Knut Baumann

List of Publications by Year
in descending order

68 papers	2,887 citations	126858 33 h-index	168321 53 g-index
74 all docs	74 docs citations	74 times ranked	3907 citing authors

#	Article	IF	Citations
1	Maximum Unbiased Validation (MUV) Data Sets for Virtual Screening Based on PubChem Bioactivity Data. Journal of Chemical Information and Modeling, 2009, 49, 169-184.	2.5	283
2	Cross-validation as the objective function for variable-selection techniques. TrAC - Trends in Analytical Chemistry, 2003, 22, 395-406.	5.8	213
3	Towards a Detailed Understanding of Bacterial Metabolismâ€"Spectroscopic Characterization ofStaphylococcus Epidermidis. ChemPhysChem, 2007, 8, 124-137.	1.0	201
4	Evaluation of arene ruthenium(<scp>ii</scp>) N-heterocyclic carbene complexes as organometallics interacting with thiol and selenol containing biomolecules. Dalton Transactions, 2013, 42, 1657-1666.	1.6	118
5	Novel strategies for the formulation and processing of poorly water-soluble drugs. European Journal of Pharmaceutics and Biopharmaceutics, 2018, 126, 40-56.	2.0	110
6	Reliable estimation of prediction errors for QSAR models under model uncertainty using double cross-validation. Journal of Cheminformatics, 2014, 6, 47.	2.8	109
7	Chemoinformatic Classification Methods and their Applicability Domain. Molecular Informatics, 2016, 35, 160-180.	1.4	102
8	ErG:Â 2D Pharmacophore Descriptions for Scaffold Hopping. Journal of Chemical Information and Modeling, 2006, 46, 208-220.	2.5	100
9	An Alignment-Independent Versatile Structure Descriptor for QSAR and QSPR Based on the Distribution of Molecular Features. Journal of Chemical Information and Computer Sciences, 2002, 42, 26-35.	2.8	98
10	10-Iodo-11H-indolo[3,2-c]quinoline-6-carboxylic Acids Are Selective Inhibitors of DYRK1A. Journal of Medicinal Chemistry, 2015, 58, 3131-3143.	2.9	87
11	Inhibitors of Cysteine Proteases. Current Topics in Medicinal Chemistry, 2006, 6, 331-353.	1.0	79
12	Structureâ^'Activity Relationships in a Series of Bisquaternary Bisphthalimidine Derivatives Modulating the Muscarinic M2-Receptor Allosterically. Journal of Medicinal Chemistry, 2000, 43, 2155-2164.	2.9	67
13	Gaussian mixture discriminant analysis for the single-cell differentiation of bacteria using micro-Raman spectroscopy. Chemometrics and Intelligent Laboratory Systems, 2009, 96, 159-171.	1.8	67
14	Validation tools for variable subset regression. Journal of Computer-Aided Molecular Design, 2004, 18, 549-562.	1.3	63
15	Mapping Property Distributions of Molecular Surfaces:â€‰ Algorithm and Evaluation of a Novel 3D Quantitative Structureâ^'Activity Relationship Technique. Journal of Medicinal Chemistry, 2003, 46, 1390-1407.	2.9	61
16	Chance Correlation in Variable Subset Regression: Influence of the Objective Function, the Selection Mechanism, and Ensemble Averaging. QSAR and Combinatorial Science, 2005, 24, 1033-1046.	1.5	61
17	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. Journal of Medicinal Chemistry, 2010, 53, 2433-2442.	2.9	61
18	A gold(<scp>i</scp>) biscarbene complex with improved activity as a TrxR inhibitor and cytotoxic drug: comparative studies with different gold metallodrugs. Metallomics, 2019, 11, 533-545.	1.0	58

