

Knut Baumann

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

56
papers

2,441
citations

31
h-index

49
g-index

74
ext. papers

2,737
ext. citations

5.2
avg, IF

5.19
L-index

#	Paper	IF	Citations
56	Evaluating High-Variance Leaves as Uncertainty Measure for Random Forest Regression. <i>Molecules</i> , 2021 , 26,	4.8	1
55	Formulation of Cannabidiol in Colloidal Lipid Carriers. <i>Molecules</i> , 2021 , 26,	4.8	7
54	A gold(i) biscarbene complex with improved activity as a TrxR inhibitor and cytotoxic drug: comparative studies with different gold metallodrugs. <i>Metallomics</i> , 2019 , 11, 533-545	4.5	44
53	Screening for linearly and nonlinearly related variables in predictive cheminformatic models. <i>Journal of Chemometrics</i> , 2018 , 32, e3009	1.6	7
52	Novel strategies for the formulation and processing of poorly water-soluble drugs. <i>European Journal of Pharmaceutics and Biopharmaceutics</i> , 2018 , 126, 40-56	5.7	73
51	xMaP-An Interpretable Alignment-Free Four-Dimensional Quantitative Structure-Activity Relationship Technique Based on Molecular Surface Properties and Conformer Ensembles. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 165-181	6.1	11
50	A Diverse Benchmark Based on 3D Matched Molecular Pairs for Validating Scoring Functions. <i>ACS Omega</i> , 2018 , 3, 5704-5714	3.9	9
49	Efficiency of different measures for defining the applicability domain of classification models. <i>Journal of Cheminformatics</i> , 2017 , 9, 44	8.6	26
48	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. <i>Journal of Cheminformatics</i> , 2016 , 8, 18	8.6	
47	Chemoinformatic Classification Methods and their Applicability Domain. <i>Molecular Informatics</i> , 2016 , 35, 160-80	3.8	70
46	Data quality in drug discovery: the role of analytical performance in ligand binding assays. <i>Journal of Computer-Aided Molecular Design</i> , 2015 , 29, 847-65	4.2	32
45	10-iodo-11H-indolo[3,2-c]quinoline-6-carboxylic acids are selective inhibitors of DYRK1A. <i>Journal of Medicinal Chemistry</i> , 2015 , 58, 3131-43	8.3	70
44	Granule mobility, fusion frequency and insulin secretion are differentially affected by insulinotropic stimuli. <i>Traffic</i> , 2015 , 16, 493-509	5.7	6
43	Recent progress in tight junction modulation for improving bioavailability. <i>Expert Opinion on Drug Discovery</i> , 2014 , 9, 367-81	6.2	18
42	inSARa: intuitive and interactive SAR interpretation by reduced graphs and hierarchical MCS-based network navigation. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 1578-95	6.1	7
41	Observer-independent quantification of insulin granule exocytosis and pre-exocytotic mobility by TIRF microscopy. <i>Microscopy and Microanalysis</i> , 2014 , 20, 206-18	0.5	4
40	Reliable estimation of prediction errors for QSAR models under model uncertainty using double cross-validation. <i>Journal of Cheminformatics</i> , 2014 , 6, 47	8.6	86

39	Reliable estimation of externally validated prediction errors for QSAR models. <i>Journal of Cheminformatics</i> , 2013 , 5,	8.6	78
38	Evaluation of arene ruthenium(II) N-heterocyclic carbene complexes as organometallics interacting with thiol and selenol containing biomolecules. <i>Dalton Transactions</i> , 2013 , 42, 1657-66	4.3	99
37	2-Anilino-4-(benzimidazol-2-yl)pyrimidines--a multikinase inhibitor scaffold with antiproliferative activity toward cancer cell lines. <i>European Journal of Medicinal Chemistry</i> , 2012 , 53, 254-63	6.8	35
36	Bidirectional insulin granule turnover in the submembrane space during K(+) depolarization-induced secretion. <i>Traffic</i> , 2011 , 12, 1166-78	5.7	9
35	Comparison of established and novel purity tests for the quality control of heparin by means of a set of 177 heparin samples. <i>Analytical and Bioanalytical Chemistry</i> , 2011 , 399, 605-20	4.4	33
34	From catalysts to bioactive organometallics: do Grubbs catalysts trigger biological effects?. <i>ChemMedChem</i> , 2011 , 6, 2142-5	3.7	36
33	Identification of 2-anilino-9-methoxy-5,7-dihydro-6H-pyrimido[5,4-d][1]benzazepin-6-ones as dual PLK1/VEGF-R2 kinase inhibitor chemotypes by structure-based lead generation. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 2433-42	8.3	45
32	Enzyme kinetics and hit validation in fluorimetric protease assays. <i>Current Topics in Medicinal Chemistry</i> , 2010 , 10, 368-82	3	28
31	Composition of OSCS-contaminated heparin occurring in 2008 in batches on the German market. <i>European Journal of Pharmaceutical Sciences</i> , 2010 , 40, 297-304	5.1	36
30	QSAR guided synthesis of simplified antiplasmodial analogs of naphthylisoquinoline alkaloids. <i>European Journal of Medicinal Chemistry</i> , 2010 , 45, 5370-83	6.8	8
29	Gaussian mixture discriminant analysis for the single-cell differentiation of bacteria using micro-Raman spectroscopy. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2009 , 96, 159-171	3.8	58
28	A small-molecule inhibitor of Nipah virus envelope protein-mediated membrane fusion. <i>Journal of Medicinal Chemistry</i> , 2009 , 52, 4257-65	8.3	31
27	Maximum unbiased validation (MUV) data sets for virtual screening based on PubChem bioactivity data. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 169-84	6.1	208
26	Impact of benchmark data set topology on the validation of virtual screening methods: exploration and quantification by spatial statistics. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 704-18	6.1	25
25	Cis-Configured aziridines are new pseudo-irreversible dual-mode inhibitors of <i>Candida albicans</i> secreted aspartic protease 2. <i>ChemMedChem</i> , 2008 , 3, 302-15	3.7	17
24	Comparison of Cyclodextrin-Dipeptide Inclusion Complexes in the Absence and Presence of Urea by Means of Capillary Electrophoresis, Nuclear Magnetic Resonance and Molecular Modeling. <i>European Journal of Organic Chemistry</i> , 2007 , 2007, 2921-2930	3.2	29
23	Towards a detailed understanding of bacterial metabolism--spectroscopic characterization of <i>Staphylococcus epidermidis</i> . <i>ChemPhysChem</i> , 2007 , 8, 124-37	3.2	167
22	Aziridide-based inhibitors of cathepsin L: synthesis, inhibition activity, and docking studies. <i>ChemMedChem</i> , 2006 , 1, 1126-41	3.7	53

