Irini Doytchinova

List of Publications by Citations

109 papers	4,857 citations	31 h-index	68 g-index
116 ext. papers	6,019 ext. citations	4.1 avg, IF	5.86 L-index

#	Paper	IF	Citations
109	VaxiJen: a server for prediction of protective antigens, tumour antigens and subunit vaccines. *BMC Bioinformatics*, **2007**, 8, 4	3.6	1001
108	AllerTOP v.2--a server for in silico prediction of allergens. *Journal of Molecular Modeling*, **2014**, 20, 2278	2	305
107	AllergenFP: allergenicity prediction by descriptor fingerprints. *Bioinformatics*, **2014**, 30, 846-51	7.2	249
106	T-cell epitope vaccine design by immunoinformatics. *Open Biology*, **2013**, 3, 120139	7	241
105	Hydrazones of 1,2-benzisothiazole hydrazides: synthesis, antimicrobial activity and QSAR investigations. *European Journal of Medicinal Chemistry*, **2002**, 37, 553-64	6.8	215
104	MHCPred: A server for quantitative prediction of peptide-MHC binding. *Nucleic Acids Research*, **2003**, 31, 3621-4	20.1	188
103	AllerTOP--a server for in silico prediction of allergens. *BMC Bioinformatics*, **2013**, 14 Suppl 6, S4	3.6	156
102	In silico identification of supertypes for class II MHCs. *Journal of Immunology*, **2005**, 174, 7085-95	5.3	151
101	Synthesis and antiproliferative activity of benzo[d]isothiazole hydrazones. *European Journal of Medicinal Chemistry*, **2006**, 41, 624-32	6.8	128
100	JenPep: a database of quantitative functional peptide data for immunology. *Bioinformatics*, **2002**, 18, 434-9	7.2	128
99	EpiJen: a server for multistep T cell epitope prediction. *BMC Bioinformatics*, **2006**, 7, 131	3.6	118
98	Toward the quantitative prediction of T-cell epitopes: coMFA and coMSIA studies of peptides with affinity for the class I MHC molecule HLA-A*0201. *Journal of Medicinal Chemistry*, **2001**, 44, 3572-81	8.3	115
97	Identifiying human MHC supertypes using bioinformatic methods. *Journal of Immunology*, **2004**, 172, 4314-23	5.3	106
96	Identifying candidate subunit vaccines using an alignment-independent method based on principal amino acid properties. *Vaccine*, **2007**, 25, 856-66	4.1	102
95	Additive method for the prediction of protein-peptide binding affinity. Application to the MHC class I molecule HLA-A*0201. *Journal of Proteome Research*, **2002**, 1, 263-72	5.6	77
94	Synthesis of some new S-triazine based chalcones and their derivatives as potent antimicrobial agents. *European Journal of Medicinal Chemistry*, **2010**, 45, 510-8	6.8	73
93	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, 2263-70	7.2	68

92	JenPep: a novel computational information resource for immunobiology and vaccinology. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1276-87		65
91	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, 7495-502	5.3	63
90	Galantamine derivatives with indole moiety: Docking, design, synthesis and acetylcholinesterase inhibitory activity. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 5382-9	3.4	59
89	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, 505-18	4.2	55
88	MHCPred 2.0: an updated quantitative T-cell epitope prediction server. *Applied Bioinformatics*, **2006** , 5, 55-61		53
87	EpiTOP--a proteochemometric tool for MHC class II binding prediction. *Bioinformatics*, **2010**, 26, 2066-8	7.2	43
86	Analysis of peptide-protein binding using amino acid descriptors: prediction and experimental verification for human histocompatibility complex HLA-A0201. *Journal of Medicinal Chemistry*, **2005**, 48, 7418-25	8.3	43
85	Quantitative online prediction of peptide binding to the major histocompatibility complex. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 195-207	2.8	43
84	Towards the chemometric dissection of peptide--HLA-A*0201 binding affinity: comparison of local and global QSAR models. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 203-12	4.2	43
83	Quantitative approaches to computational vaccinology. *Immunology and Cell Biology*, **2002**, 80, 270-9	5	40
82	Peptide binding prediction for the human class II MHC allele HLA-DP2: a molecular docking approach. *BMC Structural Biology*, **2011**, 11, 32	2.7	38
81	EpiDOCK: a molecular docking-based tool for MHC class II binding prediction. *Protein Engineering, Design and Selection*, **2013**, 26, 631-4	1.9	36
80	Transporter associated with antigen processing preselection of peptides binding to the MHC: a bioinformatic evaluation. *Journal of Immunology*, **2004**, 173, 6813-9	5.3	35
79	The HLA-A2-supermotif: a QSAR definition. *Organic and Biomolecular Chemistry*, **2003**, 1, 2648-54	3.9	31
78	Class I T-cell epitope prediction: improvements using a combination of proteasome cleavage, TAP affinity, and MHC binding. *Molecular Immunology*, **2006**, 43, 2037-44	4.3	28
77	A comparative molecular similarity index analysis (CoMSIA) study identifies an HLA-A2 binding supermotif. *Journal of Computer-Aided Molecular Design*, **2002**, 16, 535-44	4.2	27
76	Novel camphane-based anti-tuberculosis agents with nanomolar activity. *European Journal of Medicinal Chemistry*, **2013**, 70, 372-9	6.8	24
75	Peptide binding to the HLA-DRB1 supertype: a proteochemometrics analysis. *European Journal of Medicinal Chemistry*, **2010**, 45, 236-43	6.8	24

