# Knut Baumann

## List of Publications by Citations



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|---|---|---|---|
| 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 | Maximum unbiased validation (MUV) data sets for virtual screening based on PubChem bioactivity data. *Journal of Chemical Information and Modeling*, **2009**, 49, 169-84 | 6.1 | 208 |
| 55 | Cross-validation as the objective function for variable-selection techniques. *TrAC - Trends in Analytical Chemistry*, **2003**, 22, 395-406 | 14.6 | 182 |
| 54 | Towards a detailed understanding of bacterial metabolism--spectroscopic characterization of Staphylococcus epidermidis. *ChemPhysChem*, **2007**, 8, 124-37 | 3.2 | 167 |
| 53 | Evaluation of arene ruthenium(II) N-heterocyclic carbene complexes as organometallics interacting with thiol and selenol containing biomolecules. *Dalton Transactions*, **2013**, 42, 1657-66 | 4.3 | 99 |
| 52 | Reliable estimation of prediction errors for QSAR models under model uncertainty using double cross-validation. *Journal of Cheminformatics*, **2014**, 6, 47 | 8.6 | 86 |
| 51 | 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 | | 86 |
| 50 | Reliable estimation of externally validated prediction errors for QSAR models. *Journal of Cheminformatics*, **2013**, 5, | 8.6 | 78 |
| 49 | Inhibitors of cysteine proteases. *Current Topics in Medicinal Chemistry*, **2006**, 6, 331-53 | 3 | 74 |
| 48 | Novel strategies for the formulation and processing of poorly water-soluble drugs. *European Journal of Pharmaceutics and Biopharmaceutics*, **2018**, 126, 40-56 | 5.7 | 73 |
| 47 | ErG: 2D pharmacophore descriptions for scaffold hopping. *Journal of Chemical Information and Modeling*, **2006**, 46, 208-20 | 6.1 | 72 |
| 46 | 10-iodo-11H-indolo[3,2-c]quinoline-6-carboxylic acids are selective inhibitors of DYRK1A. *Journal of Medicinal Chemistry*, **2015**, 58, 3131-43 | 8.3 | 70 |
| 45 | Chemoinformatic Classification Methods and their Applicability Domain. *Molecular Informatics*, **2016**, 35, 160-80 | 3.8 | 70 |
| 44 | 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 | | 60 |
| 43 | Structure-activity relationships in a series of bisquaternary bisphthalimidine derivatives modulating the muscarinic M(2)-receptor allosterically. *Journal of Medicinal Chemistry*, **2000**, 43, 2155-64 | 8.3 | 60 |
| 42 | Gaussian mixture discriminant analysis for the single-cell differentiation of bacteria using micro-Raman spectroscopy. *Chemometrics and Intelligent Laboratory Systems*, **2009**, 96, 159-171 | 3.8 | 58 |
| 41 | Validation tools for variable subset regression. *Journal of Computer-Aided Molecular Design*, **2004**, 18, 549-62 | 4.2 | 58 |
| 40 | Mapping property distributions of molecular surfaces: algorithm and evaluation of a novel 3D quantitative structure-activity relationship technique. *Journal of Medicinal Chemistry*, **2003**, 46, 1390-407 | 8.3 | 55 |

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| 39 | Aziridide-based inhibitors of cathepsin L: synthesis, inhibition activity, and docking studies. *ChemMedChem*, **2006**, 1, 1126-41 | 3.7 | 53 |
| 38 | 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. *Journal of Medicinal Chemistry*, **2005**, 48, 6832-42 | 8.3 | 49 |
| 37 | 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, 2433-42 | 8.3 | 45 |
| 36 | A gold(i) biscarbene complex with improved activity as a TrxR inhibitor and cytotoxic drug: comparative studies with different gold metallodrugs. *Metallomics*, **2019**, 11, 533-545 | 4.5 | 44 |
| 35 | 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, 5365-9 | 2.9 | 39 |
| 34 | 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, 7208-12 | 16.4 | 37 |
| 33 | Appropriate calibration functions for capillary electrophoresis II. Heteroscedasticity and its consequences. *Journal of Chromatography A*, **1995**, 700, 9-20 | 4.5 | 37 |
| 32 | From catalysts to bioactive organometallics: do Grubbs catalysts trigger biological effects?. *ChemMedChem*, **2011**, 6, 2142-5 | 3.7 | 36 |
| 31 | Composition of OSCS-contaminated heparin occurring in 2008 in batches on the German market. *European Journal of Pharmaceutical Sciences*, **2010**, 40, 297-304 | 5.1 | 36 |
| 30 | Synthesis, biological activity, and docking studies of new acetylcholinesterase inhibitors of the bispyridinium type. *Archiv Der Pharmazie*, **2003**, 336, 523-40 | 4.3 | 36 |
| 29 | NMR Spectroscopic and Molecular Modelling Studies on Cyclodextrin□Dipeptide Inclusion Complexes. *European Journal of Organic Chemistry*, **2005**, 2005, 1578-1589 | 3.2 | 36 |
| 28 | 2-Anilino-4-(benzimidazol-2-yl)pyrimidines--a multikinase inhibitor scaffold with antiproliferative activity toward cancer cell lines. *European Journal of Medicinal Chemistry*, **2012**, 53, 254-63 | 6.8 | 35 |
| 27 | 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, 605-20 | 4.4 | 33 |
| 26 | Data quality in drug discovery: the role of analytical performance in ligand binding assays. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 847-65 | 4.2 | 32 |
| 25 | A small-molecule inhibitor of Nipah virus envelope protein-mediated membrane fusion. *Journal of Medicinal Chemistry*, **2009**, 52, 4257-65 | 8.3 | 31 |
| 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. *European Journal of Organic Chemistry*, **2007**, 2007, 2921-2930 | 3.2 | 29 |
| 23 | Enzyme kinetics and hit validation in fluorimetric protease assays. *Current Topics in Medicinal Chemistry*, **2010**, 10, 368-82 | 3 | 28 |
| 22 | Efficiency of different measures for defining the applicability domain of classification models. *Journal of Cheminformatics*, **2017**, 9, 44 | 8.6 | 26 |

