Bernard Testa

List of Publications by Year
in descending order

102 papers	3,532 citations	196777 29 h-index	169272 56 g-index
156 all docs	156 docs citations	156 times ranked	4039 citing authors

#	Article	IF	Citations
1	MetaQSAR: An Integrated Database Engine to Manage and Analyze Metabolic Data. Journal of Medicinal Chemistry, 2018, 61, 1019-1030.	2.9	18
2	Prediction of the Formation of Reactive Metabolites by A Novel Classifier Approach Based on Enrichment Factor Optimization (EFO) as Implemented in the VEGA Program. Molecules, 2018, 23, 2955.	1.7	9
3	Emerging Chemodiversity and Stereoisomerism in Acyclic Mono- and Dichloroalkanes. Chemistry and Biodiversity, 2018, 15, e1800421.	1.0	0
4	Binding Space Concept: A New Approach To Enhance the Reliability of Docking Scores and Its Application to Predicting Butyrylcholinesterase Hydrolytic Activity. Journal of Chemical Information and Modeling, 2017, 57, 1691-1702.	2.5	31
5	Emergent chemodiversity: The case of stereoisomerism in acyclic alkanes. Chirality, 2017, 29, 415-421.	1.3	2
6	Mechanisms and pharmaceutical consequences of processes of stereoisomerisation â€" A didactic excursion. European Journal of Pharmaceutical Sciences, 2016, 88, 101-123.	1.9	14
7	Types of stereoselectivity in drug metabolism: a heuristic approach. Drug Metabolism Reviews, 2015, 47, 239-251.	1.5	15
8	Predicting drug metabolism: experiment and/or computation?. Nature Reviews Drug Discovery, 2015, 14, 387-404.	21.5	355
9	Esters of Pyrazinoic Acid Are Active against Pyrazinamide-Resistant Strains of Mycobacterium tuberculosis and Other Naturally Resistant Mycobacteria In Vitro and Ex Vivo within Macrophages. Antimicrobial Agents and Chemotherapy, 2015, 59, 7693-7699.	1.4	17
10	Small Molecules as Exemplars of Emergent Properties and Diversification into the â€˜Adjacent Possibleâ€™. Chemistry and Biodiversity, 2014, 11, 1309-1329.	1.0	4
11	Organic Stereochemistry. Part 8. Helvetica Chimica Acta, 2013, 96, 1409-1451.	1.0	10
12	Organic Stereochemistry. Part 7. Helvetica Chimica Acta, 2013, 96, 1203-1234.	1.0	7
13	Organic Stereochemistry. Part 1. Symmetry Elements and Operations, Classification of Stereoisomers. Helvetica Chimica Acta, 2013, 96, 4-30.	1.0	8
14	Organic Stereochemistry. Part 2. Helvetica Chimica Acta, 2013, 96, 159-188.	1.0	21
15	Simulations in Evolution. III. Randomness as a Generator of Opportunities. Chemistry and Biodiversity, 2013, 10, 62-72.	1.0	0
16	Organic Stereochemistry: Guiding Principles and Bio-Medicinal Relevance. Helvetica Chimica Acta, 2013, 96, 1-3.	1.0	1
17	Organic Stereochemistry. Part 3. Helvetica Chimica Acta, 2013, 96, 351-374.	1.0	35
18	Organic Stereochemistry. Part 4. Helvetica Chimica Acta, 2013, 96, 564-623.	1.0	17

