

Ola Engkvist

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

139
papers

4,660
citations

37
h-index

65
g-index

181
ext. papers

6,121
ext. citations

7.1
avg, IF

6.11
L-index

#	Paper	IF	Citations
139	The rise of deep learning in drug discovery. <i>Drug Discovery Today</i> , 2018 , 23, 1241-1250	8.8	650
138	Molecular de-novo design through deep reinforcement learning. <i>Journal of Cheminformatics</i> , 2017 , 9, 48	8.6	352
137	Application of Generative Autoencoder in De Novo Molecular Design. <i>Molecular Informatics</i> , 2018 , 37, 1700123	3.8	174
136	Accurate Intermolecular Potentials Obtained from Molecular Wave Functions: Bridging the Gap between Quantum Chemistry and Molecular Simulations. <i>Chemical Reviews</i> , 2000 , 100, 4087-108	68.1	160
135	Structure and vibrational dynamics of the benzene dimer. <i>Journal of Chemical Physics</i> , 1999 , 111, 572-583	3.9	140
134	Characterization of a conserved structural determinant controlling protein kinase sensitivity to selective inhibitors. <i>Chemistry and Biology</i> , 2004 , 11, 691-701		114
133	On the Integration of Drug Design Methods for Drug Repurposing. <i>Frontiers in Pharmacology</i> , 2017 , 8, 298	5.6	109
132	Uracil Dimer: Potential Energy and Free Energy Surfaces. Ab Initio beyond Hartree-Fock and Empirical Potential Studies. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 6921-6926	2.8	100
131	Beyond size, ionization state, and lipophilicity: influence of molecular topology on absorption, distribution, metabolism, excretion, and toxicity for druglike compounds. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 3667-77	8.3	96
130	Molecular modeling of the second extracellular loop of G-protein coupled receptors and its implication on structure-based virtual screening. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 71, 599-620	4.2	89
129	Computational prediction of chemical reactions: current status and outlook. <i>Drug Discovery Today</i> , 2018 , 23, 1203-1218	8.8	83
128	HTS explorer. <i>Journal of Cheminformatics</i> , 2014 , 6,	8.6	78
127	Hit series selection in noisy HTS data: clustering techniques, statistical tests and data visualisations. <i>Journal of Cheminformatics</i> , 2014 , 6,	8.6	78
126	Benzene trimer and benzene tetramer: Structures and properties determined by the nonempirical model (NEMO) potential calibrated from the CCSD(T) benzene dimer energies. <i>Journal of Chemical Physics</i> , 1999 , 110, 5758-5762	3.9	78
125	A de novo molecular generation method using latent vector based generative adversarial network. <i>Journal of Cheminformatics</i> , 2019 , 11, 74	8.6	78
124	Target prediction utilising negative bioactivity data covering large chemical space. <i>Journal of Cheminformatics</i> , 2015 , 7, 51	8.6	76
123	Randomized SMILES strings improve the quality of molecular generative models. <i>Journal of Cheminformatics</i> , 2019 , 11, 71	8.6	74

122	Minimum information about a bioactive entity (MIABE). <i>Nature Reviews Drug Discovery</i> , 2011 , 10, 661-9	64.1	69
121	Exploring the GDB-13 chemical space using deep generative models. <i>Journal of Cheminformatics</i> , 2019 , 11, 20	8.6	67
120	Multifingerprint based similarity searches for targeted class compound selection. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 1201-13	6.1	59
119	Molecular representations in AI-driven drug discovery: a review and practical guide. <i>Journal of Cheminformatics</i> , 2020 , 12, 56	8.6	59
118	BIGCHEM: Challenges and Opportunities for Big Data Analysis in Chemistry. <i>Molecular Informatics</i> , 2016 , 35, 615-621	3.8	59
117	ExCAPE-DB: an integrated large scale dataset facilitating Big Data analysis in chemogenomics. <i>Journal of Cheminformatics</i> , 2017 , 9, 17	8.6	56
116	Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis. <i>Journal of Medicinal Chemistry</i> , 2020 , 63, 8667-8682	8.3	53
115	Building attention and edge message passing neural networks for bioactivity and physical-chemical property prediction. <i>Journal of Cheminformatics</i> , 2020 , 12, 1	8.6	51
114	Investigation of the relationship between topology and selectivity for druglike molecules. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 7709-14	8.3	50
113	Comparison of molecular fingerprint methods on the basis of biological profile data. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 338-47	6.1	48
112	In silico prediction of unbound brain-to-plasma concentration ratio using machine learning algorithms. <i>Journal of Molecular Graphics and Modelling</i> , 2011 , 29, 985-95	2.8	48
111	Intermolecular Potential for the 1,2-Dimethoxyethane-Water Complex. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 6950-6957		48
110	Direct steering of de novo molecular generation with descriptor conditional recurrent neural networks. <i>Nature Machine Intelligence</i> , 2020 , 2, 254-265	22.5	47
109	SMILES-based deep generative scaffold decorator for de-novo drug design. <i>Journal of Cheminformatics</i> , 2020 , 12, 38	8.6	45
108	On the origin of the gauche effect. A quantum chemical study of 1,2-difluoroethane. <i>Chemical Physics Letters</i> , 1997 , 265, 19-23	2.5	45
107	Prediction of CNS activity of compound libraries using substructure analysis. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 155-60		43
106	High-throughput, in silico prediction of aqueous solubility based on one- and two-dimensional descriptors. <i>Journal of Chemical Information and Computer Sciences</i> , 2002 , 42, 1247-9		43
105	REINVENT 2.0: An AI Tool for De Novo Drug Design. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 5918-5922	6.1	42

