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	Detection of NDM-1/5 and OXA-48 co-producing extensively drug-resistant hypervirulent Klebsiella pneumoniae in Northern Italy. Journal of Global Antimicrobial Resistance, 2022, 28, 146-150.	0.9	15
2	Whole genome sequencing of isoniazid monoresistant clinical isolates of Mycobacterium tuberculosis reveals novel genetic polymorphisms. Tuberculosis, 2022, 133, 102173.	0.8	1
3	Rapid SARS-CoV-2 Intra-Host and Within-Household Emergence of Novel Haplotypes. Viruses, 2022, 14, 399.	1.5	5
4	The 2021 WHO catalogue of Mycobacterium tuberculosis complex mutations associated with drug resistance: a genotypic analysis. Lancet Microbe, The, 2022, 3, e265-e273.	3.4	114
5	Whole genome sequencing of multidrug-resistant Mycobacterium tuberculosis isolates collected in the Czech Republic, 2005â€“2020. Scientific Reports, 2022, 12, 7149.	1.6	14
6	Tuning Local Hydration Enables a Deeper Understanding of Proteinâ€“Ligand Binding: The PP1-Src Kinase Case. Journal of Physical Chemistry Letters, 2021, 12, 49-58.	2.1	5
7	Adaptive nanopores: A bioinspired label-free approach for protein sequencing and identification. Nano Research, 2021, 14, 328-333.	5.8	9
8	Role of Epistasis in Amikacin, Kanamycin, Bedaquiline, and Clofazimine Resistance in Mycobacterium tuberculosis Complex. Antimicrobial Agents and Chemotherapy, 2021, 65, e0116421.	1.4	35
9	Enhanced Molecular Dynamics Method to Efficiently Increase the Discrimination Capability of Computational Proteinâ€“Protein Docking. Journal of Chemical Theory and Computation, 2021, 17, 7271-7280.	2.3	6
10	Characterization of Genomic Variants Associated with Resistance to Bedaquiline and Delamanid in Naive Mycobacterium tuberculosis Clinical Strains. Journal of Clinical Microbiology, 2020, 58, .	1.8	46
11	GenomegaMap: Within-Species Genome-Wide dN/dS Estimation from over 10,000 Genomes. Molecular Biology and Evolution, 2020, 37, 2450-2460.	3.5	25
12	NanoShaperâ€“VMD interface: computing and visualizing surfaces, pockets and channels in molecular systems. Bioinformatics, 2019, 35, 1241-1243.	1.8	23
13	BiKi Life Sciences: A New Suite for Molecular Dynamics and Related Methods in Drug Discovery. Journal of Chemical Information and Modeling, 2018, 58, 219-224.	2.5	48
14	Fast Dynamic Docking Guided by Adaptive Electrostatic Bias: The MD-Binding Approach. Journal of Chemical Theory and Computation, 2018, 14, 1727-1736.	2.3	40
15	dMM-PBSA: A New HADDOCK Scoring Function for Protein-Peptide Docking. Frontiers in Molecular Biosciences, 2016, 3, 46.	1.6	67
16	A Novel HRAS Mutation Independently Contributes to Left Ventricular Hypertrophy in a Family with a Known MYH7 Mutation. PLoS ONE, 2016, 11, e0168501.	1.1	13
17	AurkA controls self-renewal of breast cancer-initiating cells promoting wnt3a stabilization through suppression of miR-128. Scientific Reports, 2016, 6, 28436.	1.6	25
18	Metadynamics Simulations Rationalise the Conformational Effects Induced by Nâ€Methylation of RGD Cyclic Hexapeptides. Chemistry - A European Journal, 2015, 21, 14165-14170.	1.7	20

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19	Investigating Drugâ€“Target Association and Dissociation Mechanisms Using Metadynamics-Based Algorithms. Accounts of Chemical Research, 2015, 48, 277-285.	7.6	134
20	GMXPBSA 2.1: A GROMACS tool to perform MM/PBSA and computational alanine scanning. Computer Physics Communications, 2015, 186, 105-107.	3.0	72
21	Identification of a novel de novo deletion in RAF1 associated with biventricular hypertrophy in Noonan syndrome. American Journal of Medical Genetics, Part A, 2014, 164, 2069-2073.	0.7	5