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19	Organic Stereochemistry. Partâ€...5. Helvetica Chimica Acta, 2013, 96, 747-798.	1.0	19
20	Organic Stereochemistry. Partâ€...6. Helvetica Chimica Acta, 2013, 96, 1005-1030.	1.0	6
21	To Monty Kier, A Friendly Tribute. Current Computer-Aided Drug Design, 2012, 8, 85-86.	0.8	1
22	Reactions and enzymes in the metabolism of drugs and other xenobiotics. Drug Discovery Today, 2012, 17, 549-560.	3.2	183
23	Molecular properties and structure-permeation relations revisited. Journal of Pharmacy and Pharmacology, 2011, 50, 106-106.	1.2	0
24	Nicotinate Esters: Their Binding to and Hydrolysis by Human Serum Albumin. Journal of Pharmacy and Pharmacology, 2011, 44, 745-749.	1.2	9
25	The influence of conformational factors on the metabolic conjugation of aryloxyacetates. Journal of Pharmacy and Pharmacology, 2011, 38, 14-18.	1.2	9
26	Influence of Lipophilicity and Chirality on the Selectivity of Ligands for Î²1- and Î²2-Adrenoceptors. Journal of Pharmacy and Pharmacology, 2011, 40, 609-612.	1.2	18
27	Chemodiversity and molecular plasticity: recognition processes as explored by property spaces. Future Medicinal Chemistry, 2011, 3, 995-1010.	1.1	11
28	Dispersal (Entropy) and Recognition (Information) as Foundations of Emergence and Dissolvence. Entropy, 2009, 11, 993-1000.	1.1	10
29	Simulations in Evolution. II. Relative Fitness and the Propagation of Mutants. Chemistry and Biodiversity, 2009, 6, 356-368.	1.0	2
30	The Biochemistry of Drug Metabolism - An Introduction. Chemistry and Biodiversity, 2009, 6, 591-684.	1.0	58
31	Drug Metabolism for the Perplexed Medicinal Chemist. Chemistry and Biodiversity, 2009, 6, 2055-2070.	1.0	30
32	Atomic Diversity, Molecular Diversity, and Chemical Diversity: The Concept of Chemodiversity. Chemistry and Biodiversity, 2009, 6, 1145-1151.	1.0	10
33	Partition Coefficient and Molecular Flexibility: The Concept of Lipophilicity Space. Chemistry and Biodiversity, 2009, 6, 1152-1169.	1.0	24
34	Prodrugs: bridging pharmacodynamic/pharmacokinetic gaps. Current Opinion in Chemical Biology, 2009, 13, 338-344.	2.8	78
35	The Biochemistry of Drug Metabolism â€“ An Introduction. Chemistry and Biodiversity, 2008, 5, 2171-2336.	1.0	102
36	Computational Approaches to Lipophilicity: Methods and Applications. Reviews in Computational Chemistry, 2007, , 241-315.	1.5	45

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37	The Biochemistry of Drug Metabolism - An Introduction. Chemistry and Biodiversity, 2007, 4, 257-405.	1.0	139
38	The Biochemistry of Drug Metabolism â€“ An Introduction. Chemistry and Biodiversity, 2007, 4, 2031-2122.	1.0	68
39	Variation, Natural Selection, and Information Content â€“ A Simulation. Chemistry and Biodiversity, 2007, 4, 2458-2472.	1.0	3
40	The Biochemistry of Drug Metabolism â€“ An Introduction. Chemistry and Biodiversity, 2006, 3, 1053-1101.	1.0	79
41	Predicting Drug Metabolism - An Evaluation of the Expert SystemMETEOR. Chemistry and Biodiversity, 2005, 2, 872-885.	1.0	73
42	Musings on ADME Predictions and Structure-Activity Relations. Chemistry and Biodiversity, 2005, 2, 1411-1427.	1.0	21
43	Prodrug research: futile or fertile?. Biochemical Pharmacology, 2004, 68, 2097-2106.	2.0	106
44	Lipophilicity Measurement by Reversed-Phase High-Performance Liquid Chromatography (RP-HPLC): A Comparison of Two Stationary Phases Based on Retention Mechanisms. Helvetica Chimica Acta, 2004, 87, 2866-2876.	1.0	35
45	A Cellular Automata Model of Water Structuring by a Chiral Solute. Journal of Chemical Information and Computer Sciences, 2002, 42, 712-716.	2.8	3
46	Development of molecular hydrogen-bonding potentials (MHBPs) and their application to structureâ€“permeation relations. Journal of Molecular Graphics and Modelling, 2001, 19, 521-535.	1.3	31
47	Emergence and Dissolvence in the Self-organisation of Complex Systems. Entropy, 2000, 2, 1-25.	1.1	25
48	Predicting Bloodâ^'Brain Barrier Permeation from Three-Dimensional Molecular Structure. Journal of Medicinal Chemistry, 2000, 43, 2204-2216.	2.9	428
49	Monoamine oxidase inhibitory properties of some benzazoles: Structure-; Activity relationships. AAPS PharmSci, 1999, 1, 1-4.	1.3	65
50	Complex systems in drug research: I. The chemical levels. Complexity, 1996, 1, 29-36.	0.9	6
51	Complex systems in drug research: II. The ligand-active site-water confluence as a complex system. Complexity, 1996, 1, 37-42.	0.9	9
52	Lipophilicity in molecular modeling. Pharmaceutical Research, 1996, 13, 335-343.	1.7	145
53	Kinetics and Mechanisms of Racemization: 5-Substituted Hydantoins (= Imidazolidine-2,4-diones) as Models of Chiral Drugs. Helvetica Chimica Acta, 1996, 79, 767-778.	1.0	25
54	Racemization, enantiomerization, diastereomerization, and epimerization: Their meaning and pharmacological significance. Chirality, 1995, 7, 396-400.	1.3	149