104	Applying Mondrian Cross-Conformal Prediction To Estimate Prediction Confidence on Large Imbalanced Bioactivity Data Sets. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 1591-1598	6.1	38
103	Adsorption of water on the NaCl(001) surface. III. Monte Carlo simulations at ambient temperatures. <i>Journal of Chemical Physics</i> , 2000 , 112, 6827-6833	3.9	38
102	Ligand-based target prediction with signature fingerprints. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 2647-53	6.1	35
101	Datasets and their influence on the development of computer assisted synthesis planning tools in the pharmaceutical domain. <i>Chemical Science</i> , 2020 , 11, 154-168	9.4	35
100	A method to calculate the probability distribution for systems with large energy barriers. <i>Chemical Physics</i> , 1996 , 213, 63-76	2.3	34
99	AiZynthFinder: a fast, robust and flexible open-source software for retrosynthetic planning. <i>Journal of Cheminformatics</i> , 2020 , 12, 70	8.6	34
98	Heart regeneration: opportunities and challenges for drug discovery with novel chemical and therapeutic methods or agents. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 4056-75	16.4	32
97	A fast virtual screening filter for cytochrome P450 3A4 inhibition liability of compound libraries. <i>QSAR and Combinatorial Science</i> , 2002 , 21, 249-256		32
96	Adsorption of water on NaCl(001). I. Intermolecular potentials and low temperature structures. <i>Journal of Chemical Physics</i> , 1999 , 110, 12089-12096	3.9	32
95	Physicochemical property profiles of marketed drugs, clinical candidates and bioactive compounds. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009 , 19, 6943-7	2.9	31
94	A comparative analysis of the molecular topologies for drugs, clinical candidates, natural products, human metabolites and general bioactive compounds. <i>MedChemComm</i> , 2012 , 3, 312-321	5	30
93	Adsorption of water on the MgO(001) surface. <i>Surface Science</i> , 1999 , 437, 239-248	1.8	29
92	Annotating Human P-Glycoprotein Bioassay Data. <i>Molecular Informatics</i> , 2012 , 31, 599-609	3.8	27
91	Developments in computational studies of crystallization and morphology applied to urea. <i>Physical Chemistry Chemical Physics</i> , 2000 , 2, 3017-3027	3.6	27
90	Hoogsteen and Stacked Structures of the 9-Methyladenine-Methylthymine Pair Are Populated Equally at Experimental Conditions: Ab Initio and Molecular Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 1197-1202	2.8	27
89	Small molecule inducers of ABCA1 and apoE that act through indirect activation of the LXR pathway. <i>Journal of Lipid Research</i> , 2018 , 59, 830-842	6.3	26
88	Applications of Deep-Learning in Exploiting Large-Scale and Heterogeneous Compound Data in Industrial Pharmaceutical Research. <i>Frontiers in Pharmacology</i> , 2019 , 10, 1303	5.6	26
87	Exploring in silico prediction of the unbound brain-to-plasma drug concentration ratio: model validation, renewal, and interpretation. <i>Journal of Pharmaceutical Sciences</i> , 2015 , 104, 1197-206	3.9	24

