

Ruth Brenk

List of Publications by Year in descending order

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58
papers

2,806
citations

172457

29
h-index

182427

51
g-index

69
all docs

69
docs citations

69
times ranked

3800
citing authors

#	ARTICLE	IF	CITATIONS
1	Riboswitches as Drug Targets for Antibiotics. <i>Antibiotics</i> , 2021, 10, 45.	3.7	53
2	DrugPred_RNA – A Tool for Structure-Based Druggability Predictions for RNA Binding Sites. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4068-4081.	5.4	5
3	Fragment-Based Drug Discovery for RNA Targets. <i>ChemMedChem</i> , 2021, 16, 2588-2603.	3.2	11
4	An Experimental Toolbox for Structure-Based Hit Discovery for <i>Pseudomonas aeruginosa</i> FabF, a Promising Target for Antibiotics. <i>ChemMedChem</i> , 2021, 16, 2715-2726.	3.2	6
5	Crystal structure of <i>Pseudomonas aeruginosa</i> FabB C161A, a template for structure-based design for new antibiotics. <i>F1000Research</i> , 2021, 10, 1102.	1.6	0
6	How To Design Selective Ligands for Highly Conserved Binding Sites: A Case Study Using <i>N-Myristoyltransferase</i> as a Model System. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 2095-2113.	6.4	10
7	Targeting the Class A Carbapenemase GES-5 via Virtual Screening. <i>Biomolecules</i> , 2020, 10, 304.	4.0	1
8	Identification of a potential allosteric site of Golgi β -mannosidase II using computer-aided drug design. <i>PLoS ONE</i> , 2019, 14, e0216132.	2.5	5
9	In silico identification and experimental validation of hits active against KPC-2 β -lactamase. <i>PLoS ONE</i> , 2018, 13, e0203241.	2.5	9
10	A Molecular Hybridization Approach for the Design of Potent, Highly Selective, and Brain-Penetrant <i>N-Myristoyltransferase</i> Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 8374-8389.	6.4	41
11	Structure-Based Discovery of Small Molecules Binding to RNA. <i>Topics in Medicinal Chemistry</i> , 2017, , 47-77.	0.8	8
12	Ligand design for riboswitches, an emerging target class for novel antibiotics. <i>Future Medicinal Chemistry</i> , 2017, 9, 1649-1662.	2.3	16
13	Design and Synthesis of Brain Penetrant Trypanocidal <i>N-Myristoyltransferase</i> Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 9790-9806.	6.4	14
14	Development of Small-Molecule <i>Trypanosoma brucei N-Myristoyltransferase</i> Inhibitors: Discovery and Optimisation of a Novel Binding Mode. <i>ChemMedChem</i> , 2015, 10, 1821-1836.	3.2	20
15	Structures of <i>Pseudomonas aeruginosa</i> β -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. <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2015, 71, 1020-1026.	0.8	4
16	Cytotoxicity of cardiotonic steroids in sensitive and multidrug-resistant leukemia cells and the link with Na ⁺ /K ⁺ -ATPase. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2015, 150, 97-111.	2.5	40
17	To Hit or Not to Hit, That Is the Question – Genome-wide Structure-Based Druggability Predictions for <i>Pseudomonas aeruginosa</i> Proteins. <i>PLoS ONE</i> , 2015, 10, e0137279.	2.5	9
18	Quantitative structure-activity relationship and molecular docking of artemisinin derivatives to vascular endothelial growth factor receptor 1. <i>Anticancer Research</i> , 2015, 35, 1929-34.	1.1	14

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19	Increasing the Coverage of Medicinal Chemistry-Relevant Space in Commercial Fragments Screening. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 79-85.	5.4	19
20	Lead Optimization of a Pyrazole Sulfonamide Series of <i>Trypanosoma brucei</i> N-Myristoyltransferase Inhibitors: Identification and Evaluation of CNS Penetrant Compounds as Potential Treatments for Stage 2 Human African Trypanosomiasis. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 9855-9869.	6.4	57
21	The Design and Synthesis of Potent and Selective Inhibitors of <i>Trypanosoma brucei</i> Glycogen Synthase Kinase 3 for the Treatment of Human African Trypanosomiasis. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 7536-7549.	6.4	28
22	Structure-Based Virtual Screening for the Identification of RNA-Binding Ligands. <i>Methods in Molecular Biology</i> , 2014, 1103, 127-139.	0.9	8
23	Allosteric Competitive Inhibitors of the Glucose-1-phosphate Thymidyltransferase (RmlA) from <i>Pseudomonas aeruginosa</i> . <i>ACS Chemical Biology</i> , 2013, 8, 387-396.	3.4	39
24	Locating Sweet Spots for Screening Hits and Evaluating Pan-Assay Interference Filters from the Performance Analysis of Two Lead-like Libraries. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 534-544.	5.4	22
25	Structural Insights into the Mechanism and Inhibition of the $\hat{1}^2$ -Hydroxydecanoyl-Acyl Carrier Protein Dehydratase from <i>Pseudomonas aeruginosa</i> . <i>Journal of Molecular Biology</i> , 2013, 425, 365-377.	4.2	30
26	De Novo Design of Protein Kinase Inhibitors by in Silico Identification of Hinge Region-Binding Fragments. <i>ACS Chemical Biology</i> , 2013, 8, 1044-1052.	3.4	47
27	From On-Target to Off-Target Activity: Identification and Optimisation of <i>Trypanosoma brucei</i> GSK3 Inhibitors and Their Characterisation as Anti- <i>Trypanosoma brucei</i> Drug Discovery Lead Molecules. <i>ChemMedChem</i> , 2013, 8, 1127-1137.	3.2	30
28	Discovery of a Novel Class of Orally Active Trypanocidal N-Myristoyltransferase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 140-152.	6.4	102
29	IspE Inhibitors Identified by a Combination of In Silico and In Vitro High-Throughput Screening. <i>PLoS ONE</i> , 2012, 7, e35792.	2.5	18
30	Mining the ChEMBL Database: An Efficient Chemoinformatics Workflow for Assembling an Ion Channel-Focused Screening Library. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2449-2454.	5.4	41
31	Probing the Dynamic Nature of Water Molecules and Their Influences on Ligand Binding in a Model Binding Site. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2581-2594.	5.4	19
32	DrugPred: A Structure-Based Approach To Predict Protein Druggability Developed Using an Extensive Nonredundant Data Set. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2829-2842.	5.4	82
33	Design, Synthesis and Biological Evaluation of Novel Inhibitors of <i>Trypanosoma brucei</i> Pteridine Reductase...1. <i>ChemMedChem</i> , 2011, 6, 302-308.	3.2	39
34	Optimisation of the Anti- <i>Trypanosoma brucei</i> Activity of the Opioid Agonist U50488. <i>ChemMedChem</i> , 2011, 6, 1832-1840.	3.2	7
35	Identification of Inhibitors of the <i>Leishmania</i> cdc2-Related Protein Kinase CRK3. <i>ChemMedChem</i> , 2011, 6, 2214-2224.	3.2	45
36	Novel Ligands for a Purine Riboswitch Discovered by RNA-Ligand Docking. <i>Chemistry and Biology</i> , 2011, 18, 324-335.	6.0	93

