Gisbert Schneider

List of Publications by Year in Descending Order

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	De Novo Molecular Design with Chemical Language Models. *Methods in Molecular Biology*, **2022**, 2390, 207-232	1.4	1
451	Perplexity-Based Molecule Ranking and Bias Estimation of Chemical Language Models.. *Journal of Chemical Information and Modeling*, **2022**,	6.1	4
450	Quantum machine-learning for medicinal chemistry.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	4
449	Identification of novel off targets of baricitinib and tofacitinib by machine learning with a focus on thrombosis and viral infection.. *Scientific Reports*, **2022**, 12, 7843	4.9	1
448	TBIO-08. The molecular basis for rational targeting of FGFR-driven growth and invasiveness in pediatric brain tumors. *Neuro-Oncology*, **2022**, 24, i184-i184	1	
447	QMugs, quantum mechanical properties of drug-like molecules. *Scientific Data*, **2022**, 9,	8.2	4
446	Geometric deep learning on molecular representations. *Nature Machine Intelligence*, **2021**, 3, 1023-1032	22.5	15
445	Computer-Aided Design and Synthesis of a New Class of PEX14 Inhibitors: Substituted 2,3,4,5-Tetrahydrobenzo[F][1,4]oxazepines as Potential New Trypanocidal Agents. *Journal of Chemical Information and Modeling*, **2021**, 61, 5256-5268	6.1	
444	Artificial intelligence in drug discovery: recent advances and future perspectives. *Expert Opinion on Drug Discovery*, **2021**, 16, 949-959	6.2	27
443	POS0091 OFF-TARGET PROFILING OF JANUS KINASE (JAK) INHIBITORS IN RHEUMATOID ARTHRITIS: A COMPUTER-BASED APPROACH FOR DRUG SAFETY STUDIES AND REPURPOSING. *Annals of the Rheumatic Diseases*, **2021**, 80, 255.2-255	2.4	
442	Combining generative artificial intelligence and on-chip synthesis for de novo drug design. *Science Advances*, **2021**, 7,	14.3	15
441	Learning from Nature: From a Marine Natural Product to Synthetic Cyclooxygenase-1 Inhibitors by Automated De Novo Design. *Advanced Science*, **2021**, 8, e2100832	13.6	5
440	Beam Search for Automated Design and Scoring of Novel ROR Ligands with Machine Intelligence*. *Angewandte Chemie - International Edition*, **2021**, 60, 19477-19482	16.4	7
439	High-mass MALDI-MS unravels ligand-mediated G protein-coupling selectivity to GPCRs. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	2
438	Engineering of a functional tocopherol transfer protein. *Redox Biology*, **2021**, 38, 101773	11.3	1
437	Molecular Scaffold Hopping via Holistic Molecular Representation. *Methods in Molecular Biology*, **2021**, 2266, 11-35	1.4	3
436	Coloring Molecules with Explainable Artificial Intelligence for Preclinical Relevance Assessment. *Journal of Chemical Information and Modeling*, **2021**, 61, 1083-1094	6.1	10

435	Beam-Search zum automatisierten Entwurf und Scoring neuer ROR-Liganden mithilfe maschineller Intelligenz**. *Angewandte Chemie*, **2021**, 133, 19626-19632	3.6	
434	Bioaffinity Screening with a Rapid and Sample-Efficient Autosampler for Native Electrospray Ionization Mass Spectrometry. *Analytical Chemistry*, **2021**, 93, 13342-13350	7.8	0
433	A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151	58.5	36
432	Introducing the CSP Analyzer: A novel Machine Learning-based application for automated analysis of two-dimensional NMR spectra in NMR fragment-based screening. *Computational and Structural Biotechnology Journal*, **2020**, 18, 603-611	6.8	6
431	Virtual Screening and Design with Machine Intelligence Applied to Pim-1 Kinase Inhibitors. *Molecular Informatics*, **2020**, 39, e2000109	3.8	5