86	Understanding Cytotoxicity and Cytostaticity in a High-Throughput Screening Collection. <i>ACS Chemical Biology</i> , 2016 , 11, 3007-3023	4.9	22
85	Monte Carlo Simulation Study of Short Poly(ethylene oxide) Chains at Different Concentrations. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 1631-1633	3.4	22
84	Cheminformatics in Drug Discovery, an Industrial Perspective. <i>Molecular Informatics</i> , 2018 , 37, e18000413.8	13.8	22
83	Has Drug Design Augmented by Artificial Intelligence Become a Reality?. <i>Trends in Pharmacological Sciences</i> , 2019 , 40, 806-809	13.2	20
82	Memory-assisted reinforcement learning for diverse molecular de novo design. <i>Journal of Cheminformatics</i> , 2020 , 12, 68	8.6	20
81	Molecular topology analysis of the differences between drugs, clinical candidate compounds, and bioactive molecules. <i>Journal of Chemical Information and Modeling</i> , 2010 , 50, 2141-50	6.1	19
80	Orthologue chemical space and its influence on target prediction. <i>Bioinformatics</i> , 2018 , 34, 72-79	7.2	18
79	Graph networks for molecular design. <i>Machine Learning: Science and Technology</i> , 2021 , 2, 025023	5.1	18
78	Combining structural and bioactivity-based fingerprints improves prediction performance and scaffoldhopping capability. <i>Journal of Cheminformatics</i> , 2019 , 11, 54	8.6	17
77	Phenotypic Screen for Cardiac Regeneration Identifies Molecules with Differential Activity in Human Epicardium-Derived Cells versus Cardiac Fibroblasts. <i>ACS Chemical Biology</i> , 2017 , 12, 132-141	4.9	16
76	Does Big Data Exist in medicinal chemistry, and if so, how can it be harnessed?. <i>Future Medicinal Chemistry</i> , 2016 , 8, 1801-1806	4.1	15
75	Identification of Compounds That Interfere with High-Throughput Screening Assay Technologies. <i>ChemMedChem</i> , 2019 , 14, 1795-1802	3.7	15
74	Open PHACTS computational protocols for target validation of cellular phenotypic screens: knowing the knowns. <i>MedChemComm</i> , 2016 , 7, 1237-1244	5	15
73	Retrosynthetic accessibility score (RAScore) - rapid machine learned synthesizability classification from AI driven retrosynthetic planning. <i>Chemical Science</i> , 2021 , 12, 3339-3349	9.4	15
72	On the Relationship between Molecular Hit Rates in High-Throughput Screening and Molecular Descriptors. <i>Journal of Biomolecular Screening</i> , 2014 , 19, 727-37		14
71	Methylated uracil dimers: potential energy and free energy surfaces. <i>Physical Chemistry Chemical Physics</i> , 2000 , 2, 2419-2424	3.6	14
70	AI-assisted synthesis prediction. <i>Drug Discovery Today: Technologies</i> , 2019 , 32-33, 65-72	7.1	14
69	Application of Bioactivity Profile-Based Fingerprints for Building Machine Learning Models. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 962-972	6.1	14

68	The convergence of artificial intelligence and chemistry for improved drug discovery. <i>Future Medicinal Chemistry</i> , 2018 , 10, 2573-2576	4.1	14
67	Using the BioAssay Ontology for analyzing high-throughput screening data. <i>Journal of Biomolecular Screening</i> , 2015 , 20, 402-15		13
66	Investigating Pharmacological Similarity by Charting Chemical Space. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 2375-90	6.1	13
65	Systematic exploration of dual-acting modulators from a combined medicinal chemistry and biology perspective. <i>Journal of Medicinal Chemistry</i> , 2013 , 56, 1197-210	8.3	13
64	ProSAR: a new methodology for combinatorial library design. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 603-14	6.1	12
63	A Monte Carlo simulation study of the temperature dependence for the conformation distribution of 1,2-dimethoxyethane in water. <i>Journal of Chemical Physics</i> , 1997 , 106, 2411-2417	3.9	12
62	Theoretical study of intermolecular potential energy surface for HCl dimer: Example of nonspherical atom-atom exchange repulsion interaction. <i>Journal of Computational Chemistry</i> , 1998 , 19, 1816-1825	3.5	12
61	Industry-scale application and evaluation of deep learning for drug target prediction. <i>Journal of Cheminformatics</i> , 2020 , 12, 26	8.6	12
60	Artificial intelligence and automation in computer aided synthesis planning. <i>Reaction Chemistry and Engineering</i> , 2021 , 6, 27-51	4.9	11
59	Molecular optimization by capturing chemist's intuition using deep neural networks. <i>Journal of Cheminformatics</i> , 2021 , 13, 26	8.6	11
58	Uncertainty quantification in drug design. <i>Drug Discovery Today</i> , 2021 , 26, 474-489	8.8	10
57	"Ring Breaker": Neural Network Driven Synthesis Prediction of the Ring System Chemical Space. <i>Journal of Medicinal Chemistry</i> , 2020 , 63, 8791-8808	8.3	9
56	The Role of Historical Bioactivity Data in the Deconvolution of Phenotypic Screens. <i>Journal of Biomolecular Screening</i> , 2014 , 19, 696-706		9
55	Comparative Study of Deep Generative Models on Chemical Space Coverage. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 2572-2581	6.1	9
54	Utility of Resazurin, Horseradish Peroxidase, and NMR Assays to Identify Redox-Related False-Positive Behavior in High-Throughput Screens. <i>Assay and Drug Development Technologies</i> , 2018 , 16, 171-191	2.1	8
53	Theory of Poly(ethylene glycol) in Solution. <i>ACS Symposium Series</i> , 1997 , 16-30	0.4	8
52	Comparison of Chemical Structure and Cell Morphology Information for Multitask Bioactivity Predictions. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 1444-1456	6.1	8
51	A comparison between the NEMO intermolecular water potential and ab initio quantum chemical calculations for the water trimer tetramer. <i>Molecular Physics</i> , 1997 , 90, 277-287	1.7	7

