Deep learning for molecular designâ€”a review of the st

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Citation Report

#	Article	IF	Citations
1	Deep Convolutional Generative Adversarial Network (dcGAN) Models for Screening and Design of Small Molecules Targeting Cannabinoid Receptors. Molecular Pharmaceutics, 2019, 16, 4451-4460.	2.3	43
2	Convolutional Neural Networks for the Design and Analysis of Non-Fullerene Acceptors. Journal of Chemical Information and Modeling, 2019, 59, 4993-5001.	2.5	29
3	Deep learning enables rapid identification of potent DDR1 kinase inhibitors. Nature Biotechnology, 2019, 37, 1038-1040.	9.4	671
4	Identification Schemes for Metalâ€“Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. Crystal Growth and Design, 2019, 19, 6682-6697.	1.4	123
5	Deep Reinforcement Learning for Multiparameter Optimization in de novo Drug Design. Journal of Chemical Information and Modeling, 2019, 59, 3166-3176.	2.5	130
6	On failure modes in molecule generation and optimization. Drug Discovery Today: Technologies, 2019, 32-33, 55-63.	4.0	59
7	Deep Learning for Deep Chemistry: Optimizing the Prediction of Chemical Patterns. Frontiers in Chemistry, 2019, 7, 809.	1.8	106
8	Attribute driven inverse materials design using deep learning Bayesian framework. Npj Computational Materials, 2019, 5, .	3.5	29
9	Applications of Deep-Learning in Exploiting Large-Scale and Heterogeneous Compound Data in Industrial Pharmaceutical Research. Frontiers in Pharmacology, 2019, 10, 1303.	1.6	38
10	Autonomous Discovery in the Chemical Sciences Partâ€…I: Progress. Angewandte Chemie - International Edition, 2020, 59, 22858-22893.	7.2	180
11	Autonomous Discovery in the Chemical Sciences Partâ€…II: Outlook. Angewandte Chemie - International Edition, 2020, 59, 23414-23436.	7.2	139
12	Autonome Entdeckung in den chemischen Wissenschaften, Teilâ€…I: Fortschritt. Angewandte Chemie, 2020, 132, 23054-23091.	1.6	11
13	Autonome Entdeckung in den chemischen Wissenschaften, Teil II: Ausblick. Angewandte Chemie, 2020, 132, 23620-23643.	1.6	4
14	Constrained Bayesian optimization for automatic chemical design using variational autoencoders. Chemical Science, 2020, 11, 577-586.	3.7	159
15	Quantitative Structureâ€“Selectivity Relationships in Enantioselective Catalysis: Past, Present, and Future. Chemical Reviews, 2020, 120, 1620-1689.	23.0	117
16	De novo generation of hit-like molecules from gene expression signatures using artificial intelligence. Nature Communications, 2020, 11, 10.	5.8	253
17	Compressed graph representation for scalable molecular graph generation. Journal of Cheminformatics, 2020, 12, 58.	2.8	11
18	Artificial neural networks for the prediction of solvation energies based on experimental and computational data. Physical Chemistry Chemical Physics, 2020, 22, 24359-24364.	1.3	15

#	Article	IF	Citations
19	Electronic Structure Modeling of Metalâ€“Organic Frameworks. Chemical Reviews, 2020, 120, 8641-8715.	23.0	149
20	Transfer Learning for Drug Discovery. Journal of Medicinal Chemistry, 2020, 63, 8683-8694.	2.9	178
21	Machine learning the ropes: principles, applications and directions in synthetic chemistry. Chemical Society Reviews, 2020, 49, 6154-6168.	18.7	148
22	Machine Learning for Electronically Excited States of Molecules. Chemical Reviews, 2021, 121, 9873-9926.	23.0	207
23	A Recommender System for Inverse Design of Polycarbonates and Polyesters. Macromolecules, 2020, 53, 10847-10854.	2.2	9
24	Photoswitching Molecular Junctions: Platforms and Electrical Properties. ChemPhysChem, 2020, 21, 2368-2383.	1.0	17
25	Inverse design of two-dimensional graphene/h-BN hybrids by a regressional and conditional GAN. Carbon, 2020, 169, 9-16.	5.4	35
26	Exploring chemical space using natural language processing methodologies for drug discovery. Drug Discovery Today, 2020, 25, 689-705.	3.2	68
27	Relevant Applications of Generative Adversarial Networks in Drug Design and Discovery: Molecular De Novo Design, Dimensionality Reduction, and De Novo Peptide and Protein Design. Molecules, 2020, 25, 3250.	1.7	51
28	Comprehensive Prediction of Molecular Recognition in a Combinatorial Chemical Space Using Machine Learning. ACS Combinatorial Science, 2020, 22, 500-508.	3.8	9
29	Generative Model for Proposing Drug Candidates Satisfying Anticancer Properties Using a Conditional Variational Autoencoder. ACS Omega, 2020, 5, 18642-18650.	1.6	19
30	A machine-learning-assisted study of the permeability of small drug-like molecules across lipid membranes. Physical Chemistry Chemical Physics, 2020, 22, 19687-19696.	1.3	17
31	Structure prediction of crystals, surfaces and nanoparticles. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190600.	1.6	26
32	Transfer Learning as Tool to Enhance Predictions of Molecular Properties Based on 2D Projections. Advanced Theory and Simulations, 2020, 3, 2000148.	1.3	7
33	EvoMol: a flexible and interpretable evolutionary algorithm for unbiased de novo molecular generation. Journal of Cheminformatics, 2020, 12, 55.	2.8	29
34	Continuous Molecular Representations of Ionic Liquids. Journal of Physical Chemistry B, 2020, 124, 8347-8357.	1.2	12
35	Scaffold-Constrained Molecular Generation. Journal of Chemical Information and Modeling, 2020, 60, 5637-5646.	2.5	32
36	Illuminating elite patches of chemical space. Chemical Science, 2020, 11, 11485-11491.	3.7	12

