Ruth Brenk

List of Publications by Year
in descending order

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58	2,806	172457	182427
papers	citations	29 h-index	51 g-index

69	69	69	3800
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Lessons Learnt from Assembling Screening Libraries for Drug Discovery for Neglected Diseases. ChemMedChem, 2008, 3, 435-444.	3.2	409
2	N-myristoyltransferase inhibitors as new leads to treat sleeping sickness. Nature, 2010, 464, 728-732.	27.8	272
3	Nucleophilic catalysis of acylhydrazone equilibration for protein-directed dynamic covalent chemistry. Nature Chemistry, 2010, 2, 490-497.	13.6	170
4	Virtual Screening for Submicromolar Leads of tRNA-guanine Transglycosylase Based on a New Unexpected Binding Mode Detected by Crystal Structure Analysis. Journal of Medicinal Chemistry, 2003, 46, 1133-1143.	6.4	110
5	Decoys for Docking. Journal of Medicinal Chemistry, 2005, 48, 3714-3728.	6.4	107
6	Discovery of a Novel Class of Orally Active Trypanocidal N-Myristoyltransferase Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 140-152.	6.4	102
7	One Scaffold, Three Binding Modes: Novel and Selective Pteridine Reductase 1 Inhibitors Derived from Fragment Hits Discovered by Virtual Screening. Journal of Medicinal Chemistry, 2009, 52, 4454-4465.	6.4	96
8	Nucleosomes can invade DNA territories occupied by their neighbors. Nature Structural and Molecular Biology, 2009, 16, 151-158.	8.2	95
9	Novel Ligands for a Purine Riboswitch Discovered by RNA-Ligand Docking. Chemistry and Biology, 2011, 18, 324-335.	6.0	93
10	Design, Synthesis, and Biological Evaluation of 3,4-Diarylmaleimides as Angiogenesis Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 1271-1281.	6.4	89
11	DrugPred: A Structure-Based Approach To Predict Protein Druggability Developed Using an Extensive Nonredundant Data Set. Journal of Chemical Information and Modeling, 2011, 51, 2829-2842.	5.4	82
12	Probing Molecular Docking in a Charged Model Binding Site. Journal of Molecular Biology, 2006, 357, 1449-1470.	4.2	61
13	Crystal Structures of tRNA-guanine Transglycosylase (TGT) in Complex with Novel and Potent Inhibitors Unravel Pronounced Induced-fit Adaptations and Suggest Dimer Formation Upon Substrate Binding. Journal of Molecular Biology, 2007, 370, 492-511.	4.2	57
14	Lead Optimization of a Pyrazole Sulfonamide Series of Trypanosoma brucei N-Myristoyltransferase Inhibitors: Identification and Evaluation of CNS Penetrant Compounds as Potential Treatments for Stage 2 Human African Trypanosomiasis. Journal of Medicinal Chemistry, 2014, 57, 9855-9869.	6.4	57
15	Riboswitches as Drug Targets for Antibiotics. Antibiotics, 2021, 10, 45.	3.7	53
16	De Novo Design of Protein Kinase Inhibitors by in Silico Identification of Hinge Region-Binding Fragments. ACS Chemical Biology, 2013, 8, 1044-1052.	3.4	47
17	Identification of Inhibitors of the Leishmania cdc2â€Related Protein Kinase CRK3. ChemMedChem, 2011, 6, 2214-2224.	3.2	45
18	Here Be Dragons: Docking and Screening in an Uncharted Region of Chemical Space. Journal of Biomolecular Screening, 2005, 10, 667-674.	2.6	42