21	Inhibitors of cysteine proteases. <i>Current Topics in Medicinal Chemistry</i> , 2006 , 6, 331-53	3	74
20	ErG: 2D pharmacophore descriptions for scaffold hopping. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 208-20	6.1	72
19	A new lead for nonpeptidic active-site-directed inhibitors of the severe acute respiratory syndrome coronavirus main protease discovered by a combination of screening and docking methods. <i>Journal of Medicinal Chemistry</i> , 2005 , 48, 6832-42	8.3	49
18	Structure-based validation of the 3D-QSAR technique MaP. <i>Journal of Chemical Information and Modeling</i> , 2005 , 45, 739-49	6.1	8
17	Screening of electrophilic compounds yields an aziridinyl peptide as new active-site directed SARS-CoV main protease inhibitor. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005 , 15, 5365-9	2.9	39
16	NMR Spectroscopic and Molecular Modelling Studies on CyclodextrinDipeptide Inclusion Complexes. <i>European Journal of Organic Chemistry</i> , 2005 , 2005, 1578-1589	3.2	36
15	Charge interactions do the job: a combined statistical and combinatorial approach to finding artificial receptors for binding tetrapeptides in water. <i>Angewandte Chemie - International Edition</i> , 2005 , 44, 7208-12	16.4	37
14	Chance Correlation in Variable Subset Regression: Influence of the Objective Function, the Selection Mechanism, and Ensemble Averaging. <i>QSAR and Combinatorial Science</i> , 2005 , 24, 1033-1046		60
13	Validation tools for variable subset regression. <i>Journal of Computer-Aided Molecular Design</i> , 2004 , 18, 549-62	4.2	58
12	Probing the pharmacophore for allosteric ligands of muscarinic M2 receptors: SAR and QSAR studies in a series of bisquaternary salts of caracurine V and related ring systems. <i>Journal of Medicinal Chemistry</i> , 2004 , 47, 3561-71	8.3	21
11	Synthesis and biological activity of pyridinium-type acetylcholinesterase inhibitors. <i>Journal of Pharmacy and Pharmacology</i> , 2003 , 55, 1397-404	4.8	12
10	Evaluation of extended parameter sets for the 3D-QSAR technique MaP: implications for interpretability and model quality exemplified by antimalarially active naphthylisoquinoline alkaloids. <i>Journal of Computer-Aided Molecular Design</i> , 2003 , 17, 347-65	4.2	20
9	Synthesis, biological activity, and docking studies of new acetylcholinesterase inhibitors of the bispyridinium type. <i>Archiv Der Pharmazie</i> , 2003 , 336, 523-40	4.3	36
8	Cross-validation as the objective function for variable-selection techniques. <i>TrAC - Trends in Analytical Chemistry</i> , 2003 , 22, 395-406	14.6	182
7	Determination of clotrimazole in mice plasma by capillary electrophoresis. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2003 , 30, 1879-87	3.5	9
6	Mapping property distributions of molecular surfaces: algorithm and evaluation of a novel 3D quantitative structure-activity relationship technique. <i>Journal of Medicinal Chemistry</i> , 2003 , 46, 1390-407	8.3	55
5	Distance Profiles (DiP): A translationally and rotationally invariant 3D structure descriptor capturing steric properties of molecules. <i>QSAR and Combinatorial Science</i> , 2002 , 21, 507-519		13
4	An alignment-independent versatile structure descriptor for QSAR and QSPR based on the distribution of molecular features. <i>Journal of Chemical Information and Computer Sciences</i> , 2002 , 42, 26-35		86

3	Structure-activity relationships in a series of bisquaternary bisphthalimidine derivatives modulating the muscarinic M(2)-receptor allosterically. <i>Journal of Medicinal Chemistry</i> , 2000 , 43, 2155-64	8.3	60
2	Accord for Excel. <i>Journal of Chemical Information and Computer Sciences</i> , 1997 , 37, 413-414		0
1	Appropriate calibration functions for capillary electrophoresis II. Heteroscedasticity and its consequences. <i>Journal of Chromatography A</i> , 1995 , 700, 9-20	4.5	37