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55	Low configurational stability of amfepramone and cathinone: Mechanism and kinetics of chiral inversion. Chirality, 1995, 7, 469-473.	1.3	21
56	The Many Faces of Pharmaceutical Research. Pharmaceutical Research, 1995, 12, 1247-1247.	1.7	2
57	The temperature dependence of steady-state kinetics: What can be learned about pig liver esterase stereospecificity?. Chirality, 1994, 6, 11-16.	1.3	10
58	The so-called ?interconversion? of stereoisomeric drugs: An attempt at clarification. Chirality, 1993, 5, 105-111.	1.3	80
59	Structure-metabolism relationships in the hydrolysis of nicotinate esters by rat liver and brain subcellular fractions. Pharmaceutical Research, 1991, 08, 832-839.	1.7	25
60	The concept of molecular structure in structureâ€“activity relationship studies and drug design. Medicinal Research Reviews, 1991, 11, 35-48.	5.0	61
61	On flying wedges, crashing wedges, and perspective-blind stereochemists. Chirality, 1991, 3, 159-160.	1.3	4
62	[31] Molecular electrostatic potentials for characterizing drug-biosystem interactions. Methods in Enzymology, 1991, 203, 638-677.	0.4	38
63	Mechanisms of inhibition of xenobiotic-metabolizing enzymes. Xenobiotica, 1990, 20, 1129-1137.	0.5	12
64	Pattern recognition study of QSAR substituent descriptors. Journal of Computer-Aided Molecular Design, 1989, 3, 111-132.	1.3	48
65	Mechanisms of chiral recognition in xenobiotic metabolism and drug-receptor interactions. Chirality, 1989, 1, 7-9.	1.3	37
66	The interaction of substituted benzamides with brain benzodiazepine binding sites in vitro. British Journal of Pharmacology, 1988, 94, 1234-1240.	2.7	5
67	Metabolic chiral inversion of anti-inflammatory 2-arylpropionates: Lack of reaction in liver homogenates, and study of methine proton acidity. Xenobiotica, 1988, 18, 533-543.	0.5	33
68	In vitroInhibition by Stiripentol of Rat Brain Cytochrome P-450-Mediated Naphthalene Hydroxylation. Xenobiotica, 1988, 18, 1097-1106.	0.5	21
69	The chromatographic analysis of enantiomers in drug metabolism studies. Xenobiotica, 1986, 16, 265-279.	0.5	49
70	The Prediction of Substituent Interactions in the Lipophilicity of Disubstituted Benzenes using RP-HPLC. QSAR and Combinatorial Science, 1985, 4, 69-77.	1.4	38
71	Isomerisation and urinary excretion of proxibarbal and valofan in man; a preliminary study. European Journal of Drug Metabolism and Pharmacokinetics, 1984, 9, 117-122.	0.6	7
72	PCILO and CD. Conformational study of sulpiride, a dopamine antagonist. Helvetica Chimica Acta, 1981, 64, 2183-2188.	1.0	18

