Paolo Benedetti

List of Publications by Year
in descending order

18	587	687363 13	752698 20
papers	citations	h-index	g-index

20	20	20	1011
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	FLAP: GRID Molecular Interaction Fields in Virtual Screening. Validation using the DUD Data Set. Journal of Chemical Information and Modeling, 2010, 50, 1442-1450.	5.4	94
2	Non-invasive identification of organic materials in wall paintings by fiber optic reflectance infrared spectroscopy: a statistical multivariate approach. Analytical and Bioanalytical Chemistry, 2009, 395, 2097-2106.	3.7	70
3	Fiber-Optic Fourier Transform Mid-Infrared Reflectance Spectroscopy: A Suitable Technique for in Situ Studies of Mural Paintings. Applied Spectroscopy, 2007, 61, 293-299.	2.2	65
4	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.	5.4	65
5	Isozyme-Specific Ligands for O-acetylserine sulfhydrylase, a Novel Antibiotic Target. PLoS ONE, 2013, 8, e77558.	2.5	43
6	Exposition and reactivity optimization to predict sites of metabolism in chemicals. Drug Discovery Today: Technologies, 2013, 10, e155-e165.	4.0	40
7	Design, synthesis and in vitro antitumor activity of new trans 2-[2-(heteroaryl)vinyl]-1,3-dimethylimidazolium iodides. Bioorganic and Medicinal Chemistry, 2004, 12, 1689-1695.	3.0	33
8	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.	6.4	29
9	Targeting Cystalysin, a Virulence Factor of Treponema denticolaâ€Supported Periodontitis. ChemMedChem, 2014, 9, 1501-1511.	3.2	26
10	GRIND/ALMOND investigations on CysLT1 receptor antagonists of the quinolinyl(bridged)aryl type. Bioorganic and Medicinal Chemistry, 2004, 12, 3607-3617.	3.0	22
11	Inhibitor of Ovarian Cancer Cells Growth by Virtual Screening: A New Thiazole Derivative Targeting Human Thymidylate Synthase. Journal of Medicinal Chemistry, 2012, 55, 10272-10276.	6.4	20
12	Structure-based rationalization of antitumor drugs mechanism of action by a MIF approach. European Journal of Medicinal Chemistry, 2004, 39, 281-289.	5.5	18
13	GBR Compounds and Mepyramines as Cocaine Abuse Therapeutics:Â Chemometric Studies on Selectivity Using Grid Independent Descriptors (GRIND). Journal of Medicinal Chemistry, 2002, 45, 1577-1584.	6.4	17
14	Discovering New Casein Kinase 1d Inhibitors with an Innovative Molecular Dynamics Enabled Virtual Screening Workflow. ACS Medicinal Chemistry Letters, 2019, 10, 487-492.	2.8	10
15	First virtual screening and experimental validation of inhibitors targeting GES-5 carbapenemase. Journal of Computer-Aided Molecular Design, 2019, 33, 295-305.	2.9	9
16	Human dopamine transporter: the first implementation of a combined in silico/in vitro approach revealing the substrate and inhibitor specificities. Journal of Biomolecular Structure and Dynamics, 2019, 37, 291-306.	3.5	8
17	Distant collaboration in drug discovery: the LINK3D project. Journal of Computer-Aided Molecular Design, 2002, 16, 809-818.	2.9	4
18	The CARSO procedure in process optimization. Journal of Chemometrics, 2003, 17, 9-15.	1.3	2