Emanuele Carosati

List of Publications by Year
in descending order

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42	2,223	236612	253896
papers	citations	25 h-index	43 g-index

48	48	48	3276
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Combining machine learning and quantum mechanics yields more <scp>chemically aware</scp> molecular descriptors for medicinal chemistry applications. Journal of Computational Chemistry, 2021, 42, 2068-2078.	1.5	6
2	Side-Chain Modified Ergosterol and Stigmasterol Derivatives as Liver X Receptor Agonists. Journal of Medicinal Chemistry, 2017, 60, 6548-6562.	2.9	21
3	ADME-Space: a new tool for medicinal chemists to explore ADME properties. Scientific Reports, 2017, 7, 6359.	1.6	58
4	Understanding Oxadiazolothiazinone Biological Properties: Negative Inotropic Activity versus Cytochrome P450-Mediated Metabolism. Journal of Medicinal Chemistry, 2016, 59, 3340-3352.	2.9	10
5	Discovery of Novel, Potent, and Specific Cellâ€Death Inducers in the Jurkat Acute Lymphoblastic Leukemia Cell Line. ChemMedChem, 2015, 10, 1700-1706.	1.6	0
6	Synthesis and L-type calcium channel blocking activity of new chiral oxadiazolothiazinones. European Journal of Medicinal Chemistry, 2015, 92, 481-489.	2.6	4
7	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
8	Targeting Cystalysin, a Virulence Factor of Treponema denticolaâ€Supported Periodontitis. ChemMedChem, 2014, 9, 1501-1511.	1.6	26
9	Large, chemically diverse dataset of logP measurements for benchmarking studies. European Journal of Pharmaceutical Sciences, 2013, 48, 21-29.	1.9	42
10	Modelling cytochromes P450 binding modes to predict P450 inhibition, metabolic stability and isoform selectivity. Drug Discovery Today: Technologies, 2013, 10, e167-e175.	4.0	15
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.	2.9	20
12	Absolute configuration and biological profile of two thiazinooxadiazol-3-ones with L-type calcium channel activity: a study of the structural effects. Organic and Biomolecular Chemistry, 2012, 10, 8994.	1.5	9
13	1,4-Dihydropyridine Scaffold in Medicinal Chemistry, The Story So Far And Perspectives (Part 2): Action in Other Targets and Antitargets. Current Medicinal Chemistry, 2012, 19, 4306-4323.	1.2	104
14	Ligand Promiscuity between the Efflux Pumps Human P-Glycoprotein and S. aureus NorA. ACS Medicinal Chemistry Letters, 2012, 3, 248-251.	1.3	20
15	QSAR Modeling and Data Mining Link Torsades de Pointes Risk to the Interplay of Extent of Metabolism, Active Transport, and hERG Liability. Molecular Pharmaceutics, 2012, 9, 2290-2301.	2.3	33
16	Pyrazolo[4,3-c][1,2]benzothiazines 5,5-Dioxide: A Promising New Class of Staphylococcus aureus NorA Efflux Pump Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 3568-3572.	2.9	82
17	Discovery of Novel Inhibitors of the NorA Multidrug Transporter of Staphylococcus aureus. Journal of Medicinal Chemistry, 2011, 54, 354-365.	2.9	67
18	1,4-Dihydropyridine Scaffold in Medicinal Chemistry, The Story so Far And Perspectives (Part 1): Action in Ion Channels and GPCRs. Current Medicinal Chemistry, 2011, 18, 4901-4922.	1.2	86

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19	The flavonoid scaffold as a template for the design of modulators of the vascular Ca_v1.2 channels. British Journal of Pharmacology, 2011, 164, 1684-1697.	2.7	40
20	A Novel Approach for Predicting P-Glycoprotein (ABCB1) Inhibition Using Molecular Interaction Fields. Journal of Medicinal Chemistry, 2011, 54, 1740-1751.	2.9	141
21	From 6-Aminoquinolone Antibacterials to 6-Amino-7-thiopyranopyridinylquinolone Ethyl Esters as Inhibitors of Staphylococcus aureus Multidrug Efflux Pumps. Journal of Medicinal Chemistry, 2010, 53, 4466-4480.	2.9	41
22	IAP antagonists: promising candidates for cancer therapy. Drug Discovery Today, 2010, 15, 210-219.	3.2	85
23	Transporterâ€Mediated Efflux Influences CNS Side Effects: ABCB1, from Antitarget to Target. Molecular Informatics, 2010, 29, 16-26.	1.4	35
24	Ligand-based virtual screening and ADME-tox guided approach to identify triazolo-quinoxalines as folate cycle inhibitors. Bioorganic and Medicinal Chemistry, 2010, 18, 7773-7785.	1.4	20
25	Homodimeric Enzymes as Drug Targets. Current Medicinal Chemistry, 2010, 17, 826-846.	1.2	45
26	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
27	On the catalytic role of the active site residue E121 of E. coli l-aspartate oxidase. Biochimie, 2010, 92, 1335-1342.	1.3	13
28	Stereoselective Behavior of the Functional Diltiazem Analogue 1-[(4-Chlorophenyl)sulfonyl]-2-(2-thienyl)pyrrolidine, a New L-Type Calcium Channel Blocker. Journal of Medicinal Chemistry, 2009, 52, 6637-6648.	2.9	10
29	L-Type Calcium Channel Blockers: From Diltiazem to 1,2,4-Oxadiazol-5-ones via Thiazinooxadiazol-3-one Derivatives. Journal of Medicinal Chemistry, 2009, 52, 2352-2362.	2.9	29
30	Integrating Crystallography into Early Metabolism Studies. NATO Science for Peace and Security Series A: Chemistry and Biology, 2009, , 63-77.	0.5	0
31	Discovery of Novel and Cardioselective Diltiazem-like Calcium Channel Blockers via Virtual Screening. Journal of Medicinal Chemistry, 2008, 51, 5552-5565.	2.9	27
32	Diltiazem Analogues: The Last Ten Years on Structure Activity Relationships. Current Medicinal Chemistry, 2007, 14, 279-287.	1.2	26
33	Virtual Screening for Novel Openers of Pancreatic KATPChannels. Journal of Medicinal Chemistry, 2007, 50, 2117-2126.	2.9	46
34	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
35	Calcium Channel Antagonists Discovered by a Multidisciplinary Approach. Journal of Medicinal Chemistry, 2006, 49, 5206-5216.	2.9	61
36	Binding studies and GRIND/ALMOND-based 3D QSAR analysis of benzothiazine type KATP-channel openers. Bioorganic and Medicinal Chemistry, 2005, 13, 5581-5591.	1.4	21

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37	MetaSite:Â Understanding Metabolism in Human Cytochromes from the Perspective of the Chemist. Journal of Medicinal Chemistry, 2005, 48, 6970-6979.	2.9	466
38	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
39	A New Class of Selective Myocardial Calcium Channel Modulators. 2. Role of the Acetal Chain in Oxadiazol-3-one Derivatives. Journal of Medicinal Chemistry, 2005, 48, 2445-2456.	2.9	37
40	Peptide studies by means of principal properties of amino acids derived from MIF descriptors. Journal of Chemometrics, 2004, 18, 146-155.	0.7	49
41	Hydrogen Bonding Interactions of Covalently Bonded Fluorine Atoms:Â From Crystallographic Data to a New Angular Function in the GRID Force Field. Journal of Medicinal Chemistry, 2004, 47, 5114-5125.	2.9	218
42	THREE-DIMENSIONAL QUANTITATIVE STRUCTURE-PROPERTY RELATIONSHIPS. , 2003, , 405-416.		7