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73	Novel Pathways in Drug Metabolism. Xenobiotica, 1978, 8, 1-25.	0.5	43
74	A Reappraisal of the Stereoselective Metabolism of Nicotine to Nicotine-l'-N-oxide. Xenobiotica, 1976, 6, 553-556.	0.5	16
75	The Role of Plasma Protein Binding in Drug Discovery. , 0, , 119-141.		17
76	Accelerated Stability Profiling in Drug Discovery. , 0, , 281-306.		3
77	TheBioPrintÂ® Approach for the Evaluation of ADMET Properties: Application to the Prediction of Cytochrome P450 2D6 Inhibition. , 0, , 395-415.		1
78	High-Throughput Solubility, Permeability, and the MAD PAMPA Model. , 0, , 221-241.		8
79	Physicochemical Characterization of the Solid State in Drug Development. , 0, , 307-329.		1
80	Cell Culture Absorption Modelsâ€“ State of the Art. , 0, , 71-78.		2
81	In vivo Pharmacokinetic Profiling of Drugs. , 0, , 143-152.		0
82	In vitro, in vivo, andin silico Approaches to Predict Induction of Drug Metabolism. , 0, , 93-103.		0
83	Lipid Bilayers in ADME: Permeation Barriers and Distribution Compartments. , 0, , 203-220.		3
84	Prediction of Site of Metabolism in Humans: Case Studies of Cytochromes P450 2C9, 2D6, and 3A4. , 0, , 367-379.		0
85	Property-Based Lead Optimization. , 0, , 25-45.		0
86	Automated Parallel Synthesis in Support of Early Drug Discovery: Balancing Accessibility of Chemistry with the Design of Drug-Like Libraries. , 0, , 153-163.		0
87	The Concept of Property Space: The Case of Acetylcholine. , 0, , 353-365.		0
88	Educational and Communication Issues Related to Profiling Compounds for Their Drug-Like Properties. , 0, , 459-465.		0
89	Metabolic Studies in Drug Research and Development. , 0, , 79-92.		0
90	Coordination of Uptake and Efflux Transporters in Drug Disposition. , 0, , 105-117.		0

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91	Pharmaceutical Research: For What, for Whom? Science and Social Policies. , 0, , 1-24.		1
92	Present and Future Significance of ADMET Profiling in Industrial Drug Research. , 0, , 467-479.		0
93	Membranesâ€“ from Barriers to Magic Bullets. , 0, , 47-70.		0
94	New Insights into the Lipophilicity of Ionized Species. , 0, , 165-185.		4
95	Calculation of Lipophilicity: A Classification of Methods. , 0, , 331-352.		2
96	Physicochemical and Biological Profiling in Drug Research. ElogD7.4 20,000 Compounds Later: Refinements, Observations, and Applications. , 0, , 187-201.		3
97	Using Computer Reasoning about Qualitative and Quantitative Information to Predict Metabolism and Toxicity. , 0, , 417-429.		6
98	Correlations between PAMPA Permeability and logP. , 0, , 243-257.		6
99	Physiologically Based Pharmacokinetic Models. , 0, , 431-439.		0
100	Processing of Biopharmaceutical Profiling Data in Drug Discovery. , 0, , 441-458.		10
101	Use of Pharmacophores in Predictive ADME. , 0, , 381-393.		0
102	Predicting the Intestinal Solubility of Poorly Soluble Drugs. , 0, , 259-280.		21