Francesco L Gervasio

List of Publications by Year
in descending order

126	10,168	38742	37204
papers	citations	50 h-index	96 g-index

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

#	Article	IF	Citations
1	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
2	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
3	Efficient Reconstruction of Complex Free Energy Landscapes by Multiple Walkers Metadynamicsâ€. Journal of Physical Chemistry B, 2006, 110, 3533-3539.	2.6	511
4	From A to B in free energy space. Journal of Chemical Physics, 2007, 126, 054103.	3.0	476
5	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
6	Assessing the Accuracy of Metadynamicsâ€. Journal of Physical Chemistry B, 2005, 109, 6714-6721.	2.6	446
7	The Role of Protein Loops and Linkers in Conformational Dynamics and Allostery. Chemical Reviews, 2016, 116, 6391-6423.	47.7	302
8	Flexible Docking in Solution Using Metadynamics. Journal of the American Chemical Society, 2005, 127, 2600-2607.	13.7	266
9	Stacking and T-shape Competition in Aromaticâ^'Aromatic Amino Acid Interactions. Journal of the American Chemical Society, 2002, 124, 6133-6143.	13.7	233
10	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
11	Electronic Structure of Wet DNA. Physical Review Letters, 2002, 89, 108102.	7.8	157
12	Understanding Cryptic Pocket Formation in Protein Targets by Enhanced Sampling Simulations. Journal of the American Chemical Society, 2016, 138, 14257-14263.	13.7	151
13	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
14	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
15	New advances in metadynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 771-779.	14.6	136
16	Role of glutamine synthetase in angiogenesis beyond glutamine synthesis. Nature, 2018, 561, 63-69.	27.8	136
17	Investigating Drugâ€“Target Association and Dissociation Mechanisms Using Metadynamics-Based Algorithms. Accounts of Chemical Research, 2015, 48, 277-285.	15.6	134
18	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

#	Article	IF	Citations
19	Molecular Mechanism of SSR128129E, an Extracellularly Acting, Small-Molecule, Allosteric Inhibitor of FGF Receptor Signaling. Cancer Cell, 2013, 23, 489-501.	16.8	125
20	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
21	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
22	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
23	Investigating Cryptic Binding Sites by Molecular Dynamics Simulations. Accounts of Chemical Research, 2020, 53, 654-661.	15.6	106
24	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
25	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
26	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
27	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
28	Investigating biological systems using first principles Carâ€“Parrinello molecular dynamics simulations. Current Opinion in Structural Biology, 2007, 17, 149-156.	5.7	90
29	Exploring Complex Proteinâ^Ligand Recognition Mechanisms with Coarse Metadynamics. Journal of Physical Chemistry B, 2009, 113, 4807-4816.	2.6	77
30	Enabling multiscale modeling in systems medicine. Genome Medicine, 2014, 6, 21.	8.2	76
31	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
32	The nature of intermolecular interactions between aromatic amino acid residues. Proteins: Structure, Function and Bioinformatics, 2002, 48, 117-125.	2.6	72
33	The architecture of EGFRâ€™s basal complexes reveals autoinhibition mechanisms in dimers and oligomers. Nature Communications, 2018, 9, 4325.	12.8	71
34	Influence of DNA Structure on the Reactivity of the Guanine Radical Cation. Chemistry - A European Journal, 2004, 10, 4846-4852.	3.3	70
35	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
36	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