430	Filovirus Antiviral Activity of Cationic Amphiphilic Drugs Is Associated with Lipophilicity and Ability To Induce Phospholipidosis. *Antimicrobial Agents and Chemotherapy*, **2020**, 64,	5.9	8
429	Generative molecular design in low data regimes. *Nature Machine Intelligence*, **2020**, 2, 171-180	22.5	44
428	Shape Similarity by Fractal Dimensionality: An Application in the de novo Design of (-)-Englerin A Mimetics. *ChemMedChem*, **2020**, 15, 566-570	3.7	3
427	Interaction analysis of glycoengineered antibodies with CD16a: a native mass spectrometry approach. *MAbs*, **2020**, 12, 1736975	6.6	3
426	A novel FRET peptide assay reveals efficient Helicobacter pylori HtrA inhibition through zinc and copper binding. *Scientific Reports*, **2020**, 10, 10563	4.9	5
425	AI reflections in 2019. *Nature Machine Intelligence*, **2020**, 2, 2-9	22.5	1
424	Bidirectional Molecule Generation with Recurrent Neural Networks. *Journal of Chemical Information and Modeling*, **2020**, 60, 1175-1183	6.1	39
423	Rethinking drug design in the artificial intelligence era. *Nature Reviews Drug Discovery*, **2020**, 19, 353-364	64.1	179
422	Structural insights into the interaction of botulinum neurotoxin a with its neuronal receptor SV2C. *Toxicon*, **2020**, 175, 36-43	2.8	2
421	Drug discovery with explainable artificial intelligence. *Nature Machine Intelligence*, **2020**, 2, 573-584	22.5	116
420	Morphing of Amphipathic Helices to Explore the Activity and Selectivity of Membranolytic Antimicrobial Peptides. *Biochemistry*, **2020**, 59, 3772-3781	3.2	2
419	Identification of Synthetic Activators of Cancer Cell Migration by Hybrid Deep Learning. *ChemBioChem*, **2020**, 21, 500-507	3.8	0
418	SIG-02. RATIONAL TARGETING OF PRO-INVASIVE FGFR SIGNALING IN MEDULLOBLASTOMA. *Neuro-Oncology*, **2019**, 21, ii113-ii113	1	1

417	Identification of Chemokine Ligands by Biochemical Fragmentation and Simulated Peptide Evolution. *Angewandte Chemie - International Edition*, **2019**, 58, 7138-7142	16.4	1
416	Design of Natural-Product-Inspired Multitarget Ligands by Machine Learning. *ChemMedChem*, **2019**, 14, 1129-1134	3.7	21
415	De novo design of anticancer peptides by ensemble artificial neural networks. *Journal of Molecular Modeling*, **2019**, 25, 112	2	25
414	Automated De Novo Drug Design: Are We Nearly There Yet?. *Angewandte Chemie - International Edition*, **2019**, 58, 10792-10803	16.4	60
413	Automated De Novo Drug Design: Are We Nearly There Yet?. *Angewandte Chemie*, **2019**, 131, 10906-10917	3.6	9
412	In silico design and optimization of selective membranolytic anticancer peptides. *Scientific Reports*, **2019**, 9, 11282	4.9	23
411	Concepts of Artificial Intelligence for Computer-Assisted Drug Discovery. *Chemical Reviews*, **2019**, 119, 10520-10594	68.1	243
410	Automated de novo molecular design by hybrid machine intelligence and rule-driven chemical synthesis. *Nature Machine Intelligence*, **2019**, 1, 307-315	22.5	30
409	Machine learning models for hydrogen bond donor and acceptor strengths using large and diverse training data generated by first-principles interaction free energies. *Journal of Cheminformatics*, **2019**, 11, 59	8.6	8
408	Identifizierung von Chemokinliganden durch biochemische Rezeptorfragmentierung und simulierte Peptidevolution. *Angewandte Chemie*, **2019**, 131, 7212-7216	3.6	
407	[Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Molecular Design With Long Short-Term Memory Networks. *Journal of Computer Aided Chemistry*, **2019**, 20, 35-42	0.2	
406	Molecular Design with Generative Long Short-term Memory. *Chimia*, **2019**, 73, 1006-1011	1.3	12