#	Article	IF	Citations
37	A Review of Deep Learning Methods for Antibodies. Antibodies, 2020, 9, 12.	1.2	40
38	Machine-Learning Coupled Cluster Properties through a Density Tensor Representation. Journal of Physical Chemistry A, 2020, 124, 4861-4871.	1.1	21
39	Direct steering of de novo molecular generation with descriptor conditional recurrent neural networks. Nature Machine Intelligence, 2020, 2, 254-265.	8.3	124
40	CReM: chemically reasonable mutations framework for structure generation. Journal of Cheminformatics, 2020, 12, 28.	2.8	42
41	kGCN: a graph-based deep learning framework for chemical structures. Journal of Cheminformatics, 2020, 12, 32.	2.8	55
42	Artificial intelligence in chemistry and drug design. Journal of Computer-Aided Molecular Design, 2020, 34, 709-715.	1.3	79
43	Role of Artificial Intelligence and Machine Learning in Nanosafety. Small, 2020, 16, e2001883.	5.2	86
44	Efficient sampling of high-energy states by machine learning force fields. Physical Chemistry Chemical Physics, 2020, 22, 14364-14374.	1.3	3
45	Big-Data Science in Porous Materials: Materials Genomics and Machine Learning. Chemical Reviews, 2020, 120, 8066-8129.	23.0	284
46	Molecular generation targeting desired electronic properties via deep generative models. Nanoscale, 2020, 12, 6744-6758.	2.8	27
47	Deep Generative Models for 3D Linker Design. Journal of Chemical Information and Modeling, 2020, 60, 1983-1995.	2.5	126
48	The power of deep learning to ligand-based novel drug discovery. Expert Opinion on Drug Discovery, 2020, 15, 755-764.	2.5	44
49	In silico toxicology: From structureâ€“activity relationships towards deep learning and adverse outcome pathways. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1475.	6.2	80
50	Deep learning and knowledge-based methods for computer-aided molecular designâ€”toward a unified approach: State-of-the-art and future directions. Computers and Chemical Engineering, 2020, 141, 107005.	2.0	67
51	Generative adversarial networks (GAN) based efficient sampling of chemical composition space for inverse design of inorganic materials. Npj Computational Materials, 2020, 6, .	3.5	117
52	ChEMBL-Likeness Score and Database GDBChEMBL. Frontiers in Chemistry, 2020, 8, 46.	1.8	33
53	Machine-Learning-Assisted De Novo Design of Organic Molecules and Polymers: Opportunities and Challenges. Polymers, 2020, 12, 163.	2.0	95
54	Synergistic Approach of Ultrafast Spectroscopy and Molecular Simulations in the Characterization of Intramolecular Charge Transfer in Push-Pull Molecules. Molecules, 2020, 25, 430.	1.7	24

#	Article	IF	Citations
55	GEN: highly efficient SMILES explorer using autodidactic generative examination networks. Journal of Cheminformatics, 2020, 12, 22.	2.8	23
56	Hard-threshold neural network-based prediction of organic synthetic outcomes. BMC Chemical Engineering, 2020, 2, .	3.4	1
57	Exploring Novel Biologically-Relevant Chemical Space Through Artificial Intelligence: The NCATS ASPIRE Program. Frontiers in Robotics and AI, 2019, 6, 143.	2.0	4
58	A Structure-Based Platform for Predicting Chemical Reactivity. CheM, 2020, 6, 1379-1390.	5.8	154
59	Machine-enabled inverse design of inorganic solid materials: promises and challenges. Chemical Science, 2020, 11, 4871-4881.	3.7	88
60	Evolving the Materials Genome: How Machine Learning Is Fueling the Next Generation of Materials Discovery. Annual Review of Materials Research, 2020, 50, 1-25.	4.3	49
61	Augmenting Molecular Images with Vector Representations as a Featurization Technique for Drug Classification. , 2020, , .		1
62	Deep computational pathology in breast cancer. Seminars in Cancer Biology, 2021, 72, 226-237.	4.3	30
63	Machine learning-accelerated quantum mechanics-based atomistic simulations for industrial applications. Journal of Computer-Aided Molecular Design, 2021, 35, 557-586.	1.3	29
64	Uncertainty quantification in drug design. Drug Discovery Today, 2021, 26, 474-489.	3.2	39
65	Target-Specific Drug Design Method Combining Deep Learning and Water Pharmacophore. Journal of Chemical Information and Modeling, 2021, 61, 36-45.	2.5	9
66	Improvement of the Structure Generator DAECS with Respect to Structural Diversity. Molecular Informatics, 2021, 40, 2000225.	1.4	2
67	Design and Synthesis of DDR1 Inhibitors with a Desired Pharmacophore Using Deep Generative Models. ChemMedChem, 2021, 16, 955-958.	1.6	21
68	Generative deep learning for macromolecular structure and dynamics. Current Opinion in Structural Biology, 2021, 67, 170-177.	2.6	26
69	High-Throughput Molecular Dynamics Simulations and Validation of Thermophysical Properties of Polymers for Various Applications. ACS Applied Polymer Materials, 2021, 3, 620-630.	2.0	35
70	De novo generation of optically active small organic molecules using Monte Carlo tree search combined with recurrent neural network. Journal of Computational Chemistry, 2021, 42, 136-143.	1.5	8
71	Artificial intelligence in drug discovery: applications and techniques. Briefings in Bioinformatics, 2022, 23, .	3.2	44
72	De novo molecular drug design benchmarking. RSC Medicinal Chemistry, 2021, 12, 1273-1280.	1.7	7

