Irina Moreira

List of Publications by Year
in descending order

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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	Network biology and artificial intelligence drive the understanding of the multidrug resistance phenotype in cancer. Drug Resistance Updates, 2022, 60, 100811.	6.5	13
2	Using machineâ€learningâ€driven approaches to boost hotâ€spot's knowledge. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	2
3	Discovery of Virus-Host interactions using bioinformatic tools. Methods in Cell Biology, 2022, , .	0.5	2
4	Aberrant hippocampal transmission and behavior in mice with a stargazin mutation linked to intellectual disability. Molecular Psychiatry, 2022, 27, 2457-2469.	4.1	3
5	Class A and C GPCR dimers in neurodegenerative diseases. Current Neuropharmacology, 2022, 20, .	1.4	2
6	SARS-CoV-2 Membrane Protein: From Genomic Data to Structural New Insights. International Journal of Molecular Sciences, 2022, 23, 2986.	1.8	15
7	Targeting GPCRs Via Multi-Platforms Arrays and AI. , 2021, , .		0
8	Integrated in Silico and Experimental Approach towards the Design of a Novel Recombinant Protein Containing an Anti-HER2 scFv. International Journal of Molecular Sciences, 2021, 22, 3547.	1.8	10
9	The Treasury Chest of Text Mining: Piling Available Resources for Powerful Biomedical Text Mining. Biochem, 2021, 1, 60-80.	0.5	7
10	Decoding Partner Specificity of Opioid Receptor Family. Frontiers in Molecular Biosciences, 2021, 8, 715215.	1.6	3
11	MENSAdb: a thorough structural analysis of membrane protein dimers. Database: the Journal of Biological Databases and Curation, 2021, 2021, .	1.4	2
12	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
13	Predicting Hot Spots Using a Deep Neural Network Approach. Methods in Molecular Biology, 2021, 2190, 267-288.	0.4	2
14	SicknessMiner: a deep-learning-driven text-mining tool to abridge disease-disease associations. BMC Bioinformatics, 2021, 22, 482.	1.2	4
15	In Silico End-to-End Proteinâ€“Ligand Interaction Characterization Pipeline: The Case of SARS-CoV-2. ACS Synthetic Biology, 2021, 10, 3209-3235.	1.9	9
16	Prediction and targeting of GPCR oligomer interfaces. Progress in Molecular Biology and Translational Science, 2020, 169, 105-149.	0.9	13
17	An overview of dataâ€driven HADDOCK strategies in CAPRI rounds 38â€45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1029-1036.	1.5	11
18	Understanding the Binding Specificity of G-Protein Coupled Receptors toward G-Proteins and Arrestins: Application to the Dopamine Receptor Family. Journal of Chemical Information and Modeling, 2020, 60, 3969-3984.	2.5	8

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19	SPOTONE: Hot Spots on Protein Complexes with Extremely Randomized Trees via Sequence-Only Features. International Journal of Molecular Sciences, 2020, 21, 7281.	1.8	12
20	Computational modeling on mitochondrial channel nanotoxicity. Nano Today, 2020, 34, 100913.	6.2	7
21	The Central Role of Non-Structural Protein 1 (NS1) in Influenza Biology and Infection. International Journal of Molecular Sciences, 2020, 21, 1511.	1.8	39
22	An Overview of Antiretroviral Agents for Treating HIV Infection in Paediatric Population. Current Medicinal Chemistry, 2020, 27, 760-794.	1.2	5
23	Dynamical Rearrangement of Human Epidermal Growth Factor Receptor 2 upon Antibody Binding: Effects on the Dimerization. Biomolecules, 2019, 9, 706.	1.8	6
24	A Complete Assessment of Dopamine Receptor- Ligand Interactions through Computational Methods. Molecules, 2019, 24, 1196.	1.7	23
25	Structural Characterization of Membrane Protein Dimers. Methods in Molecular Biology, 2019, 1958, 403-436.	0.4	1
26	Computer-Aided Drug Design Approaches to Study Key Therapeutic Targets in Alzheimerâ€™s Disease. Neuromethods, 2018, , 61-106.	0.2	2
27	Performance of HADDOCK and a simple contact-based proteinâ€“ligand binding affinity predictor in the D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 175-185.	1.3	97
28	Modulation of Protein-Protein Interactions for the Development of Effective Therapeutics - From a Joint Perspective of Experiment and Computation. Current Topics in Medicinal Chemistry, 2018, 18, 645-646.	1.0	1
29	Prediction and Targeting of Interaction Interfaces in G-protein Coupled Receptor Oligomers. Current Topics in Medicinal Chemistry, 2018, 18, 714-746.	1.0	18
30	Computational Approaches in Antibody-drug Conjugate Optimization for Targeted Cancer Therapy. Current Topics in Medicinal Chemistry, 2018, 18, 1091-1109.	1.0	11
31	In Silico Studies Targeting G-protein Coupled Receptors for Drug Research Against Parkinsonâ€™s Disease. Current Neuropharmacology, 2018, 16, 786-848.	1.4	18
32	Spoton: A Machine-Learning Approach for Hot-Spot Determination. Biophysical Journal, 2017, 112, 45a.	0.2	0
33	SpotOn: High Accuracy Identification of Protein-Protein Interface Hot-Spots. Scientific Reports, 2017, 7, 8007.	1.6	77
34	Membrane proteins structures: A review on computational modeling tools. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 2021-2039.	1.4	87
35	Computational studies of G protein-coupled receptor complexes: Structure and dynamics. Methods in Cell Biology, 2017, 142, 205-245.	0.5	7
36	A Machine Learning Approach for Hot-Spot Detection at Protein-Protein Interfaces. International Journal of Molecular Sciences, 2016, 17, 1215.	1.8	46

