Giulia Rossetti

List of Publications by Year
in descending order

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92 papers	2,382 citations	218381 26 h-index	243296 44 g-index
101 all docs	101 docs citations	101 times ranked	3816 citing authors

#	Article	IF	Citations
1	Sodium Channels and Local Anestheticsâ€"Old Friends With New Perspectives. Frontiers in Pharmacology, 2022, 13, 837088.	1.6	13
2	Multiple Poses and Thermodynamics of Ligands Targeting Protein Surfaces: The Case of Furosemide Binding to mitoNEET in Aqueous Solution. Frontiers in Cell and Developmental Biology, 2022, 10, 886568.	1.8	3
3	Molecular Dynamics-Assisted Interpretation of Experimentally Determined Intrinsically Disordered Protein Conformational Components: The Case of Human Î±-Synuclein. Journal of Physical Chemistry B, 2022, 126, 3632-3639.	1.2	7
4	An anti-diabetic drug targets NEET (CISD) proteins through destabilization of their [2Fe-2S] clusters. Communications Biology, 2022, 5, 437.	2.0	8
5	Aromaticity at position 39 in Î±â€synuclein: A modulator of amyloid fibril assembly and membraneâ€bound conformations. Protein Science, 2022, 31, .	3.1	7
6	The Interplay of Cholesterol and Ligand Binding in hTSPO from Classical Molecular Dynamics Simulations. Molecules, 2021, 26, 1250.	1.7	5
7	Combining Different Docking Engines and Consensus Strategies to Design and Validate Optimized Virtual Screening Protocols for the SARS-CoV-2 3CL Protease. Molecules, 2021, 26, 797.	1.7	14
8	A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. ACS Pharmacology and Translational Science, 2021, 4, 1079-1095.	2.5	44
9	Binding of Androgen- and Estrogen-Like Flavonoids to Their Cognate (Non)Nuclear Receptors: A Comparison by Computational Prediction. Molecules, 2021, 26, 1613.	1.7	20
10	Identification of Inhibitors of SARS-CoV-2 3CL-Pro Enzymatic Activity Using a Small Molecule in Vitro Repurposing Screen. ACS Pharmacology and Translational Science, 2021, 4, 1096-1110.	2.5	101
11	Nintedanib targets KIT D816V neoplastic cells derived from induced pluripotent stem cells of systemic mastocytosis. Blood, 2021, 137, 2070-2084.	0.6	21
12	Expanding the boundaries of ligandâ€"target modeling by exascale calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1535.	6.2	13
13	Evaluation of 3â€•and 4â€Phenoxybenzamides as Selective Inhibitors of the Monoâ€ADPâ€Ribosyltransferase PARP10. ChemistryOpen, 2021, 10, 939-948.	0.9	4
14	Role and Perspective of Molecular Simulation-Based Investigation of RNAâ€"Ligand Interaction: From Small Molecules and Peptides to Photoswitchable RNA Binding. Molecules, 2021, 26, 3384.	1.7	3
15	Dynorphin Neuropeptides Decrease Apparent Proton Affinity of ASIC1a by Occluding the Acidic Pocket. Journal of Medicinal Chemistry, 2021, 64, 13299-13311.	2.9	8
16	The two redox states of the human NEET proteinsâ€™ [2Feâ€"2S] clusters. Journal of Biological Inorganic Chemistry, 2021, 26, 763-774.	1.1	6
17	The MID1 Protein: A Promising Therapeutic Target in Huntingtonâ€™s Disease. Frontiers in Genetics, 2021, 12, 761714.	1.1	7
18	Structural and Biochemical Analysis of the Dual Inhibition of MG-132 against SARS-CoV-2 Main Protease (Mpro/3CLpro) and Human Cathepsin-L. International Journal of Molecular Sciences, 2021, 22, 11779.	1.8	47