#	Article	IF	Citations
37	Molecular basis of engineered meganuclease targeting of the endogenous human RAG1 locus. Nucleic Acids Research, 2011, 39, 729-743.	14.5	63
38	Density Functional Calculation of Structural and Vibrational Properties of Glycerol. Journal of Physical Chemistry A, 2000, 104, 5351-5357.	2.5	62
39	Conformational Changes and Gating at the Selectivity Filter of Potassium Channels. Journal of the American Chemical Society, 2008, 130, 9474-9480.	13.7	61
40	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
41	Protein CoAlation and antioxidant function of coenzyme A in prokaryotic cells. Biochemical Journal, 2018, 475, 1909-1937.	3.7	60
42	Bifunctional Catalysis by Natural Cinchona Alkaloids: A Mechanism Explained. Chemistry - A European Journal, 2009, 15, 7913-7921.	3.3	59
43	Towards a Molecular Understanding of the Link between Imatinib Resistance and Kinase Conformational Dynamics. PLoS Computational Biology, 2015, 11, e1004578.	3.2	59
44	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
45	Molecular engineering of polymersome surface topology. Science Advances, 2016, 2, e1500948.	10.3	56
46	Charge Localization in DNA Fibers. Physical Review Letters, 2005, 94, 158103.	7.8	53
47	Exploring the Gating Mechanism in the ClC Chloride Channel via Metadynamics. Journal of Molecular Biology, 2006, 361, 390-398.	4.2	53
48	Solvent Effects on Charge Spatial Extent in DNA and Implications for Transfer. Physical Review Letters, 2007, 99, 058104.	7.8	53
49	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
50	Double Proton Coupled Charge Transfer in DNA. Angewandte Chemie - International Edition, 2006, 45, 5606-5609.	13.8	52
51	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
52	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
53	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
54	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

#	Article	IF	Citations
55	Conformational Changes and Free Energies in a Proline Isomerase. Journal of Chemical Theory and Computation, 2014, 10, 4169-4174.	5.3	46
56	Exploring Cryptic Pockets Formation in Targets of Pharmaceutical Interest with SWISH. Journal of Chemical Theory and Computation, 2018, 14, 3321-3331.	5.3	45
57	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
58	Allosteric communication in class A Î²-lactamases occurs via cooperative coupling of loop dynamics. ELife, 2021, 10, .	6.0	44
59	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
60	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
61	Efficient Numerical Reconstruction of Protein Folding Kinetics with Partial Path Sampling and Pathlike Variables. Physical Review Letters, 2013, 110, 108106.	7.8	41
62	Is the T-Shaped Toluene Dimer a Stable Intermolecular Complex?. Journal of Physical Chemistry A, 2002, 106, 2945-2948.	2.5	40
63	A Variational Definition of Electrostatic Potential Derived Charges. Journal of Physical Chemistry B, 2004, 108, 7963-7968.	2.6	40
64	Insight into the Folding Inhibition of the HIV-1 Protease by a Small Peptide. Biophysical Journal, 2007, 93, 2813-2821.	0.5	40
65	DNA-binding protects p53 from interactions with cofactors involved in transcription-independent functions. Nucleic Acids Research, 2016, 44, gkw770.	14.5	40
66	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
67	A Threeâ€Site Mechanism for Agonist/Antagonist Selective Binding to Vasopressin Receptors. Angewandte Chemie - International Edition, 2016, 55, 8008-8012.	13.8	38
68	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
69	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
70	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
71	Density functional calculation of structure and vibrational spectra of polyenes. Journal of Chemical Physics, 1999, 110, 3241-3250.	3.0	35
72	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

#	Article	IF	Citations
73	Assessment of the model refinement category in CASP12. Proteins: Structure, Function and Bioinformatics, 2018, 86, 152-167.	2.6	33
74	Conformational Distribution of Gas-phase Glycerol. Journal of Physical Chemistry A, 2000, 104, 11220-11222.	2.5	32
75	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
76	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
77	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
78	A Multiscale Simulation Approach to Modeling Drugâ€"Protein Binding Kinetics. Journal of Chemical Theory and Computation, 2018, 14, 6093-6101.	5.3	29
79	Understanding Ligand Binding Selectivity in a Prototypical GPCR Family. Journal of Chemical Information and Modeling, 2019, 59, 2830-2836.	5.4	28
80	Defining the architecture of KPC-2 Carbapenemase:Âidentifying allosteric networks to fight antibiotics resistance. Scientific Reports, 2018, 8, 12916.	3.3	27
81	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
82	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
83	BioSimSpace: An interoperable Python framework for biomolecular simulation. Journal of Open Source Software, 2019, 4, 1831.	4.6	26
84	Defining an Optimal Metric for the Path Collective Variables. Journal of Chemical Theory and Computation, 2019, 15, 25-32.	5.3	25
85	Non-specific proteinâ€"DNA interactions control I-CreI target binding and cleavage. Nucleic Acids Research, 2012, 40, 6936-6945.	14.5	24
86	Structural basis of the effect of activating mutations on the EGF receptor. ELife, 2021, 10, .	6.0	24
87	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
88	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
89	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
90	New Insights in Protein Kinase Conformational Dynamics. Current Topics in Medicinal Chemistry, 2012, 12, 1889-1895.	2.1	22