74	Quantitative structure-activity relationships and the prediction of MHC supermotifs. *Methods*, **2004**, 34, 444-53	4.6	24
73	Proteomics in Vaccinology and Immunobiology: An Informatics Perspective of the Immunone. *Journal of Biomedicine and Biotechnology*, **2003**, 2003, 267-290		23
72	Aminothiazole derivatives with antidegenerative activity on cartilage. *Bioorganic and Medicinal Chemistry*, **2003**, 11, 2983-9	3.4	23
71	Toward prediction of class II mouse major histocompatibility complex peptide binding affinity: in silico bioinformatic evaluation using partial least squares, a robust multivariate statistical technique. *Journal of Chemical Information and Modeling*, **2006**, 46, 1491-502	6.1	22
70	Predicting class I major histocompatibility complex (MHC) binders using multivariate statistics: comparison of discriminant analysis and multiple linear regression. *Journal of Chemical Information and Modeling*, **2007**, 47, 234-8	6.1	21
69	Docking-based design and synthesis of galantamine-camphane hybrids as inhibitors of acetylcholinesterase. *Chemical Biology and Drug Design*, **2017**, 90, 709-718	2.9	20
68	Molecular Docking Study on Galantamine Derivatives as Cholinesterase Inhibitors. *Molecular Informatics*, **2015**, 34, 394-403	3.8	19
67	Quantitative structure--plasma protein binding relationships of acidic drugs. *Journal of Pharmaceutical Sciences*, **2012**, 101, 4627-41	3.9	19
66	Reversed-phase high-performance liquid chromatography for evaluating the distribution of pharmaceutical substances in suppository base-phosphate buffer system. *Journal of Pharmaceutical and Biomedical Analysis*, **2000**, 23, 955-64	3.5	18
65	Novel hits for acetylcholinesterase inhibition derived by docking-based screening on ZINC database. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2018**, 33, 768-776	5.6	17
64	MHC Class II Binding Prediction-A Little Help from a Friend. *Journal of Biomedicine and Biotechnology*, **2010**, 2010, 705821		17
63	In silico prediction of peptide binding affinity to class I mouse major histocompatibility complexes: a comparative molecular similarity index analysis (CoMSIA) study. *Journal of Chemical Information and Modeling*, **2005**, 45, 1415-23	6.1	17
62	Modeling the peptide-T cell receptor interaction by the comparative molecular similarity indices analysis-soft independent modeling of class analogy technique. *Journal of Medicinal Chemistry*, **2006**, 49, 2193-9	8.3	17
61	A comparative molecular similarity indices (CoMSIA) study of peptide binding to the HLA-A3 superfamily. *Bioorganic and Medicinal Chemistry*, **2003**, 11, 2307-11	3.4	17
60	Topical anal fissure treatment: placebo-controlled study of mononitrate and trinitrate therapies. *International Journal of Colorectal Disease*, **2009**, 24, 461-4	3	16
59	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, 3274-83	3.9	16
58	Prediction of steady-state volume of distribution of acidic drugs by quantitative structure-pharmacokinetics relationships. *Journal of Pharmaceutical Sciences*, **2012**, 101, 1253-66	3.9	15
57	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	2.7	15

