Ola Engkvist

List of Publications by Year in Descending Order

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	Fast prediction of distances between synthetic routes with deep learning. *Machine Learning: Science and Technology*, **2022**, 3, 015018	5.1	0
138	Has Artificial Intelligence Impacted Drug Discovery?. *Methods in Molecular Biology*, **2022**, 2390, 153-176	1.4	2
137	Transformer-based molecular optimization beyond matched molecular pairs.. *Journal of Cheminformatics*, **2022**, 14, 18	8.6	2
136	Novel endosomolytic compounds enable highly potent delivery of antisense oligonucleotides.. *Communications Biology*, **2022**, 5, 185	6.7	3
135	DockStream: a docking wrapper to enhance de novo molecular design. *Journal of Cheminformatics*, **2021**, 13, 89	8.6	1
134	Artificial applicability labels for improving policies in retrosynthesis prediction. *Machine Learning: Science and Technology*, **2021**, 2, 017001	5.1	0
133	Comparison of Chemical Structure and Cell Morphology Information for Multitask Bioactivity Predictions. *Journal of Chemical Information and Modeling*, **2021**, 61, 1444-1456	6.1	8
132	Graph networks for molecular design. *Machine Learning: Science and Technology*, **2021**, 2, 025023	5.1	18
131	Comparative Study of Deep Generative Models on Chemical Space Coverage. *Journal of Chemical Information and Modeling*, **2021**, 61, 2572-2581	6.1	9
130	Artificial intelligence and automation in computer aided synthesis planning. *Reaction Chemistry and Engineering*, **2021**, 6, 27-51	4.9	11
129	Uncertainty quantification in drug design. *Drug Discovery Today*, **2021**, 26, 474-489	8.8	10
128	An Introduction to Systems Medicine Applied to Drug Discovery **2021**, 128		
127	Parallel Capsule Networks for Classification of White Blood Cells. *Lecture Notes in Computer Science* , **2021**, 743-752	0.9	
126	Public-Private Partnerships: Compound and Data Sharing in Drug Discovery and Development. *SLAS Discovery*, **2021**, 26, 604-619	3.4	2
125	Molecular optimization by capturing chemist's intuition using deep neural networks. *Journal of Cheminformatics*, **2021**, 13, 26	8.6	11
124	De novo design with deep generative models based on 3D similarity scoring. *Bioorganic and Medicinal Chemistry*, **2021**, 44, 116308	3.4	1
123	Clustering of Synthetic Routes Using Tree Edit Distance. *Journal of Chemical Information and Modeling*, **2021**, 61, 3899-3907	6.1	0

122	Probabilistic Random Forest improves bioactivity predictions close to the classification threshold by taking into account experimental uncertainty. *Journal of Cheminformatics*, **2021**, 13, 62	8.6	0
121	Collaborative virtual screening to elaborate an imidazo[1,2-]pyridine hit series for visceral leishmaniasis. *RSC Medicinal Chemistry*, **2021**, 12, 384-393	3.5	4
120	Retrosynthetic accessibility score (RAscore) - rapid machine learned synthesizability classification from AI driven retrosynthetic planning. *Chemical Science*, **2021**, 12, 3339-3349	9.4	15
119	Practical notes on building molecular graph generative models. *Applied AI Letters*, **2020**, 1,	1.2	5
118	"Ring Breaker": Neural Network Driven Synthesis Prediction of the Ring System Chemical Space. *Journal of Medicinal Chemistry*, **2020**, 63, 8791-8808	8.3	9
117	Axl receptor tyrosine kinase is a regulator of apolipoprotein E. *Molecular Brain*, **2020**, 13, 66	4.5	5
116	Direct steering of de novo molecular generation with descriptor conditional recurrent neural networks. *Nature Machine Intelligence*, **2020**, 2, 254-265	22.5	47
115	SMILES-based deep generative scaffold decorator for de-novo drug design. *Journal of Cheminformatics*, **2020**, 12, 38	8.6	45
114	Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis. *Journal of Medicinal Chemistry*, **2020**, 63, 8667-8682	8.3	53
113	Multisolvent Models for Solvation Free Energy Predictions Using 3D-RISM Hydration Thermodynamic Descriptors. *Journal of Chemical Information and Modeling*, **2020**, 60, 2977-2988	6.1	6
112	Building attention and edge message passing neural networks for bioactivity and physical-chemical property prediction. *Journal of Cheminformatics*, **2020**, 12, 1	8.6	51
111	Datasets and their influence on the development of computer assisted synthesis planning tools in the pharmaceutical domain. *Chemical Science*, **2020**, 11, 154-168	9.4	35
110	Memory-assisted reinforcement learning for diverse molecular de novo design. *Journal of Cheminformatics*, **2020**, 12, 68	8.6	20
109	AiZynthFinder: a fast, robust and flexible open-source software for retrosynthetic planning. *Journal of Cheminformatics*, **2020**, 12, 70	8.6	34
108	REINVENT 2.0: An AI Tool for De Novo Drug Design. *Journal of Chemical Information and Modeling*, **2020**, 60, 5918-5922	6.1	42
107	Comparison of Scaling Methods to Obtain Calibrated Probabilities of Activity for Protein-Ligand Predictions. *Journal of Chemical Information and Modeling*, **2020**, 60, 4546-4559	6.1	4
106	Molecular representations in AI-driven drug discovery: a review and practical guide. *Journal of Cheminformatics*, **2020**, 12, 56	8.6	59
105	Pluripotent Stem Cell-Derived Hepatocytes Phenotypic Screening Reveals Small Molecules Targeting the CDK2/4-C/EBP□DGAT2 Pathway Preventing ER-Stress Induced Lipid Accumulation. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	2