22	Underwater acoustic positioning system for the SMO and KM3NeT - Italia projects. , 2014, , .		3
23	The trigger and data acquisition for the NEMO-Phase 2 tower. , 2014, , .		3
24	Oxidation-induced Structural Changes of Ceruloplasmin Foster NGR Motif Deamidation That Promotes Integrin Binding and Signaling. Journal of Biological Chemistry, 2014, 289, 3736-3748.	1.6	28
25	GMXPBSA 2.0: A GROMACS tool to perform MM/PBSA and computational alanine scanning. Computer Physics Communications, 2014, 185, 2920-2929.	3.0	76
26	NMR and Computational Methods in the Structural and Dynamic Characterization of Ligand-Receptor Interactions. Advances in Experimental Medicine and Biology, 2014, 805, 271-304.	0.8	8
27	muma, An R Package for Metabolomics Univariate and Multivariate Statistical Analysis. Current Metabolomics, 2013, 1, 180-189.	0.5	93
28	Abstract 5081: Development and characterization of a new antiangiogenic peptide targeting tumor vessels.. , 2013, , .		0
29	Solvent effects of the structures of prenucleation aggregates of carbamazepine. CrystEngComm, 2012, 14, 7115.	1.3	58
30	Exploring PHD Fingers and H3K4me0 Interactions with Molecular Dynamics Simulations and Binding Free Energy Calculations: AIRE-PHD1, a Comparative Study. PLoS ONE, 2012, 7, e46902.	1.1	80
31	Molecular Dynamics Reveal that isoDGRâ€Containing Cyclopeptides Are True Î±vÎ²3 Antagonists Unable To Promote Integrin Allostery and Activation. Angewandte Chemie - International Edition, 2012, 51, 7702-7705.	7.2	37
32	Use of Metadynamics in the Design of isoDGRâ€Based Î±vÎ²3 Antagonists To Fineâ€Tune the Conformational Ensemble. Angewandte Chemie - International Edition, 2011, 50, 1832-1836.	7.2	33
33	2D TRâ€NOESY Experiments Interrogate and Rank Ligandâ€“Receptor Interactions in Living Human Cancer Cells. Angewandte Chemie - International Edition, 2010, 49, 1071-1074.	7.2	40
34	Nephrocystin-1 Forms a Complex with Polycystin-1 via a Polyproline Motif/SH3 Domain Interaction and Regulates the Apoptotic Response in Mammals. PLoS ONE, 2010, 5, e12719.	1.1	25
35	Abstract 748: Development and application of novelin silicomethods in the discovery and characterization of integrins antagonists. , 2010, , .		0
36	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. Nucleic Acids Research, 2009, 37, 2951-2961.	6.5	79

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37	Determination of Proteinâ€“Ligand Binding Modes Using Complexation-Induced Changes in 1H NMR Chemical Shift. Journal of Medicinal Chemistry, 2008, 51, 2512-2517.	2.9	34
38	Structural Basis for the Interaction of isoDGR with the RGD-binding Site of Î±vÎ²3 Integrin. Journal of Biological Chemistry, 2008, 283, 19757-19768.	1.6	93
39	Glycyrrhizin Binds to High-Mobility Group Box 1 Protein and Inhibits Its Cytokine Activities. Chemistry and Biology, 2007, 14, 431-441.	6.2	484
40	Tailbiter: a new amide foldamer. Chemical Communications, 2005, , 3691.	2.2	34
41	A 1H NMR study of crystal nucleation in solution. CrystEngComm, 2004, 6, 489.	1.3	70
42	Supported ruthenium nanoparticles on polyorganophosphazenes: preparation, structural and catalytic studies. Inorganica Chimica Acta, 2003, 352, 61-71.	1.2	37
43	Fluoro- or Trifluoromethyl-Substituted Benzyl and Phenethyl Alcohols: Substrates for Metal-Mediated Site-Selective Functionalization. European Journal of Organic Chemistry, 2002, 2002, 2508.	1.2	13
44	Fluorophenols and (Trifluoromethyl)phenols as Substrates of Site-Selective Metalation Reactions: To Protect or not To Protect. European Journal of Organic Chemistry, 2001, 2001, 2911.	1.2	33
45	Plasma viscosity: Relation to age, atherogenic diet and suloctidil. Pharmacological Research Communications, 1981, 13, 765-767.	0.2	2