#	Article	IF	Citations
73	Data-driven algorithms for inverse design of polymers. Soft Matter, 2021, 17, 7607-7622.	1.2	39
74	TSNet: predicting transition state structures with tensor field networks and transfer learning. Chemical Science, 2021, 12, 10022-10040.	3.7	28
75	Determination of Leaf Water Content with a Portable NIRS System Based on Deep Learning and Information Fusion Analysis. Transactions of the ASABE, 2021, 64, 127-135.	1.1	15
76	Predicting chemical reaction outcomes: A grammar ontologyâ€based transformer framework. AICHE Journal, 2021, 67, e17190.	1.8	27
77	Physically inspired deep learning of molecular excitations and photoemission spectra. Chemical Science, 2021, 12, 10755-10764.	3.7	35
78	Transformer neural network for protein-specific de novo drug generation as a machine translation problem. Scientific Reports, 2021, 11, 321.	1.6	96
79	A review on machine learning algorithms for the ionic liquid chemical space. Chemical Science, 2021, 12, 6820-6843.	3.7	80
80	Independent Vector Analysis for Molecular Data Fusion: Application to Property Prediction and Knowledge Discovery of Energetic Materials. , 2021, , .		6
81	Transmol: repurposing a language model for molecular generation. RSC Advances, 2021, 11, 25921-25932.	1.7	4
82	Generative chemistry: drug discovery with deep learning generative models. Journal of Molecular Modeling, 2021, 27, 71.	0.8	63
83	Defining and Exploring Chemical Spaces. Trends in Chemistry, 2021, 3, 133-145.	4.4	60
84	Selectivity in organocatalysisâ€”From qualitative to quantitative predictive models. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1518.	6.2	23
85	The Playbooks of Medicinal Chemistry Design Moves. Journal of Chemical Information and Modeling, 2021, 61, 729-742.	2.5	11
86	Learning Atomic Interactions through Solvation Free Energy Prediction Using Graph Neural Networks. Journal of Chemical Information and Modeling, 2021, 61, 689-698.	2.5	21
87	Discovery of novel chemical reactions by deep generative recurrent neural network. Scientific Reports, 2021, 11, 3178.	1.6	40
88	Machine learning for molecular thermodynamics. Chinese Journal of Chemical Engineering, 2021, 31, 227-239.	1.7	16
89	SMILES Pair Encoding: A Data-Driven Substructure Tokenization Algorithm for Deep Learning. Journal of Chemical Information and Modeling, 2021, 61, 1560-1569.	2.5	41
90	Artificial Intelligence and Early Detection of Pancreatic Cancer. Pancreas, 2021, 50, 251-279.	0.5	71

#	Article	IF	Citations
91	Deep Learning Optical Spectroscopy Based on Experimental Database: Potential Applications to Molecular Design. Jacs Au, 2021, 1, 427-438.	3.6	61
92	Diversity oriented Deep Reinforcement Learning for targeted molecule generation. Journal of Cheminformatics, 2021, 13, 21.	2.8	36
93	MolFinder: an evolutionary algorithm for the global optimization of molecular properties and the extensive exploration of chemical space using SMILES. Journal of Cheminformatics, 2021, 13, 24.	2.8	26
94	Graph networks for molecular design. Machine Learning: Science and Technology, 2021, 2, 025023.	2.4	74
95	Discovering Relationships between OSDAs and Zeolites through Data Mining and Generative Neural Networks. ACS Central Science, 2021, 7, 858-867.	5.3	57
96	Artificial intelligence in oncology: From bench to clinic. Seminars in Cancer Biology, 2022, 84, 113-128.	4.3	16
97	Beyond Tolerance Factor: Using Deep Learning for Prediction Formability of ABX3 Perovskite Structures. Advanced Theory and Simulations, 2021, 4, 2100021.	1.3	5
98	Artificial intelligence in drug discovery: recent advances and future perspectives. Expert Opinion on Drug Discovery, 2021, 16, 949-959.	2.5	128
99	Machine learning discovery of high-temperature polymers. Patterns, 2021, 2, 100225.	3.1	51
100	Critical assessment of AI in drug discovery. Expert Opinion on Drug Discovery, 2021, 16, 937-947.	2.5	25
101	Active discovery of organic semiconductors. Nature Communications, 2021, 12, 2422.	5.8	66
102	Challenges and Perspectives in the Discovery of Dengue Virus Entry Inhibitors. Current Medicinal Chemistry, 2022, 29, 719-740.	1.2	2
103	Comparison of structure- and ligand-based scoring functions for deep generative models: a GPCR case study. Journal of Cheminformatics, 2021, 13, 39.	2.8	33
104	Research on University Product System under Computer Science Aided Operation. , 2021, , .		0
105	Enabling rapid COVID-19 small molecule drug design through scalable deep learning of generative models. International Journal of High Performance Computing Applications, 2021, 35, 469-482.	2.4	21
106	Automated Generation of Novel Fragments Using Screening Data, a Dual SMILES Autoencoder, Transfer Learning and Syntax Correction. Journal of Chemical Information and Modeling, 2021, 61, 2547-2559.	2.5	11
107	Inferring experimental procedures from text-based representations of chemical reactions. Nature Communications, 2021, 12, 2573.	5.8	28
109	De novo molecular design and generative models. Drug Discovery Today, 2021, 26, 2707-2715.	3.2	107