104	Industry-scale application and evaluation of deep learning for drug target prediction. *Journal of Cheminformatics*, **2020**, 12, 26	8.6	12
103	Exploring the GDB-13 chemical space using deep generative models. *Journal of Cheminformatics*, **2019**, 11, 20	8.6	67
102	Accurate Hit Estimation for Iterative Screening Using Venn-ABERS Predictors. *Journal of Chemical Information and Modeling*, **2019**, 59, 1230-1237	6.1	5
101	Combining structural and bioactivity-based fingerprints improves prediction performance and scaffold hopping capability. *Journal of Cheminformatics*, **2019**, 11, 54	8.6	17
100	Has Drug Design Augmented by Artificial Intelligence Become a Reality?. *Trends in Pharmacological Sciences*, **2019**, 40, 806-809	13.2	20
99	Identification of Compounds That Interfere with High-Throughput Screening Assay Technologies. *ChemMedChem*, **2019**, 14, 1795-1802	3.7	15
98	Attention and Edge Memory Convolution for Bioactivity Prediction. *Lecture Notes in Computer Science*, **2019**, 752-757	0.9	1
97	Neural Network Guided Tree-Search Policies for Synthesis Planning. *Lecture Notes in Computer Science*, **2019**, 721-724	0.9	1
96	Improving Deep Generative Models with Randomized SMILES. *Lecture Notes in Computer Science*, **2019**, 747-751	0.9	1
95	AI-assisted synthesis prediction. *Drug Discovery Today: Technologies*, **2019**, 32-33, 65-72	7.1	14
94	A de novo molecular generation method using latent vector based generative adversarial network. *Journal of Cheminformatics*, **2019**, 11, 74	8.6	78
93	Randomized SMILES strings improve the quality of molecular generative models. *Journal of Cheminformatics*, **2019**, 11, 71	8.6	74
92	Applications of Deep-Learning in Exploiting Large-Scale and Heterogeneous Compound Data in Industrial Pharmaceutical Research. *Frontiers in Pharmacology*, **2019**, 10, 1303	5.6	26
91	Bioinformatic Approaches in the Understanding of Mechanism of Action (MoA). *Methods and Principles in Medicinal Chemistry*, **2019**, 323-363	0.4	2
90	High-content phenotypic assay for proliferation of human iPSC-derived cardiomyocytes identifies L-type calcium channels as targets. *Journal of Molecular and Cellular Cardiology*, **2019**, 127, 204-214	5.8	7
89	Application of Bioactivity Profile-Based Fingerprints for Building Machine Learning Models. *Journal of Chemical Information and Modeling*, **2019**, 59, 962-972	6.1	14
88	Computational prediction of chemical reactions: current status and outlook. *Drug Discovery Today*, **2018**, 23, 1203-1218	8.8	83
87	Utility of Resazurin, Horseradish Peroxidase, and NMR Assays to Identify Redox-Related False-Positive Behavior in High-Throughput Screens. *Assay and Drug Development Technologies*, **2018**, 16, 171-191	2.1	8

