The rise of deep learning in drug discovery

DOI: 10.1016/j.drudis.2018.01.039
Drug Discovery Today, 2018, 23, 1241-1250.

#	Paper	IF	Citations
852	Understanding Medication Nonadherence from Social Media: A Sentiment-Enriched Deep Learning Approach. **2017**,		2
851	Comparing and Validating Machine Learning Models for Mycobacterium tuberculosis Drug Discovery. **2018**, 15, 4346-4360		66
850	Prediction of Compound Profiling Matrices Using Machine Learning. **2018**, 3, 4713-4723		23
849	Uses of Artificial Intelligence in Health. **2018**,		
848	Learning Framework in the Industrial Age 4.0 in Higher Education. **2018**,		4
847	A System for Learning Atoms Based on Long Short-Term Memory Recurrent Neural Networks. **2018** ,		6
846	An overview of neural networks for drug discovery and the inputs used. **2018**, 13, 1091-1102		18
845	A review on machine learning methods for in silico toxicity prediction. **2018**, 36, 169-191		37
844	Potential of quantum computing for drug discovery. **2018**, 62, 6:1-6:20		47
843	Precision pharmacotherapy: psychiatry's future direction in preventing, diagnosing, and treating mental disorders. **2018**, 11, 211-222		17
842	The convergence of artificial intelligence and chemistry for improved drug discovery. **2018**, 10, 2573-2576		14
841	Artificial Intelligence in Drug Design. **2018**, 23,		107
840	Prediction of Compound Profiling Matrices, Part II: Relative Performance of Multitask Deep Learning and Random Forest Classification on the Basis of Varying Amounts of Training Data. **2018**, 3, 12033-12040		12
839	Deep Learning in Drug Discovery and Medicine; Scratching the Surface. **2018**, 23,		38
838	Graphic Encoding of Macromolecules for Efficient High-Throughput Analysis. **2018**,		3
837	How far have decision tree models come for data mining in drug discovery?. **2018**, 13, 1067-1069		9
836	Entangled Conditional Adversarial Autoencoder for de Novo Drug Discovery. **2018**, 15, 4398-4405		99

835	Novel applications of Machine Learning in cheminformatics. **2018**, 10, 46		2
834	Recent applications of machine learning in medicinal chemistry. **2018**, 28, 2807-2815		59
833	G-quadruplex virtual drug screening: A review. **2018**, 152, 134-148		27
832	Insight Analysis of Promiscuous Estrogen Receptor Ligand Binding by a Novel Machine Learning Scheme. **2018**, 31, 799-813		3
831	Machine learning in chemoinformatics and drug discovery. *Drug Discovery Today*, **2018**, 23, 1538-1546	8.8	382
830	Comparing Multiple Machine Learning Algorithms and Metrics for Estrogen Receptor Binding Prediction. **2018**, 15, 4361-4370		80
829	Accelerating Drugs Discovery with Deep Reinforcement Learning. **2018**,		2
828	Expanding the medicinal chemistry synthetic toolbox. **2018**, 17, 709-727		223
827	Discovering Highly Potent Molecules from an Initial Set of Inactives Using Iterative Screening. **2018**, 58, 2000-2014		21
826	Drug-Induced Rhabdomyolysis Atlas (DIRA) for idiosyncratic adverse drug reaction management. *Drug Discovery Today*, **2019**, 24, 9-15	8.8	12
825	Learning for Personalized Medicine: A Comprehensive Review From a Deep Learning Perspective. **2019**, 12, 194-208		25
824	Delfos: deep learning model for prediction of solvation free energies in generic organic solvents. **2019**, 10, 8306-8315		28
823	Reaction-Based Enumeration, Active Learning, and Free Energy Calculations To Rapidly Explore Synthetically Tractable Chemical Space and Optimize Potency of Cyclin-Dependent Kinase 2 Inhibitors. **2019**, 59, 3782-3793		33
822	Deep learning in drug discovery: opportunities, challenges and future prospects. *Drug Discovery Today*, **2019**, 24, 2017-2032	8.8	101
821	From Target to Drug: Generative Modeling for the Multimodal Structure-Based Ligand Design. **2019**, 16, 4282-4291		29
820	Securing the future of research computing in the biosciences. **2019**, 15, e1006958		1
819	Concepts of Artificial Intelligence for Computer-Assisted Drug Discovery. **2019**, 119, 10520-10594		243
818	Parkinson's Disease Detection Using Isosurfaces-Based Features and Convolutional Neural Networks. **2019**, 13, 48		30

