

Alexander Hillisch

List of Publications by Year in descending order

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51
papers

3,094
citations

172457

29
h-index

214800

47
g-index

59
all docs

59
docs citations

59
times ranked

3625
citing authors

#	ARTICLE	IF	CITATIONS
1	Utility of homology models in the drug discovery process. Drug Discovery Today, 2004, 9, 659-669.	6.4	265
2	Discovery of BAY 9448862: A Nonsteroidal Antagonist of the Mineralocorticoid Receptor for the Treatment of Cardiorenal Diseases. ChemMedChem, 2012, 7, 1385-1403.	3.2	194
3	Recent advances in FRET: distance determination in protein-DNA complexes. Current Opinion in Structural Biology, 2001, 11, 201-207.	5.7	185
4	Dissecting Physiological Roles of Estrogen Receptor α and β with Potent Selective Ligands from Structure-Based Design. Molecular Endocrinology, 2004, 18, 1599-1609.	3.7	158
5	A New Mode of Mineralocorticoid Receptor Antagonism by a Potent and Selective Nonsteroidal Molecule. Journal of Biological Chemistry, 2010, 285, 29932-29940.	3.4	157
6	Improving the hit-to-lead process: data-driven assessment of drug-like and lead-like screening hits. Drug Discovery Today, 2006, 11, 175-180.	6.4	156
7	The Lab Oddity Prevails: Discovery of Pan-CDK Inhibitor (1 <i>R</i> ,2 <i>R</i>)-4-(4-((1 <i>R</i> ,2 <i>R</i>)-2-hydroxy-1-methylpropyl)oxy)-5-(trifluoromethyl)cyclopropylsulfonamide (BAY...1000394) for the Treatment of Cancer. ChemMedChem, 2013, 8, 1067-1085.	5.4	156
8	Binding Free Energy Calculations for Lead Optimization: Assessment of Their Accuracy in an Industrial Drug Design Context. Journal of Chemical Theory and Computation, 2014, 10, 3331-3344.	5.3	139
9	Conception and pharmacodynamic profile of drospirenone. Steroids, 2003, 68, 891-905.	1.8	119
10	Finerenone Impedes Aldosterone-dependent Nuclear Import of the Mineralocorticoid Receptor and Prevents Genomic Recruitment of Steroid Receptor Coactivator-1. Journal of Biological Chemistry, 2015, 290, 21876-21889.	3.4	116
11	Impact of isotype-selective estrogen receptor agonists on ovarian function. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 5129-5134.	7.1	111
12	In-silico ADMET Traffic Lights as a Tool for the Prioritization of HTS Hits. ChemMedChem, 2006, 1, 1229-1236.	3.2	100
13	Bayer's in silico ADMET platform: a journey of machine learning over the past two decades. Drug Discovery Today, 2020, 25, 1702-1709.	6.4	92
14	Best of Both Worlds: Combining Pharma Data and State of the Art Modeling Technology To Improve in Silico PK Prediction. Journal of Chemical Information and Modeling, 2015, 55, 389-397.	5.4	87
15	DNA Bending Induced by High Mobility Group Proteins Studied by Fluorescence Resonance Energy Transfer. Biochemistry, 1999, 38, 12150-12158.	2.5	72
16	Global structure similarities of intact and nicked DNA complexed with IHF measured in solution by fluorescence resonance energy transfer. Nucleic Acids Research, 1999, 27, 4619-4625.	14.5	71
17	CypScore: Quantitative Prediction of Reactivity toward Cytochromes P450 Based on Semiempirical Molecular Orbital Theory. ChemMedChem, 2009, 4, 657-669.	3.2	69
18	Computational Chemistry in the Pharmaceutical Industry: From Childhood to Adolescence. ChemMedChem, 2015, 10, 1958-1962.	3.2	65