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19	Mining the ChEMBL Database: An Efficient Chemoinformatics Workflow for Assembling an Ion Channel-Focused Screening Library. Journal of Chemical Information and Modeling, 2011, 51, 2449-2454.	5.4	41
20	A Molecular Hybridization Approach for the Design of Potent, Highly Selective, and Brain-Penetrant N-Myristoyltransferase Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 8374-8389.	6.4	41
21	Cytotoxicity of cardiotonic steroids in sensitive and multidrug-resistant leukemia cells and the link with Na+/K+-ATPase. Journal of Steroid Biochemistry and Molecular Biology, 2015, 150, 97-111.	2.5	40
22	Design, Synthesis and Biological Evaluation of Novel Inhibitors of Trypanosoma brucei Pteridine Reductaseâ€...1. ChemMedChem, 2011, 6, 302-308.	3.2	39
23	Allosteric Competitive Inhibitors of the Glucose-1-phosphate Thymidylyltransferase (RmlA) from Pseudomonas aeruginosa. ACS Chemical Biology, 2013, 8, 387-396.	3.4	39
24	De Novo Design, Synthesis, and In Vitro Evaluation of Inhibitors for Prokaryotic tRNA-Guanine Transglycosylase: A Dramatic Sulfur Effect on Binding Affinity. ChemBioChem, 2002, 3, 250-253.	2.6	38
25	Identification of novel inhibitors of UDP-Glc 4â€²-epimerase, a validated drug target for african sleeping sickness. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 5744-5747.	2.2	37
26	The small molecule tool (S)-(â^')-blebbistatin: novel insights of relevance to myosin inhibitor design. Organic and Biomolecular Chemistry, 2008, 6, 2076.	2.8	37
27	Crystallographic Study of Inhibitors of tRNA-guanine Transglycosylase Suggests a New Structure-based Pharmacophore for Virtual Screening. Journal of Molecular Biology, 2004, 338, 55-75.	4.2	35
28	Synthesis, Biological Evaluation, and Crystallographic Studies of Extended Guanine-Based (lin-Benzoguanine) Inhibitors for tRNA-Guanine Transglycosylase (TGT). Helvetica Chimica Acta, 2006, 89, 573-597.	1.6	31
29	Flexible Adaptations in the Structure of the tRNA-Modifying Enzyme tRNA-Guanine Transglycosylase and Their Implications for Substrate Selectivity, Reaction Mechanism and Structure-Based Drug Design. ChemBioChem, 2003, 4, 1066-1077.	2.6	30
30	Structural Insights into the Mechanism and Inhibition of the Î²-Hydroxydecanoyl-Acyl Carrier Protein Dehydratase from Pseudomonas aeruginosa. Journal of Molecular Biology, 2013, 425, 365-377.	4.2	30
31	From Onâ€Target to Offâ€Target Activity: Identification and Optimisation of Trypanosoma brucei GSK3 Inhibitors and Their Characterisation as Antiâ€Trypanosoma brucei Drug Discovery Lead Molecules. ChemMedChem, 2013, 8, 1127-1137.	3.2	30
32	The Design and Synthesis of Potent and Selective Inhibitors ofTrypanosoma bruceiGlycogen Synthase Kinase 3 for the Treatment of Human African Trypanosomiasis. Journal of Medicinal Chemistry, 2014, 57, 7536-7549.	6.4	28
33	Virtual fragment screening for novel inhibitors of 6-phosphogluconate dehydrogenase. Bioorganic and Medicinal Chemistry, 2010, 18, 5056-5062.	3.0	26
34	Synthesis andIn Vitro Evaluation of 2-Aminoquinazolin-4(3H)-one-Based Inhibitors for tRNA-Guanine Transglycosylase (TGT). Helvetica Chimica Acta, 2004, 87, 1333-1356.	1.6	25
35	Locating Sweet Spots for Screening Hits and Evaluating Pan-Assay Interference Filters from the Performance Analysis of Two Lead-like Libraries. Journal of Chemical Information and Modeling, 2013, 53, 534-544.	5.4	22
36	Development of Smallâ€Molecule Trypanosoma brucei Nâ€Myristoyltransferase Inhibitors: Discovery and Optimisation of a Novel Binding Mode. ChemMedChem, 2015, 10, 1821-1836.	3.2	20

