Gisbert Schneider

List of Publications by Citations

452 papers	18,862 citations	65 h-index	119 g-index
515 ext. papers	21,754 ext. citations	6.8 avg, IF	7.38 L-index

#	Paper	IF	Citations
452	Designing antimicrobial peptides: form follows function. *Nature Reviews Drug Discovery*, **2011**, 11, 37-51	64.1	1190
451	Counting on natural products for drug design. *Nature Chemistry*, **2016**, 8, 531-41	17.6	592
450	Computer-based de novo design of drug-like molecules. *Nature Reviews Drug Discovery*, **2005**, 4, 649-63	64.1	583
449	Scaffold-Hopping by Topological Pharmacophore Search: A Contribution to Virtual Screening. *Angewandte Chemie - International Edition*, **1999**, 38, 2894-2896	16.4	529
448	Comparison of support vector machine and artificial neural network systems for drug/nondrug classification. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1882-9		402
447	Virtual screening: an endless staircase?. *Nature Reviews Drug Discovery*, **2010**, 9, 273-6	64.1	368
446	Deep Learning in Drug Discovery. *Molecular Informatics*, **2016**, 35, 3-14	3.8	360
445	Automating drug discovery. *Nature Reviews Drug Discovery*, **2018**, 17, 97-113	64.1	275
444	Development of a virtual screening method for identification of "frequent hitters" in compound libraries. *Journal of Medicinal Chemistry*, **2002**, 45, 137-42	8.3	258
443	Predicting drug metabolism: experiment and/or computation?. *Nature Reviews Drug Discovery*, **2015**, 14, 387-404	64.1	255
442	Scaffold architecture and pharmacophoric properties of natural products and trade drugs: application in the design of natural product-based combinatorial libraries. *ACS Combinatorial Science*, **2001**, 3, 284-9		245
441	Concepts of Artificial Intelligence for Computer-Assisted Drug Discovery. *Chemical Reviews*, **2019**, 119, 10520-10594	68.1	243
440	PocketPicker: analysis of ligand binding-sites with shape descriptors. *Chemistry Central Journal*, **2007**, 1, 7		228
439	Virtual screening and fast automated docking methods. *Drug Discovery Today*, **2002**, 7, 64-70	8.8	228
438	Virtual screening and fast automated docking methods. *Drug Discovery Today*, **2002**, 7, 64-70	8.8	214
437	Helicobacter pylori HtrA is a new secreted virulence factor that cleaves E-cadherin to disrupt intercellular adhesion. *EMBO Reports*, **2010**, 11, 798-804	6.5	211
436	Generative Recurrent Networks for De Novo Drug Design. *Molecular Informatics*, **2018**, 37, 1700111	3.8	184