56	Docking-based Design of Galantamine Derivatives with Dual-site Binding to Acetylcholinesterase. *Molecular Informatics*, **2016**, 35, 278-85	3.8	15
55	MHC Class II Binding Prediction by Molecular Docking. *Molecular Informatics*, **2011**, 30, 368-75	3.8	14
54	Antimycobacterial activity of chiral aminoalcohols with camphane scaffold. *European Journal of Medicinal Chemistry*, **2014**, 81, 150-7	6.8	13
53	Phenolic derivatives in raspberry (Rubus L.) germplasm collection in Bulgaria. *Biochemical Systematics and Ecology*, **2013**, 50, 419-427	1.4	13
52	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	3.7	13
51	Synthetic piperine amide analogs with antimycobacterial activity. *Chemical Biology and Drug Design*, **2018**, 91, 763-768	2.9	13
50	HLA-DP2 binding prediction by molecular dynamics simulations. *Protein Science*, **2011**, 20, 1918-28	6.3	12
49	VaxiJen Dataset of Bacterial Immunogens: An Update. *Current Computer-Aided Drug Design*, **2019**, 15, 398-400	1.4	12
48	Associations between Milk and Egg Allergens and the HLA-DRB1/DQ Polymorphism: A Bioinformatics Approach. *International Archives of Allergy and Immunology*, **2016**, 169, 33-9	3.7	11
47	Quantitative Structure Activity Relationship Study on Saponins as Cytotoxicity Enhancers. *Letters in Drug Design and Discovery*, **2014**, 12, 166-171	0.8	11
46	Proteochemometrics-Based Prediction of Peptide Binding to HLA-DP Proteins. *Journal of Chemical Information and Modeling*, **2018**, 58, 297-304	6.1	11
45	Immunogenicity Prediction by VaxiJen: A Ten Year Overview. *Journal of Proteomics and Bioinformatics*, **2017**, 10,	2.1	10
44	Quantitative structure--clearance relationships of acidic drugs. *Molecular Pharmaceutics*, **2013**, 10, 3758-68	5.8	10
43	2D and 3D QSAR analysis of some valproic acid metabolites and analogues as anticonvulsant agents. *Pharmaceutical Research*, **2000**, 17, 727-32	4.5	10
42	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	5.1	10
41	Galantamine-Curcumin Hybrids as Dual-Site Binding Acetylcholinesterase Inhibitors. *Molecules*, **2020**, 25,	4.8	10
40	Design, Synthesis, and Antimycobacterial Activity of Novel Theophylline-7-Acetic Acid Derivatives With Amino Acid Moieties. *Chemical Biology and Drug Design*, **2016**, 87, 335-41	2.9	10
39	Bone protective effects of purified extract from Ruscus aculeatus on ovariectomy-induced osteoporosis in rats. *Food and Chemical Toxicology*, **2019**, 132, 110668	4.7	9

