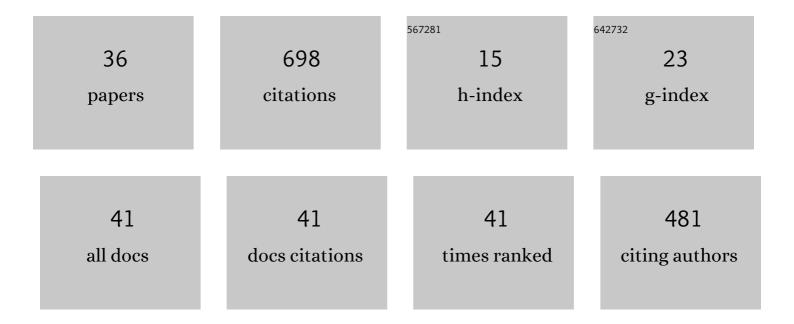
## Monica L FernÃ;ndez-Quintero

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Paratope states in solution improve structure prediction and docking. Structure, 2022, 30, 430-440.e3.	3.3	8
2	Explicit solvation thermodynamics in ionic solution: extending grid inhomogeneous solvation theory to solvation free energy of salt–water mixtures. Journal of Computer-Aided Molecular Design, 2022, 36, 101-116.	2.9	8
3	CDR loop interactions can determine heavy and light chain pairing preferences in bispecific antibodies. MAbs, 2022, 14, 2024118.	5.2	4
4	Comparing Antibody Interfaces to Inform Rational Design of New Antibody Formats. Frontiers in Molecular Biosciences, 2022, 9, 812750.	3.5	4
5	Broadly neutralizing antibodies target a haemagglutinin anchor epitope. Nature, 2022, 602, 314-320.	27.8	78
6	Calcium current modulation by the γ1 subunit depends on alternative splicing of CaV1.1. Journal of General Physiology, 2022, 154, .	1.9	4
7	Essential role of a conserved aspartate for the enzymatic activity of plasmanylethanolamine desaturase. Cellular and Molecular Life Sciences, 2022, 79, 214.	5.4	2
8	Grid inhomogeneous solvation theory for cross-solvation in rigid solvents. Journal of Chemical Physics, 2022, 156, .	3.0	3
9	Nanobody Paratope Ensembles in Solution Characterized by MD Simulations and NMR. International Journal of Molecular Sciences, 2022, 23, 5419.	4.1	6
10	Conformational Ensembles of Antibodies Determine Their Hydrophobicity. Biophysical Journal, 2021, 120, 143-157.	0.5	23
11	Ensembles in solution as a new paradigm for antibody structure prediction and design. MAbs, 2021, 13, 1923122.	5.2	19
12	Structural determinants of voltage-gating properties in calcium channels. ELife, 2021, 10, .	6.0	18
13	<i>CACNA1I</i> gain-of-function mutations differentially affect channel gating and cause neurodevelopmental disorders. Brain, 2021, 144, 2092-2106.	7.6	26
14	Conformational Shifts of Stacked Heteroaromatics: Vacuum vs. Water Studied by Machine Learning. Frontiers in Chemistry, 2021, 9, 641610.	3.6	1
15	Mutation of Framework Residue H71 Results in Different Antibody Paratope States in Solution. Frontiers in Immunology, 2021, 12, 630034.	4.8	17
16	Shark Antibody Variable Domains Rigidify Upon Affinity Maturation—Understanding the Potential of Shark Immunoglobulins as Therapeutics. Frontiers in Molecular Biosciences, 2021, 8, 639166.	3.5	9
17	Implementation of the Freely Jointed Chain Model to Assess Kinetics and Thermodynamics of Thermosensitive Coil–Globule Transition by Markov States. Journal of Physical Chemistry B, 2021, 125, 4898-4909.	2.6	4
18	Pore mutation N617D in the skeletal muscle DHPR blocks Ca2+ influx due to atypical high-affinity Ca2+ binding. ELife, 2021, 10, .	6.0	5

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IF # ARTICLE CITATIONS Cav1.4 dysfunction and congenital stationary night blindness type 2. Pflugers Archiv European Journal 2.8 of Physiology, 2021, 473, 1437-1454. Germline-Dependent Antibody Paratope States and Pairing Specific VH-VL Interface Dynamics. Frontiers 20 4.8 11 in Immunology, 2021, 12, 675655. Ion-pair interactions between voltage-sensing domain IV and pore domain I regulate CaV1.1 gating. Biophysical Journal, 2021, 120, 4429-4441. V/sub>H</sub> $\hat{a}$ +V/sub>L</sub> interdomain dynamics observed by computer simulations and NMR. 22 2.6 28 Proteins: Structure, Function and Bioinformatics, 2020, 88, 830-839. Local and Global Rigidification Upon Antibody Affinity Maturation. Frontiers in Molecular 3.5 29 Biosciences, 2020, 7, 182. T-Cell Receptor CDR3 Loop Conformations in Solution Shift the Relative  $V\hat{I}\pm -V\hat{I}^2$  Domain Distributions. 24 4.8 17 Frontiers in Immunology, 2020, 11, 1440. Polyreactive Broadly Neutralizing B cells Are Selected to Provide Defense against Pandemic Threat Influenza Viruses. Immunity, 2020, 53, 1230-1244.e5. 14.3 61 Antibodies exhibit multiple paratope states influencing VH–VL domain orientations. Communications 26 4.4 38 Biology, 2020, 3, 589. Surprisingly Fast Interface and Elbow Angle Dynamics of Antigen-Binding Fragments. Frontiers in 3.5 Molecular Biosciences, 2020, 7, 609088. T-Cell Receptor Variable Î<sup>2</sup> Domains Rigidify During Affinity Maturation. Scientific Reports, 2020, 10, 28 3.3 20 4472. STACKED – <u>S</u>olvation <u>T</u>heory of <u>A</u>romatic <u>C</u>omplexes as <u>K</u>ey for <u>E</u>stimating <u>D</u>rug Binding. Journal of Chemical Information and Modeling, 2020, 60, 5.4 10 2304-2313. Antibody CDR loops as ensembles in solution vs. canonical clusters from X-ray structures. MAbs, 30 5.2 34 2020, 12, 1744328. pH-Induced Local Unfolding of the Phl p 6 Pollen Allergen From cpH-MD. Frontiers in Molecular 3.5 Biosciences, 2020, 7, 603644. CDR-H3 loop ensemble in solution – conformational selection upon antibody binding. MAbs, 2019, 11, 32 5.2 49 1077-1088. Conformational selection of allergen-antibody complexesâ€"surface plasticity of paratopes and epitopes. Protein Engineering, Design and Selection, 2019, 32, 513-523. 33 2.1 Antibody humanizationâ€"the Influence of the antibody framework on the CDR-H3 loop ensemble in 34 2.1 17 solution. Protein Engineering, Design and Selection, 2019, 32, 411-422. Transitions of CDR-L3 Loop Canonical Cluster Conformations on the Micro-to-Millisecond Timescale. 4.8 Frontiers in Immunology, 2019, 10, 2652. Characterizing the Diversity of the CDR-H3 Loop Conformational Ensembles in Relationship to 36 4.8 73 Antibody Binding Properties. Frontiers in Immunology, 2018, 9, 3065.