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| 21 | 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, 704-18 | 6.1 | 25 |
| 20 | 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. *Journal of Medicinal Chemistry*, **2004**, 47, 3561-71 | 8.3 | 21 |
| 19 | 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, 347-65 | 4.2 | 20 |
| 18 | Recent progress in tight junction modulation for improving bioavailability. *Expert Opinion on Drug Discovery*, **2014**, 9, 367-81 | 6.2 | 18 |
| 17 | Cis-Configured aziridines are new pseudo-irreversible dual-mode inhibitors of Candida albicans secreted aspartic protease 2. *ChemMedChem*, **2008**, 3, 302-15 | 3.7 | 17 |
| 16 | Distance Profiles (DiP): A translationally and rotationally invariant 3D structure descriptor capturing steric properties of molecules. *QSAR and Combinatorial Science*, **2002**, 21, 507-519 | | 13 |
| 15 | Synthesis and biological activity of pyridinium-type acetylcholinesterase inhibitors. *Journal of Pharmacy and Pharmacology*, **2003**, 55, 1397-404 | 4.8 | 12 |
| 14 | xMaP-An Interpretable Alignment-Free Four-Dimensional Quantitative Structure-Activity Relationship Technique Based on Molecular Surface Properties and Conformer Ensembles. *Journal of Chemical Information and Modeling*, **2018**, 58, 165-181 | 6.1 | 11 |
| 13 | Bidirectional insulin granule turnover in the submembrane space during K(+) depolarization-induced secretion. *Traffic*, **2011**, 12, 1166-78 | 5.7 | 9 |
| 12 | Determination of clotrimazole in mice plasma by capillary electrophoresis. *Journal of Pharmaceutical and Biomedical Analysis*, **2003**, 30, 1879-87 | 3.5 | 9 |
| 11 | A Diverse Benchmark Based on 3D Matched Molecular Pairs for Validating Scoring Functions. *ACS Omega*, **2018**, 3, 5704-5714 | 3.9 | 9 |
| 10 | QSAR guided synthesis of simplified antiplasmodial analogs of naphthylisoquinoline alkaloids. *European Journal of Medicinal Chemistry*, **2010**, 45, 5370-83 | 6.8 | 8 |
| 9 | Structure-based validation of the 3D-QSAR technique MaP. *Journal of Chemical Information and Modeling*, **2005**, 45, 739-49 | 6.1 | 8 |
| 8 | Screening for linearly and nonlinearly related variables in predictive cheminformatic models. *Journal of Chemometrics*, **2018**, 32, e3009 | 1.6 | 7 |
| 7 | inSARa: intuitive and interactive SAR interpretation by reduced graphs and hierarchical MCS-based network navigation. *Journal of Chemical Information and Modeling*, **2014**, 54, 1578-95 | 6.1 | 7 |
| 6 | Formulation of Cannabidiol in Colloidal Lipid Carriers. *Molecules*, **2021**, 26, | 4.8 | 7 |
| 5 | Granule mobility, fusion frequency and insulin secretion are differentially affected by insulinotropic stimuli. *Traffic*, **2015**, 16, 493-509 | 5.7 | 6 |
| 4 | Observer-independent quantification of insulin granule exocytosis and pre-exocytotic mobility by TIRF microscopy. *Microscopy and Microanalysis*, **2014**, 20, 206-18 | 0.5 | 4 |

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| 3 | Evaluating High-Variance Leaves as Uncertainty Measure for Random Forest Regression. *Molecules*, **2021**, 26, | 4.8 | 1 |
| 2 | Accord for Excel. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 413-414 | | 0 |
| 1 | 11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18 | 8.6 | |