435	Rethinking drug design in the artificial intelligence era. *Nature Reviews Drug Discovery*, **2020**, 19, 353-364	64.1	179
434	Scaffold diversity of natural products: inspiration for combinatorial library design. *Natural Product Reports*, **2008**, 25, 892-904	15.1	178
433	De novo design of molecular architectures by evolutionary assembly of drug-derived building blocks. *Journal of Computer-Aided Molecular Design*, **2000**, 14, 487-94	4.2	178
432	Deciphering apicoplast targeting signals--feature extraction from nuclear-encoded precursors of Plasmodium falciparum apicoplast proteins. *Gene*, **2001**, 280, 19-26	3.8	177
431	Identifying the macromolecular targets of de novo-designed chemical entities through self-organizing map consensus. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 4067-72	11.5	169
430	Artificial neural networks for computer-based molecular design. *Progress in Biophysics and Molecular Biology*, **1998**, 70, 175-222	4.7	160
429	Optimized Particle Swarm Optimization (OPSO) and its application to artificial neural network training. *BMC Bioinformatics*, **2006**, 7, 125	3.6	156
428	De Novo Design of Bioactive Small Molecules by Artificial Intelligence. *Molecular Informatics*, **2018**, 37, 1700153	3.8	155
427	A virtual screening method for prediction of the HERG potassium channel liability of compound libraries. *ChemBioChem*, **2002**, 3, 455-9	3.8	152
426	DOGS: reaction-driven de novo design of bioactive compounds. *PLoS Computational Biology*, **2012**, 8, e1002380	5	151
425	Dual-display of small molecules enables the discovery of ligand pairs and facilitates affinity maturation. *Nature Chemistry*, **2015**, 7, 241-9	17.6	143
424	Support vector machine applications in bioinformatics. *Applied Bioinformatics*, **2003**, 2, 67-77		127
423	An unusual ERAD-like complex is targeted to the apicoplast of Plasmodium falciparum. *Eukaryotic Cell*, **2009**, 8, 1134-45		125
422	Scaffold-Hopping: How Far Can You Jump?. *QSAR and Combinatorial Science*, **2006**, 25, 1162-1171		123
421	Distinct roles of secreted HtrA proteases from gram-negative pathogens in cleaving the junctional protein and tumor suppressor E-cadherin. *Journal of Biological Chemistry*, **2012**, 287, 10115-10120	5.4	122
420	Drug discovery with explainable artificial intelligence. *Nature Machine Intelligence*, **2020**, 2, 573-584	22.5	116
419	Collection of Bioactive Reference Compounds for Focused Library Design. *QSAR and Combinatorial Science*, **2003**, 22, 713-718		112
418	Chemically Advanced Template Search (CATS) for Scaffold-Hopping and Prospective Target Prediction for 'Orphan' Molecules. *Molecular Informatics*, **2013**, 32, 133-138	3.8	109

417	Active-learning strategies in computer-assisted drug discovery. *Drug Discovery Today*, **2015**, 20, 458-65	8.8	108
416	Properties and prediction of mitochondrial transit peptides from Plasmodium falciparum. *Molecular and Biochemical Parasitology*, **2003**, 132, 59-66	1.9	105
415	The rational design of amino acid sequences by artificial neural networks and simulated molecular evolution: de novo design of an idealized leader peptidase cleavage site. *Biophysical Journal*, **1994**, 66, 335-44	2.9	105
414	Revealing the macromolecular targets of complex natural products. *Nature Chemistry*, **2014**, 6, 1072-8	17.6	100
413	Prediction of type III secretion signals in genomes of gram-negative bacteria. *PLoS ONE*, **2009**, 4, e5917	3.7	95
412	Recurrent Neural Network Model for Constructive Peptide Design. *Journal of Chemical Information and Modeling*, **2018**, 58, 472-479	6.1	90
411	Self-organizing maps in drug discovery: compound library design, scaffold-hopping, repurposing. *Current Medicinal Chemistry*, **2009**, 16, 258-66	4.3	90
410	Advances in the prediction of protein targeting signals. *Proteomics*, **2004**, 4, 1571-80	4.8	90
409	Flux (1): a virtual synthesis scheme for fragment-based de novo design. *Journal of Chemical Information and Modeling*, **2006**, 46, 699-707	6.1	88
408	De novo drug design. *Methods in Molecular Biology*, **2011**, 672, 299-323	1.4	87
407	Discovery of small-molecule interleukin-2 inhibitors from a DNA-encoded chemical library. *Chemistry - A European Journal*, **2012**, 18, 7729-37	4.8	83
406	De Novo Design at the Edge of Chaos. *Journal of Medicinal Chemistry*, **2016**, 59, 4077-86	8.3	81
405	Scaffold-hopping potential of ligand-based similarity concepts. *ChemMedChem*, **2006**, 1, 181-5	3.7	80
404	Peptide lineup against Gram-negative bacterial infection First-in-class peptide inhibitor of H. pylori HtrA. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
403	Target prediction by cascaded self-organizing maps for ligand de-orphaning and side-effect investigation. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
402	Visualization and virtual screening in molecular property spaces. *Journal of Cheminformatics*, **2011**, 3,	8.6	78
401	Feature-extraction from endopeptidase cleavage sites in mitochondrial targeting peptides **1998**, 30, 49-60		77
400	Accessing new chemical entities through microfluidic systems. *Angewandte Chemie - International Edition*, **2014**, 53, 5750-8	16.4	76