405	Synthetic Activators of Cell Migration Designed by Constructive Machine Learning. *ChemistryOpen*, **2019**, 8, 1303-1308	2.3	6
404	Discovery of Novel Molecular Frameworks of Farnesoid X Receptor Modulators by Ensemble Machine Learning. *ChemistryOpen*, **2019**, 8, 3	2.3	0
403	Discovery of Novel Molecular Frameworks of Farnesoid X Receptor Modulators by Ensemble Machine Learning. *ChemistryOpen*, **2019**, 8, 7-14	2.3	1
402	In Silico Target Prediction for Small Molecules. *Methods in Molecular Biology*, **2019**, 1888, 273-309	1.4	15
401	Simulated Molecular Evolution for Anticancer Peptide Design. *Angewandte Chemie - International Edition*, **2019**, 58, 1674-1678	16.4	10
400	Simulated Molecular Evolution for Anticancer Peptide Design. *Angewandte Chemie*, **2019**, 131, 1688-1693	3.6	

399	Gaussian Process Regression Models for the Prediction of Hydrogen Bond Acceptor Strengths. *Molecular Informatics*, **2019**, 38, e1800115	3.8	7
398	Designing Anticancer Peptides by Constructive Machine Learning. *ChemMedChem*, **2018**, 13, 1300-1302	3.7	44
397	Future Perspectives of Computational Drug Design **2018**, 405-416		
396	Recurrent Neural Network Model for Constructive Peptide Design. *Journal of Chemical Information and Modeling*, **2018**, 58, 472-479	6.1	90
395	De Novo Design of Bioactive Small Molecules by Artificial Intelligence. *Molecular Informatics*, **2018**, 37, 1700153	3.8	155
394	Total Synthesis of Ripostatin B and Structure-Activity Relationship Studies on Ripostatin Analogs. *Journal of Organic Chemistry*, **2018**, 83, 7150-7172	4.2	17
393	Binding Specificities of Nanobody–Membrane Protein Complexes Obtained from Chemical Cross-Linking and High-Mass MALDI Mass Spectrometry. *Analytical Chemistry*, **2018**, 90, 5306-5313	7.8	8
392	Generative Recurrent Networks for De Novo Drug Design. *Molecular Informatics*, **2018**, 37, 1700111	3.8	184
391	Quantification of hydrolyzed peptides and proteins by amino acid fluorescence. *Journal of Peptide Science*, **2018**, 24, e3113	2.1	9
390	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
389	Lipophilicity prediction of peptides and peptide derivatives by consensus machine learning. *MedChemComm*, **2018**, 9, 1538-1546	5	13
388	Scaffold hopping from natural products to synthetic mimetics by holistic molecular similarity. *Communications Chemistry*, **2018**, 1,	6.3	29
387	Scaffold hopping from synthetic RXR modulators by virtual screening and design. *MedChemComm*, **2018**, 9, 1289-1292	5	13
386	Computer-Assisted Discovery of Retinoid X Receptor Modulating Natural Products and Isofunctional Mimetics. *Journal of Medicinal Chemistry*, **2018**, 61, 5442-5447	8.3	28
385	Automating drug discovery. *Nature Reviews Drug Discovery*, **2018**, 17, 97-113	64.1	275
384	Scaffold-Hopping from Synthetic Drugs by Holistic Molecular Representation. *Scientific Reports*, **2018**, 8, 16469	4.9	17
383	Tuning artificial intelligence on the de novo design of natural-product-inspired retinoid X receptor modulators. *Communications Chemistry*, **2018**, 1,	6.3	44
382	MetScore: Site of Metabolism Prediction Beyond Cytochrome P450 Enzymes. *ChemMedChem*, **2018**, 13, 2281-2289	3.7	17

381	Polypharmacological Drug-target Inference for Chemogenomics. *Molecular Informatics*, **2018**, 37, e1800050	3.8	6
380	Combined Proteomic and In Silico Target Identification Reveal a Role for 5-Lipoxygenase in Developmental Signaling Pathways. *Cell Chemical Biology*, **2018**, 25, 1095-1106.e23	8.2	10
379	Hybrid Network Model for "Deep Learning" of Chemical Data: Application to Antimicrobial Peptides. *Molecular Informatics*, **2017**, 36, 1600011	3.8	31
