Alexander Hillisch

List of Publications by Year
in descending order

51	3,094	172207	214527
papers	citations	29 h-index	47 g-index

59	59	59	3625
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Machine Learning Applied to the Modeling of Pharmacological and ADMET Endpoints. Methods in Molecular Biology, 2022, 2390, 61-101.	0.4	3
2	Target 2035 â€“ update on the quest for a probe for every protein. RSC Medicinal Chemistry, 2022, 13, 13-21.	1.7	39
3	CACHE (Critical Assessment of Computational Hit-finding Experiments): A publicâ€“private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295.	13.8	22
4	Druggability Assessment for Selected Serine Proteases in a Pharmaceutical Industry Setting. ChemMedChem, 2020, 15, 2010-2018.	1.6	5
5	Design, Synthesis, and Pharmacological Characterization of a Neutral, Non-Prodrug Thrombin Inhibitor with Good Oral Pharmacokinetics. Journal of Medicinal Chemistry, 2020, 63, 12574-12594.	2.9	15
6	Structureâ€“Permeability Relationship of Semipeptidic Macrocyclesâ€”Understanding and Optimizing Passive Permeability and Efflux Ratio. Journal of Medicinal Chemistry, 2020, 63, 6774-6783.	2.9	22
7	Bayerâ€™s in silico ADMET platform: a journey of machine learning over the past two decades. Drug Discovery Today, 2020, 25, 1702-1709.	3.2	92
8	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. Journal of Chemical Information and Modeling, 2019, 59, 4893-4905.	2.5	52
9	An approach towards enhancement of a screening library: The Next Generation Library Initiative (NGLI) at Bayer â€” against all odds?. Drug Discovery Today, 2019, 24, 668-672.	3.2	43
10	Reliable and Performant Identification of Low-Energy Conformers in the Gas Phase and Water. Journal of Chemical Information and Modeling, 2018, 58, 1005-1020.	2.5	22
11	Computational Chemistry in the Pharmaceutical Industry: From Childhood to Adolescence. ChemMedChem, 2015, 10, 1958-1962.	1.6	65
12	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.	1.6	116
13	Best of Both Worlds: Combining Pharma Data and State of the Art Modeling Technology To Improve in Silico pK_a Prediction. Journal of Chemical Information and Modeling, 2015, 55, 389-397.	2.5	87
14	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.	2.3	139
15	The Lab Oddity Prevails: Discovery of Panâ€CDK Inhibitor (R)â€Sâ€Cyclopropylâ€Sâ€(4â€{[4â€{[(1R,2R)â€2â€hydroxyâ€1â€methylpropyl]oxy}â€5â€(trifluo (BAYâ€…1000394) for the Treatment of Cancer. ChemMedChem, 2013, 8, 1067-1085.		
16	Discovery of BAY 94â€8862: A Nonsteroidal Antagonist of the Mineralocorticoid Receptor for the Treatment of Cardiorenal Diseases. ChemMedChem, 2012, 7, 1385-1403.	1.6	194
17	Rendezvous in chemical space? Comparing the small molecule compound libraries of Bayer and Schering. Drug Discovery Today, 2011, 16, 636-641.	3.2	24
18	Utility of protein structures in overcoming ADMET-related issues of drug-like compounds. Drug Discovery Today, 2011, 16, 530-538.	3.2	42