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37	Understanding the Differential Selectivity of Arrestins toward the Phosphorylation State of the Receptor. ACS Chemical Neuroscience, 2016, 7, 1212-1224.	1.7	18
38	General AMBER Force Field Parameters for Diphenyl Diselenides and Diphenyl Ditellurides. Journal of Physical Chemistry A, 2016, 120, 4389-4400.	1.1	22
39	Re(I) and Tc(I) Complexes for Targeting Nitric Oxide Synthase: Influence of the Chelator in the Affinity for the Enzyme. Chemical Biology and Drug Design, 2015, 86, 1072-1086.	1.5	8
40	Solvent Accessible Surface Area-Based Hot-Spot Detection Methods for Proteinâ€“Protein and Proteinâ€“Nucleic Acid Interfaces. Journal of Chemical Information and Modeling, 2015, 55, 1077-1086.	2.5	33
41	A new scoring function for proteinâ€“protein docking that identifies native structures with unprecedented accuracy. Physical Chemistry Chemical Physics, 2015, 17, 2378-2387.	1.3	14
42	The Role of Water Occlusion for the Definition of a Protein Binding Hot-Spot. Current Topics in Medicinal Chemistry, 2015, 15, 2068-2079.	1.0	14
43	Structural features of the G-protein/GPCR interactions. Biochimica Et Biophysica Acta - General Subjects, 2014, 1840, 16-33.	1.1	100
44	Hot-Spots Detection - Application to a Variety of Different Protein-Based Systems. Biophysical Journal, 2014, 106, 697a.	0.2	0
45	Are hot-spots occluded from water?. Journal of Biomolecular Structure and Dynamics, 2014, 32, 186-197.	2.0	11
46	Dynamic Structure of NGF and proNGF Complexed with p75NTR: Pro-Peptide Effect. Journal of Chemical Information and Modeling, 2014, 54, 2051-2067.	2.5	4
47	Solventâ€accessible surface area: How well can be applied to hotâ€spot detection?. Proteins: Structure, Function and Bioinformatics, 2014, 82, 479-490.	1.5	22
48	CompASM: an Amber-VMD alanine scanning mutagenesis plug-in. Highlights in Theoretical Chemistry, 2014, , 81-87.	0.0	1
49	Evolution of Drug Resistance: Insight on TEM β-Lactamases Structure and Activity and β-Lactam Antibiotics. Mini-Reviews in Medicinal Chemistry, 2014, 14, 111-122.	1.1	44
50	Computational Alanine Scanning Mutagenesis: MM-PBSA vs TI. Journal of Chemical Theory and Computation, 2013, 9, 1311-1319.	2.3	67
51	Computational Alanine Scanning Mutagenesisâ€”An Improved Methodological Approach for Proteinâ€“DNA Complexes. Journal of Chemical Theory and Computation, 2013, 9, 4243-4256.	2.3	32
52	Ligand-Induced Structural Changes in TEM-1 Probed by Molecular Dynamics and Relative Binding Free Energy Calculations. Journal of Chemical Information and Modeling, 2013, 53, 2648-2658.	2.5	7
53	Extending the applicability of the O-ring theory to proteinâ€“DNA complexes. Computational Biology and Chemistry, 2013, 44, 31-39.	1.1	7
54	Are Hot-Spots Occluded from Water?. Biophysical Journal, 2013, 104, 505a.	0.2	0

