

Irina Moreira

List of Publications by Year in descending order

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Version: 2024-02-01

85
papers

2,826
citations

279487

23
h-index

182168

51
g-index

95
all docs

95
docs citations

95
times ranked

4053
citing authors

#	ARTICLE	IF	CITATIONS
1	Hot spots-A review of the protein-protein interface determinant amino-acid residues. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 68, 803-812.	1.5	639
2	Allosteric communication between protomers of dopamine class A GPCR dimers modulates activation. <i>Nature Chemical Biology</i> , 2009, 5, 688-695.	3.9	323
3	Computational alanine scanning mutagenesis—An improved methodological approach. <i>Journal of Computational Chemistry</i> , 2007, 28, 644-654.	1.5	230
4	Protein—protein docking dealing with the unknown. <i>Journal of Computational Chemistry</i> , 2010, 31, 317-342.	1.5	100
5	Identification of a small-molecule inhibitor of the PICK1 PDZ domain that inhibits hippocampal LTP and LTD. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 413-418.	3.3	100
6	Structural features of the G-protein/GPCR interactions. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2014, 1840, 16-33.	1.1	100
7	Performance of HADDOCK and a simple contact-based protein—ligand binding affinity predictor in the D3R Grand Challenge 2. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 175-185.	1.3	97
8	Vascular Endothelial Growth Factor (VEGF) Inhibition - A Critical Review. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2007, 7, 223-245.	0.9	90
9	Membrane proteins structures: A review on computational modeling tools. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 2021-2039.	1.4	87
10	SpotOn: High Accuracy Identification of Protein-Protein Interface Hot-Spots. <i>Scientific Reports</i> , 2017, 7, 8007.	1.6	77
11	Computational Alanine Scanning Mutagenesis: MM-PBSA vs TI. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1311-1319.	2.3	67
12	Unraveling the Importance of Protein—Protein Interaction:—Application of a Computational Alanine-Scanning Mutagenesis to the Study of the IgG1 Streptococcal Protein G (C2 Fragment) Complex. <i>Journal of Physical Chemistry B</i> , 2006, 110, 10962-10969.	1.2	60
13	A Machine Learning Approach for Hot-Spot Detection at Protein-Protein Interfaces. <i>International Journal of Molecular Sciences</i> , 2016, 17, 1215.	1.8	46
14	Evolution of Drug Resistance: Insight on TEM—Lactamases Structure and Activity and—Lactam Antibiotics. <i>Mini-Reviews in Medicinal Chemistry</i> , 2014, 14, 111-122.	1.1	44
15	The Central Role of Non-Structural Protein 1 (NS1) in Influenza Biology and Infection. <i>International Journal of Molecular Sciences</i> , 2020, 21, 1511.	1.8	39
16	Unravelling Hot Spots: a comprehensive computational mutagenesis study. <i>Theoretical Chemistry Accounts</i> , 2006, 117, 99-113.	0.5	35
17	Understanding the importance of the aromatic amino-acid residues as hot-spots. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013, 1834, 404-414.	1.1	34
18	Solvent Accessible Surface Area-Based Hot-Spot Detection Methods for Protein—Protein and Protein—Nucleic Acid Interfaces. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1077-1086.	2.5	33