#	Article	IF	Citations
110	Perspective on integrating machine learning into computational chemistry and materials science. Journal of Chemical Physics, 2021, 154, 230903.	1.2	107
111	Applying Deutschâ€™s concept of good explanations to artificial intelligence and neuroscience â€“ An initial exploration. Cognitive Systems Research, 2021, 67, 9-17.	1.9	1
112	How Deep Learning Tools Can Help Protein Engineers Find Good Sequences. Journal of Physical Chemistry B, 2021, 125, 6440-6450.	1.2	7
113	Computational catalysis for metal-organic frameworks: An overview. Coordination Chemistry Reviews, 2021, 436, 213777.	9.5	34
114	Data Science in Chemical Engineering: Applications to Molecular Science. Annual Review of Chemical and Biomolecular Engineering, 2021, 12, 15-37.	3.3	9
115	Efficient Search for Energetically Favorable Molecular Conformations against Metastable States via Gray-Box Optimization. Journal of Chemical Theory and Computation, 2021, 17, 5419-5427.	2.3	8
116	Structure-Based de Novo Molecular Generator Combined with Artificial Intelligence and Docking Simulations. Journal of Chemical Information and Modeling, 2021, 61, 3304-3313.	2.5	41
117	Artificial Intelligence in Chemistry: Current Trends and Future Directions. Journal of Chemical Information and Modeling, 2021, 61, 3197-3212.	2.5	80
118	Chemical language models enable navigation in sparsely populated chemical space. Nature Machine Intelligence, 2021, 3, 759-770.	8.3	48
120	Reinforcement learning applied to metamaterial design. Journal of the Acoustical Society of America, 2021, 150, 321-338.	0.5	27
121	De novo design with deep generative models based on 3D similarity scoring. Bioorganic and Medicinal Chemistry, 2021, 44, 116308.	1.4	14
122	Machine Learning in Chemical Product Engineering: The State of the Art and a Guide for Newcomers. Processes, 2021, 9, 1456.	1.3	28
123	Molecular design in drug discovery: a comprehensive review of deep generative models. Briefings in Bioinformatics, 2021, 22, .	3.2	61
124	Molecular Generators and Optimizers Failure Modes. Malaysian Journal of Medical and Biological Research, 2021, 8, 53-62.	0.2	1
125	Comparing classification modelsâ€”a practical tutorial. Journal of Computer-Aided Molecular Design, 2022, 36, 381-389.	1.3	6
126	Using molecular embeddings in QSAR modeling: does it make a difference?. Briefings in Bioinformatics, 2022, 23, .	3.2	14
127	Kinase Inhibitor Scaffold Hopping with Deep Learning Approaches. Journal of Chemical Information and Modeling, 2021, 61, 4900-4912.	2.5	11
128	GenUI: interactive and extensible open source software platform for de novo molecular generation and cheminformatics. Journal of Cheminformatics, 2021, 13, 73.	2.8	7

#	Article	IF	Citations
129	Generic and specific recurrent neural network models: Applications for large and small scale biopharmaceutical upstream processes. Biotechnology Reports (Amsterdam, Netherlands), 2021, 31, e00640.	2.1	12
130	Machine learning, artificial intelligence, and data science breaking into drug design and neglected diseases. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1513.	6.2	21
131	Multilabel Classification Models for the Prediction of Cross-Coupling Reaction Conditions. Journal of Chemical Information and Modeling, 2021, 61, 156-166.	2.5	34
132	Machine-learning Applications to Membrane Active Peptides. , 2021, , 198-207.		1
133	Sparse Convolutions on Continuous Domains for Point Cloud and Event Stream Networks. Lecture Notes in Computer Science, 2021, , 400-416.	1.0	1
134	Computational Approaches for De Novo Drug Design: Past, Present, and Future. Methods in Molecular Biology, 2021, 2190, 139-165.	0.4	26
135	Artificial Intelligence in Drug Discovery: A Comprehensive Review of Data-driven and Machine Learning Approaches. Biotechnology and Bioprocess Engineering, 2020, 25, 895-930.	1.4	43
136	Machine Learning in Science â€“ A Role for Mechanical Sympathy?. RSC Theoretical and Computational Chemistry Series, 2020, , 109-135.	0.7	2
137	cheML.io: an online database of ML-generated molecules. RSC Advances, 2020, 10, 45189-45198.	1.7	4
138	Deep learning and generative methods in cheminformatics and chemical biology: navigating small molecule space intelligently. Biochemical Journal, 2020, 477, 4559-4580.	1.7	29
139	Machine learning and excited-state molecular dynamics. Machine Learning: Science and Technology, 2020, 1, 043001.	2.4	50
140	Self-referencing embedded strings (SELFIES): A 100% robust molecular string representation. Machine Learning: Science and Technology, 2020, 1, 045024.	2.4	272
144	CRYSPNet: Crystal structure predictions via neural networks. Physical Review Materials, 2020, 4, .	0.9	26
145	Chemical space exploration: how genetic algorithms find the needle in the haystack. PeerJ Physical Chemistry, 0, 2, e11.	0.0	25
146	Computational anti-COVID-19 drug design: progress and challenges. Briefings in Bioinformatics, 2022, 23, .	3.2	8
147	Multiobjective Reinforcement Learning in Optimized Drug Design. , 2021, , .		0
148	IMPECCABLE: Integrated Modeling PipelinE for COVID Cure by Assessing Better LEads. , 2021, , .		13
149	Intelligent host engineering for metabolic flux optimisation in biotechnology. Biochemical Journal, 2021, 478, 3685-3721.	1.7	8