399	Voyages to the (un)known: adaptive design of bioactive compounds. *Trends in Biotechnology*, **2009**, 27, 18-26	15.1	76
398	Simple 2,4-diacylphloroglucinols as classic transient receptor potential-6 activators--identification of a novel pharmacophore. *Molecular Pharmacology*, **2010**, 77, 368-77	4.3	74
397	Comparison of correlation vector methods for ligand-based similarity searching. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 687-98	4.2	74
396	Virtual Screening for Bioactive Molecules by Evolutionary De Novo Design. *Angewandte Chemie - International Edition*, **2000**, 39, 4130-4133	16.4	74
395	Properties and Architecture of Drugs and Natural Products Revisited. *Current Chemical Biology*, **2007**, 1, 115-127	0.4	74
394	Identification and functional analysis of cyclooxygenase-1 as a molecular target of boswellic acids. *Biochemical Pharmacology*, **2008**, 75, 503-13	6	73
393	Processing and classification of chemical data inspired by insect olfaction. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 20285-9	11.5	70
392	Combining in vitro and in vivo pharmacokinetic data for prediction of hepatic drug clearance in humans by artificial neural networks and multivariate statistical techniques. *Journal of Medicinal Chemistry*, **1999**, 42, 5072-6	8.3	70
391	A collection of robust organic synthesis reactions for in silico molecule design. *Journal of Chemical Information and Modeling*, **2011**, 51, 3093-8	6.1	69
390	Pseudoreceptor models in drug design: bridging ligand- and receptor-based virtual screening. *Nature Reviews Drug Discovery*, **2008**, 7, 667-77	64.1	69
389	Prediction of hepatic metabolic clearance: comparison and assessment of prediction models. *Clinical Pharmacokinetics*, **2001**, 40, 553-63	6.2	69
388	Ligand-based combinatorial design of selective purinergic receptor (A2A) antagonists using self-organizing maps. *ACS Combinatorial Science*, **2003**, 5, 233-7		65
387	Trends in virtual combinatorial library design. *Current Medicinal Chemistry*, **2002**, 9, 2095-101	4.3	65
386	Prediction of extracellular proteases of the human pathogen Helicobacter pylori reveals proteolytic activity of the Hp1018/19 protein HtrA. *PLoS ONE*, **2008**, 3, e3510	3.7	64
385	Multi-objective molecular de novo design by adaptive fragment prioritization. *Angewandte Chemie - International Edition*, **2014**, 53, 4244-8	16.4	63
384	Privileged Structures Revisited. *Angewandte Chemie - International Edition*, **2017**, 56, 7971-7974	16.4	61
383	Identification of natural-product-derived inhibitors of 5-lipoxygenase activity by ligand-based virtual screening. *Journal of Medicinal Chemistry*, **2007**, 50, 2640-6	8.3	61
382	The molecular mechanism of the inhibition by licofelone of the biosynthesis of 5-lipoxygenase products. *British Journal of Pharmacology*, **2007**, 152, 471-80	8.6	61