50	High-content phenotypic assay for proliferation of human iPSC-derived cardiomyocytes identifies L-type calcium channels as targets. <i>Journal of Molecular and Cellular Cardiology</i> , 2019 , 127, 204-214	5.8	7
49	Multisolvant Models for Solvation Free Energy Predictions Using 3D-RISM Hydration Thermodynamic Descriptors. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 2977-2988	6.1	6
48	Innovation in Small-Molecule-Druggable Chemical Space: Where are the Initial Modulators of New Targets Published?. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 2741-2753	6.1	5
47	Accurate Hit Estimation for Iterative Screening Using Venn-ABERS Predictors. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 1230-1237	6.1	5
46	Compound Properties and their Influence on Drug Quality 2015 , 379-393		5
45	Practical notes on building molecular graph generative models. <i>Applied AI Letters</i> , 2020 , 1,	1.2	5
44	Axl receptor tyrosine kinase is a regulator of apolipoprotein E. <i>Molecular Brain</i> , 2020 , 13, 66	4.5	5
43	Transporter assays and assay ontologies: useful tools for drug discovery. <i>Drug Discovery Today: Technologies</i> , 2014 , 12, e47-54	7.1	4
42	Comparison of Scaling Methods to Obtain Calibrated Probabilities of Activity for Protein-Ligand Predictions. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 4546-4559	6.1	4
41	Collaborative virtual screening to elaborate an imidazo[1,2-]pyridine hit series for visceral leishmaniasis. <i>RSC Medicinal Chemistry</i> , 2021 , 12, 384-393	3.5	4
40	Extending Protein Target Prediction Models to Include Functional Effects. <i>Frontiers in Pharmacology</i> , 2018 , 9, 613	5.6	3
39	Mining Molecular Pharmacological Effects from Biomedical Text: a Case Study for Eliciting Anti-Obesity/Diabetes Effects of Chemical Compounds. <i>Molecular Informatics</i> , 2014 , 33, 332-42	3.8	3
38	On the Relation between Retention Indexes and the Interaction between the Solute and the Column in Gas/Liquid Chromatography. <i>Journal of Chemical Information and Computer Sciences</i> , 1996 , 36, 1153-1161		3
37	Novel endosomolytic compounds enable highly potent delivery of antisense oligonucleotides.. <i>Communications Biology</i> , 2022 , 5, 185	6.7	3
36	Evaluation guidelines for machine learning tools in the chemical sciences. <i>Nature Reviews Chemistry</i> ,	34.6	3
35	Herzregeneration: Chancen und Aufgaben für die Wirkstoff-Forschung mit neuartigen chemischen und therapeutischen Methoden oder Agentien. <i>Angewandte Chemie</i> , 2014 , 126, 4138-4159	3.6	2
34	Merged Multiple Ligands. <i>Methods and Principles in Medicinal Chemistry</i> , 2017 , 247-274	0.4	2
33	Combinatorial library design from reagent pharmacophore fingerprints. <i>Methods in Molecular Biology</i> , 2011 , 685, 135-52	1.4	2