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19	Computational Alanine Scanning Mutagenesis—An Improved Methodological Approach for Protein–DNA Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4243-4256.	2.3	32
20	Hot Spot Occlusion from Bulk Water: A Comprehensive Study of the Complex between the Lysozyme HEL and the Antibody FVD1.3. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2697-2706.	1.2	31
21	Structure–activity relationships of a small-molecule inhibitor of the PDZ domain of PICK1. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 4281.	1.5	31
22	Accuracy of the numerical solution of the Poisson–Boltzmann equation. <i>Computational and Theoretical Chemistry</i> , 2005, 729, 11-18.	1.5	29
23	A Complete Assessment of Dopamine Receptor- Ligand Interactions through Computational Methods. <i>Molecules</i> , 2019, 24, 1196.	1.7	23
24	Solvent-accessible surface area: How well can be applied to hot-spot detection?. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 479-490.	1.5	22
25	General AMBER Force Field Parameters for Diphenyl Diselenides and Diphenyl Ditellurides. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4389-4400.	1.1	22
26	Hot spot computational identification: Application to the complex formed between the hen egg white lysozyme (HEL) and the antibody HyHEL-10. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 299-310.	1.0	21
27	Protein–protein recognition: a computational mutagenesis study of the MDM2–P53 complex. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 533-542.	0.5	21
28	Detailed microscopic study of the full zipA:FtsZ interface. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 63, 811-821.	1.5	19
29	Understanding the Differential Selectivity of Arrestins toward the Phosphorylation State of the Receptor. <i>ACS Chemical Neuroscience</i> , 2016, 7, 1212-1224.	1.7	18
30	Prediction and Targeting of Interaction Interfaces in G-protein Coupled Receptor Oligomers. <i>Current Topics in Medicinal Chemistry</i> , 2018, 18, 714-746.	1.0	18
31	In Silico Studies Targeting G-protein Coupled Receptors for Drug Research Against Parkinson's Disease. <i>Current Neuropharmacology</i> , 2018, 16, 786-848.	1.4	18
32	SARS-CoV-2 Membrane Protein: From Genomic Data to Structural New Insights. <i>International Journal of Molecular Sciences</i> , 2022, 23, 2986.	1.8	15
33	Insights into the structural determinants for selective inhibition of nitric oxide synthase isoforms. <i>Journal of Molecular Modeling</i> , 2013, 19, 1537-1551.	0.8	14
34	A new scoring function for protein–protein docking that identifies native structures with unprecedented accuracy. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2378-2387.	1.3	14
35	The Role of Water Occlusion for the Definition of a Protein Binding Hot-Spot. <i>Current Topics in Medicinal Chemistry</i> , 2015, 15, 2068-2079.	1.0	14
36	CompASM: an Amber-VMD alanine scanning mutagenesis plug-in. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	13

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37	Theoretical studies on the binding of rhenium(I) complexes to inducible nitric oxide synthase. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 45, 13-25.	1.3	13
38	Prediction and targeting of GPCR oligomer interfaces. <i>Progress in Molecular Biology and Translational Science</i> , 2020, 169, 105-149.	0.9	13
39	Network biology and artificial intelligence drive the understanding of the multidrug resistance phenotype in cancer. <i>Drug Resistance Updates</i> , 2022, 60, 100811.	6.5	13
40	New designs for MRI contrast agents. <i>Journal of Computer-Aided Molecular Design</i> , 2003, 17, 463-473.	1.3	12
41	Backbone Importance for Protein-Protein Binding. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 885-893.	2.3	12
42	SPOTONE: Hot Spots on Protein Complexes with Extremely Randomized Trees via Sequence-Only Features. <i>International Journal of Molecular Sciences</i> , 2020, 21, 7281.	1.8	12
43	Are hot-spots occluded from water?. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014, 32, 186-197.	2.0	11
44	An overview of data-driven HADDOCK strategies in CAPRI rounds 38-45. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 1029-1036.	1.5	11
45	Computational Approaches in Antibody-drug Conjugate Optimization for Targeted Cancer Therapy. <i>Current Topics in Medicinal Chemistry</i> , 2018, 18, 1091-1109.	1.0	11
46	Integrated in Silico and Experimental Approach towards the Design of a Novel Recombinant Protein Containing an Anti-HER2 scFv. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3547.	1.8	10
47	In Silico End-to-End Protein-Ligand Interaction Characterization Pipeline: The Case of SARS-CoV-2. <i>ACS Synthetic Biology</i> , 2021, 10, 3209-3235.	1.9	9
48	The Evolutionary Portrait of Metazoan NAD Salvage. <i>PLoS ONE</i> , 2013, 8, e64674.	1.1	8
49	Re(I) and Tc(I) Complexes for Targeting Nitric Oxide Synthase: Influence of the Chelator in the Affinity for the Enzyme. <i>Chemical Biology and Drug Design</i> , 2015, 86, 1072-1086.	1.5	8
50	Understanding the Binding Specificity of G-Protein Coupled Receptors toward G-Proteins and Arrestins: Application to the Dopamine Receptor Family. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3969-3984.	2.5	8
51	Ligand-Induced Structural Changes in TEM-1 Probed by Molecular Dynamics and Relative Binding Free Energy Calculations. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2648-2658.	2.5	7
52	Extending the applicability of the O-ring theory to protein-DNA complexes. <i>Computational Biology and Chemistry</i> , 2013, 44, 31-39.	1.1	7
53	Computational studies of G protein-coupled receptor complexes: Structure and dynamics. <i>Methods in Cell Biology</i> , 2017, 142, 205-245.	0.5	7
54	Computational modeling on mitochondrial channel nanotoxicity. <i>Nano Today</i> , 2020, 34, 100913.	6.2	7