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19	Aziridide-Based Inhibitors of Cathepsinâ€…L: Synthesis, Inhibition Activity, and Docking Studies. ChemMedChem, 2006, 1, 1126-1141.	1.6	56
20	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 Methodsâ€“. Journal of Medicinal Chemistry, 2005, 48, 6832-6842.	2.9	55
21	Composition of OSCS-contaminated heparin occurring in 2008 in batches on the German market. European Journal of Pharmaceutical Sciences, 2010, 40, 297-304.	1.9	47
22	Efficiency of different measures for defining the applicability domain of classification models. Journal of Cheminformatics, 2017, 9, 44.	2.8	44
23	Appropriate calibration functions for capillary electrophoresis II. Heteroscedasticity and its consequences. Journal of Chromatography A, 1995, 700, 9-20.	1.8	42
24	Screening of electrophilic compounds yields an aziridinyl peptide as new active-site directed SARS-CoV main protease inhibitor. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 5365-5369.	1.0	42
25	Charge Interactions Do the Job: A Combined Statistical and Combinatorial Approach to Finding Artificial Receptors for Binding Tetrapeptides in Water. Angewandte Chemie - International Edition, 2005, 44, 7208-7212.	7.2	42
26	2-Anilino-4-(benzimidazol-2-yl)pyrimidines â€“ A multikinase inhibitor scaffold with antiproliferative activity toward cancer cell lines. European Journal of Medicinal Chemistry, 2012, 53, 254-263.	2.6	41
27	A Small-Molecule Inhibitor of Nipah Virus Envelope Protein-Mediated Membrane Fusion. Journal of Medicinal Chemistry, 2009, 52, 4257-4265.	2.9	39
28	Data quality in drug discovery: the role of analytical performance in ligand binding assays. Journal of Computer-Aided Molecular Design, 2015, 29, 847-865.	1.3	39
29	Synthesis, Biological Activity, and Docking Studies of New Acetylcholinesterase Inhibitors of the Bispyridinium Type. Archiv Der Pharmazie, 2003, 336, 523-540.	2.1	37
30	NMR Spectroscopic and Molecular Modelling Studies on Cyclodextrin-Dipeptide Inclusion Complexes. European Journal of Organic Chemistry, 2005, 2005, 1578-1589.	1.2	37
31	Enzyme Kinetics and Hit Validation in Fluorimetric Protease Assays. Current Topics in Medicinal Chemistry, 2010, 10, 368-382.	1.0	37
32	Comparison of established and novel purity tests for the quality control of heparin by means of a set of 177 heparin samples. Analytical and Bioanalytical Chemistry, 2011, 399, 605-620.	1.9	37
33	From Catalysts to Bioactive Organometallics: Do Grubbs Catalysts Trigger Biological Effects?. ChemMedChem, 2011, 6, 2142-2145.	1.6	37
34	Comparison of Cyclodextrin-Dipeptide Inclusion Complexes in the Absence and Presence of Urea by Means of Capillary Electrophoresis, Nuclear Magnetic Resonance and Molecular Modeling. European Journal of Organic Chemistry, 2007, 2007, 2921-2930.	1.2	30
35	Impact of Benchmark Data Set Topology on the Validation of Virtual Screening Methods: Exploration and Quantification by Spatial Statistics. Journal of Chemical Information and Modeling, 2008, 48, 704-718.	2.5	30
36	Evaluation of extended parameter sets for the 3D-QSAR technique MaP: implications for interpretability and model quality exemplified by antimalarially active naphthylisoquinoline alkaloids. Journal of Computer-Aided Molecular Design, 2003, 17, 347-365.	1.3	25

