Francesco L Gervasio

List of Publications by Year
in descending order

126	10,168	38738 50	37202 96
papers	citations	h-index	g-index

153	153	153	10458
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mechanistic Insights into the Ligand-Induced Unfolding of an RNA G-Quadruplex. Journal of the American Chemical Society, 2022, 144, 935-950.	13.7	21
2	Beyond Structure. Imaging Protein Dynamics at Physiological Temperatures. Biophysical Journal, 2021, 120, 173a.	0.5	0
3	Allosteric communication in class A Î²-lactamases occurs via cooperative coupling of loop dynamics. ELife, 2021, 10, .	6.0	44
4	Structural basis of the effect of activating mutations on the EGF receptor. ELife, 2021, 10, .	6.0	24
5	Concurrent mutations in RNA-dependent RNA polymerase and spike protein emerged as the epidemiologically most successful SARS-CoV-2 variant. Scientific Reports, 2021, 11, 13705.	3.3	45
6	Amphiphilic Histidine-Based Oligopeptides Exhibit pH-Reversible Fibril Formation. ACS Macro Letters, 2021, 10, 984-989.	4.8	8
7	Aromatic side-chain flips orchestrate the conformational sampling of functional loops in human histone deacetylase 8. Chemical Science, 2021, 12, 9318-9327.	7.4	5
8	Liquid-Phase Electron Microscopy in Structural Protein Studies. Microscopy and Microanalysis, 2021, 27, 89-90.	0.4	0
9	Imaging Protein Dynamics in Liquid Water. Microscopy and Microanalysis, 2021, 27, 15-16.	0.4	0
10	A different perspective for nonphotochemical quenching in plant antenna complexes. Nature Communications, 2021, 12, 7152.	12.8	22
11	Combining Machine Learning and Enhanced Sampling Techniques for Efficient and Accurate Calculation of Absolute Binding Free Energies. Journal of Chemical Theory and Computation, 2020, 16, 4641-4654.	5.3	26
12	A combined activation mechanism for the glucagon receptor. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 15414-15422.	7.1	49
13	Investigating Cryptic Binding Sites by Molecular Dynamics Simulations. Accounts of Chemical Research, 2020, 53, 654-661.	15.6	106
14	Unravelling the effect of the E545K mutation on PI3KÎ± kinase. Chemical Science, 2020, 11, 3511-3515.	7.4	17
15	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
16	Modulating Ligand Dissociation through Methyl Isomerism in Accessory Sites: Binding of Retinol to Cellular Carriers. Journal of Physical Chemistry Letters, 2019, 10, 7333-7339.	4.6	5
17	Editorial: Machine Learning in Biomolecular Simulations. Frontiers in Molecular Biosciences, 2019, 6, 76.	3.5	4
18	The Role of Post-translational Modifications on the Energy Landscape of Huntingtin N-Terminus. Frontiers in Molecular Biosciences, 2019, 6, 95.	3.5	19