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19	Enhanced Sampling Approach to the Induced-Fit Docking Problem in Proteinâ€“Ligand Binding: The Case of Mono-ADP-Ribosylation Hydrolase Inhibitors. Journal of Chemical Theory and Computation, 2021, 17, 7899-7911.	2.3	17
20	Role of Tyr-39 for the Structural Features of Î±-Synuclein and for the Interaction with a Strong Modulator of Its Amyloid Assembly. International Journal of Molecular Sciences, 2020, 21, 5061.	1.8	4
21	Impact of Cholesterol on the Stability of Monomeric and Dimeric Forms of the Translocator Protein TSPO: A Molecular Simulation Study. Molecules, 2020, 25, 4299.	1.7	6
22	CGMD Platform: Integrated Web Servers for the Preparation, Running, and Analysis of Coarse-Grained Molecular Dynamics Simulations. Molecules, 2020, 25, 5934.	1.7	14
23	Murine cytomegalovirus infection exacerbates complex IV deficiency in a model of mitochondrial disease. PLoS Genetics, 2020, 16, e1008604.	1.5	1
24	Challenges in RNA Regulation in Huntington's Disease: Insights from Computational Studies. Israel Journal of Chemistry, 2020, 60, 681-693.	1.0	0
25	Modeling the allosteric modulation on a G-Protein Coupled Receptor: the case of M2 muscarinic Acetylcholine Receptor in complex with LY211960. Scientific Reports, 2020, 10, 3037.	1.6	6
26	Receptors' Mosaics and Allostery for Pharmacology. Biophysical Journal, 2020, 118, 521a-522a.	0.2	0
27	In silico/inÂvitro screening and hit evaluation identified new phenothiazine anti-prion derivatives. European Journal of Medicinal Chemistry, 2020, 196, 112295.	2.6	7
28	Chiral Analogues of PFI-1 as BET Inhibitors and Their Functional Role in Myeloid Malignancies. ACS Medicinal Chemistry Letters, 2020, 11, 1928-1934.	1.3	25
29	RhoA regulates translation of the Nogo-A decoy SPARC in white matter-invading glioblastomas. Acta Neuropathologica, 2019, 138, 275-293.	3.9	6
30	Investigating targets for neuropharmacological intervention by molecular dynamics simulations. Biochemical Society Transactions, 2019, 47, 909-918.	1.6	1
31	Structural Determinants of the Prion Protein N-Terminus and Its Adducts with Copper Ions. International Journal of Molecular Sciences, 2019, 20, 18.	1.8	42
32	Deregulated Splicing Is a Major Mechanism of RNA-Induced Toxicity in Huntington's Disease. Journal of Molecular Biology, 2019, 431, 1869-1877.	2.0	57
33	High-throughput screening discovers antifibrotic properties of haloperidol by hindering myofibroblast activation. JCI Insight, 2019, 4, .	2.3	17
34	Reducing Mutant Huntingtin Protein Expression in Living Cells by a Newly Identified RNA CAG Binder. ACS Chemical Neuroscience, 2018, 9, 1399-1408.	1.7	29
35	Nucleolar-nucleoplasmic shuttling of TARG1 and its control by DNA damage-induced poly-ADP-ribosylation and by nucleolar transcription. Scientific Reports, 2018, 8, 6748.	1.6	32
36	Effect ofin vivopost-translational modifications of the HMGB1 protein upon binding to platinated DNA: a molecular simulation study. Nucleic Acids Research, 2018, 46, 11687-11697.	6.5	15