#	Article	IF	Citations
91	Intrinsically active MEK variants are differentially regulated by proteinases and phosphatases. Scientific Reports, 2018, 8, 11830.	3.3	22
92	A different perspective for nonphotochemical quenching in plant antenna complexes. Nature Communications, 2021, 12, 7152.	12.8	22
93	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
94	Cyclin-dependent kinases: bridging their structure and function through computations. Future Medicinal Chemistry, 2011, 3, 1551-1559.	2.3	19
95	The Role of Post-translational Modifications on the Energy Landscape of Huntingtin N-Terminus. Frontiers in Molecular Biosciences, 2019, 6, 95.	3.5	19
96	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
97	Unravelling the effect of the E545K mutation on PI3KÎ± kinase. Chemical Science, 2020, 11, 3511-3515.	7.4	17
98	Conformational Selection versus Induced Fit in Kinases: The Case of PI3Kâ€Î³. Angewandte Chemie - International Edition, 2012, 51, 642-646.	13.8	16
99	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
100	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
101	DFT modeling of biological systems. Physica Status Solidi (B): Basic Research, 2006, 243, 2500-2515.	1.5	15
102	Multiple Routes and Milestones in the Folding of HIVâ€“1 Protease Monomer. PLoS ONE, 2010, 5, e13208.	2.5	15
103	The Structure of the Pro-domain of Mouse proNGF in Contact with the NGF Domain. Structure, 2019, 27, 78-89.e3.	3.3	15
104	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
105	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
106	A Threeâ€Site Mechanism for Agonist/Antagonist Selective Binding to Vasopressin Receptors. Angewandte Chemie, 2016, 128, 8140-8144.	2.0	11
107	Backbone assignment of the tyrosine kinase Src catalytic domain in complex with imatinib. Biomolecular NMR Assignments, 2011, 5, 221-224.	0.8	10
108	Charge localisation and hopping in DNA. Molecular Simulation, 2007, 33, 57-60.	2.0	9

#	Article	IF	Citations
109	Amphiphilic Histidine-Based Oligopeptides Exhibit pH-Reversible Fibril Formation. ACS Macro Letters, 2021, 10, 984-989.	4.8	8
110	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
111	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
112	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
113	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
114	Editorial: Machine Learning in Biomolecular Simulations. Frontiers in Molecular Biosciences, 2019, 6, 76.	3.5	4
115	Charge transfer mechanism in a PolydGpdCp fiber and in wet DNA. Computer Physics Communications, 2007, 177, 27-29.	7.5	3
116	Recent Progress in Free Energy Methods. , 2017, , 34-50.		3
117	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1
118	Protein Conformational Plasticity: the â€œoff-onâ€•Switching Movement in Cdk5. AIP Conference Proceedings, 2007, , .	0.4	0
119	Non-Native Structure in the Unfolded Ensemble of a Prototypical Î²-Hairpin. Biophysical Journal, 2009, 96, 78a-79a.	0.5	0
120	Multiple Routes and Milestones in the Folding of HIV-1 Protease Monomer. Biophysical Journal, 2010, 98, 199a.	0.5	0
121	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
122	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
123	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
124	Beyond Structure. Imaging Protein Dynamics at Physiological Temperatures. Biophysical Journal, 2021, 120, 173a.	0.5	0
125	Liquid-Phase Electron Microscopy in Structural Protein Studies. Microscopy and Microanalysis, 2021, 27, 89-90.	0.4	0
126	Imaging Protein Dynamics in Liquid Water. Microscopy and Microanalysis, 2021, 27, 15-16.	0.4	0