378	De-orphaning the marine natural product (±)-marinopyrrole A by computational target prediction and biochemical validation. *Chemical Communications*, **2017**, 53, 2272-2274	5.8	27
377	modlAMP: Python for antimicrobial peptides. *Bioinformatics*, **2017**, 33, 2753-2755	7.2	46
376	Exploring the Structural Space of the Galectin-1-Ligand Interaction. *ChemBioChem*, **2017**, 18, 1477-1481	3.8	2
375	Privileged Structures Revisited. *Angewandte Chemie - International Edition*, **2017**, 56, 7971-7974	16.4	61
374	Active learning for computational chemogenomics. *Future Medicinal Chemistry*, **2017**, 9, 381-402	4.1	54
373	Site of Metabolism Prediction Based on ab initio Derived Atom Representations. *ChemMedChem*, **2017**, 12, 606-612	3.7	19
372	Macromolecular target prediction by self-organizing feature maps. *Expert Opinion on Drug Discovery*, **2017**, 12, 271-277	6.2	22
371	Discovery of a Novel Inhibitor of the Hedgehog Signaling Pathway through Cell-based Compound Discovery and Target Prediction. *Angewandte Chemie*, **2017**, 129, 13201-13205	3.6	4
370	Discovery of a Novel Inhibitor of the Hedgehog Signaling Pathway through Cell-based Compound Discovery and Target Prediction. *Angewandte Chemie - International Edition*, **2017**, 56, 13021-13025	16.4	17
369	A Computational Method for Unveiling the Target Promiscuity of Pharmacologically Active Compounds. *Angewandte Chemie - International Edition*, **2017**, 56, 11520-11524	16.4	33
368	Peptide-Membrane Interaction between Targeting and Lysis. *ACS Chemical Biology*, **2017**, 12, 2254-2259	4.9	10
367	Privilegierte Strukturen neu betrachtet. *Angewandte Chemie*, **2017**, 129, 8079-8083	3.6	8
366	A Computational Method for Unveiling the Target Promiscuity of Pharmacologically Active Compounds. *Angewandte Chemie*, **2017**, 129, 11678-11682	3.6	7
365	Rational Design of Membrane-Pore-Forming Peptides. *Small*, **2017**, 13, 1701316	11	17
364	Characterisation of anticancer peptides at the single-cell level. *Lab on A Chip*, **2017**, 17, 2933-2940	7.2	21

363	Matrix-based Molecular Descriptors for Prospective Virtual Compound Screening. *Molecular Informatics*, **2017**, 36, 1600091	3.8	16
362	Scoring of de novo Designed Chemical Entities by Macromolecular Target Prediction. *Molecular Informatics*, **2017**, 36, 1600110	3.8	5
361	New use of an old drug: inhibition of breast cancer stem cells by benztropine mesylate. *Oncotarget*, **2017**, 8, 1007-1022	3.3	19
360	The quantum chemical search for novel materials and the issue of data processing: The InfoMol project. *Journal of Computational Science*, **2016**, 15, 65-73	3.4	3
359	Identification of E-cadherin signature motifs functioning as cleavage sites for Helicobacter pylori HtrA. *Scientific Reports*, **2016**, 6, 23264	4.9	56
358	Membranolytic anticancer peptides. *MedChemComm*, **2016**, 7, 2232-2245	5	44
357	Deorphaning the Macromolecular Targets of the Natural Anticancer Compound Doliculide. *Angewandte Chemie*, **2016**, 128, 12596-12599	3.6	2
356	Coping with Complexity in Ligand-Based De Novo Design. *ACS Symposium Series*, **2016**, 143-158	0.4	1
355	Calcium binding protects E-cadherin from cleavage by Helicobacter pylori HtrA. *Gut Pathogens*, **2016**, 8, 29	5.4	19
354	Von komplexen Naturstoffen zu synthetisch leicht zugänglichen Mimetika mithilfe von computergestütztem De-novo-Design. *Angewandte Chemie*, **2016**, 128, 6901-6904	3.6	11
353	From Complex Natural Products to Simple Synthetic Mimetics by Computational De Novo Design. *Angewandte Chemie - International Edition*, **2016**, 55, 6789-92	16.4	36
