# Andrea Zaliani

List of Publications by Year
in descending order

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|---|---|---|---|
| 41<br>papers | 2,355<br>citations | 331670<br>21<br>h-index | 315739<br>38<br>g-index |
| 51<br>all docs | 51<br>docs citations | 51<br>times ranked | 3227<br>citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Minimal information for chemosensitivity assays (MICHA): a next-generation pipeline to enable the FAIRification of drug screening experiments. Briefings in Bioinformatics, 2022, 23, . | 6.5 | 7 |
| 2 | The blood-brain barrier is dysregulated in COVID-19 and serves as a CNS entry route for SARS-CoV-2. Stem Cell Reports, 2022, 17, 307-320. | 4.8 | 138 |
| 3 | A hybrid approach unveils drug repurposing candidates targeting an Alzheimer pathophysiology mechanism. Patterns, 2022, 3, 100433. | 5.9 | 13 |
| 4 | SASC: A simple approach to synthetic cohorts for generating longitudinal observational patient cohorts from COVID-19 clinical data. Patterns, 2022, 3, 100453. | 5.9 | 4 |
| 5 | Natural Compounds Inhibit SARS-CoV-2 nsp13 Unwinding and ATPase Enzyme Activities. ACS Pharmacology and Translational Science, 2022, 5, 226-239. | 4.9 | 43 |
| 6 | Cytopathic SARS-CoV-2 screening on VERO-E6 cells in a large-scale repurposing effort. Scientific Data, 2022, 9, . | 5.3 | 17 |
| 7 | A SARS-CoV-2 cytopathicity dataset generated by high-content screening of a large drug repurposing collection. Scientific Data, 2021, 8, 70. | 5.3 | 65 |
| 8 | A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. ACS Pharmacology and Translational Science, 2021, 4, 1079-1095. | 4.9 | 44 |
| 9 | Identification of Inhibitors of SARS-CoV-2 3CL-Pro Enzymatic Activity Using a Small Molecule in Vitro Repurposing Screen. ACS Pharmacology and Translational Science, 2021, 4, 1096-1110. | 4.9 | 101 |
| 10 | X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. Science, 2021, 372, 642-646. | 12.6 | 240 |
| 11 | A method for the rational selection of drug repurposing candidates from multimodal knowledge harmonization. Scientific Reports, 2021, 11, 11049. | 3.3 | 12 |
| 12 | Data-science based analysis of perceptual spaces of odors in olfactory loss. Scientific Reports, 2021, 11, 10595. | 3.3 | 3 |
| 13 | Structural and Biochemical Analysis of the Dual Inhibition of MG-132 against SARS-CoV-2 Main Protease (Mpro/3CLpro) and Human Cathepsin-L. International Journal of Molecular Sciences, 2021, 22, 11779. | 4.1 | 47 |
| 14 | Machine Learning Based Prediction of COVID-19 Mortality Suggests Repositioning of Anticancer Drug for Treating Severe Cases. Artificial Intelligence in the Life Sciences, 2021, 1, 100020. | 2.2 | 6 |
| 15 | Discovery of Protein-Protein Interaction Inhibitors by Integrating Protein Engineering and Chemical Screening Platforms. Cell Chemical Biology, 2020, 27, 1441-1451.e7. | 5.2 | 13 |
| 16 | Novel nanomolar imidazo[4,5-b]pyridines as selective nitric oxide synthase (iNOS) inhibitors: SAR and structural insights. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 4228-4232. | 2.2 | 30 |
| 17 | Synthesis and biological evaluation of novel (4 or 5-aryl)pyrazolyl-indoles as inhibitors of interleukin-2 inducible T-cell kinase (ITK). Bioorganic and Medicinal Chemistry, 2010, 18, 4547-4559. | 3.0 | 31 |
| 18 | Spiro-Annelated Zn-Phthalocyanine: A Novel Building Block for Molecular Architecture?. Synthesis, 2010, 2010, 3569-3575. | 2.3 | 0 |

