

Elisa Fadda

List of Publications by Year in descending order

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38
papers

2,481
citations

471509

17
h-index

345221

36
g-index

45
all docs

45
docs citations

45
times ranked

5061
citing authors

#	ARTICLE	IF	CITATIONS
1	Beyond Shielding: The Roles of Glycans in the SARS-CoV-2 Spike Protein. ACS Central Science, 2020, 6, 1722-1734.	11.3	727
2	Circulating SARS-CoV-2 spike N439K variants maintain fitness while evading antibody-mediated immunity. Cell, 2021, 184, 1171-1187.e20.	28.9	541
3	SARS-CoV-2 simulations go exascale to predict dramatic spike opening and cryptic pockets across the proteome. Nature Chemistry, 2021, 13, 651-659.	13.6	190
4	Molecular simulations of carbohydrates and protein-carbohydrate interactions: motivation, issues and prospects. Drug Discovery Today, 2010, 15, 596-609.	6.4	165
5	Presentation, presentation, presentation! Molecular-level insight into linker effects on glycan array screening data. Glycobiology, 2014, 24, 17-25.	2.5	80
6	Fine-tuning the spike: role of the nature and topology of the glycan shield in the structure and dynamics of the SARS-CoV-2 S. Chemical Science, 2022, 13, 386-395.	7.4	58
7	The case for post-predictional modifications in the AlphaFold Protein Structure Database. Nature Structural and Molecular Biology, 2021, 28, 869-870.	8.2	54
8	Structure and binding analysis of Polyporus squamosus lectin in complex with the Neu5Ac1±2-6Gal1±2-4GlcNAc human-type influenza receptor. Glycobiology, 2011, 21, 973-984.	2.5	53
9	Electrostatic control of proton pumping in cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2008, 1777, 277-284.	1.0	47
10	Sequence-to-structure dependence of isolated IgG Fc complex biantennary N-glycans: a molecular dynamics study. Glycobiology, 2019, 29, 94-103.	2.5	45
11	Role of the XPA protein in the NER pathway: A perspective on the function of structural disorder in macromolecular assembly. Computational and Structural Biotechnology Journal, 2016, 14, 78-85.	4.1	38
12	The Influence of N-Linked Glycans on the Molecular Dynamics of the HIV-1 gp120 V3 Loop. PLoS ONE, 2013, 8, e80301.	2.5	35
13	A chromatin-independent role of Polycomb-like 1 to stabilize p53 and promote cellular quiescence. Genes and Development, 2015, 29, 2231-2243.	5.9	32
14	On the Role of Water Models in Quantifying the Binding Free Energy of Highly Conserved Water Molecules in Proteins: The Case of Concanavalin A. Journal of Chemical Theory and Computation, 2011, 7, 3391-3398.	5.3	31
15	Acidity of a Cu-Bound Histidine in the Binuclear Center of CytochromecOxidase. Journal of Physical Chemistry B, 2005, 109, 22629-22640.	2.6	27
16	Principles of SARS-CoV-2 glycosylation. Current Opinion in Structural Biology, 2022, 75, 102402.	5.7	27
17	Time-dependent density functional theory as a foundation for a firmer understanding of sum-over-states density functional perturbation theory: ?Loc.3? approximation. International Journal of Quantum Chemistry, 2003, 91, 67-83.	2.0	20
18	Lower rim isoxazole-calix[4]arene derivatives as fluorescence sensors for copper(II) ions. Tetrahedron, 2015, 71, 9223-9233.	1.9	18

#	ARTICLE	IF	CITATIONS
19	How and why plants and human N-glycans are different: Insight from molecular dynamics into the α -glycoblocks architecture of complex carbohydrates. <i>Beilstein Journal of Organic Chemistry</i> , 2020, 16, 2046-2056.	2.2	18
20	Molecular simulations of complex carbohydrates and glycoconjugates. <i>Current Opinion in Chemical Biology</i> , 2022, 69, 102175.	6.1	17
21	On the molecular basis of uracil recognition in DNA: comparative study of T-A versus U-A structure, dynamics and open base pair kinetics. <i>Nucleic Acids Research</i> , 2011, 39, 767-780.	14.5	16
22	Aminoquinoline Fluorescent Labels Obstruct Efficient Removal of α -N-Glycan Core \pm (1 \pm 6) Fucose by Bovine Kidney α -Fucosidase (BKF). <i>Journal of Proteome Research</i> , 2017, 16, 4237-4243.	3.7	16
23	$^{14,15}\text{N}$ NMR Shielding Constants from Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9924-9930.	2.5	15
24	An atomistic perspective on antibody-dependent cellular cytotoxicity quenching by core-fucosylation of IgG1 Fc N-glycans from enhanced sampling molecular dynamics. <i>Glycobiology</i> , 2020, 30, 407-414.	2.5	14
25	Defining the structural origin of the substrate sequence independence of O-GlcNAcase using a combination of molecular docking and dynamics simulation. <i>Glycobiology</i> , 2014, 24, 85-96.	2.5	13
26	Calculating Binding Free Energies for Protein-Carbohydrate Complexes. <i>Methods in Molecular Biology</i> , 2015, 1273, 431-465.	0.9	13
27	Conformational Determinants for the Recruitment of ERCC1 by XPA in the Nucleotide Excision Repair (NER) Pathway: Structure and Dynamics of the XPA Binding Motif. <i>Biophysical Journal</i> , 2013, 104, 2503-2511.	0.5	12
28	Molecular basis of proton uptake in single and double mutants of cytochrome <i>c</i> oxidase. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 234102.	1.8	11
29	The transient manifold structure of the p53 extreme C-terminal domain: insight into disorder, recognition, and binding promiscuity by molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 21287-21296.	2.8	11
30	NMR shieldings from sum-over-states density-functional-perturbation theory: Further testing of the Loc.3 approximation. <i>Journal of Chemical Physics</i> , 2003, 118, 6758-6768.	3.0	10
31	Contribution of the empirical dispersion correction on the conformation of short alanine peptides obtained by gas-phase QM calculations. <i>Canadian Journal of Chemistry</i> , 2013, 91, 859-865.	1.1	9
32	Oligomannose α -N-Glycans 3D Architecture and Its Response to the Fc β 3R1IIa Structural Landscape. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2607-2616.	2.6	9
33	Reply to α -Comment on Acidity of a Cu-bound Histidine in the Binuclear Center of Cytochrome <i>c</i> Oxidase. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17288-17289.	2.6	6
34	The role of conformational selection in the molecular recognition of the wild type and mutants α -XPA β 780 peptides by α -ERCC1. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 1341-1351.	2.6	4
35	Computational Modeling in Glycoscience. , 2021, , 374-404.		3
36	Synthesis and characterisation of new copper(II) coordination polymers constructed from pyrazine-tetrazole ligands with the formation of a water cluster. <i>Supramolecular Chemistry</i> , 2016, 28, 707-719.	1.2	2

#	ARTICLE	IF	CITATIONS
37	Binding Free Energies of Conformationally Disordered Peptides Through Extensive Sampling and End-Point Methods. <i>Methods in Molecular Biology</i> , 2019, 2039, 229-242.	0.9	1
38	Understanding the Structure and Function of Viral Glycosylation by Molecular Simulations: State-of-the-Art and Recent Case Studies. , 2021, , 405-415.		1