352	Robust molecular representations for modelling and design derived from atomic partial charges. *Chemical Communications*, **2016**, 52, 681-4	5.8	23
351	De Novo Design at the Edge of Chaos. *Journal of Medicinal Chemistry*, **2016**, 59, 4077-86	8.3	81
350	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
349	Spotting and designing promiscuous ligands for drug discovery. *Chemical Communications*, **2016**, 52, 1135-8	5.8	27
348	Characterisation of worldwide Helicobacter pylori strains reveals genetic conservation and essentiality of serine protease HtrA. *Molecular Microbiology*, **2016**, 99, 925-44	4.1	48
347	Counting on natural products for drug design. *Nature Chemistry*, **2016**, 8, 531-41	17.6	592
346	Sparse Neural Network Models of Antimicrobial Peptide-Activity Relationships. *Molecular Informatics*, **2016**, 35, 606-614	3.8	12

345	Deorphaning the Macromolecular Targets of the Natural Anticancer Compound Doliculide. *Angewandte Chemie - International Edition*, **2016**, 55, 12408-11	16.4	26
344	Designing Multi-target Compound Libraries with Gaussian Process Models. *Molecular Informatics*, **2016**, 35, 192-8	3.8	5
343	Deep Learning in Drug Discovery. *Molecular Informatics*, **2016**, 35, 3-14	3.8	360
342	Multidimensional de novo design reveals 5-HT2B receptor-selective ligands. *Angewandte Chemie - International Edition*, **2015**, 54, 1551-5	16.4	36
341	In Silico Screening **2015**, 141-160		0
340	Chemography of natural product space. *Planta Medica*, **2015**, 81, 429-35	3.1	23
339	Fragmentation of GW4064 led to a highly potent partial farnesoid X receptor agonist with improved drug-like properties. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 3490-8	3.4	15
338	Predicting drug metabolism: experiment and/or computation?. *Nature Reviews Drug Discovery*, **2015**, 14, 387-404	64.1	255
337	Repurposing de novo designed entities reveals phosphodiesterase 3B and cathepsin L modulators. *Chemical Communications*, **2015**, 51, 7478-81	5.8	10
336	Multidimensional Design of Anticancer Peptides. *Angewandte Chemie - International Edition*, **2015**, 54, 10370-4	16.4	28
335	Boswellic acids target the human immune system-modulating antimicrobial peptide LL-37. *Pharmacological Research*, **2015**, 102, 53-60	10.2	12
334	Multidimensional De Novo Design Reveals 5-HT2B Receptor-Selective Ligands. *Angewandte Chemie*, **2015**, 127, 1571-1575	3.6	8
333	Active-learning strategies in computer-assisted drug discovery. *Drug Discovery Today*, **2015**, 20, 458-65	8.8	108
332	Attractors in Sequence Space: Peptide Morphing by Directed Simulated Evolution. *Molecular Informatics*, **2015**, 34, 709-714	3.8	5
331	Computer-assisted quantification of motile and invasive capabilities of cancer cells. *Scientific Reports*, **2015**, 5, 15338	4.9	13
330	Revealing the Macromolecular Targets of Fragment-Like Natural Products. *Angewandte Chemie*, **2015**, 127, 10662-10666	3.6	19
329	De-novo-Fragmententwurf f□ die Wirkstoffforschung und chemische Biologie. *Angewandte Chemie* , **2015**, 127, 15294-15298	3.6	5
328	Aryl Bis-Sulfonamide Inhibitors of IspF from Arabidopsis thaliana and Plasmodium falciparum. *ChemMedChem*, **2015**, 10, 2090-8	3.7	15

327	De Novo Fragment Design for Drug Discovery and Chemical Biology. *Angewandte Chemie - International Edition*, **2015**, 54, 15079-83	16.4	25
326	Fragment-Based De Novo Design Reveals a Small-Molecule Inhibitor of Helicobacter Pylori HtrA. *Angewandte Chemie - International Edition*, **2015**, 54, 10244-8	16.4	28
325	Revealing the Macromolecular Targets of Fragment-Like Natural Products. *Angewandte Chemie - International Edition*, **2015**, 54, 10516-20	16.4	47
