

# Andrea Spitaleri

## List of Publications by Year in descending order

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45  
papers

2,141  
citations

257357

24  
h-index

243529

44  
g-index

54  
all docs

54  
docs citations

54  
times ranked

3549  
citing authors

#	ARTICLE	IF	CITATIONS
1	Glycyrrhizin Binds to High-Mobility Group Box 1 Protein and Inhibits Its Cytokine Activities. <i>Chemistry and Biology</i> , 2007, 14, 431-441.	6.2	484
2	Investigating Drug-Target Association and Dissociation Mechanisms Using Metadynamics-Based Algorithms. <i>Accounts of Chemical Research</i> , 2015, 48, 277-285.	7.6	134
3	The 2021 WHO catalogue of <i>Mycobacterium tuberculosis</i> complex mutations associated with drug resistance: a genotypic analysis. <i>Lancet Microbe</i> , The, 2022, 3, e265-e273.	3.4	114
4	Structural Basis for the Interaction of isoDGR with the RGD-binding Site of $\alpha_3\beta_1$ Integrin. <i>Journal of Biological Chemistry</i> , 2008, 283, 19757-19768.	1.6	93
5	muma, An R Package for Metabolomics Univariate and Multivariate Statistical Analysis. <i>Current Metabolomics</i> , 2013, 1, 180-189.	0.5	93
6	Exploring PHD Fingers and H3K4me0 Interactions with Molecular Dynamics Simulations and Binding Free Energy Calculations: AIRE-PHD1, a Comparative Study. <i>PLoS ONE</i> , 2012, 7, e46902.	1.1	80
7	The solution structure of the first PHD finger of autoimmune regulator in complex with non-modified histone H3 tail reveals the antagonistic role of H3R2 methylation. <i>Nucleic Acids Research</i> , 2009, 37, 2951-2961.	6.5	79
8	GMXPBSA 2.0: A GROMACS tool to perform MM/PBSA and computational alanine scanning. <i>Computer Physics Communications</i> , 2014, 185, 2920-2929.	3.0	76
9	GMXPBSA 2.1: A GROMACS tool to perform MM/PBSA and computational alanine scanning. <i>Computer Physics Communications</i> , 2015, 186, 105-107.	3.0	72
10	A 1H NMR study of crystal nucleation in solution. <i>CrystEngComm</i> , 2004, 6, 489.	1.3	70
11	dMM-PBSA: A New HADDOCK Scoring Function for Protein-Peptide Docking. <i>Frontiers in Molecular Biosciences</i> , 2016, 3, 46.	1.6	67
12	Solvent effects of the structures of prenucleation aggregates of carbamazepine. <i>CrystEngComm</i> , 2012, 14, 7115.	1.3	58
13	BiKi Life Sciences: A New Suite for Molecular Dynamics and Related Methods in Drug Discovery. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 219-224.	2.5	48
14	Characterization of Genomic Variants Associated with Resistance to Bedaquiline and Delamanid in Naive <i>Mycobacterium tuberculosis</i> Clinical Strains. <i>Journal of Clinical Microbiology</i> , 2020, 58, .	1.8	46
15	2D TR-NOESY Experiments Interrogate and Rank Ligand-Receptor Interactions in Living Human Cancer Cells. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1071-1074.	7.2	40
16	Fast Dynamic Docking Guided by Adaptive Electrostatic Bias: The MD-Binding Approach. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1727-1736.	2.3	40
17	Supported ruthenium nanoparticles on polyorganophosphazenes: preparation, structural and catalytic studies. <i>Inorganica Chimica Acta</i> , 2003, 352, 61-71.	1.2	37
18	Molecular Dynamics Reveal that isoDGR-Containing Cyclopeptides Are True $\alpha_3\beta_1$ Antagonists Unable To Promote Integrin Allosteric Activation. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 7702-7705.	7.2	37