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37	Virtual fragment screening for novel inhibitors of 6-phosphogluconate dehydrogenase. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 5056-5062.	3.0	26
38	N-myristoyltransferase inhibitors as new leads to treat sleeping sickness. <i>Nature</i> , 2010, 464, 728-732.	27.8	272
39	Nucleophilic catalysis of acylhydrazone equilibration for protein-directed dynamic covalent chemistry. <i>Nature Chemistry</i> , 2010, 2, 490-497.	13.6	170
40	Nucleosomes can invade DNA territories occupied by their neighbors. <i>Nature Structural and Molecular Biology</i> , 2009, 16, 151-158.	8.2	95
41	A Structure-Based Approach to Ligand Discovery for 2-C-Methyl-erythritol-2,4-cyclodiphosphate Synthase: A Target for Antimicrobial Therapy. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 2531-2542.	6.4	19
42	One Scaffold, Three Binding Modes: Novel and Selective Pteridine Reductase 1 Inhibitors Derived from Fragment Hits Discovered by Virtual Screening. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 4454-4465.	6.4	96
43	Lessons Learnt from Assembling Screening Libraries for Drug Discovery for Neglected Diseases. <i>ChemMedChem</i> , 2008, 3, 435-444.	3.2	409
44	The small molecule tool (S)-(α)-blebbistatin: novel insights of relevance to myosin inhibitor design. <i>Organic and Biomolecular Chemistry</i> , 2008, 6, 2076.	2.8	37
45	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. <i>Journal of Molecular Biology</i> , 2007, 370, 492-511.	4.2	57
46	Design, Synthesis, and Biological Evaluation of 3,4-Diarylmaleimides as Angiogenesis Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 1271-1281.	6.4	89
47	Probing Molecular Docking in a Charged Model Binding Site. <i>Journal of Molecular Biology</i> , 2006, 357, 1449-1470.	4.2	61
48	Identification of novel inhibitors of UDP-Glc 4-epimerase, a validated drug target for african sleeping sickness. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 5744-5747.	2.2	37
49	Synthesis, Biological Evaluation, and Crystallographic Studies of Extended Guanine-Based (lin-Benzoguanine) Inhibitors for tRNA-Guanine Transglycosylase (TGT). <i>Helvetica Chimica Acta</i> , 2006, 89, 573-597.	1.6	31
50	Here Be Dragons: Docking and Screening in an Uncharted Region of Chemical Space. <i>Journal of Biomolecular Screening</i> , 2005, 10, 667-674.	2.6	42
51	Decoys for Docking. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 3714-3728.	6.4	107
52	Synthesis and In Vitro Evaluation of 2-Aminoquinazolin-4(3H)-one-Based Inhibitors for tRNA-Guanine Transglycosylase (TGT). <i>Helvetica Chimica Acta</i> , 2004, 87, 1333-1356.	1.6	25
53	Crystallographic Study of Inhibitors of tRNA-guanine Transglycosylase Suggests a New Structure-based Pharmacophore for Virtual Screening. <i>Journal of Molecular Biology</i> , 2004, 338, 55-75.	4.2	35
54	From Hit to Lead: De Novo Design Based on Virtual Screening Hits of Inhibitors of tRNA-Guanine Transglycosylase, a Putative Target of Shigellosis Therapy. <i>Helvetica Chimica Acta</i> , 2003, 86, 1435-1452.	1.6	16

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55	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. <i>ChemBioChem</i> , 2003, 4, 1066-1077.	2.6	30
56	Virtual Screening for Submicromolar Leads of tRNA-guanine Transglycosylase Based on a New Unexpected Binding Mode Detected by Crystal Structure Analysis. <i>Journal of Medicinal Chemistry</i> , 2003, 46, 1133-1143.	6.4	110
57	De Novo Design, Synthesis, and In Vitro Evaluation of Inhibitors for Prokaryotic tRNA-Guanine Transglycosylase: A Dramatic Sulfur Effect on Binding Affinity. <i>ChemBioChem</i> , 2002, 3, 250-253.	2.6	38
58	Crystal structure of <i>Pseudomonas aeruginosa</i> FabB C161A, a template for structure-based design for new antibiotics. <i>F1000Research</i> , 0, 10, 1102.	1.6	0