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19	Understanding Ligand Binding Selectivity in a Prototypical GPCR Family. Journal of Chemical Information and Modeling, 2019, 59, 2830-2836.	5.4	28
20	Structure and Dynamics of the EGF Receptor as Revealed by Experiments and Simulations and Its Relevance to Non-Small Cell Lung Cancer. Cells, 2019, 8, 316.	4.1	35
21	Importance of the Force Field Choice in Capturing Functionally Relevant Dynamics in the von Willebrand Factor. Journal of Physical Chemistry Letters, 2019, 10, 1928-1934.	4.6	32
22	The Structure of the Pro-domain of Mouse proNGF in Contact with the NGF Domain. Structure, 2019, 27, 78-89.e3.	3.3	15
23	Defining an Optimal Metric for the Path Collective Variables. Journal of Chemical Theory and Computation, 2019, 15, 25-32.	5.3	25
24	BioSimSpace: An interoperable Python framework for biomolecular simulation. Journal of Open Source Software, 2019, 4, 1831.	4.6	26
25	Protein CoAlation and antioxidant function of coenzyme A in prokaryotic cells. Biochemical Journal, 2018, 475, 1909-1937.	3.7	60
26	Assessment of the model refinement category in CASP12. Proteins: Structure, Function and Bioinformatics, 2018, 86, 152-167.	2.6	33
27	The architecture of EGFRâ€™s basal complexes reveals autoinhibition mechanisms in dimers and oligomers. Nature Communications, 2018, 9, 4325.	12.8	71
28	A Multiscale Simulation Approach to Modeling Drugâ€“Protein Binding Kinetics. Journal of Chemical Theory and Computation, 2018, 14, 6093-6101.	5.3	29
29	Role of glutamine synthetase in angiogenesis beyond glutamine synthesis. Nature, 2018, 561, 63-69.	27.8	136
30	Defining the architecture of KPC-2 Carbapenemase:Âidentifying allosteric networks to fight antibiotics resistance. Scientific Reports, 2018, 8, 12916.	3.3	27
31	Exploring Cryptic Pockets Formation in Targets of Pharmaceutical Interest with SWISH. Journal of Chemical Theory and Computation, 2018, 14, 3321-3331.	5.3	45
32	Intrinsically active MEK variants are differentially regulated by proteinases and phosphatases. Scientific Reports, 2018, 8, 11830.	3.3	22
33	An Efficient Metadynamics-Based Protocol To Model the Binding Affinity and the Transition State Ensemble of G-Protein-Coupled Receptor Ligands. Journal of Chemical Information and Modeling, 2017, 57, 1210-1217.	5.4	114
34	Investigating allosteric effects on the functional dynamics of Î²2-adrenergic ternary complexes with enhanced-sampling simulations. Chemical Science, 2017, 8, 4019-4026.	7.4	42
35	Conformational transition of FGFR kinase activation revealed by site-specific unnatural amino acid reporter and single molecule FRET. Scientific Reports, 2017, 7, 39841.	3.3	6
36	Recent Progress in Free Energy Methods. , 2017, , 34-50.		3

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37	Changes in the free-energy landscape of p38Î± MAP kinase through its canonical activation and binding events as studied by enhanced molecular dynamics simulations. ELife, 2017, 6, .	6.0	65
38	A Threeâ€Site Mechanism for Agonist/Antagonist Selective Binding to Vasopressin Receptors. Angewandte Chemie - International Edition, 2016, 55, 8008-8012.	13.8	38
39	An Allosteric Cross-Talk Between the Activation Loop and the ATP Binding Site Regulates the Activation of Src Kinase. Scientific Reports, 2016, 6, 24235.	3.3	36
40	DNA-binding protects p53 from interactions with cofactors involved in transcription-independent functions. Nucleic Acids Research, 2016, 44, gkw770.	14.5	40
41	Bidirectional Allosteric Communication between the ATP-Binding Site and the Regulatory PIF Pocket in PDK1 Protein Kinase. Cell Chemical Biology, 2016, 23, 1193-1205.	5.2	65
42	Understanding Cryptic Pocket Formation in Protein Targets by Enhanced Sampling Simulations. Journal of the American Chemical Society, 2016, 138, 14257-14263.	13.7	151
43	Conformational Selection and Induced Fit Mechanisms in the Binding of an Anticancer Drug to the c-Src Kinase. Scientific Reports, 2016, 6, 24439.	3.3	53
44	Molecular engineering of polymersome surface topology. Science Advances, 2016, 2, e1500948.	10.3	56
45	Changes in the folding landscape of the WW domain provide a molecular mechanism for an inherited genetic syndrome. Scientific Reports, 2016, 6, 30293.	3.3	13
46	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1
47	A Threeâ€Site Mechanism for Agonist/Antagonist Selective Binding to Vasopressin Receptors. Angewandte Chemie, 2016, 128, 8140-8144.	2.0	11
48	The Role of Protein Loops and Linkers in Conformational Dynamics and Allostery. Chemical Reviews, 2016, 116, 6391-6423.	47.7	302
49	Modeling the effect of pathogenic mutations on the conformational landscape of protein kinases. Current Opinion in Structural Biology, 2016, 37, 108-114.	5.7	16
50	The Effect of Mutations on Drug Sensitivity and Kinase Activity of Fibroblast Growth Factor Receptors: A Combined Experimental and Theoretical Study. EBioMedicine, 2015, 2, 194-204.	6.1	60
51	New Insights into the Molecular Mechanism of E-Cadherin-Mediated Cell Adhesion by Free Energy Calculations. Journal of Chemical Theory and Computation, 2015, 11, 1354-1359.	5.3	7
52	The Effect of a Widespread Cancer-Causing Mutation on the Inactive to Active Dynamics of the B-Raf Kinase. Journal of the American Chemical Society, 2015, 137, 5280-5283.	13.7	37
53	From residue coevolution to protein conformational ensembles and functional dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 13567-13572.	7.1	116
54	Investigating Drugâ€“Target Association and Dissociation Mechanisms Using Metadynamics-Based Algorithms. Accounts of Chemical Research, 2015, 48, 277-285.	15.6	134

