# 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 | 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 |
| 2 | Principles of SARS-CoV-2 glycosylation. Current Opinion in Structural Biology, 2022, 75, 102402. | 5.7 | 27 |
| 3 | Molecular simulations of complex carbohydrates and glycoconjugates. Current Opinion in Chemical Biology, 2022, 69, 102175. | 6.1 | 17 |
| 4 | Understanding the Structure and Function of Viral Glycosylation by Molecular Simulations: State-of-the-Art and Recent Case Studies. , 2021, , 405-415. | | 1 |
| 5 | Oligomannose N-Glycans 3D Architecture and Its Response to the FcÎ³RIIIa Structural Landscape. Journal of Physical Chemistry B, 2021, 125, 2607-2616. | 2.6 | 9 |
| 6 | Circulating SARS-CoV-2 spike N439K variants maintain fitness while evading antibody-mediated immunity. Cell, 2021, 184, 1171-1187.e20. | 28.9 | 541 |
| 7 | 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 |
| 8 | Computational Modeling in Glycoscience. , 2021, , 374-404. | | 3 |
| 9 | The case for post-predictional modifications in the AlphaFold Protein Structure Database. Nature Structural and Molecular Biology, 2021, 28, 869-870. | 8.2 | 54 |
| 10 | An atomistic perspective on antibody-dependent cellular cytotoxicity quenching by core-fucosylation of IgG1 Fc N-glycans from enhanced sampling molecular dynamics. Glycobiology, 2020, 30, 407-414. | 2.5 | 14 |
| 11 | How and why plants and human N-glycans are different: Insight from molecular dynamics into the â€œglycoblocksâ€•architecture of complex carbohydrates. Beilstein Journal of Organic Chemistry, 2020, 16, 2046-2056. | 2.2 | 18 |
| 12 | Beyond Shielding: The Roles of Glycans in the SARS-CoV-2 Spike Protein. ACS Central Science, 2020, 6, 1722-1734. | 11.3 | 727 |
| 13 | Binding Free Energies of Conformationally Disordered Peptides Through Extensive Sampling and End-Point Methods. Methods in Molecular Biology, 2019, 2039, 229-242. | 0.9 | 1 |
| 14 | Sequence-to-structure dependence of isolated IgG Fc complex biantennaryN-glycans: a molecular dynamics study. Glycobiology, 2019, 29, 94-103. | 2.5 | 45 |
| 15 | The transient manifold structure of the p53 extreme C-terminal domain: insight into disorder, recognition, and binding promiscuity by molecular dynamics simulations. Physical Chemistry Chemical Physics, 2017, 19, 21287-21296. | 2.8 | 11 |
| 16 | Aminoquinoline Fluorescent Labels Obstruct Efficient Removal of N-Glycan Core Î±(1â€“6) Fucose by Bovine Kidney Î±-<scp>l</scp>-Fucosidase (BKF). Journal of Proteome Research, 2017, 16, 4237-4243. | 3.7 | 16 |
| 17 | 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 |
| 18 | Synthesis and characterisation of new copper(II) coordination polymers constructed from pyrazineâ€“tetrazole ligands with the formation of a water cluster. Supramolecular Chemistry, 2016, 28, 707-719. | 1.2 | 2 |

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|---|---|---|---|
| 19 | The role of conformational selection in the molecular recognition of the wild type and mutants <scp>XPA</scp><sub>67â€80</sub> peptides by <scp>ERCC</scp>1. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1341-1351. | 2.6 | 4 |
| 20 | Lower rim isoxazole-calix[4]arene derivatives as fluorescence sensors for copper(II) ions. Tetrahedron, 2015, 71, 9223-9233. | 1.9 | 18 |
| 21 | 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 |
| 22 | Calculating Binding Free Energies for Proteinâ€“Carbohydrate Complexes. Methods in Molecular Biology, 2015, 1273, 431-465. | 0.9 | 13 |
| 23 | Defining the structural origin of the substrate sequence independence of O-GlcNAcase using a combination of molecular docking and dynamics simulation. Glycobiology, 2014, 24, 85-96. | 2.5 | 13 |
| 24 | Presentation, presentation, presentation! Molecular-level insight into linker effects on glycan array screening data. Glycobiology, 2014, 24, 17-25. | 2.5 | 80 |
| 25 | Contribution of the empirical dispersion correction on the conformation of short alanine peptides obtained by gas-phase QM calculations. Canadian Journal of Chemistry, 2013, 91, 859-865. | 1.1 | 9 |
| 26 | Conformational Determinants for the Recruitment of ERCC1 by XPA in the Nucleotide Excision Repair (NER) Pathway: Structure and Dynamics of the XPA Binding Motif. Biophysical Journal, 2013, 104, 2503-2511. | 0.5 | 12 |
| 27 | 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 |
| 28 | 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 |
| 29 | Molecular basis of proton uptake in single and double mutants of cytochromecoxidase. Journal of Physics Condensed Matter, 2011, 23, 234102. | 1.8 | 11 |
| 30 | Structure and binding analysis of Polyporus squamosus lectin in complex with the Neu5AcÎ±2-6GalÎ²1-4GlcNAc human-type influenza receptor. Glycobiology, 2011, 21, 973-984. | 2.5 | 53 |
| 31 | On the molecular basis of uracil recognition in DNA: comparative study of T-A versus U-A structure, dynamics and open base pair kinetics. Nucleic Acids Research, 2011, 39, 767-780. | 14.5 | 16 |
| 32 | Molecular simulations of carbohydrates and proteinâ€“carbohydrate interactions: motivation, issues and prospects. Drug Discovery Today, 2010, 15, 596-609. | 6.4 | 165 |
| 33 | Electrostatic control of proton pumping in cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2008, 1777, 277-284. | 1.0 | 47 |
| 34 | Reply to â€œComment on Acidity of a Cu-bound Histidine in the Binuclear Center of Cytochrome c Oxidaseâ€• Journal of Physical Chemistry B, 2006, 110, 17288-17289. | 2.6 | 6 |
| 35 | Acidity of a Cu-Bound Histidine in the Binuclear Center of CytochromecOxidase. Journal of Physical Chemistry B, 2005, 109, 22629-22640. | 2.6 | 27 |
| 36 | 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 |

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|---|---|---|---|
| 37 | 14,15N NMR Shielding Constants from Density Functional Theory. Journal of Physical Chemistry A, 2003, 107, 9924-9930. | 2.5 | 15 |
| 38 | NMR shieldings from sum-over-states density-functional-perturbation theory: Further testing of the â€œLoc.3â€•approximation. Journal of Chemical Physics, 2003, 118, 6758-6768. | 3.0 | 10 |