86	The rise of deep learning in drug discovery. *Drug Discovery Today*, **2018**, 23, 1241-1250	8.8	650
85	Application of Generative Autoencoder in De Novo Molecular Design. *Molecular Informatics*, **2018**, 37, 1700123	3.8	174
84	Small molecule inducers of ABCA1 and apoE that act through indirect activation of the LXR pathway. *Journal of Lipid Research*, **2018**, 59, 830-842	6.3	26
83	Orthologue chemical space and its influence on target prediction. *Bioinformatics*, **2018**, 34, 72-79	7.2	18
82	Extending Protein Target Prediction Models to Include Functional Effects. *Frontiers in Pharmacology*, **2018**, 9, 613	5.6	3
81	The convergence of artificial intelligence and chemistry for improved drug discovery. *Future Medicinal Chemistry*, **2018**, 10, 2573-2576	4.1	14
80	Cheminformatics in Drug Discovery, an Industrial Perspective. *Molecular Informatics*, **2018**, 37, e1800041	3.8	22
79	Applying Mondrian Cross-Conformal Prediction To Estimate Prediction Confidence on Large Imbalanced Bioactivity Data Sets. *Journal of Chemical Information and Modeling*, **2017**, 57, 1591-1598	6.1	38
78	ExCAPE-DB: an integrated large scale dataset facilitating Big Data analysis in chemogenomics. *Journal of Cheminformatics*, **2017**, 9, 17	8.6	56
77	Innovation in Small-Molecule-Druggable Chemical Space: Where are the Initial Modulators of New Targets Published?. *Journal of Chemical Information and Modeling*, **2017**, 57, 2741-2753	6.1	5
76	Merged Multiple Ligands. *Methods and Principles in Medicinal Chemistry*, **2017**, 247-274	0.4	2
75	Phenotypic Screen for Cardiac Regeneration Identifies Molecules with Differential Activity in Human Epicardium-Derived Cells versus Cardiac Fibroblasts. *ACS Chemical Biology*, **2017**, 12, 132-141	4.9	16
74	Molecular de-novo design through deep reinforcement learning. *Journal of Cheminformatics*, **2017**, 9, 48	8.6	352
73	On the Integration of Drug Design Methods for Drug Repurposing. *Frontiers in Pharmacology*, **2017**, 8, 298	5.6	109
72	Understanding Cytotoxicity and Cytostaticity in a High-Throughput Screening Collection. *ACS Chemical Biology*, **2016**, 11, 3007-3023	4.9	22
71	Does SBig DataSexist in medicinal chemistry, and if so, how can it be harnessed?. *Future Medicinal Chemistry*, **2016**, 8, 1801-1806	4.1	15
70	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18	8.6	
69	Chemistry-Driven Target Identification. *Methods and Principles in Medicinal Chemistry*, **2016**, 63-92	0.4	

68	Open PHACTS computational protocols for target validation of cellular phenotypic screens: knowing the knowns. *MedChemComm*, **2016**, 7, 1237-1244	5	15
67	BIGCHEM: Challenges and Opportunities for Big Data Analysis in Chemistry. *Molecular Informatics*, **2016**, 35, 615-621	3.8	59
66	Using the BioAssay Ontology for analyzing high-throughput screening data. *Journal of Biomolecular Screening*, **2015**, 20, 402-15		13
65	Compound Properties and their Influence on Drug Quality **2015**, 379-393		5
64	Target prediction utilising negative bioactivity data covering large chemical space. *Journal of Cheminformatics*, **2015**, 7, 51	8.6	76
63	Investigating Pharmacological Similarity by Charting Chemical Space. *Journal of Chemical Information and Modeling*, **2015**, 55, 2375-90	6.1	13
62	In Silico Tools for Predicting Brain Exposure of Drugs **2015**, 167-187		1
61	Exploring in silico prediction of the unbound brain-to-plasma drug concentration ratio: model validation, renewal, and interpretation. *Journal of Pharmaceutical Sciences*, **2015**, 104, 1197-206	3.9	24
60	Heart regeneration: opportunities and challenges for drug discovery with novel chemical and therapeutic methods or agents. *Angewandte Chemie - International Edition*, **2014**, 53, 4056-75	16.4	32
59	Ligand-based target prediction with signature fingerprints. *Journal of Chemical Information and Modeling*, **2014**, 54, 2647-53	6.1	35
58	The Role of Historical Bioactivity Data in the Deconvolution of Phenotypic Screens. *Journal of Biomolecular Screening*, **2014**, 19, 696-706		9
57	HTS explorer. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
56	Hit series selection in noisy HTS data: clustering techniques, statistical tests and data visualisations. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
55	Transporter assays and assay ontologies: useful tools for drug discovery. *Drug Discovery Today: Technologies*, **2014**, 12, e47-54	7.1	4
54	Herzregeneration: Chancen und Aufgaben f□die Wirkstoff-Forschung mit neuartigen chemischen und therapeutischen Methoden oder Agentien. *Angewandte Chemie*, **2014**, 126, 4138-4159	3.6	2
53	Mining Molecular Pharmacological Effects from Biomedical Text: a Case Study for Eliciting Anti-Obesity/Diabetes Effects of Chemical Compounds. *Molecular Informatics*, **2014**, 33, 332-42	3.8	3
52	On the Relationship between Molecular Hit Rates in High-Throughput Screening and Molecular Descriptors. *Journal of Biomolecular Screening*, **2014**, 19, 727-37		14
51	Investigation of the influence of molecular topology on ligand binding. *Journal of Molecular Graphics and Modelling*, **2013**, 40, 22-9	2.8	0