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55	Towards a Molecular Understanding of the Link between Imatinib Resistance and Kinase Conformational Dynamics. PLoS Computational Biology, 2015, 11, e1004578.	3.2	59
56	Phosphatidylinositol 4,5-bisphosphate triggers activation of focal adhesion kinase by inducing clustering and conformational changes. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E3177-86.	7.1	111
57	The SH2 Domain Regulates c-Abl Kinase Activation by a Cyclin-Like Mechanism and Remodulation of the Hinge Motion. PLoS Computational Biology, 2014, 10, e1003863.	3.2	26
58	Enabling multiscale modeling in systems medicine. Genome Medicine, 2014, 6, 21.	8.2	76
59	Conformational Changes and Free Energies in a Proline Isomerase. Journal of Chemical Theory and Computation, 2014, 10, 4169-4174.	5.3	46
60	The Free Energy Contribution of SH3 and SH2 in c-Abl 1b Autoinhibition Mechanism via a Computational Structure-Based Model. Biophysical Journal, 2014, 106, 253a-254a.	0.5	0
61	The Mechanism of Allosteric Coupling in Choline Kinaseâ€…Î±1 Revealed by the Action of a Rationally Designed Inhibitor. Angewandte Chemie - International Edition, 2013, 52, 4582-4586.	13.8	36
62	Inhibition of Tumor Angiogenesis and Growth by a Small-Molecule Multi-FGF Receptor Blocker with Allosteric Properties. Cancer Cell, 2013, 23, 477-488.	16.8	138
63	Molecular Mechanism of SSR128129E, an Extracellularly Acting, Small-Molecule, Allosteric Inhibitor of FGF Receptor Signaling. Cancer Cell, 2013, 23, 489-501.	16.8	125
64	Efficient Numerical Reconstruction of Protein Folding Kinetics with Partial Path Sampling and Pathlike Variables. Physical Review Letters, 2013, 110, 108106.	7.8	41
65	Effects of oncogenic mutations on the conformational free-energy landscape of EGFR kinase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 10616-10621.	7.1	143
66	Non-specific proteinâ€“DNA interactions control I-CreI target binding and cleavage. Nucleic Acids Research, 2012, 40, 6936-6945.	14.5	24
67	New Insights in Protein Kinase Conformational Dynamics. Current Topics in Medicinal Chemistry, 2012, 12, 1889-1895.	2.1	22
68	Using Metadynamics and Path Collective Variables to Study Ligand Binding and Induced Conformational Transitions. Methods in Molecular Biology, 2012, 819, 501-513.	0.9	30
69	Assessing the Performance of Metadynamics and Path Variables in Predicting the Binding Free Energies of p38 Inhibitors. Journal of Chemical Theory and Computation, 2012, 8, 1165-1170.	5.3	39
70	Dynamics of Large-Scale Protein Conformational Transition and Docking Events using a Hybrid All-Atom Structure Based Model. Biophysical Journal, 2012, 102, 260a-261a.	0.5	0
71	The Different Flexibility of c-Src and c-Abl Kinases Regulates the Accessibility of a Druggable Inactive Conformation. Journal of the American Chemical Society, 2012, 134, 2496-2499.	13.7	91
72	New advances in metadynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 771-779.	14.6	136