381	Peptide design by artificial neural networks and computer-based evolutionary search. *Proceedings of the National Academy of Sciences of the United States of America*, **1998**, 95, 12179-84	11.5	61
380	Automated De Novo Drug Design: Are We Nearly There Yet?. *Angewandte Chemie - International Edition*, **2019**, 58, 10792-10803	16.4	60
379	Combining on-chip synthesis of a focused combinatorial library with computational target prediction reveals imidazopyridine GPCR ligands. *Angewandte Chemie - International Edition*, **2014**, 53, 582-5	16.4	60
378	Identification of human cathepsin G as a functional target of boswellic acids from the anti-inflammatory remedy frankincense. *Journal of Immunology*, **2009**, 183, 3433-42	5.3	60
377	Species-specific inhibition of APOBEC3C by the prototype foamy virus protein bet. *Journal of Biological Chemistry*, **2009**, 284, 5819-26	5.4	60
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375	2,4-Diaminopyrimidines as histamine H4 receptor ligands--Scaffold optimization and pharmacological characterization. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 7186-96	3.4	57
374	Phenotype-based high-content chemical library screening identifies statins as inhibitors of in vivo lymphangiogenesis. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, E2665-74	11.5	57
373	Identification of E-cadherin signature motifs functioning as cleavage sites for Helicobacter pylori HtrA. *Scientific Reports*, **2016**, 6, 23264	4.9	56
372	Flux (2): comparison of molecular mutation and crossover operators for ligand-based de novo design. *Journal of Chemical Information and Modeling*, **2007**, 47, 656-67	6.1	56
371	Nonlinear dimensionality reduction and mapping of compound libraries for drug discovery. *Journal of Molecular Graphics and Modelling*, **2012**, 34, 108-17	2.8	55
370	Active learning for computational chemogenomics. *Future Medicinal Chemistry*, **2017**, 9, 381-402	4.1	54
369	Common non-epigenetic drugs as epigenetic modulators. *Trends in Molecular Medicine*, **2013**, 19, 742-53	11.5	54
368	Kernel approach to molecular similarity based on iterative graph similarity. *Journal of Chemical Information and Modeling*, **2007**, 47, 2280-6	6.1	54
367	SVM-based feature selection for characterization of focused compound collections. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 993-9		54
366	Aminothiazole-featured pirinixic acid derivatives as dual 5-lipoxygenase and microsomal prostaglandin E2 synthase-1 inhibitors with improved potency and efficiency in vivo. *Journal of Medicinal Chemistry*, **2013**, 56, 9031-44	8.3	52
365	Enabling future drug discovery by de novo design. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 742-759	7.9	51
364	Predicting compound selectivity by self-organizing maps: cross-activities of metabotropic glutamate receptor antagonists. *ChemMedChem*, **2006**, 1, 1066-8	3.7	51

363	Context-based identification of protein-protein interfaces and "hot-spot" residues. *Chemistry and Biology*, **2011**, 18, 344-53		50
362	Hyperforin is a novel type of 5-lipoxygenase inhibitor with high efficacy in vivo. *Cellular and Molecular Life Sciences*, **2009**, 66, 2759-71	10.3	48
361	Fuzzy pharmacophore models from molecular alignments for correlation-vector-based virtual screening. *Journal of Medicinal Chemistry*, **2004**, 47, 4653-64	8.3	48
360	Grundgerüstwechsel (Scaffold-Hopping) durch topologische Pharmakophorsuche: ein Beitrag zum virtuellen Screening. *Angewandte Chemie*, **1999**, 111, 3068-3070	3.6	48
359	Development of artificial neural filters for pattern recognition in protein sequences. *Journal of Molecular Evolution*, **1993**, 36, 586-95	3.1	48
358	Characterisation of worldwide Helicobacter pylori strains reveals genetic conservation and essentiality of serine protease HtrA. *Molecular Microbiology*, **2016**, 99, 925-44	4.1	48
357	Revealing the Macromolecular Targets of Fragment-Like Natural Products. *Angewandte Chemie - International Edition*, **2015**, 54, 10516-20	16.4	47
356	Inhibitors of Helicobacter pylori protease HtrA found by 'virtual ligand' screening combat bacterial invasion of epithelia. *PLoS ONE*, **2011**, 6, e17986	3.7	47
355	From machine learning to natural product derivatives that selectively activate transcription factor PPARgamma. *ChemMedChem*, **2010**, 5, 191-4	3.7	47
354	Local structural motifs of protein backbones are classified by self-organizing neural networks. *Protein Engineering, Design and Selection*, **1996**, 9, 833-42	1.9	47
353	modlAMP: Python for antimicrobial peptides. *Bioinformatics*, **2017**, 33, 2753-2755	7.2	46
352	Structure-activity relationship of nonacidic quinazolinone inhibitors of human microsomal prostaglandin synthase 1 (mPGES 1). *Journal of Medicinal Chemistry*, **2012**, 55, 3792-803	8.3	46
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350	Concept of combinatorial de novo design of drug-like molecules by particle swarm optimization. *Chemical Biology and Drug Design*, **2008**, 72, 16-26	2.9	45
349	A hierarchical clustering approach for large compound libraries. *Journal of Chemical Information and Modeling*, **2005**, 45, 807-15	6.1	45
348	A neural network model for the prediction of membrane-spanning amino acid sequences. *Protein Science*, **1994**, 3, 1597-601	6.3	45
347	Generative molecular design in low data regimes. *Nature Machine Intelligence*, **2020**, 2, 171-180	22.5	44
346	Designing Anticancer Peptides by Constructive Machine Learning. *ChemMedChem*, **2018**, 13, 1300-1302	3.7	44

