Giulia Palermo

List of Publications by Year
in descending order

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69 papers	2,718 citations	172457 29 h-index	197818 49 g-index
75 all docs	75 docs citations	75 times ranked	2886 citing authors

#	Article	IF	Citations
1	Structural and dynamic insights into the HNH nuclease of divergent Cas9 species. Journal of Structural Biology, 2022, 214, 107814.	2.8	8
2	Multi-microsecond molecular dynamics unveils the mechanism of DNA traversal within CRISPR-Cas12a. Biophysical Journal, 2022, 121, 322a.	0.5	0
3	Emerging Methods and Applications to Decrypt Allostery in Proteins and Nucleic Acids. Journal of Molecular Biology, 2022, 434, 167518.	4.2	18
4	Structural Basis for Reduced Dynamics of Three Engineered HNH Endonuclease Lys-to-Ala Mutants for the Clustered Regularly Interspaced Short Palindromic Repeat (CRISPR)-Associated 9 (CRISPR/Cas9) Enzyme. Biochemistry, 2022, 61, 785-794.	2.5	12
5	Celebrating Women of Color in Computational Chemistry. Journal of Chemical Information and Modeling, 2022, 62, 3133-3134.	5.4	0
6	Enhancement of CRISPR/Cas12a trans-cleavage activity using hairpin DNA reporters. Nucleic Acids Research, 2022, 50, 8377-8391.	14.5	41
7	Dynamics and mechanisms of CRISPR-Cas9 through the lens of computational methods. Current Opinion in Structural Biology, 2022, 75, 102400.	5.7	14
8	Establishing the allosteric mechanism in <scp>CRISPRâ€Cas9</scp>. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1503.	14.6	35
9	Foldingâ€uponâ€Repair DNA Nanoswitches for Monitoring the Activity of DNA Repair Enzymes. Angewandte Chemie - International Edition, 2021, 60, 7283-7289.	13.8	27
10	Cooperative Dynamics of REC-Nuc Lobes Prime Cas12a for DNA Processing. Biophysical Journal, 2021, 120, 16a-17a.	0.5	0
11	Foldingâ€uponâ€Repair DNA Nanoswitches for Monitoring the Activity of DNA Repair Enzymes. Angewandte Chemie, 2021, 133, 7359-7365.	2.0	10
12	Role of Electrostatic Hotspots in the Selectivity of Complement Control Proteins Toward Human and Bovine Complement Inhibition. Frontiers in Molecular Biosciences, 2021, 8, 618068.	3.5	1
13	Gaussian accelerated molecular dynamics: Principles and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1521.	14.6	127
14	Systems Biology Modeling of the Complement System Under Immune Susceptible Pathogens. Frontiers in Physics, 2021, 9, .	2.1	4
15	Cover Image, Volume 11, Issue 3. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1532.	14.6	0
16	Molecular Dynamics to Predict Cryo-EM: Capturing Transitions and Short-Lived Conformational States of Biomolecules. Frontiers in Molecular Biosciences, 2021, 8, 641208.	3.5	18
17	Controlled Trafficking of Multiple and Diverse Cations Prompts Nucleic Acid Hydrolysis. ACS Catalysis, 2021, 11, 8786-8797.	11.2	8
18	Frontiers of metal-coordinating drug design. Expert Opinion on Drug Discovery, 2021, 16, 497-511.	5.0	28