#	Article	IF	Citations
150	Curated Database and Preliminary AutoML QSAR Model for 5-HT1A Receptor. Pharmaceutics, 2021, 13, 1711.	2.0	7
151	Screening of Î²1- and Î²2-Adrenergic Receptor Modulators through Advanced Pharmacoinformatics and Machine Learning Approaches. International Journal of Molecular Sciences, 2021, 22, 11191.	1.8	3
152	Multi-constraint molecular generation based on conditional transformer, knowledge distillation and reinforcement learning. Nature Machine Intelligence, 2021, 3, 914-922.	8.3	73
153	Kernel Methods for Predicting Yields of Chemical Reactions. Journal of Chemical Information and Modeling, 2022, 62, 2077-2092.	2.5	27
154	Adversarial Deep Evolutionary Learning for Drug Design. , 2021, , .		2
155	Application advances of deep learning methods for de novo drug design and molecular dynamics simulation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1581.	6.2	49
156	Generative Deep Learning for Targeted Compound Design. Journal of Chemical Information and Modeling, 2021, 61, 5343-5361.	2.5	57
157	Grand challenges on accelerating discovery in catalysis. Catalysis Today, 2022, 387, 140-142.	2.2	5
158	Coexistence and Phase Behavior of Solventâ€“Polystyrene-Grafted Gold Nanoparticle Systems. Macromolecules, 2021, 54, 10435-10446.	2.2	4
160	ScaffComb: A Phenotypeâ€Based Framework for Drug Combination Virtual Screening in Largeâ€Scale Chemical Datasets. Advanced Science, 2021, 8, e2102092.	5.6	7
161	Uncovering the Folding Landscape of RNA Secondary Structure Using Deep Graph Embeddings. , 2020, , .		4
162	AIScaffold: A Web-Based Tool for Scaffold Diversification Using Deep Learning. Journal of Chemical Information and Modeling, 2021, 61, 1-6.	2.5	8
163	Convolutional neural networks for the design and analysis of nonfullerene acceptors. , 2022, , 231-256.		25
164	Goal-directed generation of new molecules by AI methods. , 2022, , 39-67.		0
165	Bayesian optimization for chemical products and functional materials. Current Opinion in Chemical Engineering, 2022, 36, 100728.	3.8	43
166	Smart manufacturing enabled by continuous monitoring and control of polymer characteristics. , 2020, , 257-308.		0
170	Predicting Antimicrobial Activity of Conjugated Oligoelectrolyte Molecules via Machine Learning. Journal of the American Chemical Society, 2021, 143, 18917-18931.	6.6	17
171	Artificial Intelligence, Machine Learning, and Deep Learning in Real-Life Drug Design Cases. Methods in Molecular Biology, 2022, 2390, 383-407.	0.4	12

#	Article	IF	Citations
172	Ultrahigh Throughput Proteinâ€“Ligand Docking with Deep Learning. Methods in Molecular Biology, 2022, 2390, 301-319.	0.4	3
173	Deep Learning Applied to Ligand-Based De Novo Drug Design. Methods in Molecular Biology, 2022, 2390, 273-299.	0.4	20
174	Deep Learning in Structure-Based Drug Design. Methods in Molecular Biology, 2022, 2390, 261-271.	0.4	5
175	Applications of Artificial Intelligence in Drug Design: Opportunities and Challenges. Methods in Molecular Biology, 2022, 2390, 1-59.	0.4	11
178	Machine learning to empower electrohydrodynamic processing. Materials Science and Engineering C, 2022, 132, 112553.	3.8	12
179	MassGenie: A Transformer-Based Deep Learning Method for Identifying Small Molecules from Their Mass Spectra. Biomolecules, 2021, 11, 1793.	1.8	29
180	Artificial Intelligence for Autonomous Molecular Design: A Perspective. Molecules, 2021, 26, 6761.	1.7	11
181	MERMAID: an open source automated hit-to-lead method based on deep reinforcement learning. Journal of Cheminformatics, 2021, 13, 94.	2.8	10
182	A deep generative model enables automated structure elucidation of novel psychoactive substances. Nature Machine Intelligence, 2021, 3, 973-984.	8.3	28
183	Highâ€Throughput Experimentation and Computational Freeway Lanes for Accelerated Battery Electrolyte and Interface Development Research. Advanced Energy Materials, 2022, 12, 2102678.	10.2	40
184	Simulation of deep eutectic solvents: Progress to promises. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1598.	6.2	22
185	Reinforcement Learning of Molecule Optimization with Bayesian Neural Networks. Computational Molecular Bioscience, 2021, 11, 69-83.	0.6	1
186	DeepGAN: Generating Molecule for Drug Discovery Based on Generative Adversarial Network. , 2021, , .		2
187	De Novo Drug Property Prediction using Graph Convolutional Neural Networks. , 2021, , .		3
188	Integration of Machine Learning and Coarse-Grained Molecular Simulations for Polymer Materials: Physical Understandings and Molecular Design. Frontiers in Chemistry, 2021, 9, 820417.	1.8	17
190	Towards artificial intelligence at scale in the chemical industry. AICHE Journal, 2022, 68, .	1.8	12
191	Prediction of the photoelectrochemical performance of hematite electrodes using analytical data. Analyst, The, 2022, 147, 1313-1320.	1.7	4
192	Predicting compositional changes of organicâ€“inorganic hybrid materials with Augmented CycleGAN. , 2022, 1, 255-265.		3