345	Membranolytic anticancer peptides. *MedChemComm*, **2016**, 7, 2232-2245	5	44
344	Standardization of WT1 mRNA quantitation for minimal residual disease monitoring in childhood AML and implications of WT1 gene mutations: a European multicenter study. *Leukemia*, **2009**, 23, 1472-9	10.7	44
343	SmiLib v2.0: A Java-Based Tool for Rapid Combinatorial Library Enumeration. *QSAR and Combinatorial Science*, **2007**, 26, 407-410		44
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341	Crystal structures of mouse class II alcohol dehydrogenase reveal determinants of substrate specificity and catalytic efficiency. *Journal of Molecular Biology*, **2000**, 302, 441-53	6.5	44
340	Tuning artificial intelligence on the de novo design of natural-product-inspired retinoid X receptor modulators. *Communications Chemistry*, **2018**, 1,	6.3	44
339	Extending the structure-activity relationship of anthranilic acid derivatives as farnesoid X receptor modulators: development of a highly potent partial farnesoid X receptor agonist. *Journal of Medicinal Chemistry*, **2014**, 57, 8035-55	8.3	42
338	Scaffold hopping by "fuzzy" pharmacophores and its application to RNA targets. *ChemBioChem*, **2007**, 8, 1932-6	3.8	41
337	Mapping of protein surface cavities and prediction of enzyme class by a self-organizing neural network. *Protein Engineering, Design and Selection*, **2000**, 13, 83-8	1.9	41
336	Form follows function: shape analysis of protein cavities for receptor-based drug design. *Proteomics*, **2009**, 9, 451-9	4.8	40
335	Benzodioxoles: novel cannabinoid-1 receptor inverse agonists for the treatment of obesity. *Journal of Medicinal Chemistry*, **2008**, 51, 2115-27	8.3	39
334	Predicting olfactory receptor neuron responses from odorant structure. *Chemistry Central Journal*, **2007**, 1, 11		39
333	Bidirectional Molecule Generation with Recurrent Neural Networks. *Journal of Chemical Information and Modeling*, **2020**, 60, 1175-1183	6.1	39
332	Adhesion, invasion, and agglutination mediated by two trimeric autotransporters in the human uropathogen Proteus mirabilis. *Infection and Immunity*, **2010**, 78, 4882-94	3.7	38
331	Model structure of APOBEC3C reveals a binding pocket modulating ribonucleic acid interaction required for encapsidation. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 12079-84	11.5	38
330	The state of the art of chemical biology. *ChemBioChem*, **2009**, 10, 16-29	3.8	38
329	Dimerization of human 5-lipoxygenase. *Biological Chemistry*, **2011**, 392, 1097-111	4.5	38
328	Neighborhood-preserving visualization of adaptive structure-activity landscapes: application to drug discovery. *Angewandte Chemie - International Edition*, **2011**, 50, 11633-6	16.4	37