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37	A Structure-Based Approach to Ligand Discovery for 2C-Methyl-<scp>d</scp>-erythritol-2,4-cyclodiphosphate Synthase: A Target for Antimicrobial Therapy. Journal of Medicinal Chemistry, 2009, 52, 2531-2542.	6.4	19
38	Probing the Dynamic Nature of Water Molecules and Their Influences on Ligand Binding in a Model Binding Site. Journal of Chemical Information and Modeling, 2011, 51, 2581-2594.	5.4	19
39	Increasing the Coverage of Medicinal Chemistry-Relevant Space in Commercial Fragments Screening. Journal of Chemical Information and Modeling, 2014, 54, 79-85.	5.4	19
40	IspE Inhibitors Identified by a Combination of In Silico and In Vitro High-Throughput Screening. PLoS ONE, 2012, 7, e35792.	2.5	18
41	From Hit to Lead: De Novo Design Based on Virtual Screening Hits of Inhibitors of tRNA-Guanine Transglycosylase, a Putative Target of Shigellosis Therapy. Helvetica Chimica Acta, 2003, 86, 1435-1452.	1.6	16
42	Ligand design for riboswitches, an emerging target class for novel antibiotics. Future Medicinal Chemistry, 2017, 9, 1649-1662.	2.3	16
43	Design and Synthesis of Brain Penetrant Trypanocidal N-Myristoyltransferase Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 9790-9806.	6.4	14
44	Quantitative structure-activity relationship and molecular docking of artemisinin derivatives to vascular endothelial growth factor receptor 1. Anticancer Research, 2015, 35, 1929-34.	1.1	14
45	Fragmentâ€Based Drug Discovery for RNA Targets. ChemMedChem, 2021, 16, 2588-2603.	3.2	11
46	How To Design Selective Ligands for Highly Conserved Binding Sites: A Case Study Using N-Myristoyltransferases as a Model System. Journal of Medicinal Chemistry, 2020, 63, 2095-2113.	6.4	10
47	In silico identification and experimental validation of hits active against KPC-2 Î²-lactamase. PLoS ONE, 2018, 13, e0203241.	2.5	9
48	To Hit or Not to Hit, That Is the Question â€“ Genome-wide Structure-Based Druggability Predictions for Pseudomonas aeruginosa Proteins. PLoS ONE, 2015, 10, e0137279.	2.5	9
49	Structure-Based Discovery of Small Molecules Binding to RNA. Topics in Medicinal Chemistry, 2017, , 47-77.	0.8	8
50	Structure-Based Virtual Screening for the Identification of RNA-Binding Ligands. Methods in Molecular Biology, 2014, 1103, 127-139.	0.9	8
51	Optimisation of the Antiâ€Trypanosoma brucei Activity of the Opioid Agonist U50488. ChemMedChem, 2011, 6, 1832-1840.	3.2	7
52	An Experimental Toolbox for Structureâ€Based Hit Discovery for P.â€¦aeruginosa FabF, a Promising Target for Antibiotics. ChemMedChem, 2021, 16, 2715-2726.	3.2	6
53	Identification of a potential allosteric site of Golgi Î±-mannosidase II using computer-aided drug design. PLoS ONE, 2019, 14, e0216132.	2.5	5
54	DrugPred_RNAâ€"A Tool for Structure-Based Druggability Predictions for RNA Binding Sites. Journal of Chemical Information and Modeling, 2021, 61, 4068-4081.	5.4	5

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55	Structures ofPseudomonas aeruginosaÎ²-ketoacyl-(acyl-carrier-protein) synthase II (FabF) and a C164Q mutant provide templates for antibacterial drug discovery and identify a buried potassium ion and a ligand-binding site that is an artefact of the crystal form. Acta Crystallographica Section F, Structural Biology Communications, 2015, 71, 1020-1026.	0.8	4
56	Targeting the Class A Carbapenemase GES-5 via Virtual Screening. Biomolecules, 2020, 10, 304.	4.0	1
57	Crystal structure of Pseudomonas aeruginosa FabB C161A, a template for structure-based design for new antibiotics. F1000Research, 2021, 10, 1102.	1.6	0
58	Crystal structure of Pseudomonas aeruginosa FabB C161A, a template for structure-based design for new antibiotics. F1000Research, 0, 10, 1102.	1.6	0