324	Fragment-Based De Novo Design Reveals a Small-Molecule Inhibitor of Helicobacter Pylori HtrA. *Angewandte Chemie*, **2015**, 127, 10382-10386	3.6	6
323	Mehrdimensionaler Entwurf von Antikrebspeptiden. *Angewandte Chemie*, **2015**, 127, 10512-10516	3.6	2
322	Structural insights on cholesterol endosynthesis: Binding of squalene and 2,3-oxidosqualene to supernatant protein factor. *Journal of Structural Biology*, **2015**, 190, 261-70	3.4	19
321	Unraveling the Activation Mechanism of Taspase1 which Controls the Oncogenic AF4-MLL Fusion Protein. *EBioMedicine*, **2015**, 2, 386-95	8.8	7
320	Dual-display of small molecules enables the discovery of ligand pairs and facilitates affinity maturation. *Nature Chemistry*, **2015**, 7, 241-9	17.6	143
319	In Silico Adoption of an Orphan Nuclear Receptor NR4A1. *PLoS ONE*, **2015**, 10, e0135246	3.7	5
318	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
317	Binding to large enzyme pockets: small-molecule inhibitors of trypanothione reductase. *ChemMedChem*, **2014**, 9, 1880-91	3.7	34
316	Future De Novo Drug Design. *Molecular Informatics*, **2014**, 33, 397-402	3.8	22
315	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
314	Accessing new chemical entities through microfluidic systems. *Angewandte Chemie - International Edition*, **2014**, 53, 5750-8	16.4	76
313	Identifizierung von Pyrrolopyrazinen als polypotente Liganden mit Antimalariawirkung. *Angewandte Chemie*, **2014**, 126, 7199-7204	3.6	2
312	Fractal Dimensions of Macromolecular Structures. *Molecular Informatics*, **2014**, 33, 588-596	3.8	9
311	Revealing the macromolecular targets of complex natural products. *Nature Chemistry*, **2014**, 6, 1072-8	17.6	100
310	Inhibiting HtrA protease by addressing a computationally predicted allosteric ligand binding site. *Chemical Science*, **2014**, 5, 3583-3590	9.4	22

309	Multi-objective molecular de novo design by adaptive fragment prioritization. *Angewandte Chemie - International Edition*, **2014**, 53, 4244-8	16.4	63
308	Vanillin-derived antiproliferative compounds influence Plk1 activity. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 5063-9	2.9	11
307	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
306	Peptide lineup against Gram-negative bacterial infection First-in-class peptide inhibitor of H. pylori HtrA. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
305	Target prediction by cascaded self-organizing maps for ligand de-orphaning and side-effect investigation. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
304	Identification of pirinixic acid derivatives bearing a 2-aminothiazole moiety combines dual PPAR/ activation and dual 5-LO/mPGES-1 inhibition. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 3757-63	2.9	10
303	Targeting dynamic pockets of HIV-1 protease by structure-based computational screening for allosteric inhibitors. *Journal of Chemical Information and Modeling*, **2014**, 54, 987-91	6.1	23
302	Anthranilic acid derivatives as novel ligands for farnesoid X receptor (FXR). *Bioorganic and Medicinal Chemistry*, **2014**, 22, 2447-60	3.4	24
301	Deorphaning pyrrolopyrazines as potent multi-target antimalarial agents. *Angewandte Chemie - International Edition*, **2014**, 53, 7079-84	16.4	27
300	Breaking the data barrier in computational medicinal chemistry. *Future Medicinal Chemistry*, **2014**, 6, 245-6	4.1	0
299	Combinatorial chemistry by ant colony optimization. *Future Medicinal Chemistry*, **2014**, 6, 267-80	4.1	15
298	Kombination von On-Chip-Synthese einer fokussierten kombinatorischen Bibliothek mit computergestützter Vorhersage der biologischen Aktivität enthüllt Imidazopyridine als GPCR-Liganden. *Angewandte Chemie*, **2014**, 126, 593-596	3.6	15