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19	Enhanced specificity mutations perturb allosteric signaling in CRISPR-Cas9. ELife, 2021, 10, .	6.0	27
20	Allosteric Motions of the CRISPRâ€“Cas9 HNH Nuclease Probed by NMR and Molecular Dynamics. Journal of the American Chemical Society, 2020, 142, 1348-1358.	13.7	78
21	NMR and computational methods for molecular resolution of allosteric pathways in enzyme complexes. Biophysical Reviews, 2020, 12, 155-174.	3.2	35
22	Fighting COVID-19 Using Molecular Dynamics Simulations. ACS Central Science, 2020, 6, 1654-1656.	11.3	50
23	Editorial: Multiscale Modeling From Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations. Frontiers in Molecular Biosciences, 2020, 7, 194.	3.5	8
24	Catalytic Mechanism of Non-Target DNA Cleavage in CRISPR-Cas9 Revealed by Ab Initio Molecular Dynamics. ACS Catalysis, 2020, 10, 13596-13605.	11.2	63
25	Molecular Dynamics Reveals a DNA-Induced Dynamic Switch Triggering Activation of CRISPR-Cas12a. Journal of Chemical Information and Modeling, 2020, 60, 6427-6437.	5.4	43
26	Mapping the Structural and Dynamic Determinants of pH-Sensitive Heparin Binding to Granulocyte Macrophage Colony Stimulating Factor. Biochemistry, 2020, 59, 3541-3553.	2.5	4
27	Spontaneous Embedding of DNA Mismatches Within the RNA:DNA Hybrid of CRISPR-Cas9. Frontiers in Molecular Biosciences, 2020, 7, 39.	3.5	32
28	Faces of Contemporary CryoEM Information and Modeling. Journal of Chemical Information and Modeling, 2020, 60, 2407-2409.	5.4	1
29	Factor H-Inspired Design of Peptide Biomarkers of the Complement C3d Protein. ACS Medicinal Chemistry Letters, 2020, 11, 1054-1059.	2.8	3
30	Structure and Dynamics of the Acyl Chains in the Membrane Trafficking and Enzymatic Processing of Lipids. Accounts of Chemical Research, 2019, 52, 3087-3096.	15.6	35
31	Dissecting Structure and Function of DNAÂ·RNA Hybrids. CheM, 2019, 5, 1364-1366.	11.7	5
32	Disclosing the Impact of Carcinogenic SF3b Mutations on Pre-mRNA Recognition Via All-Atom Simulations. Biomolecules, 2019, 9, 633.	4.0	23
33	Women Make COMP: Mentoring the Next Generation of Women in Computational Chemistry. Journal of Chemical Information and Modeling, 2019, 59, 4061-4062.	5.4	3
34	Frontiers in CryoEM Modeling. Journal of Chemical Information and Modeling, 2019, 59, 3091-3093.	5.4	2
35	Deciphering Off-Target Effects in CRISPR-Cas9 through Accelerated Molecular Dynamics. ACS Central Science, 2019, 5, 651-662.	11.3	99
36	Understanding the mechanistic basis of non-coding RNA through molecular dynamics simulations. Journal of Structural Biology, 2019, 206, 267-279.	2.8	37

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37	The invisible dance of CRISPR-Cas9. Physics Today, 2019, 72, 30-36.	0.3	10
38	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	3.3	285
39	Structure and Dynamics of the CRISPRâ€“Cas9 Catalytic Complex. Journal of Chemical Information and Modeling, 2019, 59, 2394-2406.	5.4	59
40	Key role of the REC lobe during CRISPRâ€“Cas9 activation by â€˜sensingâ€™, â€˜regulatingâ€™, and â€˜lockingâ€™ the catalytic HNH domain. Quarterly Reviews of Biophysics, 2018, 51, .	5.7	79
41	A PAM-Induced Signalling Activates the Communication between HNH and RUVC in CRISPR-Cas9. Biophysical Journal, 2018, 114, 250a.	0.5	0
42	All-atom simulations disentangle the functional dynamics underlying gene maturation in the intron lariat spliceosome. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6584-6589.	7.1	59
43	Allosteric cross-talk in chromatin can mediate drug-drug synergy. Nature Communications, 2017, 8, 14860.	12.8	61
44	CRISPR-Cas9: Computational Insights Toward Improved Genome Editing. Biophysical Journal, 2017, 112, 72a.	0.5	0
45	Development of Site-Specific Mg²⁺â€“RNA Force Field Parameters: A Dream or Reality? Guidelines from Combined Molecular Dynamics and Quantum Mechanics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 340-352.	5.3	51
46	Computational Characterization of the Dependence of Halide Perovskite Effective Masses on Chemical Composition and Structure. Journal of Physical Chemistry C, 2017, 121, 23886-23895.	3.1	38
47	Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9. Journal of the American Chemical Society, 2017, 139, 16028-16031.	13.7	104
48	CRISPR-Cas9 conformational activation as elucidated from enhanced molecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7260-7265.	7.1	133
49	An Organometallic Compound which Exhibits a DNA Topologyâ€Dependent Oneâ€Stranded Intercalation Mode. Angewandte Chemie, 2016, 128, 7567-7570.	2.0	0
50	Molecular Mechanism of Chromatin Targeting by a Potent Anticancer Agent Acting at the Nucleosome Core Particle. Biophysical Journal, 2016, 110, 68a-69a.	0.5	0
51	The Molecular Basis for Dual Fatty Acid Amide Hydrolase (FAAH)/Cyclooxygenase (COX) Inhibition. ChemMedChem, 2016, 11, 1252-1258.	3.2	33
52	Fighting Cancer with Transition Metal Complexes: From Naked DNA to Protein and Chromatin Targeting Strategies. ChemMedChem, 2016, 11, 1199-1210.	3.2	104
53	Valence and conduction band tuning in halide perovskites for solar cell applications. Journal of Materials Chemistry A, 2016, 4, 15997-16002.	10.3	132
54	Striking Plasticity of CRISPR-Cas9 and Key Role of Non-target DNA, as Revealed by Molecular Simulations. ACS Central Science, 2016, 2, 756-763.	11.3	103