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|---|---|---|---|
| 19 | Second-generation de novo design: a view from a medicinal chemist perspective. Journal of Computer-Aided Molecular Design, 2009, 23, 593-602. | 2.9 | 27 |
| 20 | FTree query construction for virtual screening: a statistical analysis. Journal of Computer-Aided Molecular Design, 2008, 22, 111-118. | 2.9 | 4 |
| 21 | On the Art of Compiling and Using 'Drugâ€Like' Chemical Fragment Spaces. ChemMedChem, 2008, 3, 1503-1507. | 3.2 | 231 |
| 22 | A Knowledge-Based Weighting Approach to Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2006, 46, 587-596. | 5.4 | 27 |
| 23 | ErG:Â 2D Pharmacophore Descriptions for Scaffold Hopping. Journal of Chemical Information and Modeling, 2006, 46, 208-220. | 5.4 | 100 |
| 24 | A Novel Glucokinase Activator Modulates Pancreatic Islet and Hepatocyte Function. Endocrinology, 2005, 146, 3696-3701. | 2.8 | 125 |
| 25 | Identifying the binding mode of a molecular scaffold. Journal of Computer-Aided Molecular Design, 2004, 18, 23-40. | 2.9 | 8 |
| 26 | The antitumor histone deacetylase inhibitor suberoylanilide hydroxamic acid exhibits antiinflammatory properties via suppression of cytokines. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 2995-3000. | 7.1 | 484 |
| 27 | Solvation enthalpies as descriptors of structure â€“ in vitro percutaneous permeation relationship of benzoxazinones regioisomers. Il Farmaco, 2000, 55, 563-568. | 0.9 | 8 |
| 28 | Global 3D-QSAR methods: MS-WHIM and autocorrelation. Journal of Computer-Aided Molecular Design, 2000, 14, 293-306. | 2.9 | 23 |
| 29 | MS-WHIM Scores for Amino Acids:â€‰ A New 3D-Description for Peptide QSAR and QSPR Studies. Journal of Chemical Information and Computer Sciences, 1999, 39, 525-533. | 2.8 | 136 |
| 30 | The interaction of myristylated peptides with the catalytic domain of protein kinase C revealed by their sequence palindromy and the identification of a myristyl binding site. Protein Engineering, Design and Selection, 1998, 11, 803-810. | 2.1 | 9 |
| 31 | Mycobacterium tuberculosis Chaperonin 10 Stimulates Bone Resorption: A Potential Contributory Factor in Pott's Disease. Journal of Experimental Medicine, 1997, 186, 1241-1246. | 8.5 | 89 |
| 32 | A New Rational Hypothesis for the Pharmacophore of the Active Metabolite of Leflunomide, a Potent Immunosuppressive Drug. Journal of Medicinal Chemistry, 1997, 40, 2011-2016. | 6.4 | 30 |
| 33 | MS-WHIM, new 3D theoretical descriptors derived from molecular surface properties: a comparative 3D QSAR study in a series of steroids. Journal of Computer-Aided Molecular Design, 1997, 11, 79-92. | 2.9 | 96 |
| 34 | SONHICA (Simple optimized non-HIerarchical Cluster Analysis): A new tool for analysis of molecular conformations. Journal of Computational Chemistry, 1997, 18, 1295-1311. | 3.3 | 14 |
| 35 | First Synthetic Method for the Preparation of 6-Unsubstituted-2,3-dihydro-1,3-oxazin-4-ones. Journal of Organic Chemistry, 1996, 61, 3358-3361. | 3.2 | 9 |
| 36 | New conformationally constrained Xxx-Pro bicyclic mimetics. International Journal of Peptide Research and Therapeutics, 1995, 2, 161-164. | 0.1 | 2 |

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|---|---|---|---|
| 37 | Mycobacterium tuberculosis Chaperonin 10 Forms Stable Tetrameric and Heptameric Structures. Journal of Biological Chemistry, 1995, 270, 26159-26167. | 3.4 | 28 |
| 38 | Sequence and Structural Homologies Between Mycobacterium tuberculosis Chaperonin 10 and the MHC Class I/II Peptide Binding Cleft. Biochemical and Biophysical Research Communications, 1995, 211, 14-20. | 2.1 | 9 |
| 39 | Synthesis of retro-inverso peptides via Meldrumâ€™s acid derivatives: Insight on the reaction mechanism. , 1993, , 607-608. | | 0 |
| 40 | Ca++-modulators. Unusual highly stereospecific hantzsch-like cyclization: first authenticated example of 2-chloromethylene-1,2,3,4-tetrahydropyridine. Tetrahedron Letters, 1988, 29, 6335-6338. | 1.4 | 14 |
| 41 | The Blood-Brain Barrier is Dysregulated in COVID-19 and Serves as a CNS Entry Route for SARS-CoV-2. SSRN Electronic Journal, 0, , . | 0.4 | 3 |