297	Mehrdimensionales De-novo-Moleküldesign durch adaptive Fragmentauswahl. *Angewandte Chemie*, **2014**, 126, 4330-4334	3.6	8
296	Neue chemische Strukturen durch Mikrofluidiksysteme. *Angewandte Chemie*, **2014**, 126, 5858-5866	3.6	12
295	Flashback Forward: Reaction-Driven De Novo Design of Bioactive Compounds. *Synlett*, **2014**, 25, 170-178	2.2	11
294	Machine learning estimates of natural product conformational energies. *PLoS Computational Biology*, **2014**, 10, e1003400	5	26
293	Coping with polypharmacology by computational medicinal chemistry. *Chimia*, **2014**, 68, 648-53	1.3	6
292	Piloting the membranolytic activities of peptides with a self-organizing map. *ChemBioChem*, **2014**, 15, 2225-31	3.8	8

291	Steering target selectivity and potency by fragment-based de novo drug design. *Angewandte Chemie - International Edition*, **2013**, 52, 10006-9	16.4	22
290	De Novo Design: From Models to Molecules **2013**, 1-55		9
289	Pharmacophore-Based De Novo Design **2013**, 201-214		
288	Ligand-Based Molecular Design Using Pseudoreceptors **2013**, 227-244		0
287	Bioisosteres in De Novo Design **2013**, 417-435		1
286	Fragment-Based Design of Focused Compound Libraries **2013**, 349-371		2
285	Construction of Drug-Like Compounds by Markov Chains **2013**, 311-323		
284	Structure-Based De Novo Drug Design **2013**, 97-124		4
283	Hit and Lead Identification from Fragments **2013**, 143-200		1
282	3D-QSAR Approaches to De Novo Drug Design **2013**, 215-225		
281	Reaction-Driven De Novo Design: a Keystone for Automated Design of Target Family-Oriented Libraries **2013**, 245-266		2
280	Peptide Design by Nature-Inspired Algorithms **2013**, 437-465		2
279	Free Energy Methods in Ligand Design **2013**, 373-415		1
278	Coping with Combinatorial Space in Molecular Design **2013**, 325-347		3
277	De Novo Design of Ligands against Multitarget Profiles **2013**, 287-309		
276	Multiobjective De Novo Design of Synthetically Accessible Compounds **2013**, 267-285		5
275	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
274	Exhaustive proteome mining for functional MHC-I ligands. *ACS Chemical Biology*, **2013**, 8, 1876-81	4.9	10

273	Common non-epigenetic drugs as epigenetic modulators. *Trends in Molecular Medicine*, **2013**, 19, 742-53	11.5	54
272	Drugs by numbers: reaction-driven de novo design of potent and selective anticancer leads. *Angewandte Chemie - International Edition*, **2013**, 52, 4676-81	16.4	20
271	CATS for Scaffold Hopping in Medicinal Chemistry. *Methods and Principles in Medicinal Chemistry*, **2013**, 119-130	0.4	
270	De novo design - hop(p)ing against hope. *Drug Discovery Today: Technologies*, **2013**, 10, e453-60	7.1	26
269	Computational Resources for MHC Ligand Identification. *Molecular Informatics*, **2013**, 32, 326-36	3.8	6
268	De novo design and optimization of Aurora A kinase inhibitors. *Chemical Science*, **2013**, 4, 1229	9.4	22
267	Quinolin-4(1H)-imines are potent antiplasmodial drugs targeting the liver stage of malaria. *Journal of Medicinal Chemistry*, **2013**, 56, 4811-5	8.3	18
266	Synthesis and pharmacological characterization of benzenesulfonamides as dual species inhibitors of human and murine mPGES-1. *Bioorganic and Medicinal Chemistry*, **2013**, 21, 7874-83	3.4	14
265	Adaptive peptide design. *Chimia*, **2013**, 67, 859-63	1.3	3
264	Scrutinizing MHC-I binding peptides and their limits of variation. *PLoS Computational Biology*, **2013**, 9, e1003088	5	28
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