#	Article	IF	Citations
193	Inverse design of 3d molecular structures with conditional generative neural networks. Nature Communications, 2022, 13, 973.	5.8	70
194	Design of potent antimalarials with generative chemistry. Nature Machine Intelligence, 2022, 4, 180-186.	8.3	17
195	Molecular Property Prediction and Molecular Design Using a Supervised Grammar Variational Autoencoder. Journal of Chemical Information and Modeling, 2022, 62, 817-828.	2.5	7
196	A review of molecular representation in the age of machine learning. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	75
197	Machine Learningâ€“Assisted Design of Material Properties. Annual Review of Chemical and Biomolecular Engineering, 2022, 13, 235-254.	3.3	13
198	Machine intelligence for chemical reaction space. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	30
199	Generative models for molecular discovery: Recent advances and challenges. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	78
200	Deep Generative Models for Materials Discovery and Machine Learning-Accelerated Innovation. Frontiers in Materials, 2022, 9, .	1.2	19
201	De novo creation of a naked eyeâ€“detectable fluorescent molecule based on quantum chemical computation and machine learning. Science Advances, 2022, 8, eabj3906.	4.7	14
202	pyscreener: A Python Wrapper for Computational Docking Software. Journal of Open Source Software, 2022, 7, 3950.	2.0	2
203	Compoundâ€“protein interaction prediction by deep learning: Databases, descriptors and models. Drug Discovery Today, 2022, 27, 1350-1366.	3.2	23
204	Artificial Intelligent Deep Learning Molecular Generative Modeling of Scaffold-Focused and Cannabinoid CB2 Target-Specific Small-Molecule Sublibraries. Cells, 2022, 11, 915.	1.8	8
205	Uncertainty estimation in deep learningâ€based property models: Graph neural networks applied to the critical properties. AICHE Journal, 2022, 68, .	1.8	10
206	On the Value of Using 3D Shape and Electrostatic Similarities in Deep Generative Methods. Journal of Chemical Information and Modeling, 2022, 62, 1388-1398.	2.5	11
207	Machine Learning in Materials Chemistry: An Invitation. Machine Learning With Applications, 2022, 8, 100265.	3.0	12
208	Surrogate-Based Black-Box Optimization Method for Costly Molecular Properties. , 2021, , .		1
209	Conditional Wasserstein generative adversarial networks applied to acoustic metamaterial design. Journal of the Acoustical Society of America, 2021, 150, 4362-4374.	0.5	14
210	Active Site Sequence Representations of Human Kinases Outperform Full Sequence Representations for Affinity Prediction and Inhibitor Generation: 3D Effects in a 1D Model. Journal of Chemical Information and Modeling, 2022, 62, 240-257.	2.5	14

#	Article	IF	Citations
211	Comprehensive assessment of deep generative architectures for de novo drug design. Briefings in Bioinformatics, 2022, 23, .	3.2	9
212	Automated Molecule Generation using Deep Q-Learning and Graph Neural Networks. , 2021, , .		2
213	Identification of miRNA-Small Molecule Associations by Continuous Feature Representation Using Auto-Encoders. Pharmaceutics, 2022, 14, 3.	2.0	2
214	Artificial intelligence: machine learning for chemical sciences. Journal of Chemical Sciences, 2022, 134, 2.	0.7	32
215	An open-source framework for fast-yet-accurate calculation of quantum mechanical features. Physical Chemistry Chemical Physics, 2022, , .	1.3	1
216	Dataâ€Driven Materials Innovation and Applications. Advanced Materials, 2022, 34, e2104113.	11.1	51
217	Beyond Woodwardâ€“Fieser Rules: Design Principles of Property-Oriented Chromophores Based on Explainable Deep Learning Optical Spectroscopy. Journal of Chemical Information and Modeling, 2022, 62, 2933-2942.	2.5	0
218	Graph-based molecular Pareto optimisation. Chemical Science, 2022, 13, 7526-7535.	3.7	8
219	Approaches for enhancing the analysis of chemical space for drug discovery. Expert Opinion on Drug Discovery, 2022, 17, 789-798.	2.5	8
220	AI-Aided Design of Novel Targeted Covalent Inhibitors against SARS-CoV-2. Biomolecules, 2022, 12, 746.	1.8	43
221	MSNovelist: de novo structure generation from mass spectra. Nature Methods, 2022, 19, 865-870.	9.0	49
222	Design and Implementation of a Multidimensional Visualization Reconstruction System for Old Urban Spaces Based on Neural Networks. Computational Intelligence and Neuroscience, 2022, 2022, 1-12.	1.1	0
223	PSI4EDUCATION: Free and Open-Source Programing Activities for Chemical Education with Free and Open-Source Software. ACS Symposium Series, 0, , 107-122.	0.5	4
224	Use of Free Energy Methods in the Drug Discovery Industry. ACS Symposium Series, 0, , 39-66.	0.5	11
225	A transfer learning approach for reaction discovery in small data situations using generative model. IScience, 2022, 25, 104661.	1.9	4
226	Chemical engineering at crossroads. Canadian Journal of Chemical Engineering, 2022, 100, 2011-2027.	0.9	3
227	Polygrammar: Grammar for Digital Polymer Representation and Generation. Advanced Science, 2022, 9, .	5.6	13
228	Fragmentâ€based drug discoveryâ€”the importance of highâ€quality molecule libraries. Molecular Oncology, 2022, 16, 3761-3777.	2.1	31