50	Systematic exploration of dual-acting modulators from a combined medicinal chemistry and biology perspective. *Journal of Medicinal Chemistry*, **2013**, 56, 1197-210	8.3	13
49	Shouldn't enantiomeric purity be included in the minimum information about a bioactive entity? Response from the MIABE group. *Nature Reviews Drug Discovery*, **2012**, 11, 730-730	64.1	
48	An Investigation of the Relationship Between Molecular Topology and CYP3A4 Inhibition for Drug-like Compounds. *Molecular Informatics*, **2012**, 31, 719-23	3.8	
47	Annotating Human P-Glycoprotein Bioassay Data. *Molecular Informatics*, **2012**, 31, 599-609	3.8	27
46	A comparative analysis of the molecular topologies for drugs, clinical candidates, natural products, human metabolites and general bioactive compounds. *MedChemComm*, **2012**, 3, 312-321	5	30
45	Beyond size, ionization state, and lipophilicity: influence of molecular topology on absorption, distribution, metabolism, excretion, and toxicity for druglike compounds. *Journal of Medicinal Chemistry*, **2012**, 55, 3667-77	8.3	96
44	Minimum information about a bioactive entity (MIABE). *Nature Reviews Drug Discovery*, **2011**, 10, 661-9	64.1	69
43	Combinatorial library design from reagent pharmacophore fingerprints. *Methods in Molecular Biology*, **2011**, 685, 135-52	1.4	2
42	In silico prediction of unbound brain-to-plasma concentration ratio using machine learning algorithms. *Journal of Molecular Graphics and Modelling*, **2011**, 29, 985-95	2.8	48
41	Investigation of the relationship between topology and selectivity for druglike molecules. *Journal of Medicinal Chemistry*, **2010**, 53, 7709-14	8.3	50
40	Molecular topology analysis of the differences between drugs, clinical candidate compounds, and bioactive molecules. *Journal of Chemical Information and Modeling*, **2010**, 50, 2141-50	6.1	19
39	Designing a Combinatorial Library by Using Reagent Pharmacophore Fingerprint. *QSAR and Combinatorial Science*, **2009**, 28, 840-844		1
38	Physicochemical property profiles of marketed drugs, clinical candidates and bioactive compounds. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 6943-7	2.9	31
37	Comparison of molecular fingerprint methods on the basis of biological profile data. *Journal of Chemical Information and Modeling*, **2009**, 49, 338-47	6.1	48
36	ProSAR: a new methodology for combinatorial library design. *Journal of Chemical Information and Modeling*, **2009**, 49, 603-14	6.1	12
35	Molecular modeling of the second extracellular loop of G-protein coupled receptors and its implication on structure-based virtual screening. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 599-620	4.2	89
34	Multifingerprint based similarity searches for targeted class compound selection. *Journal of Chemical Information and Modeling*, **2006**, 46, 1201-13	6.1	59
33	Characterization of a conserved structural determinant controlling protein kinase sensitivity to selective inhibitors. *Chemistry and Biology*, **2004**, 11, 691-701		114