327	Multidimensional de novo design reveals 5-HT2B receptor-selective ligands. *Angewandte Chemie - International Edition*, **2015**, 54, 1551-5	16.4	36
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325	Probing the bioactivity-relevant chemical space of robust reactions and common molecular building blocks. *Journal of Chemical Information and Modeling*, **2012**, 52, 1167-78	6.1	36
324	A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151	58.5	36
323	Multi-objective active machine learning rapidly improves structure-activity models and reveals new protein-protein interaction inhibitors. *Chemical Science*, **2016**, 7, 3919-3927	9.4	35
322	Binding to large enzyme pockets: small-molecule inhibitors of trypanothione reductase. *ChemMedChem*, **2014**, 9, 1880-91	3.7	34
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320	Analysis and prediction of mitochondrial targeting peptides. *Methods in Cell Biology*, **2001**, 65, 175-87	1.8	34
319	Native Electrospray Ionization Mass Spectrometry Reveals Multiple Facets of Aptamer-Ligand Interactions: From Mechanism to Binding Constants. *Journal of the American Chemical Society*, **2018**, 140, 7486-7497	16.4	33
318	A Computational Method for Unveiling the Target Promiscuity of Pharmacologically Active Compounds. *Angewandte Chemie - International Edition*, **2017**, 56, 11520-11524	16.4	33
317	Structural properties of so-called NSAID-phospholipid-complexes. *European Journal of Pharmaceutical Sciences*, **2011**, 44, 103-16	5.1	33
316	Homology model adjustment and ligand screening with a pseudoreceptor of the human histamine H4 receptor. *ChemMedChem*, **2009**, 4, 820-7	3.7	33
315	Identification and validation of a potent type II inhibitor of inactive polo-like kinase 1. *ChemMedChem*, **2009**, 4, 1806-9	3.7	32
314	Coactosin-like protein functions as a stabilizing chaperone for 5-lipoxygenase: role of tryptophan 102. *Biochemical Journal*, **2009**, 425, 265-74	3.8	32
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312	How many potentially secreted proteins are contained in a bacterial genome?. *Gene*, **1999**, 237, 113-21	3.8	32
311	Hybrid Network Model for "Deep Learning" of Chemical Data: Application to Antimicrobial Peptides. *Molecular Informatics*, **2017**, 36, 1600011	3.8	31
310	Immunosuppressive small molecule discovered by structure-based virtual screening for inhibitors of protein-protein interactions. *Angewandte Chemie - International Edition*, **2012**, 51, 258-61	16.4	31

309	Biological impact of freezing Plk1 in its inactive conformation in cancer cells. *Cell Cycle*, **2010**, 9, 761-73	4.7	31
308	Structure-based pharmacophore screening for natural-product-derived PPARgamma agonists. *ChemBioChem*, **2009**, 10, 75-8	3.8	31
307	Virtual screening for selective allosteric mGluR1 antagonists and structure-activity relationship investigations for coumarine derivatives. *ChemMedChem*, **2007**, 2, 1763-73	3.7	31
306	Scaffold-hopping cascade yields potent inhibitors of 5-lipoxygenase. *ChemMedChem*, **2008**, 3, 1535-8	3.7	31
305	New inhibitors of the Tat-TAR RNA interaction found with a "fuzzy" pharmacophore model. *ChemBioChem*, **2005**, 6, 1119-25	3.8	31
304	Feature-extraction from endopeptidase cleavage sites in mitochondrial targeting peptides. *Proteins: Structure, Function and Bioinformatics*, **1998**, 30, 49-60	4.2	31
303	Automated de novo molecular design by hybrid machine intelligence and rule-driven chemical synthesis. *Nature Machine Intelligence*, **2019**, 1, 307-315	22.5	30
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297	Peptide design in machina: development of artificial mitochondrial protein precursor cleavage sites by simulated molecular evolution. *Biophysical Journal*, **1995**, 68, 434-47	2.9	29
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284	A class of 5-benzylidene-2-phenylthiazolinones with high potency as direct 5-lipoxygenase inhibitors. *Journal of Medicinal Chemistry*, **2011**, 54, 1943-7	8.3	27
283	Self-organizing molecular fingerprints: a ligand-based view on drug-like chemical space and off-target prediction. *Future Medicinal Chemistry*, **2009**, 1, 213-8	4.1	27
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281	Peptide design aided by neural networks: biological activity of artificial signal peptidase I cleavage sites. *Biochemistry*, **1998**, 37, 3588-93	3.2	27
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279	De novo design - hop(p)ing against hope. *Drug Discovery Today: Technologies*, **2013**, 10, e453-60	7.1	26
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276	Deorphaning the Macromolecular Targets of the Natural Anticancer Compound Doliculide. *Angewandte Chemie - International Edition*, **2016**, 55, 12408-11	16.4	26
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