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37	Role of Extracellular Loops and Membrane Lipids for Ligand Recognition in the Neuronal Adenosine Receptor Type 2A: An Enhanced Sampling Simulation Study. Molecules, 2018, 23, 2616.	1.7	13
38	Vibrational Energy in Proteins Correlates with Topology. Journal of Physical Chemistry Letters, 2018, 9, 6393-6398.	2.1	8
39	Structural Prediction of the Dimeric Form of the Mammalian Translocator Membrane Protein TSPO: A Key Target for Brain Diagnostics. International Journal of Molecular Sciences, 2018, 19, 2588.	1.8	15
40	The Conorfamide RPRFa Stabilizes the Open Conformation of Acid-Sensing Ion Channel 3 via the Nonproton Ligandâ€“Sensing Domain. Molecular Pharmacology, 2018, 94, 1114-1124.	1.0	19
41	Assessment of Intracellular Auto-Modification Levels of ARTD10 Using Mono-ADP-Ribose-Specific Macrodomains 2 and 3 of Murine Artd8. Methods in Molecular Biology, 2018, 1813, 41-63.	0.4	13
42	Proton Dynamics in Protein Mass Spectrometry. Journal of Physical Chemistry Letters, 2017, 8, 1105-1112.	2.1	34
43	The conserved macrodomains of the non-structural proteins of Chikungunya virus and other pathogenic positive strand RNA viruses function as mono-ADP-ribosylhydrolases. Scientific Reports, 2017, 7, 41746.	1.6	119
44	Sulfoximines as ATR inhibitors: Analogs of VE-821. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 2659-2662.	1.0	19
45	A covalent PIN1 inhibitor selectively targets cancer cells by a dual mechanism of action. Nature Communications, 2017, 8, 15772.	5.8	102
46	Copper(II) and the pathological H50Q Î±-synuclein mutant: Environment meets genetics. Communicative and Integrative Biology, 2017, 10, e1270484.	0.6	22
47	Molecular Dynamics Simulations of the [2Feâ€“2S] Cluster-Binding Domain of NEET Proteins Reveal Key Molecular Determinants That Induce Their Cluster Transfer/Release. Journal of Physical Chemistry B, 2017, 121, 10648-10656.	1.2	18
48	Diminazene Is a Slow Pore Blocker of Acid-Sensing Ion Channel 1a (ASIC1a). Molecular Pharmacology, 2017, 92, 665-675.	1.0	42
49	Structural Modeling of Human Prion Protein's Point Mutations. Progress in Molecular Biology and Translational Science, 2017, 150, 105-122.	0.9	5
50	Structural prediction of the interaction of the tumor suppressor p27KIP1 with cyclin A/CDK2 identifies a novel catalytically relevant determinant. BMC Bioinformatics, 2017, 18, 15.	1.2	5
51	Unifying view of mechanical and functional hotspots across class A GPCRs. PLoS Computational Biology, 2017, 13, e1005381.	1.5	7
52	Carnosine and Homocarnosine Degradation Mechanisms by the Human Carnosinase Enzyme CN1: Insights from Multiscale Simulations. Biochemistry, 2016, 55, 2772-2784.	1.2	20
53	Environmental and genetic factors support the dissociation between Î±-synuclein aggregation and toxicity. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E6506-E6515.	3.3	75
54	Conformational effects in protein electrosprayâ€ionization mass spectrometry. Mass Spectrometry Reviews, 2016, 35, 111-122.	2.8	66

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55	Intramolecular hydrophobic interactions are critical mediators of STAT5 dimerization. Scientific Reports, 2016, 6, 35454.	1.6	11
56	Conformational ensemble of human Î±-synuclein physiological form predicted by molecular simulations. Physical Chemistry Chemical Physics, 2016, 18, 5702-5706.	1.3	32
57	Binding of the Antagonist Caffeine to the Human Adenosine Receptor hA2AR in Nearly Physiological Conditions. PLoS ONE, 2015, 10, e0126833.	1.1	12
58	Insight into the Mechanism of Intramolecular Inhibition of the Catalytic Activity of Sirtuin 2 (SIRT2). PLoS ONE, 2015, 10, e0139095.	1.1	11
59	Rare FLT3 deletion mutants may provide additional treatment options to patients with AML: an approach to individualized medicine. Leukemia, 2015, 29, 2434-2438.	3.3	21
60	Computational metallomics of the anticancer drug cisplatin. Journal of Inorganic Biochemistry, 2015, 153, 231-238.	1.5	20
61	The structural impact of DNA mismatches. Nucleic Acids Research, 2015, 43, 4309-4321.	6.5	113
62	Copper Binding to the N-Terminally Acetylated, Naturally Occurring Form of Alpha-Synuclein Induces Local Helical Folding. Journal of the American Chemical Society, 2015, 137, 6444-6447.	6.6	68
63	Structural predictions of neurobiologically relevant G-protein coupled receptors and intrinsically disordered proteins. Archives of Biochemistry and Biophysics, 2015, 582, 91-100.	1.4	4
64	Molecular View of Ligands Specificity for CAG Repeats in Anti-Huntington Therapy. Journal of Chemical Theory and Computation, 2015, 11, 4911-4922.	2.3	15
65	Molecular Basis for Structural Heterogeneity of an Intrinsically Disordered Protein Bound to a Partner by Combined ESI-IM-MS and Modeling. Journal of the American Society for Mass Spectrometry, 2015, 26, 472-481.	1.2	45
66	Molecular Simulation-Based Structural Prediction of Protein Complexes in Mass Spectrometry: The Human Insulin Dimer. PLoS Computational Biology, 2014, 10, e1003838.	1.5	13
67	Developing predictive rules for coordination geometry from visible circular dichroism of copper(<scp>II</scp>) and nickel(<scp>II</scp>) ions in histidine and amide mainâ€chain complexes. FEBS Journal, 2014, 281, 3945-3954.	2.2	35
68	Molecular Dynamics Simulations Identify Time Scale of Conformational Changes Responsible for Conformational Selection in Molecular Recognition of HIV-1 Transactivation Responsive RNA. Journal of the American Chemical Society, 2014, 136, 15631-15637.	6.6	35
69	Molecular Recognition of Platinated DNA from Chromosomal HMGB1. Journal of Chemical Theory and Computation, 2014, 10, 3578-3584.	2.3	12
70	Chemosensorial G-proteins-Coupled Receptors: A Perspective from Computational Methods. Advances in Experimental Medicine and Biology, 2014, 805, 441-457.	0.8	4
71	HIV-1 Integrase Binding to its Cellular Partners: A Perspective from Computational Biology. Current Pharmaceutical Design, 2014, 20, 3412-3421.	0.9	1
72	Novel Deletion Mutants in the Juxtamembrane Domain of Fms-like Tyrosine Kinase 3 (FLT3) Induce Transformation By Release from Autoinhibition in AML. Blood, 2014, 124, 885-885.	0.6	0