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37	Probing the Pharmacophore for Allosteric Ligands of Muscarinic M2Receptors:Â SAR and QSAR Studies in a Series of Bisquaternary Salts of Caracurine V and Related Ring Systems. Journal of Medicinal Chemistry, 2004, 47, 3561-3571.	2.9	22
38	Formulation of Cannabidiol in Colloidal Lipid Carriers. Molecules, 2021, 26, 1469.	1.7	20
39	Cisâ€Configured Aziridines Are New Pseudoâ€Irreversible Dualâ€Mode Inhibitors of Candida albicans Secreted Aspartic Proteaseâ€...2. ChemMedChem, 2008, 3, 302-315.	1.6	19
40	Recent progress in tight junction modulation for improving bioavailability. Expert Opinion on Drug Discovery, 2014, 9, 367-381.	2.5	19
41	A Diverse Benchmark Based on 3D Matched Molecular Pairs for Validating Scoring Functions. ACS Omega, 2018, 3, 5704-5714.	1.6	16
42	Distance Profiles (DiP): A translationally and rotationally invariant 3D structure descriptor capturing steric properties of molecules. QSAR and Combinatorial Science, 2002, 21, 507-519.	1.4	15
43	Synthesis and biological activity of pyridinium-type acetylcholinesterase inhibitors. Journal of Pharmacy and Pharmacology, 2010, 55, 1397-1404.	1.2	13
44	Bidirectional Insulin Granule Turnover in the Submembrane Space During K⁺ Depolarizationâ€Induced Secretion. Traffic, 2011, 12, 1166-1178.	1.3	12
45	xMaPâ€”An Interpretable Alignment-Free Four-Dimensional Quantitative Structureâ€“Activity Relationship Technique Based on Molecular Surface Properties and Conformer Ensembles. Journal of Chemical Information and Modeling, 2018, 58, 165-181.	2.5	12
46	Determination of clotrimazole in mice plasma by capillary electrophoresis. Journal of Pharmaceutical and Biomedical Analysis, 2003, 30, 1879-1887.	1.4	10
47	Structure-Based Validation of the 3D-QSAR Technique MaP. Journal of Chemical Information and Modeling, 2005, 45, 739-749.	2.5	10
48	inSARa: Intuitive and Interactive SAR Interpretation by Reduced Graphs and Hierarchical MCS-Based Network Navigation. Journal of Chemical Information and Modeling, 2014, 54, 1578-1595.	2.5	10
49	QSAR guided synthesis of simplified antiplasmodial analogs of naphthylisoquinoline alkaloids. European Journal of Medicinal Chemistry, 2010, 45, 5370-5383.	2.6	9
50	Granule Mobility, Fusion Frequency and Insulin Secretion Are Differentially Affected by Insulinotropic Stimuli. Traffic, 2015, 16, 493-509.	1.3	9
51	Screening for linearly and nonlinearly related variables in predictive cheminformatic models. Journal of Chemometrics, 2018, 32, e3009.	0.7	9
52	Observer-Independent Quantification of Insulin Granule Exocytosis and Pre-Exocytotic Mobility by TIRF Microscopy. Microscopy and Microanalysis, 2014, 20, 206-218.	0.2	6
53	Evaluating High-Variance Leaves as Uncertainty Measure for Random Forest Regression. Molecules, 2021, 26, 6514.	1.7	5
54	Big Data and Deep Learning: A New Age of Molecular Informatics?. Molecular Informatics, 2017, 36, 1780132.	1.4	3

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55	Systems Approaches and Big Data in Molecular Informatics. Molecular Informatics, 2015, 34, 2-2.	1.4	2
56	Accord for Excel. Journal of Chemical Information and Computer Sciences, 1997, 37, 413-414.	2.8	1
57	QSAR & Combinatorial Science: Transition to the Future. QSAR and Combinatorial Science, 2008, 27, 5-5.	1.5	1
58	Editorial: From QSAR & Combinatorial Science to Molecular Informatics â€“ Transition into the Future and Call for Papers. QSAR and Combinatorial Science, 2009, 28, 623-624.	1.5	1
59	Molecular Informatics Going â€œFully Onlineâ€• Molecular Informatics, 2014, 33, 2-2.	1.4	1
60	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	2.8	1
61	Beyond Paclitaxel and Docetaxel. New Stabilizers of Microtubules. ChemInform, 2005, 36, no.	0.1	0
62	Structure-Based Validation of the 3D-QSAR Technique MaP.. ChemInform, 2005, 36, no.	0.1	0
63	Molecular Informatics- From Models to Molecules and Systems. Molecular Informatics, 2010, 29, 9-9.	1.4	0
64	Molecular Informatics â€“ The First Year. Molecular Informatics, 2011, 30, 3-3.	1.4	0
65	Editorial:Molecular InformaticsGaining Impact. Molecular Informatics, 2012, 31, 615-615.	1.4	0
66	Reliable estimation of externally validated prediction errors for QSAR models. Journal of Cheminformatics, 2013, 5, .	2.8	0
67	Editorial: Sustained Success of Molecular Informatics. Molecular Informatics, 2013, 32, 3-3.	1.4	0
68	Molecular Informatics: From Models to Systems and Beyond. Molecular Informatics, 2016, 35, 2-2.	1.4	0