#	ARTICLE	IF	CITATIONS
19	Oral, Direct Thrombin and Factor α -Xa Inhibitors: The Replacement for Warfarin, Leeches, and Pig Intestines?. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 4574-4590.	13.8	64
20	Prediction of Oral Bioavailability in Rats: Transferring Insights from in Vitro Correlations to (Deep) Machine Learning Models Using in Silico Model Outputs and Chemical Structure Parameters. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4893-4905.	5.4	52
21	The recognition of distorted DNA structures by HMG-D: a footprinting and molecular modelling study 1 Edited by T. Richmond. <i>Journal of Molecular Biology</i> , 1999, 294, 79-91.	4.2	43
22	An approach towards enhancement of a screening library: The Next Generation Library Initiative (NGLI) at Bayer â€” against all odds?. <i>Drug Discovery Today</i> , 2019, 24, 668-672.	6.4	43
23	Utility of protein structures in overcoming ADMET-related issues of drug-like compounds. <i>Drug Discovery Today</i> , 2011, 16, 530-538.	6.4	42
24	Comparison of different heterocyclic scaffolds as substrate analog PDE5 inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 3900-3907.	2.2	41
25	Solution Structure of a Five-Adenine Bulge Loop within a DNA Duplexâ€. <i>Biochemistry</i> , 1999, 38, 12860-12868.	2.5	40
26	Target 2035 â€” update on the quest for a probe for every protein. <i>RSC Medicinal Chemistry</i> , 2022, 13, 13-21.	3.9	39
27	Structure-based design, synthesis and in vitro characterization of potent 17 β -hydroxysteroid dehydrogenase type 1 inhibitors based on 2-substitutions of estrone and D-homo-estrone. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 6740-6744.	2.2	37
28	Fluorescence energy transfer analysis of DNA structures containing several bulges and their interaction with CAP 1 Edited by I. Tinoco. <i>Journal of Molecular Biology</i> , 2000, 302, 1081-1100.	4.2	35
29	Conformational Parameters of the Sandalwood-Odor Activity: Conformational calculations on sandalwood odor. <i>Helvetica Chimica Acta</i> , 1994, 77, 2286-2296.	1.6	30
30	Inhibitory effects of fluorine-substituted estrogens on the activity of 17 β -hydroxysteroid dehydrogenases. <i>Molecular and Cellular Endocrinology</i> , 2006, 248, 218-224.	3.2	28
31	Design of Helical Proteins for Real-Time Endoprotease Assays. <i>Analytical Biochemistry</i> , 2000, 286, 26-34.	2.4	26
32	Molecular Basis of the Interaction Specificity between the Human Glucocorticoid Receptor and Its Endogenous Steroid Ligand Cortisol. <i>ChemBioChem</i> , 2005, 6, 1110-1118.	2.6	24
33	Rendezvous in chemical space? Comparing the small molecule compound libraries of Bayer and Schering. <i>Drug Discovery Today</i> , 2011, 16, 636-641.	6.4	24
34	Entering the Era of Non-Basic P1 Site Groups: Discovery of Xarelto™ (Rivaroxaban). <i>Current Topics in Medicinal Chemistry</i> , 2010, 10, 257-269.	2.1	22
35	Reliable and Performant Identification of Low-Energy Conformers in the Gas Phase and Water. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1005-1020.	5.4	22
36	Structureâ€”Permeability Relationship of Semipeptidic Macrocyclesâ€”Understanding and Optimizing Passive Permeability and Efflux Ratio. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 6774-6783.	6.4	22

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37	CACHE (Critical Assessment of Computational Hit-finding Experiments): A public-private partnership benchmarking initiative to enable the development of computational methods for hit-finding. <i>Nature Reviews Chemistry</i> , 2022, 6, 287-295.	30.2	22
38	Transcriptional repressor CopR: Structure model-based localization of the deoxyribonucleic acid binding motif. , 2000, 38, 393-406.		17
39	The significance of the 20-carbonyl group of progesterone in steroid receptor binding: a molecular dynamics and structure-based ligand design study. <i>Steroids</i> , 2003, 68, 869-878.	1.8	17
40	Transcriptional repressor CopR: Amino acids involved in forming the dimeric interface. , 2000, 39, 408-416.		16
41	Design, Synthesis, and Pharmacological Characterization of a Neutral, Non-Prodrug Thrombin Inhibitor with Good Oral Pharmacokinetics. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 12574-12594.	6.4	15
42	Fluorescence resonance energy transfer studies of U-shaped DNA molecules. <i>Reviews in Molecular Biotechnology</i> , 2002, 82, 197-209.	2.8	14
43	Modern methods of drug discovery: An introduction. , 2003, , 1-18.		8
44	The role of protein 3D-structures in the drug discovery process. , 2003, , 157-181.		8
45	Druggability Assessment for Selected Serine Proteases in a Pharmaceutical Industry Setting. <i>ChemMedChem</i> , 2020, 15, 2010-2018.	3.2	5
46	Protein-Structure-Based Prediction of Animal Model Suitability for Pharmacodynamic Studies of Subtype-Selective Estrogens. <i>ChemMedChem</i> , 2006, 1, 1237-1248.	3.2	4
47	The remarkable influence of steroid A/B-ring junction on the Wittig olefination reaction of the 11-oxo group: Towards the synthesis of 5 α - and 5 β -oriented 1 β 3-isomers of desogestrel. <i>Steroids</i> , 1998, 63, 21-27.	1.8	3
48	Machine Learning Applied to the Modeling of Pharmacological and ADMET Endpoints. <i>Methods in Molecular Biology</i> , 2022, 2390, 61-101.	0.9	3
49	Protein Structure-Based Design, Synthesis Strategy and In Vitro Pharmacological Characterization of Estrogen Receptor $\text{ER}\alpha$ and $\text{ER}\beta$ Selective Compounds. , 2004, , 47-62.		2
50	A Practical Total Synthesis of the Microbial Alkaline Proteinase Inhibitor (MAPI). <i>ChemMedChem</i> , 2009, 4, 2054-2059.	3.2	0
51	Cover Picture: Oral, Direct Thrombin and Factor Xa Inhibitors: The Replacement for Warfarin, Leeches, and Pig Intestines? (<i>Angew. Chem. Int. Ed.</i> 20(2011)). <i>Angewandte Chemie - International Edition</i> , 2011, 50, 4519-4519.	13.8	0