38	Platinum complexes with 5-methyl-5(4-pyridyl)hydantoin and its 3-methyl derivatives: synthesis and cytotoxic activity - quantitative structure-activity relationships. *Archiv Der Pharmazie*, **2011**, 344, 209-16	4.3	9
37	Using databases and data mining in vaccinology. *Expert Opinion on Drug Discovery*, **2007**, 2, 19-35	6.2	8
36	Quantitative Structure - Pharmacokinetics Relationships Analysis of Basic Drugs: Volume of Distribution. *Journal of Pharmacy and Pharmaceutical Sciences*, **2015**, 18, 515-27	3.4	7
35	CoMFA Study on Adenosine A2A Receptor Agonists. *QSAR and Combinatorial Science*, **2001**, 20, 124-129		7
34	In silico prediction of cancer immunogens: current state of the art. *BMC Immunology*, **2018**, 19, 11	3.7	6
33	Allergenicity prediction by artificial neural networks. *Journal of Chemometrics*, **2014**, 28, 282-286	1.6	6
32	Preparation and evaluation of isosorbide mononitrate hydrogels for topical fissure treatment. *Current Drug Delivery*, **2012**, 9, 452-8	3.2	6
31	QSAR and the Prediction of T-Cell Epitopes. *Current Proteomics*, **2008**, 5, 73-95	0.7	6
30	CoMFA-based comparison of two models of binding site on adenosine A1 receptor. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 29-39	4.2	6
29	Curcumin Inhibits the Primary Nucleation of Amyloid-Beta Peptide: A Molecular Dynamics Study. *Biomolecules*, **2020**, 10,	5.9	6
28	A Novel Galantamine-Curcumin Hybrid as a Potential Multi-Target Agent against Neurodegenerative Disorders. *Molecules*, **2021**, 26,	4.8	6
27	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	1.4	5
26	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	6.2	5
25	Different approaches for determination of the attachment degree of polyethylene glycols to poly(anhydride) nanoparticles. *Drug Development and Industrial Pharmacy*, **2010**, 36, 676-80	3.6	5
24	A Cohesive and Integrated Platform for Immunogenicity Prediction. *Methods in Molecular Biology*, **2016**, 1404, 761-770	1.4	5
23	Hepato-, neuroprotective effects and QSAR studies on flavoalkaloids and flavonoids from Astragalus monspessulanus. *Biotechnology and Biotechnological Equipment*, **2019**, 33, 1434-1443	1.6	4
22	Bridging solvent molecules mediate RNase A - Ligand binding. *PLoS ONE*, **2019**, 14, e0224271	3.7	4
21	Peptide Binding Prediction to Five Most Frequent HLA-DQ Proteins - a Proteochemometric Approach. *Molecular Informatics*, **2015**, 34, 467-76	3.8	4

20	Quantitative prediction of peptide binding to HLA-DP1 protein. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **2013**, 10, 811-5	3	4
19	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, 41-9	1.4	4
18	Bacterial Immunogenicity Prediction by Machine Learning Methods. *Vaccines*, **2020**, 8,	5.3	4
17	Galantamine Derivatives as Acetylcholinesterase Inhibitors: Docking, Design, Synthesis, and Inhibitory Activity. *Neuromethods*, **2018**, 163-176	0.4	3
16	Design of novel camphane-based derivatives with antimycobacterial activity. *Journal of Molecular Graphics and Modelling*, **2014**, 51, 7-12	2.8	3
15	Adenosine A2A receptor agonists: CoMFA-based selection of the most predictive conformation. *SAR and QSAR in Environmental Research*, **2002**, 13, 227-35	3.5	3
14	Biodegradable cross-linked prodrug of the bronchial dilator Vephylline. 2. Kinetics and quantum chemical studies on the release mechanism. *Journal of Controlled Release*, **1999**, 58, 189-94	11.7	3
13	Proteochemometrics for the Prediction of Binding to the MHC Proteins. *Letters in Drug Design and Discovery*, **2016**, 14, 2-9	0.8	2
12	Discovery of a Novel Acetylcholinesterase Inhibitor by Fragment-Based Design and Virtual Screening. *Molecules*, **2021**, 26,	4.8	2
11	Proteochemometrics for the Prediction of Peptide Binding to Multiple HLA Class II Proteins. *Methods in Pharmacology and Toxicology*, **2018**, 395-404	1.1	1
10	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	2.2	1
9	An Alignment-Independent Platform for Allergenicity Prediction. *Methods in Molecular Biology*, **2020**, 2131, 147-153	1.4	1
8	The Amaryllidaceae alkaloids: an untapped source of acetylcholinesterase inhibitors. *Phytochemistry Reviews*,1	7.7	1
7	Predicting Immunogenicity Risk in Biopharmaceuticals. *Symmetry*, **2021**, 13, 388	2.7	1
6	Virtual Screening and Hit Selection of Natural Compounds as Acetylcholinesterase Inhibitors. *Molecules*, **2022**, 27, 3139	4.8	1
5	Beneficial effects of the fructus Sophorae extract on experimentally induced osteoporosis in New Zealand white rabbits. *Acta Pharmaceutica*, **2022**, 72, 289-302	3.2	0
4	In Silico QSAR-Based Predictions of Class I and Class II MHC Epitopes **2008**, 63-89		
3	Design of Multi-Epitope Vaccine against SARS-CoV-2. *Cybernetics and Information Technologies*, **2020**, 20, 185-193	1.3	

2	Immunoinformatic Analysis of Human Thyroglobulin. *Cybernetics and Information Technologies*, **2020**, 20, 194-200	1.3
1	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	1.4