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73	Chapter 14. Using Molecular Simulations and Metadynamics to Predict Binding Free Energies and Kinetics: the Case of Cox and Cdk2. RSC Drug Discovery Series, 2012, , 360-371.	0.3	0
74	Conformational Selection versus Induced Fit in Kinases: The Case of PI3Kâ€Î³. Angewandte Chemie - International Edition, 2012, 51, 642-646.	13.8	16
75	Cyclin-dependent kinases: bridging their structure and function through computations. Future Medicinal Chemistry, 2011, 3, 1551-1559.	2.3	19
76	A Simple Mechanism Underlying the Effect of Protecting Osmolytes on Protein Folding. Journal of Chemical Theory and Computation, 2011, 7, 3846-3852.	5.3	23
77	Bridging the Gap between Folding Simulations and Experiments: The Case of the Villin Headpiece. Journal of Chemical Theory and Computation, 2011, 7, 2675-2680.	5.3	11
78	A Hybrid All-Atom Structure-Based Model for Protein Folding and Large Scale Conformational Transitions. Journal of Chemical Theory and Computation, 2011, 7, 4208-4217.	5.3	23
79	Backbone assignment of the tyrosine kinase Src catalytic domain in complex with imatinib. Biomolecular NMR Assignments, 2011, 5, 221-224.	0.8	10
80	Molecular basis of engineered meganuclease targeting of the endogenous human RAG1 locus. Nucleic Acids Research, 2011, 39, 729-743.	14.5	63
81	Multiple Routes and Milestones in the Folding of HIVâ€“1 Protease Monomer. PLoS ONE, 2010, 5, e13208.	2.5	15
82	Molecular basis of cyclooxygenase enzymes (COXs) selective inhibition. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5411-5416.	7.1	187
83	Comparing the Efficiency of Biased and Unbiased Molecular Dynamics in Reconstructing the Free Energy Landscape of Met-Enkephalin. Journal of Chemical Theory and Computation, 2010, 6, 3640-3646.	5.3	51
84	Free-Energy-Based Methods for Binding Profile Determination in a Congeneric Series of CDK2 Inhibitors. Journal of Physical Chemistry B, 2010, 114, 9516-9524.	2.6	48
85	Multiple Routes and Milestones in the Folding of HIV-1 Protease Monomer. Biophysical Journal, 2010, 98, 199a.	0.5	0
86	Bifunctional Catalysis by Natural Cinchona Alkaloids: A Mechanism Explained. Chemistry - A European Journal, 2009, 15, 7913-7921.	3.3	59
87	Protein Conformational Transitions: The Closure Mechanism of a Kinase Explored by Atomistic Simulations. Journal of the American Chemical Society, 2009, 131, 244-250.	13.7	130
88	Exploring Complex Proteinâ^'Ligand Recognition Mechanisms with Coarse Metadynamics. Journal of Physical Chemistry B, 2009, 113, 4807-4816.	2.6	77
89	Non-Native Structure in the Unfolded Ensemble of a Prototypical Î²-Hairpin. Biophysical Journal, 2009, 96, 78a-79a.	0.5	0
90	The role of Li⁺, Na⁺, and K⁺ in the ligand binding inside the human acetylcholinesterase gorge. Proteins: Structure, Function and Bioinformatics, 2008, 70, 779-785.	2.6	17

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91	Metadynamics: a method to simulate rare events and reconstruct the free energy in biophysics, chemistry and material science. Reports on Progress in Physics, 2008, 71, 126601.	20.1	1,334
92	Conformational Changes and Gating at the Selectivity Filter of Potassium Channels. Journal of the American Chemical Society, 2008, 130, 9474-9480.	13.7	61
93	The Unfolded Ensemble and Folding Mechanism of the C-Terminal GB1 Î²-Hairpin. Journal of the American Chemical Society, 2008, 130, 13938-13944.	13.7	97
94	Charge localisation and hopping in DNA. Molecular Simulation, 2007, 33, 57-60.	2.0	9
95	From A to B in free energy space. Journal of Chemical Physics, 2007, 126, 054103.	3.0	476
96	Charge Localization in Stacked Radical Cation DNA Base Pairs and the Benzene Dimer Studied by Self-Interaction Corrected Density-Functional Theory. Journal of Physical Chemistry A, 2007, 111, 105-112.	2.5	46
97	Insight into the Folding Inhibition of the HIV-1 Protease by a Small Peptide. Biophysical Journal, 2007, 93, 2813-2821.	0.5	40
98	Solvent Effects on Charge Spatial Extent in DNA and Implications for Transfer. Physical Review Letters, 2007, 99, 058104.	7.8	53
99	Protein Conformational Plasticity: the â€œoff-onâ€•Switching Movement in Cdk5. AIP Conference Proceedings, 2007, , .	0.4	0
100	Charge transfer mechanism in a PolydGpdCp fiber and in wet DNA. Computer Physics Communications, 2007, 177, 27-29.	7.5	3
101	Investigating biological systems using first principles Carâ€“Parrinello molecular dynamics simulations. Current Opinion in Structural Biology, 2007, 17, 149-156.	5.7	90
102	Free-Energy Landscape for Î² Hairpin Folding from Combined Parallel Tempering and Metadynamics. Journal of the American Chemical Society, 2006, 128, 13435-13441.	13.7	458
103	Metadynamics Simulation of Prion Protein:Â Î²-Structure Stability and the Early Stages of Misfolding. Journal of the American Chemical Society, 2006, 128, 2705-2710.	13.7	105
104	Exploring the Gating Mechanism in the ClC Chloride Channel via Metadynamics. Journal of Molecular Biology, 2006, 361, 390-398.	4.2	53
105	DFT modeling of biological systems. Physica Status Solidi (B): Basic Research, 2006, 243, 2500-2515.	1.5	15
106	Efficient Reconstruction of Complex Free Energy Landscapes by Multiple Walkers Metadynamicsâ€. Journal of Physical Chemistry B, 2006, 110, 3533-3539.	2.6	511
107	Double Proton Coupled Charge Transfer in DNA. Angewandte Chemie - International Edition, 2006, 45, 5606-5609.	13.8	52
108	Charge Localization in DNA Fibers. Physical Review Letters, 2005, 94, 158103.	7.8	53