32	Has Artificial Intelligence Impacted Drug Discovery?. <i>Methods in Molecular Biology</i> , 2022 , 2390, 153-176	1.4	2
31	SMILES-Based Deep Generative Scaffold Decorator for De-Novo Drug Design		2
30	A De Novo Molecular Generation Method Using Latent Vector Based Generative Adversarial Network		2
29	A De Novo Molecular Generation Method Using Latent Vector Based Generative Adversarial Network		2
28	Direct Steering of de novo Molecular Generation using Descriptor Conditional Recurrent Neural Networks (cRNNs)		2
27	Direct Steering of de novo Molecular Generation using Descriptor Conditional Recurrent Neural Networks (cRNNs)		2
26	Building Attention and Edge Convolution Neural Networks for Bioactivity and Physical-Chemical Property Prediction		2
25	Exploring the GDB-13 Chemical Space Using Deep Generative Models		2
24	Randomized SMILES Strings Improve the Quality of Molecular Generative Models		2
23	AiZynthFinder: A Fast Robust and Flexible Open-Source Software for Retrosynthetic Planning		2
22	Pluripotent Stem Cell-Derived Hepatocytes Phenotypic Screening Reveals Small Molecules Targeting the CDK2/4-C/EBP β /DGAT2 Pathway Preventing ER-Stress Induced Lipid Accumulation. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	2
21	Bioinformatic Approaches in the Understanding of Mechanism of Action (MoA). <i>Methods and Principles in Medicinal Chemistry</i> , 2019 , 323-363	0.4	2
20	Public-Private Partnerships: Compound and Data Sharing in Drug Discovery and Development. <i>SLAS Discovery</i> , 2021 , 26, 604-619	3.4	2
19	Transformer-based molecular optimization beyond matched molecular pairs.. <i>Journal of Cheminformatics</i> , 2022 , 14, 18	8.6	2
18	In Silico Tools for Predicting Brain Exposure of Drugs 2015 , 167-187		1
17	Designing a Combinatorial Library by Using Reagent Pharmacophore Fingerprint. <i>QSAR and Combinatorial Science</i> , 2009 , 28, 840-844		1
16	DockStream: a docking wrapper to enhance de novo molecular design. <i>Journal of Cheminformatics</i> , 2021 , 13, 89	8.6	1
15	Attention and Edge Memory Convolution for Bioactivity Prediction. <i>Lecture Notes in Computer Science</i> , 2019 , 752-757	0.9	1

14	Neural Network Guided Tree-Search Policies for Synthesis Planning. <i>Lecture Notes in Computer Science</i> , 2019 , 721-724	0.9	1
13	Improving Deep Generative Models with Randomized SMILES. <i>Lecture Notes in Computer Science</i> , 2019 , 747-751	0.9	1
12	De novo design with deep generative models based on 3D similarity scoring. <i>Bioorganic and Medicinal Chemistry</i> , 2021 , 44, 116308	3.4	1
11	Investigation of the influence of molecular topology on ligand binding. <i>Journal of Molecular Graphics and Modelling</i> , 2013 , 40, 22-9	2.8	0
10	Fast prediction of distances between synthetic routes with deep learning. <i>Machine Learning: Science and Technology</i> , 2022 , 3, 015018	5.1	0
9	Artificial applicability labels for improving policies in retrosynthesis prediction. <i>Machine Learning: Science and Technology</i> , 2021 , 2, 017001	5.1	0
8	Clustering of Synthetic Routes Using Tree Edit Distance. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 3899-3907	6.1	0
7	Probabilistic Random Forest improves bioactivity predictions close to the classification threshold by taking into account experimental uncertainty. <i>Journal of Cheminformatics</i> , 2021 , 13, 62	8.6	0
6	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. <i>Journal of Cheminformatics</i> , 2016 , 8, 18	8.6	
5	Shouldn't enantiomeric purity be included in the minimum information about a bioactive entity? Response from the MIABE group. <i>Nature Reviews Drug Discovery</i> , 2012 , 11, 730-730	64.1	
4	An Investigation of the Relationship Between Molecular Topology and CYP3A4 Inhibition for Drug-like Compounds. <i>Molecular Informatics</i> , 2012 , 31, 719-23	3.8	
3	Chemistry-Driven Target Identification. <i>Methods and Principles in Medicinal Chemistry</i> , 2016 , 63-92	0.4	
2	An Introduction to Systems Medicine Applied to Drug Discovery 2021 , 128		
1	Parallel Capsule Networks for Classification of White Blood Cells. <i>Lecture Notes in Computer Science</i> , 2021 , 743-752	0.9	