#	Article	IF	Citations
230	Fundamentals of Molecular Docking and Comparative Analysis of Proteinâ€“Small-Molecule Docking Approaches. , 0, , .		1
231	Data-driven multi-objective molecular design of ionic liquid with high generation efficiency on small dataset. Materials and Design, 2022, 220, 110888.	3.3	6
232	Design, Synthesis, Docking, DFT, MD Simulation Studies of a New Nicotinamide-Based Derivative: In Vitro Anticancer and VEGFR-2 Inhibitory Effects. Molecules, 2022, 27, 4606.	1.7	69
234	Gaussian Process Regression Machine Learning Models for Photonic Sintering. Computer Aided Chemical Engineering, 2022, , 1819-1824.	0.3	3
235	A Generative Approach to Materials Discovery, Design, and Optimization. ACS Omega, 2022, 7, 25958-25973.	1.6	13
236	Dual Self-Adaptive Intelligent Optimization of Feature and Hyperparameter Determination in Constructing a DNN Based QSPR Property Prediction Model. Industrial & Engineering Chemistry Research, 2022, 61, 12052-12060.	1.8	2
237	Novel control strategies for the endocrine-disrupting effect of PAEs to pregnant women in traffic system. Science of the Total Environment, 2022, , 158269.	3.9	6
238	Self-Focusing Virtual Screening with Active Design Space Pruning. Journal of Chemical Information and Modeling, 2022, 62, 3854-3862.	2.5	12
239	Integrating concept of pharmacophore with graph neural networks for chemical property prediction and interpretation. Journal of Cheminformatics, 2022, 14, .	2.8	5
240	MolSearch. , 2022, , .		4
241	Graph-based Automated Macro-Molecule Assembly. Journal of Chemical Information and Modeling, 2022, 62, 3714-3723.	2.5	0
242	Molecular dipole moment learning via rotationally equivariant derivative kernels in molecular-orbital-based machine learning. Journal of Chemical Physics, 2022, 157, .	1.2	2
243	Broadband Acoustic Metamaterial Design via Machine Learning. Journal of Theoretical and Computational Acoustics, 2022, 30, .	0.5	6
244	A diversity maximizing active learning strategy for graph neural network models of chemical properties. Molecular Systems Design and Engineering, 2022, 7, 1697-1706.	1.7	1
245	<i>Commentary</i>: Unexpected Novel Chemical Weapon Agents Designed by Innocuous Drug-Development AI (Artificial Intelligence) Algorithm. Pharmacology & Pharmacy, 2022, 13, 225-229.	0.2	1
246	Generative Approaches for the Synthesis of Process Structures. Computer Aided Chemical Engineering, 2022, , 289-294.	0.3	2
247	Implementation of an AI-assisted fragment-generator in an open-source platform. RSC Medicinal Chemistry, 2022, 13, 1205-1211.	1.7	1
248	SMICLR: Contrastive Learning on Multiple Molecular Representations for Semisupervised and Unsupervised Representation Learning. Journal of Chemical Information and Modeling, 2022, 62, 3948-3960.	2.5	10

#	Article	IF	Citations
249	Building Chemical Property Models for Energetic Materials from Small Datasets Using a Transfer Learning Approach. Journal of Chemical Information and Modeling, 2022, 62, 5397-5410.	2.5	11
250	Assessing Deep Generative Models in Chemical Composition Space. Chemistry of Materials, 2022, 34, 9455-9467.	3.2	10
251	Graph representation learning in biomedicine and healthcare. Nature Biomedical Engineering, 2022, 6, 1353-1369.	11.6	51
252	Addressing Noise and Estimating Uncertainty in Biomedical Data through the Exploration of Chemical Space. International Journal of Molecular Sciences, 2022, 23, 12975.	1.8	0
253	AugLiChem: data augmentation library of chemical structures for machine learning. Machine Learning: Science and Technology, 2022, 3, 045015.	2.4	9
254	Application of SMILES-based molecular generative model in new drug design. Frontiers in Pharmacology, 0, 13, .	1.6	0
255	Molecular-orbital-based machine learning for open-shell and multi-reference systems with kernel addition Gaussian process regression. Journal of Chemical Physics, 2022, 157, .	1.2	3
256	Adversarial deep evolutionary learning for drug design. BioSystems, 2022, 222, 104790.	0.9	2
257	Unveiling the potential of Lichtheimia ramosa AJP11 for myco-transformation of polystyrene sulfonate and its driving molecular mechanism. Journal of Environmental Management, 2023, 325, 116579.	3.8	1
258	Generative multiscale analysis of de novo proteome-inspired molecular structures and nanomechanical optimization using a VoxelPerceiver transformer model. Journal of the Mechanics and Physics of Solids, 2023, 170, 105098.	2.3	8
259	Data-driven discovery of molecular photoswitches with multioutput Gaussian processes. Chemical Science, 2022, 13, 13541-13551.	3.7	12
260	GCN-Based Structure-Activity Relationship and DFT Studies of Staphylococcus aureus FabI Inhibitors. International Journal of Quantitative Structure-Property Relationships, 2022, 7, 1-16.	1.1	0
261	A New Theobromine-Based EGFRWT and EGFRT790M Inhibitor and Apoptosis Inducer: Design, Semi-Synthesis, Docking, DFT, MD Simulations, and In Vitro Studies. Processes, 2022, 10, 2290.	1.3	10
263	Predictive chemistry: machine learning for reaction deployment, reaction development, and reaction discovery. Chemical Science, 2023, 14, 226-244.	3.7	26
264	Cell morphology-guided de novo hit design by conditioning GANs on phenotypic image features. , 2023, 2, 91-102.		4
265	Predicting Synergistic Drug Interaction with DNN and GAT. , 2022, , .		3
266	An Improved Model for Predicting Compound Retrosynthesizability Using Machine Learning. , 2022, , .		2
267	Digital advancements in smart materials design and multifunctional coating manufacturing. Physics Open, 2023, 14, 100133.	0.7	4