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109	The Role of the Peripheral Anionic Site and Cationâ^Ï€ Interactions in the Ligand Penetration of the Human AChE Gorge. Journal of the American Chemical Society, 2005, 127, 9147-9155.	13.7	94
110	Assessing the Accuracy of Metadynamicsâ€. Journal of Physical Chemistry B, 2005, 109, 6714-6721.	2.6	446
111	Flexible Docking in Solution Using Metadynamics. Journal of the American Chemical Society, 2005, 127, 2600-2607.	13.7	266
112	Inter-residue and solvent-residue interactions in proteins: A statistical study on experimental structures. Proteins: Structure, Function and Bioinformatics, 2004, 55, 139-151.	2.6	15
113	Influence of DNA Structure on the Reactivity of the Guanine Radical Cation. Chemistry - A European Journal, 2004, 10, 4846-4852.	3.3	70
114	A Minimum Free Energy Reaction Path for the E2 Reaction between Fluoro Ethane and a Fluoride Ion. Journal of the American Chemical Society, 2004, 126, 9492-9493.	13.7	73
115	A Variational Definition of Electrostatic Potential Derived Charges. Journal of Physical Chemistry B, 2004, 108, 7963-7968.	2.6	40
116	Influence of Outer-Shell Metal Ligands on the Structural and Electronic Properties of Horse Liver Alcohol Dehydrogenase Zinc Active Site. Journal of Physical Chemistry B, 2003, 107, 6886-6892.	2.6	22
117	Electronic Structure of Wet DNA. Physical Review Letters, 2002, 89, 108102.	7.8	157
118	Is the T-Shaped Toluene Dimer a Stable Intermolecular Complex?. Journal of Physical Chemistry A, 2002, 106, 2945-2948.	2.5	40
119	Stacking and T-shape Competition in Aromaticâ^'Aromatic Amino Acid Interactions. Journal of the American Chemical Society, 2002, 124, 6133-6143.	13.7	233
120	The nature of intermolecular interactions between aromatic amino acid residues. Proteins: Structure, Function and Bioinformatics, 2002, 48, 117-125.	2.6	72
121	Determination of the Potential of Mean Force of Aromatic Amino Acid Complexes in Various Solvents Using Molecular Dynamics Simulations:Â The Case of the Tryptophanâ^'Histidine Pair. Journal of Physical Chemistry B, 2001, 105, 7835-7846.	2.6	29
122	Interaction between Aromatic Residues. Molecular Dynamics and ab Initio Exploration of the Potential Energy Surface of the Tryptophanâ^'Histidine Pair. Journal of Physical Chemistry B, 2000, 104, 1108-1114.	2.6	41
123	Density Functional Calculation of Structural and Vibrational Properties of Glycerol. Journal of Physical Chemistry A, 2000, 104, 5351-5357.	2.5	62
124	Conformational Distribution of Gas-phase Glycerol. Journal of Physical Chemistry A, 2000, 104, 11220-11222.	2.5	32
125	Density functional calculation of structure and vibrational spectra of polyenes. Journal of Chemical Physics, 1999, 110, 3241-3250.	3.0	35
126	Low-Frequency Vibrations ofall-trans-Retinal:Â Far-Infrared and Raman Spectra and Density Functional Calculations. Journal of Physical Chemistry A, 1998, 102, 2131-2136.	2.5	56