Massimo Baroni

List of Publications by Year
in descending order

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35	2,048	279487 23	395343 33
papers	citations	h-index	g-index

38	38	38	2291
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Getting Insights into Structural and Energetic Properties of Reciprocal Peptideâ€“Protein Interactions. Journal of Chemical Information and Modeling, 2022, 62, 1113-1125.	2.5	8
2	Indomethacin-based PROTACs as pan-coronavirus antiviral agents. European Journal of Medicinal Chemistry, 2021, 226, 113814.	2.6	46
3	First virtual screening and experimental validation of inhibitors targeting GES-5 carbapenemase. Journal of Computer-Aided Molecular Design, 2019, 33, 295-305.	1.3	9
4	Discovering New Casein Kinase 1d Inhibitors with an Innovative Molecular Dynamics Enabled Virtual Screening Workflow. ACS Medicinal Chemistry Letters, 2019, 10, 487-492.	1.3	10
5	From Experiments to a Fast Easy-to-Use Computational Methodology to Predict Human Aldehyde Oxidase Selectivity and Metabolic Reactions. Journal of Medicinal Chemistry, 2018, 61, 360-371.	2.9	29
6	BioGPS: Navigating biological space to predict polypharmacology, off-targeting, and selectivity. Proteins: Structure, Function and Bioinformatics, 2015, 83, 517-532.	1.5	68
7	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. Journal of Chemical Information and Modeling, 2015, 55, 2256-2274.	2.5	65
8	BioGPS Descriptors for Rational Engineering of Enzyme Promiscuity and Structure Based Bioinformatic Analysis. PLoS ONE, 2014, 9, e109354.	1.1	18
9	Playing with Opening and Closing of Heterocycles: Using the Cusmano-Ruccia Reaction to Develop a Novel Class of Oxadiazolothiazinones, Active as Calcium Channel Modulators and P-Glycoprotein Inhibitors. Molecules, 2014, 19, 16543-16572.	1.7	6
10	Flavin Monooxygenase Metabolism: Why Medicinal Chemists Should Matter. Journal of Medicinal Chemistry, 2014, 57, 6183-6196.	2.9	39
11	Exposition and reactivity optimization to predict sites of metabolism in chemicals. Drug Discovery Today: Technologies, 2013, 10, e155-e165.	4.0	40
12	Disrupting Proteinâ€“Protein Interfaces Using GRID Molecular Interaction Fields. , 2013, , 61-82.		1
13	GRID-Based Three-Dimensional Pharmacophores II: PharmBench, a Benchmark Data Set for Evaluating Pharmacophore Elucidation Methods. Journal of Chemical Information and Modeling, 2012, 52, 2599-2608.	2.5	36
14	GRID-Based Three-Dimensional Pharmacophores I: FLAPpharm, a Novel Approach for Pharmacophore Elucidation. Journal of Chemical Information and Modeling, 2012, 52, 2587-2598.	2.5	76
15	FLAP: GRID Molecular Interaction Fields in Virtual Screening. Validation using the DUD Data Set. Journal of Chemical Information and Modeling, 2010, 50, 1442-1450.	2.5	94
16	High-Throughput Virtual Screening of Proteins Using GRID Molecular Interaction Fields. Journal of Chemical Information and Modeling, 2010, 50, 155-169.	2.5	75
17	Molecular Interaction Fields and 3D-QSAR Studies of p53â^'MDM2 Inhibitors Suggest Additional Features of Ligandâ^'Target Interaction. Journal of Chemical Information and Modeling, 2010, 50, 1451-1465.	2.5	12
18	Targeting the Conformational Transitions of MDM2 and MDMX: Insights into Dissimilarities and Similarities of p53 Recognition. Journal of Chemical Information and Modeling, 2008, 48, 1999-2009.	2.5	28

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19	Virtual Screening for Novel Openers of Pancreatic KATPChannels. Journal of Medicinal Chemistry, 2007, 50, 2117-2126.	2.9	46
20	A Common Reference Framework for Analyzing/Comparing Proteins and Ligands. Fingerprints for Ligands And Proteins (FLAP):â€‰ Theory and Application. Journal of Chemical Information and Modeling, 2007, 47, 279-294.	2.5	410
21	Novel TOPP descriptors in 3D-QSAR analysis of apoptosis inducing 4-aryl-4H-chromenes: Comparison versus other 2D- and 3D-descriptors. Bioorganic and Medicinal Chemistry, 2007, 15, 6450-6462.	1.4	27
22	Comparison of Ligand-Based and Structure-Based 3D-QSAR Approaches:Â A Case Study on (Aryl-)Bridged 2-Aminobenzonitriles Inhibiting HIV-1 Reverse Transcriptase. Journal of Medicinal Chemistry, 2005, 48, 3756-3767.	2.9	45
23	Principal component analysis of some oxidative stress parameters and their relationships in hemodialytic and transplanted patients. Clinica Chimica Acta, 2005, 358, 87-94.	0.5	28
24	Peptide studies by means of principal properties of amino acids derived from MIF descriptors. Journal of Chemometrics, 2004, 18, 146-155.	0.7	49
25	Conformer- and Alignment-Independent Model for Predicting Structurally Diverse Competitive CYP2C9 Inhibitors. Journal of Medicinal Chemistry, 2004, 47, 907-914.	2.9	64
26	Chemometric Studies on the Bactericidal Activity of Quinolones via an Extended VolSurf Approach. Journal of Medicinal Chemistry, 2004, 47, 3193-3201.	2.9	39
27	The CARSO procedure in process optimization. Journal of Chemometrics, 2003, 17, 9-15.	0.7	2
28	Generating Optimal Linear PLS Estimations (GOLPE): An Advanced Chemometric Tool for Handling 3D-QSAR Problems. QSAR and Combinatorial Science, 1993, 12, 9-20.	1.4	311
29	D-Optimal Designs in QSAR. QSAR and Combinatorial Science, 1993, 12, 225-231.	1.4	68
30	GOLPE: An advanced chemometric tool for 3D QSAR problems. , 1993, , 256-259.		2
31	Predictive ability of regression models. Part I: Standard deviation of prediction errors (SDEP). Journal of Chemometrics, 1992, 6, 335-346.	0.7	120
32	Predictive ability of regression models. Part II: Selection of the best predictive PLS model. Journal of Chemometrics, 1992, 6, 347-356.	0.7	116
33	Comparison of Chemometric Models for QSAR. QSAR and Combinatorial Science, 1990, 9, 101-107.	1.4	36
34	Chemometric approach to a QSAR study of peptides behaving as NK-2 receptor antagonists. Tetrahedron Computer Methodology, 1990, 3, 379-387.	0.2	9
35	CROMATIC: Cross-Relationship Map of Cavities from Coronaviruses. Journal of Chemical Information and Modeling, 0, , .	2.5	4