#	Article	IF	Citations
268	Application of Machine Learning to the Design of Energetic Materials: Preliminary Experience and Comparison with Alternative Techniques. Propellants, Explosives, Pyrotechnics, 2023, 48, .	1.0	5
269	Perspectives of Machine Learning Development on Kerogen Molecular Model Reconstruction and Shale Oil/Gas Exploitation. Energy & Fuels, 2023, 37, 98-117.	2.5	4
270	Graph machine learning for design of highâ€octane fuels. AICHE Journal, 2023, 69, .	1.8	7
271	PETrans: De Novo Drug Design with Protein-Specific Encoding Based on Transfer Learning. International Journal of Molecular Sciences, 2023, 24, 1146.	1.8	8
272	Transferring chemical and energetic knowledge between molecular systems with machine learning. Communications Chemistry, 2023, 6, .	2.0	0
273	Molecular Generative Model via Retrosynthetically Prepared Chemical Building Block Assembly. Advanced Science, 2023, 10, .	5.6	7
274	Proteinâ€“ligand binding affinity prediction with edge awareness and supervised attention. IScience, 2023, 26, 105892.	1.9	6
276	GVA: Gated Variational Autoencoder for de novo molecule generation. , 2022, , .		0
277	A Review on Artificial Intelligence Enabled Design, Synthesis, and Process Optimization of Chemical Products for Industry 4.0. Processes, 2023, 11, 330.	1.3	11
278	Molecular Property Prediction of Modified Gedunin Using Machine Learning. Molecules, 2023, 28, 1125.	1.7	2
279	Definition and exploration of realistic chemical spaces using the connectivity and cyclic features of ChEMBL and ZINC. , 2023, 2, 736-747.		1
280	Deep Learning Methods for Small Molecule Drug Discovery: A Survey. IEEE Transactions on Artificial Intelligence, 2024, 5, 459-479.	3.4	0
282	Quantum chemical data generation as fill-in for reliability enhancement of machine-learning reaction and retrosynthesis planning. , 2023, 2, 663-673.		2
283	Identification of dominant factors contributing to photocurrent density of BiVO4 photoanodes using Machine learning. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 440, 114651.	2.0	3
284	Deep Learning based Hand-Drawn Molecular Structure Recognition and 3D Visualisation using Augmented Reality. , 2022, , .		1
285	Chemical language models for de novo drug design: Challenges and opportunities. Current Opinion in Structural Biology, 2023, 79, 102527.	2.6	15
286	Physicsâ€informed Transfer Learning for Outâ€ofâ€sample Vapor Pressure Predictions. Propellants, Explosives, Pyrotechnics, 2023, 48, .	1.0	4
287	High-throughput property-driven generative design of functional organic molecules. Nature Computational Science, 2023, 3, 139-148.	3.8	15

#	Article	IF	Citations
288	UnCorrupt SMILES: a novel approach to de novo design. Journal of Cheminformatics, 2023, 15, .	2.8	5
289	Future of computational molecular spectroscopyâ€"from supporting interpretation to leading the innovation. Physical Chemistry Chemical Physics, 2023, 25, 7090-7105.	1.3	4
290	Integrating structure-based approaches in generative molecular design. Current Opinion in Structural Biology, 2023, 79, 102559.	2.6	16
291	Treat Molecular Linear Notations as Sentences: Accurate Quantitative Structureâ€"Property Relationship Modeling via a Natural Language Processing Approach. Industrial & Engineering Chemistry Research, 2023, 62, 5336-5346.	1.8	4
293	Machine-learning accelerated annealing with fitting-search style for multicomponent alloy structure predictions. Physical Review Materials, 2023, 7, .	0.9	0
294	De novo drug design based on Stack-RNN with multi-objective reward-weighted sum and reinforcement learning. Journal of Molecular Modeling, 2023, 29, .	0.8	2
295	Testing the limits of SMILES-based de novo molecular generation with curriculum and deep reinforcement learning. Nature Machine Intelligence, 2023, 5, 386-394.	8.3	9
296	Reorganization Energy Predictions with Graph Neural Networks Informed by Low-Cost Conformers. Journal of Physical Chemistry A, 2023, 127, 3484-3489.	1.1	4
297	Regression Transformer enables concurrent sequence regression and generation for molecular language modelling. Nature Machine Intelligence, 2023, 5, 432-444.	8.3	19
298	Substituted Oligosaccharides as Protein Mimics: Deep Learning Free Energy Landscapes. Journal of Chemical Information and Modeling, 0, , .	2.5	0
299	Principles and requirements for nanomaterial representations to facilitate machine processing and cooperation with nanoinformatics tools. Journal of Cheminformatics, 2023, 15, .	2.8	3
300	Advancing Drug Discovery with Deep Learning: Harnessing Reinforcement Learning and One-Shot Learning for Molecular Design in Low-Data Situations. ACM SIGAPP Applied Computing Review: A Publication of the Special Interest Group on Applied Computing, 2023, 23, 36-48.	0.5	1
301	Direct De Novo Molecule Generation Using Probabilistic Diverse Variational Autoencoder. Lecture Notes in Networks and Systems, 2023, , 13-22.	0.5	0
306	Deep learning methodologies in drug design. , 2023, , 361-392.		0
307	Recent advances in deep learning enabled approaches for identification of molecules of therapeutics relevance. , 2023, , 503-518.		0
319	Open-Source Machine Learning in Computational Chemistry. Journal of Chemical Information and Modeling, 2023, 63, 4505-4532.	2.5	3
328	Graph Neural Networks for Molecules. Challenges and Advances in Computational Chemistry and Physics, 2023, , 21-66.	0.6	3
336	Constructive Machine Learning andÂHierarchical Multi-label Classification forÂMolecules Design. Lecture Notes in Computer Science, 2023, , 276-290.	1.0	0

#	Article	IF	Citations
354	Unlocking New Possibilities in Drug Discovery: A GAN-Based Approach. , 2023, , 135-144.		1
357	Deep learning algorithms applied to computational chemistry. Molecular Diversity, 0, , .	2.1	0
359	Graph Neural Networks for the Prediction of Molecular Structureâ€“Property Relationships. , 2023, , 159-181.		0