#	Article	IF	Citations
19	Oral, Direct Thrombin and Factorâ€...Xa Inhibitors: The Replacement for Warfarin, Leeches, and Pig Intestines?. Angewandte Chemie - International Edition, 2011, 50, 4574-4590.	7.2	64
20	Cover Picture: Oral, Direct Thrombin and Factorâ€...Xa Inhibitors: The Replacement for Warfarin, Leeches, and Pig Intestines? (Angew. Chem. Int. Ed. 20/2011). Angewandte Chemie - International Edition, 2011, 50, 4519-4519.	7.2	0
21	A New Mode of Mineralocorticoid Receptor Antagonism by a Potent and Selective Nonsteroidal Molecule. Journal of Biological Chemistry, 2010, 285, 29932-29940.	1.6	157
22	Entering the Era of Non-Basic P1 Site Groups: Discovery of Xarelto™ (Rivaroxaban). Current Topics in Medicinal Chemistry, 2010, 10, 257-269.	1.0	22
23	CypScore: Quantitative Prediction of Reactivity toward Cytochromes P450 Based on Semiempirical Molecular Orbital Theory. ChemMedChem, 2009, 4, 657-669.	1.6	69
24	A Practical Total Synthesis of the Microbial Alkaline Proteinase Inhibitor (MAPI). ChemMedChem, 2009, 4, 2054-2059.	1.6	0
25	Structure-based design, synthesis and in vitro characterization of potent 17Î²-hydroxysteroid dehydrogenase type 1 inhibitors based on 2-substitutions of estrone and D-homo-estrone. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6740-6744.	1.0	37
26	Inhibitory effects of fluorine-substituted estrogens on the activity of 17beta-hydroxysteroid dehydrogenases. Molecular and Cellular Endocrinology, 2006, 248, 218-224.	1.6	28
27	Improving the hit-to-lead process: data-driven assessment of drug-like and lead-like screening hits. Drug Discovery Today, 2006, 11, 175-180.	3.2	156
28	Inâ€...Silico ADMET Traffic Lights as a Tool for the Prioritization of HTS Hits. ChemMedChem, 2006, 1, 1229-1236.	1.6	100
29	Protein-Structure-Based Prediction of Animal Model Suitability for Pharmacodynamic Studies of Subtype-Selective Estrogens. ChemMedChem, 2006, 1, 1237-1248.	1.6	4
30	Molecular Basis of the Interaction Specificity between the Human Glucocorticoid Receptor and Its Endogenous Steroid Ligand Cortisol. ChemBioChem, 2005, 6, 1110-1118.	1.3	24
31	Comparison of different heterocyclic scaffolds as substrate analog PDE5 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 3900-3907.	1.0	41
32	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.	3.3	111
33	Dissecting Physiological Roles of Estrogen Receptor Î± and Î² with Potent Selective Ligands from Structure-Based Design. Molecular Endocrinology, 2004, 18, 1599-1609.	3.7	158
34	Utility of homology models in the drug discovery process. Drug Discovery Today, 2004, 9, 659-669.	3.2	265
35	Protein Structure-Based Design, Synthesis Strategy and In Vitro Pharmacological Characterization of Estrogen Receptor Î± and Î² Selective Compounds. , 2004, , 47-62.		2
36	Conception and pharmacodynamic profile of drospirenone. Steroids, 2003, 68, 891-905.	0.8	119

#	Article	IF	Citations
37	The significance of the 20-carbonyl group of progesterone in steroid receptor binding: a molecular dynamics and structure-based ligand design study. Steroids, 2003, 68, 869-878.	0.8	17
38	Modern methods of drug discovery: An introduction. , 2003, , 1-18.		8
39	The role of protein 3D-structures in the drug discovery process. , 2003, , 157-181.		8
40	Fluorescence resonance energy transfer studies of U-shaped DNA molecules. Reviews in Molecular Biotechnology, 2002, 82, 197-209.	2.9	14
41	Recent advances in FRET: distance determination in proteinâ€“DNA complexes. Current Opinion in Structural Biology, 2001, 11, 201-207.	2.6	185
42	Transcriptional repressor CopR: Structure model-based localization of the deoxyribonucleic acid binding motif. , 2000, 38, 393-406.		17
43	Transcriptional repressor CopR: Amino acids involved in forming the dimeric interface. , 2000, 39, 408-416.		16
44	Design of Helical Proteins for Real-Time Endoprotease Assays. Analytical Biochemistry, 2000, 286, 26-34.	1.1	26
45	Fluorescence energy transfer analysis of DNA structures containing several bulges and their interaction with CAP 1 1Edited by I. Tinoco. Journal of Molecular Biology, 2000, 302, 1081-1100.	2.0	35
46	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.	6.5	71
47	DNA Bending Induced by High Mobility Group Proteins Studied by Fluorescence Resonance Energy Transferâ€. Biochemistry, 1999, 38, 12150-12158.	1.2	72
48	Solution Structure of a Five-Adenine Bulge Loop within a DNA Duplexâ€. Biochemistry, 1999, 38, 12860-12868.	1.2	40
49	The recognition of distorted DNA structures by HMG-D: a footprinting and molecular modelling study 1 1Edited by T. Richmond. Journal of Molecular Biology, 1999, 294, 79-91.	2.0	43
50	The remarkable influence of steroid A/B-ring junction on the Wittig olefination reaction of the 11-oxo group: Towards the synthesis of 5Î±- and 5Î²-oriented Î”3-isomers of desogestrel. Steroids, 1998, 63, 21-27.	0.8	3
51	Conformational Parameters of the Sandalwood-Odor Activity: Conformational calculations on sandalwood odor. Helvetica Chimica Acta, 1994, 77, 2286-2296.	1.0	30