2019, 83, 91-102.	0.6	7
89	Protein-engineered molecules carrying GAD65 epitopes and targeting CD35 selectively down-modulate disease-associated human B lymphocytes. Clinical and Experimental Immunology, 2019, 197, 329-340.	1.1	7
90	CoMFA-based comparison of two models of binding site on adenosine A1 receptor. , 2001, 15, 29-39.		6

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91	QSAR and the Prediction of T-Cell Epitopes. Current Proteomics, 2008, 5, 73-95.	0.1	6
92	Different approaches for determination of the attachment degree of polyethylene glycols to poly(anhydride) nanoparticles. Drug Development and Industrial Pharmacy, 2010, 36, 676-680.	0.9	6
93	A Cohesive and Integrated Platform for Immunogenicity Prediction. Methods in Molecular Biology, 2016, 1404, 761-770.	0.4	6
94	Galantamine Derivatives as Acetylcholinesterase Inhibitors: Docking, Design, Synthesis, and Inhibitory Activity. Neuromethods, 2018, , 163-176.	0.2	6
95	Hepato-, neuroprotective effects and QSAR studies on flavoalkaloids and flavonoids fromAstragalus monspessulanus. Biotechnology and Biotechnological Equipment, 2019, 33, 1434-1443.	0.5	6
96	Bridging solvent molecules mediate RNase A â€“ Ligand binding. PLoS ONE, 2019, 14, e0224271.	1.1	6
97	The Amaryllidaceae alkaloids: an untapped source of acetylcholinesterase inhibitors. Phytochemistry Reviews, 2022, 21, 1415-1443.	3.1	6
98	Adenosine A 2A receptor agonists: CoMFA-based selection of the most predictive conformation. SAR and QSAR in Environmental Research, 2002, 13, 227-235.	1.0	4
99	Quantitative Prediction of Peptide Binding to HLA-DP1 Protein. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2013, 10, 811-815.	1.9	4
100	Design of novel camphane-based derivatives with antimycobacterial activity. Journal of Molecular Graphics and Modelling, 2014, 51, 7-12.	1.3	4
101	Peptide Binding Prediction to Five Most Frequent HLAâ€ĐQ Proteins â€“ a Proteochemometric Approach. Molecular Informatics, 2015, 34, 467-476.	1.4	4
102	Biodegradable cross-linked prodrug of the bronchial dilator VephyllineÂ®. 2. Kinetics and quantum chemical studies on the release mechanism. Journal of Controlled Release, 1999, 58, 189-194.	4.8	3
103	Synthesis, 5-HT1A and 5-HT2A receptor affinity and QSAR study of 1-benzhydryl-piperazine derivatives with xanthine moiety at N4. Medicinal Chemistry Research, 2012, 21, 477-486.	1.1	3
104	A Galantamineâ€“Curcumin Hybrid Decreases the Cytotoxicity of Amyloid-Beta Peptide on SH-SY5Y Cells. International Journal of Molecular Sciences, 2021, 22, 7592.	1.8	3
105	An Alignment-Independent Platform for Allergenicity Prediction. Methods in Molecular Biology, 2020, 2131, 147-153.	0.4	3
106	Proteochemometrics for the Prediction of Binding to the MHC Proteins. Letters in Drug Design and Discovery, 2016, 14, 2-9.	0.4	2
107	Proteochemometrics for the Prediction of Peptide Binding to Multiple HLA Class II Proteins. Methods in Pharmacology and Toxicology, 2018, , 395-404.	0.1	1
108	MOLECULAR DOCKING STUDY ON 1-(3-(4-BENZYLPIPERAZIN-1-YL)PROPYL)-3,7-DIMETHYL-1H-PURINE-2,6(3H,7H)-DIONE AS AN ACETYLCHOLINESTERASE INHIBITOR. CBU International Conference Proceedings, 0, 6, 898-903.	0.0	1

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109	Beneficial effects of the fructus Sophorae extract on experimentally induced osteoporosis in New Zealand white rabbits. Acta Pharmaceutica, 2022, 72, 289-302.	0.9	1
110	Computational Chemistry, Informatics, and the Discovery of Vaccines. Current Computer-Aided Drug Design, 2005, 1, 377-395.	0.8	0
111	In Silico QSAR-Based Predictions of Class I and Class II MHC Epitopes. , 2008, , 63-89.		0
112	Substrate â€“ Inositol Transporter Interactions: Molecular Docking Study. Letters in Drug Design and Discovery, 2015, 12, 622-627.	0.4	0
113	Design of Multi-Epitope Vaccine against SARS-CoV-2. Cybernetics and Information Technologies, 2020, 20, 185-193.	0.4	0
114	Immunoinformatic Analysis of Human Thyroglobulin. Cybernetics and Information Technologies, 2020, 20, 194-200.	0.4	0
115	In Silico Identification of the B-Cell and T-Cell Epitopes of the Antigenic Proteins of Staphylococcus aureus for Potential Vaccines. Methods in Molecular Biology, 2022, 2412, 439-447.	0.4	0