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55	Theoretical studies on the binding of rhenium(I) complexes to inducible nitric oxide synthase. Journal of Molecular Graphics and Modelling, 2013, 45, 13-25.	1.3	13
56	Insights into the structural determinants for selective inhibition of nitric oxide synthase isoforms. Journal of Molecular Modeling, 2013, 19, 1537-1551.	0.8	14
57	The Evolutionary Portrait of Metazoan NAD Salvage. PLoS ONE, 2013, 8, e64674.	1.1	8
58	Understanding the importance of the aromatic amino-acid residues as hot-spots. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 404-414.	1.1	34
59	Structural Determinants of a Typical Leucine-Rich Repeat Protein. Communications in Computational Physics, 2013, 13, 238-255.	0.7	5
60	CompASM: an Amber-VMD alanine scanning mutagenesis plug-in. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	13
61	Computational proteomics: from methodological developments to biological applications. , 2011, , 181-220.		0
62	Proteinâ€“protein docking dealing with the unknown. Journal of Computational Chemistry, 2010, 31, 317-342.	1.5	100
63	Identification of a small-molecule inhibitor of the PICK1 PDZ domain that inhibits hippocampal LTP and LTD. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 413-418.	3.3	100
64	Structureâ€“activity relationships of a small-molecule inhibitor of the PDZ domain of PICK1. Organic and Biomolecular Chemistry, 2010, 8, 4281.	1.5	31
65	Structural Basis of Dopamine Receptor Activation. , 2010, , 47-73.		4
66	Allosteric communication between protomers of dopamine class A GPCR dimers modulates activation. Nature Chemical Biology, 2009, 5, 688-695.	3.9	323
67	Proteinâ€“protein recognition: a computational mutagenesis study of the MDM2â€“P53 complex. Theoretical Chemistry Accounts, 2008, 120, 533-542.	0.5	21
68	Vascular Endothelial Growth Factor (VEGF) Inhibition - A Critical Review. Anti-Cancer Agents in Medicinal Chemistry, 2007, 7, 223-245.	0.9	90
69	Backbone Importance for Proteinâ”Protein Binding. Journal of Chemical Theory and Computation, 2007, 3, 885-893.	2.3	12
70	Hot Spot Occlusion from Bulk Water:Â a Comprehensive Study of the Complex between the Lysozyme HEL and the Antibody FVD1.3. Journal of Physical Chemistry B, 2007, 111, 2697-2706.	1.2	31
71	Computational alanine scanning mutagenesisâ€”An improved methodological approach. Journal of Computational Chemistry, 2007, 28, 644-654.	1.5	230
72	Hot spot computational identification: Application to the complex formed between the hen egg white lysozyme (HEL) and the antibody HyHEL-10. International Journal of Quantum Chemistry, 2007, 107, 299-310.	1.0	21

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73	Hot spots-A review of the protein-protein interface determinant amino-acid residues. Proteins: Structure, Function and Bioinformatics, 2007, 68, 803-812.	1.5	639
74	Computational Determination of the Relative Free Energy of Binding â€“ Application to Alanine Scanning Mutagenesis. Challenges and Advances in Computational Chemistry and Physics, 2007, , 305-339.	0.6	6
75	Unraveling the Importance of Proteinâ^'Protein Interaction:Â Application of a Computational Alanine-Scanning Mutagenesis to the Study of the IgG1 Streptococcal Protein G (C2 Fragment) Complex. Journal of Physical Chemistry B, 2006, 110, 10962-10969.	1.2	60
76	Detailed microscopic study of the full zipA:FtsZ interface. Proteins: Structure, Function and Bioinformatics, 2006, 63, 811-821.	1.5	19
77	Unravelling Hot Spots: a comprehensive computational mutagenesis study. Theoretical Chemistry Accounts, 2006, 117, 99-113.	0.5	35
78	Accuracy of the numerical solution of the Poissonâ€“Boltzmann equation. Computational and Theoretical Chemistry, 2005, 729, 11-18.	1.5	29
79	New designs for MRI contrast agents. Journal of Computer-Aided Molecular Design, 2003, 17, 463-473.	1.3	12
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