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55	Who Activates the Nucleophile in Ribozyme Catalysis? An Answer from the Splicing Mechanism of Group II Introns. Journal of the American Chemical Society, 2016, 138, 10374-10377.	13.7	79
56	An Organometallic Compound which Exhibits a DNA Topologyâ€Dependent Oneâ€Stranded Intercalation Mode. Angewandte Chemie - International Edition, 2016, 55, 7441-7444.	13.8	21
57	Computational Chemistry for Drug Discovery. , 2016, , 611-625.		1
58	Anandamide Hydrolysis in FAAH Reveals a Dual Strategy for Efficient Enzyme-Assisted Amide Bond Cleavage via Nitrogen Inversion. Journal of Physical Chemistry B, 2015, 119, 789-801.	2.6	36
59	Catalytic Metal Ions and Enzymatic Processing of DNA and RNA. Accounts of Chemical Research, 2015, 48, 220-228.	15.6	130
60	An optimized polyamine moiety boosts the potency of human type II topoisomerase poisons as quantified by comparative analysis centered on the clinical candidate F14512. Chemical Communications, 2015, 51, 14310-14313.	4.1	32
61	Molecular Mechanism of Ruthenium and Gold Anticancer Agents in the Allosteric Regulation of the Histone Proteins of Chromatin. Biophysical Journal, 2015, 108, 59a.	0.5	1
62	Computational insights into function and inhibition of fatty acid amide hydrolase. European Journal of Medicinal Chemistry, 2015, 91, 15-26.	5.5	40
63	Computational Chemistry for Drug Discovery. , 2015, , 1-15.		8
64	Keys to Lipid Selection in Fatty Acid Amide Hydrolase Catalysis: Structural Flexibility, Gating Residues and Multiple Binding Pockets. PLoS Computational Biology, 2015, 11, e1004231.	3.2	31
65	Wagging the Tail: Essential Role of Substrate Flexibility in FAAH Catalysis. Journal of Chemical Theory and Computation, 2013, 9, 1202-1213.	5.3	24
66	Molecular Simulations Highlight the Role of Metals in Catalysis and Inhibition of Type II Topoisomerase. Journal of Chemical Theory and Computation, 2013, 9, 857-862.	5.3	45
67	Covalent Inhibitors of Fatty Acid Amide Hydrolase: A Rationale for the Activity of Piperidine and Piperazine Aryl Ureas. Journal of Medicinal Chemistry, 2011, 54, 6612-6623.	6.4	43
68	Pushing the Frontiers of First-Principles Based Computer Simulations of Chemical and Biological Systems. Chimia, 2011, 65, 667.	0.6	22
69	Effect of Electronegative Substituents and Angular Dependence on the Heteronuclear Spinâ"Spin Coupling Constant³J_{Câ"H}: An Empirical Prediction Equation Derived by Density Functional Theory Calculations. Journal of Organic Chemistry, 2010, 75, 1982-1991.	3.2	50