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19	Role of Epistasis in Amikacin, Kanamycin, Bedaquiline, and Clofazimine Resistance in Mycobacterium tuberculosis Complex. <i>Antimicrobial Agents and Chemotherapy</i> , 2021, 65, e0116421.	1.4	35
20	Tailbiter: a new amide foldamer. <i>Chemical Communications</i> , 2005, , 3691.	2.2	34
21	Determination of Protein-Ligand Binding Modes Using Complexation-Induced Changes in <sup>1</sup> H NMR Chemical Shift. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 2512-2517.	2.9	34
22	Fluorophenols and (Trifluoromethyl)phenols as Substrates of Site-Selective Metalation Reactions: To Protect or not To Protect. <i>European Journal of Organic Chemistry</i> , 2001, 2001, 2911.	1.2	33
23	Use of Metadynamics in the Design of isoDGR-Based $\beta$ 3 Antagonists To Fine-Tune the Conformational Ensemble. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 1832-1836.	7.2	33
24	Oxidation-induced Structural Changes of Ceruloplasmin Foster NGR Motif Deamidation That Promotes Integrin Binding and Signaling. <i>Journal of Biological Chemistry</i> , 2014, 289, 3736-3748.	1.6	28
25	AurkA controls self-renewal of breast cancer-initiating cells promoting wnt3a stabilization through suppression of miR-128. <i>Scientific Reports</i> , 2016, 6, 28436.	1.6	25
26	GenomeMap: Within-Species Genome-Wide dN/dS Estimation from over 10,000 Genomes. <i>Molecular Biology and Evolution</i> , 2020, 37, 2450-2460.	3.5	25
27	Nephrocystin-1 Forms a Complex with Polycystin-1 via a Polyproline Motif/SH3 Domain Interaction and Regulates the Apoptotic Response in Mammals. <i>PLoS ONE</i> , 2010, 5, e12719.	1.1	25
28	NanoShaper-VMD interface: computing and visualizing surfaces, pockets and channels in molecular systems. <i>Bioinformatics</i> , 2019, 35, 1241-1243.	1.8	23
29	Metadynamics Simulations Rationalise the Conformational Effects Induced by N-Methylation of RGD Cyclic Hexapeptides. <i>Chemistry - A European Journal</i> , 2015, 21, 14165-14170.	1.7	20
30	Detection of NDM-1/5 and OXA-48 co-producing extensively drug-resistant hypervirulent <i>Klebsiella pneumoniae</i> in Northern Italy. <i>Journal of Global Antimicrobial Resistance</i> , 2022, 28, 146-150.	0.9	15
31	Whole genome sequencing of multidrug-resistant <i>Mycobacterium tuberculosis</i> isolates collected in the Czech Republic, 2005-2020. <i>Scientific Reports</i> , 2022, 12, 7149.	1.6	14
32	Fluoro- or Trifluoromethyl-Substituted Benzyl and Phenethyl Alcohols: Substrates for Metal-Mediated Site-Selective Functionalization. <i>European Journal of Organic Chemistry</i> , 2002, 2002, 2508.	1.2	13
33	A Novel HRAS Mutation Independently Contributes to Left Ventricular Hypertrophy in a Family with a Known MYH7 Mutation. <i>PLoS ONE</i> , 2016, 11, e0168501.	1.1	13
34	Adaptive nanopores: A bioinspired label-free approach for protein sequencing and identification. <i>Nano Research</i> , 2021, 14, 328-333.	5.8	9
35	NMR and Computational Methods in the Structural and Dynamic Characterization of Ligand-Receptor Interactions. <i>Advances in Experimental Medicine and Biology</i> , 2014, 805, 271-304.	0.8	8
36	Enhanced Molecular Dynamics Method to Efficiently Increase the Discrimination Capability of Computational Protein-Protein Docking. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7271-7280.	2.3	6

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37	Identification of a novel de novo deletion in <i>RAF1</i> associated with biventricular hypertrophy in Noonan syndrome. <i>American Journal of Medical Genetics, Part A</i> , 2014, 164, 2069-2073.	0.7	5
38	Tuning Local Hydration Enables a Deeper Understanding of Protein-Ligand Binding: The PP1- <i>Src</i> Kinase Case. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 49-58.	2.1	5
39	Rapid SARS-CoV-2 Intra-Host and Within-Household Emergence of Novel Haplotypes. <i>Viruses</i> , 2022, 14, 399.	1.5	5
40	Underwater acoustic positioning system for the SMO and KM3NeT - Italia projects. , 2014, , .		3
41	The trigger and data acquisition for the NEMO-Phase 2 tower. , 2014, , .		3
42	Plasma viscosity: Relation to age, atherogenic diet and suloctidil. <i>Pharmacological Research Communications</i> , 1981, 13, 765-767.	0.2	2
43	Whole genome sequencing of isoniazid monoresistant clinical isolates of <i>Mycobacterium tuberculosis</i> reveals novel genetic polymorphisms. <i>Tuberculosis</i> , 2022, 133, 102173.	0.8	1
44	Abstract 748: Development and application of novel in silico methods in the discovery and characterization of integrin antagonists. , 2010, , .		0
45	Abstract 5081: Development and characterization of a new antiangiogenic peptide targeting tumor vessels.. , 2013, , .		0