32	Prediction of CNS activity of compound libraries using substructure analysis. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 155-60		43
31	A fast virtual screening filter for cytochrome P450 3A4 inhibition liability of compound libraries. *QSAR and Combinatorial Science*, **2002**, 21, 249-256		32
30	High-throughput, in silico prediction of aqueous solubility based on one- and two-dimensional descriptors. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 1247-9		43
29	Hoogsteen and Stacked Structures of the 9-Methyladenine□□1-Methylthymine Pair Are Populated Equally at Experimental Conditions: Ab Initio and Molecular Dynamics Study. *Journal of Physical Chemistry A*, **2001**, 105, 1197-1202	2.8	27
28	Accurate Intermolecular Potentials Obtained from Molecular Wave Functions: Bridging the Gap between Quantum Chemistry and Molecular Simulations. *Chemical Reviews*, **2000**, 100, 4087-108	68.1	160
27	Developments in computational studies of crystallization and morphology applied to urea. *Physical Chemistry Chemical Physics*, **2000**, 2, 3017-3027	3.6	27
26	Methylated uracil dimers: potential energy and free energy surfaces. *Physical Chemistry Chemical Physics*, **2000**, 2, 2419-2424	3.6	14
25	Adsorption of water on the NaCl(001) surface. III. Monte Carlo simulations at ambient temperatures. *Journal of Chemical Physics*, **2000**, 112, 6827-6833	3.9	38
24	Adsorption of water on NaCl(001). I. Intermolecular potentials and low temperature structures. *Journal of Chemical Physics*, **1999**, 110, 12089-12096	3.9	32
23	Structure and vibrational dynamics of the benzene dimer. *Journal of Chemical Physics*, **1999**, 111, 572-583	3.9	140
22	Adsorption of water on the MgO(001) surface. *Surface Science*, **1999**, 437, 239-248	1.8	29
21	Benzene trimer and benzene tetramer: Structures and properties determined by the nonempirical model (NEMO) potential calibrated from the CCSD(T) benzene dimer energies. *Journal of Chemical Physics*, **1999**, 110, 5758-5762	3.9	78
20	Theoretical study of intermolecular potential energy surface for HCl dimer: Example of nonspherical atom□atom exchange repulsion interaction. *Journal of Computational Chemistry*, **1998**, 19, 1816-1825	3.5	12
19	Uracil Dimer: Potential Energy and Free Energy Surfaces. Ab Initio beyond Hartree□ock and Empirical Potential Studies. *Journal of Physical Chemistry A*, **1998**, 102, 6921-6926	2.8	100
18	A Monte Carlo simulation study of the temperature dependence for the conformation distribution of 1,2-dimethoxyethane in water. *Journal of Chemical Physics*, **1997**, 106, 2411-2417	3.9	12
17	A comparison between the NEMO intermolecular water potential and ab initio quantum chemical calculations for the water trimer tetramer. *Molecular Physics*, **1997**, 90, 277-287	1.7	7
16	Monte Carlo Simulation Study of Short Poly(ethylene oxide) Chains at Different Concentrations. *Journal of Physical Chemistry B*, **1997**, 101, 1631-1633	3.4	22
15	Theory of Poly(ethylene glycol) in Solution. *ACS Symposium Series*, **1997**, 16-30	0.4	8

14	On the origin of the gauche effect. A quantum chemical study of 1,2-difluoroethane. *Chemical Physics Letters*, **1997**, 265, 19-23	2.5	45
13	Intermolecular Potential for the 1,2-Dimethoxyethane−Water Complex. *The Journal of Physical Chemistry*, **1996**, 100, 6950-6957		48
12	On the Relation between Retention Indexes and the Interaction between the Solute and the Column in Gas−Liquid Chromatography. *Journal of Chemical Information and Computer Sciences*, **1996**, 36, 1153-1161		3
11	A method to calculate the probability distribution for systems with large energy barriers. *Chemical Physics*, **1996**, 213, 63-76	2.3	34
10	SMILES-Based Deep Generative Scaffold Decorator for De-Novo Drug Design		2
9	A De Novo Molecular Generation Method Using Latent Vector Based Generative Adversarial Network		2
8	A De Novo Molecular Generation Method Using Latent Vector Based Generative Adversarial Network		2
7	Direct Steering of de novo Molecular Generation using Descriptor Conditional Recurrent Neural Networks (cRNNs)		2
6	Direct Steering of de novo Molecular Generation using Descriptor Conditional Recurrent Neural Networks (cRNNs)		2
5	Building Attention and Edge Convolution Neural Networks for Bioactivity and Physical-Chemical Property Prediction		2
4	Exploring the GDB-13 Chemical Space Using Deep Generative Models		2
3	Randomized SMILES Strings Improve the Quality of Molecular Generative Models		2
2	AiZynthFinder: A Fast Robust and Flexible Open-Source Software for Retrosynthetic Planning		2
1	Evaluation guidelines for machine learning tools in the chemical sciences. *Nature Reviews Chemistry*,	34.6	3