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55	The Treasury Chest of Text Mining: Piling Available Resources for Powerful Biomedical Text Mining. <i>Biochem</i> , 2021, 1, 60-80.	0.5	7
56	Dynamical Rearrangement of Human Epidermal Growth Factor Receptor 2 upon Antibody Binding: Effects on the Dimerization. <i>Biomolecules</i> , 2019, 9, 706.	1.8	6
57	Computational Determination of the Relative Free Energy of Binding – Application to Alanine Scanning Mutagenesis. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2007, , 305-339.	0.6	6
58	Structural Determinants of a Typical Leucine-Rich Repeat Protein. <i>Communications in Computational Physics</i> , 2013, 13, 238-255.	0.7	5
59	An Overview of Antiretroviral Agents for Treating HIV Infection in Paediatric Population. <i>Current Medicinal Chemistry</i> , 2020, 27, 760-794.	1.2	5
60	Dynamic Structure of NGF and proNGF Complexed with p75NTR: Pro-Peptide Effect. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2051-2067.	2.5	4
61	Structural Basis of Dopamine Receptor Activation. , 2010, , 47-73.		4
62	SicknessMiner: a deep-learning-driven text-mining tool to abridge disease-disease associations. <i>BMC Bioinformatics</i> , 2021, 22, 482.	1.2	4
63	Decoding Partner Specificity of Opioid Receptor Family. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 715215.	1.6	3
64	Aberrant hippocampal transmission and behavior in mice with a stargazin mutation linked to intellectual disability. <i>Molecular Psychiatry</i> , 2022, 27, 2457-2469.	4.1	3
65	Computer-Aided Drug Design Approaches to Study Key Therapeutic Targets in Alzheimer’s Disease. <i>Neuromethods</i> , 2018, , 61-106.	0.2	2
66	MENSAdb: a thorough structural analysis of membrane protein dimers. <i>Database: the Journal of Biological Databases and Curation</i> , 2021, 2021, .	1.4	2
67	Predicting Hot Spots Using a Deep Neural Network Approach. <i>Methods in Molecular Biology</i> , 2021, 2190, 267-288.	0.4	2
68	Using machine-learning-driven approaches to boost hot spot's knowledge. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, .	6.2	2
69	Discovery of Virus-Host interactions using bioinformatic tools. <i>Methods in Cell Biology</i> , 2022, , .	0.5	2
70	Class A and C GPCR dimers in neurodegenerative diseases. <i>Current Neuropharmacology</i> , 2022, 20, .	1.4	2
71	Modulation of Protein-Protein Interactions for the Development of Effective Therapeutics - From a Joint Perspective of Experiment and Computation. <i>Current Topics in Medicinal Chemistry</i> , 2018, 18, 645-646.	1.0	1
72	Structural Characterization of Membrane Protein Dimers. <i>Methods in Molecular Biology</i> , 2019, 1958, 403-436.	0.4	1

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73	CompASM: an Amber-VMD alanine scanning mutagenesis plug-in. Highlights in Theoretical Chemistry, 2014, , 81-87.	0.0	1
74	Are Hot-Spots Occluded from Water?. Biophysical Journal, 2013, 104, 505a.	0.2	0
75	Hot-Spots Detection - Application to a Variety of Different Protein-Based Systems. Biophysical Journal, 2014, 106, 697a.	0.2	0
76	Spoton: A Machine-Learning Approach for Hot-Spot Determination. Biophysical Journal, 2017, 112, 45a.	0.2	0
77	Targeting GPCRs Via Multi-Platforms Arrays and AI. , 2021, , .		0
78	Guardians of the Cell: State-of-the-Art of Membrane Proteins from a Computational Point-of-View. Methods in Molecular Biology, 2021, 2315, 3-28.	0.4	0
79	Computational proteomics: from methodological developments to biological applications. , 2011, , 181-220.		0
80	Solvent Accessible Surface Area Hot-Spot Detection Method. , 0, , .		0
81	Co-evolution importance on binding Hot-Spot prediction methods. , 0, , .		0
82	Creating a valid in silico Dopamine D2-receptor model for small molecular docking studies. , 0, , .		0
83	Structural and dynamic understanding of the ghrelin receptor high constitutive activity. , 0, , .		0
84	Alpha-helical and beta-sheet membrane- membrane protein dimers: centralizing information. , 0, , .		0
85	Using big-data to understand the protein interface landscape. , 0, , .		0