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73	A Molecular Dynamics Simulation-Based Interpretation of Nuclear Magnetic Resonance Multidimensional Heteronuclear Spectra of Î±-SynucleinÂ·Dopamine Adducts. Biochemistry, 2013, 52, 6672-6683.	1.2	32
74	Ligand Binding on Intrinsic Disordered Proteins: Focus on Human Alpha-Synuclein. Biophysical Journal, 2013, 104, 379a.	0.2	0
75	Translation of HTT mRNA with expanded CAG repeats is regulated by the MID1â€“PP2A protein complex. Nature Communications, 2013, 4, 1511.	5.8	84
76	Role of Prion Disease-Linked Mutations in the Intrinsically Disordered N-Terminal Domain of the Prion Protein. Journal of Chemical Theory and Computation, 2013, 9, 5158-5167.	2.3	14
77	Dominant-negative effects in prion diseases: insights from molecular dynamics simulations on mouse prion protein chimeras. Journal of Biomolecular Structure and Dynamics, 2013, 31, 829-840.	2.0	9
78	Computational Studies on the Prion Protein. Current Topics in Medicinal Chemistry, 2013, 13, 2419-2431.	1.0	6
79	HIV-1 Tat Binding to PCAF Bromodomain: Structural Determinants from Computational Methods. Biology, 2012, 1, 277-296.	1.3	9
80	Structural Determinants of Cisplatin and Transplatin Binding to the Met-Rich Motif of Ctr1: A Computational Spectroscopy Approach. Journal of Chemical Theory and Computation, 2012, 8, 2912-2920.	2.3	27
81	Local Fluctuations and Conformational Transitions in Proteins. Journal of Chemical Theory and Computation, 2012, 8, 4775-4785.	2.3	37
82	Common Structural Traits across Pathogenic Mutants of the Human Prion Protein and Their Implications for Familial Prion Diseases. Journal of Molecular Biology, 2011, 411, 700-712.	2.0	66
83	Conformations of the Huntingtin N-term in aqueous solution from atomistic simulations. FEBS Letters, 2011, 585, 3086-3089.	1.3	24
84	Structural facets of diseaseâ€linked human prion protein mutants: A molecular dynamic study. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3270-3280.	1.5	46
85	Hydrogen Bonding Cooperativity in polyQ Î²-Sheets from First Principle Calculations. Journal of Chemical Theory and Computation, 2010, 6, 1777-1782.	2.3	17
86	Huntingtin: Stability and Interaction with Molecular Partner from Computational Biophysics Studies. Biophysical Journal, 2010, 98, 637a.	0.2	0
87	Docking Ligands on Protein Surfaces: The Case Study of Prion Protein. Journal of Chemical Theory and Computation, 2009, 5, 2565-2573.	2.3	34
88	Structural Properties of Polyglutamine Aggregates Investigated via Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 16843-16850.	1.2	19
89	Aggregation of small peptides studied by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2006, 65, 914-921.	1.5	19
90	MID1, mutated in Opitz syndrome, encodes an ubiquitin ligase that targets phosphatase 2A for degradation. Nature Genetics, 2001, 29, 287-294.	9.4	264

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91	Molecular Mechanism of Huntingtonâ€™s Disease â€” A Computational Perspective. , 0, , .		1
92	Chapter 12. Molecular Modelling and Simulations Applied to Challenging Drug Discovery Targets. Chemical Biology, 0, , 317-348.	0.1	0