817	Applicability Domain of Active Learning in Chemical Probe Identification: Convergence in Learning from Non-Specific Compounds and Decision Rule Clarification. **2019**, 24,	5
816	A deep convolutional neural network for the estimation of gas chromatographic retention indices. **2019**, 1607, 460395	23
815	Automated de novo molecular design by hybrid machine intelligence and rule-driven chemical synthesis. **2019**, 1, 307-315	30
814	Toward Explainable Anticancer Compound Sensitivity Prediction via Multimodal Attention-Based Convolutional Encoders. **2019**, 16, 4797-4806	43
813	Has Drug Design Augmented by Artificial Intelligence Become a Reality?. **2019**, 40, 806-809	20
812	STS-NLSP: A Network-Based Label Space Partition Method for Predicting the Specificity of Membrane Transporter Substrates Using a Hybrid Feature of Structural and Semantic Similarity. **2019**, 7, 306	8
811	Improving Strong-Scaling of CNN Training by Exploiting Finer-Grained Parallelism. **2019**,	14
810	Shortcuts to schistosomiasis drug discovery: The state-of-the-art. **2019**, 139-180	2
809	Rethinking Drug Repositioning and Development with Artificial Intelligence, Machine Learning, and Omics. **2019**, 23, 539-548	38
808	Process-Guided Deep Learning Predictions of Lake Water Temperature. **2019**, 55, 9173-9190	78
807	Deep Transferable Compound Representation across Domains and Tasks for Low Data Drug Discovery. **2019**, 59, 4528-4539	13
806	Machine Learning with Digital Microfluidics for Drug Discovery and Development. **2019**,	0
805	Multi-Channel CNN Based Inner-Attention for Compound Sentence Relation Classification. **2019**, 7, 141801-141809	18
804	Systems Biology of Cancer Metastasis. **2019**, 9, 109-127	85
803	Synthetic organic chemistry driven by artificial intelligence. **2019**, 3, 589-604	86
802	Novel Big Data Approach for Drug Prediction in Health Care Systems. **2019**,	5
801	Tutorial. **2019**,	1
800	ATC-NLSP: Prediction of the Classes of Anatomical Therapeutic Chemicals Using a Network-Based Label Space Partition Method. **2019**, 10, 971	13

799	Phenotypic Profiling of High Throughput Imaging Screens with Generic Deep Convolutional Features. **2019**,	3
798	DeepFunNet: Deep Learning for Gene Functional Similarity Network Construction. **2019**,	
797	Learning Drug Functions from Chemical Structures with Convolutional Neural Networks and Random Forests. **2019**, 59, 4438-4449	29
796	Deep separable convolutional network for remaining useful life prediction of machinery. **2019**, 134, 106330	102
795	Neural-based approaches to overcome feature selection and applicability domain in drug-related property prediction. **2019**, 85, 105777	5
794	LightGBM: An Effective and Scalable Algorithm for Prediction of Chemical Toxicity-Application to the Tox21 and Mutagenicity Data Sets. **2019**, 59, 4150-4158	59
793	Ontology-Based Healthcare Named Entity Recognition from Twitter Messages Using a Recurrent Neural Network Approach. **2019**, 16,	19
792	Label aided deep ranking for the automatic diagnosis of Parkinsonian syndromes. **2019**, 330, 162-171	3
791	Could advances in representation learning in Artificial Intelligence provide the new paradigm for data integration in drug discovery?. **2019**, 14, 191-194	1
790	Learning continuous and data-driven molecular descriptors by translating equivalent chemical representations. **2019**, 10, 1692-1701	152
789	Hammett neural networks: prediction of frontier orbital energies of tungsten-benzylidyne photoredox complexes. **2019**, 10, 6844-6854	6
788	KekuleScope: prediction of cancer cell line sensitivity and compound potency using convolutional neural networks trained on compound images. **2019**, 11, 41	29
787	Reliable Prediction Errors for Deep Neural Networks Using Test-Time Dropout. **2019**, 59, 3330-3339	18
786	Biomicrofluidic Systems for Hematologic Cancer Research and Clinical Applications. **2019**, 24, 457-476	6
785	Precise Modeling of the Protective Effects of Quercetin against Mycotoxin via System Identification with Neural Networks. **2019**, 20,	2
784	An exploration strategy improves the diversity of de novo ligands using deep reinforcement learning: a case for the adenosine A receptor. **2019**, 11, 35	29
783	Applications of deep learning for the analysis of medical data. **2019**, 42, 492-504	29
782	Binding affinity in drug design: experimental and computational techniques. **2019**, 14, 755-768	36

781	Deep Learning in Chemistry. **2019**, 59, 2545-2559	164
780	Comparing Deep and Machine Learning Approaches in Bioinformatics: A miRNA-Target Prediction Case Study. **2019**, 31-44	1
779	Deep Learning to Therapeutically Target Unreported Complexes. **2019**, 40, 551-554	1
778	Ovarian cancer: time to move beyond one size fits all. **2019**, 20, 754-755	2
777	Exploring the GDB-13 chemical space using deep generative models. **2019**, 11, 20	67
776	Discovering Barriers to Opioid Addiction Treatment from Social Media: A Similarity Network-Based Deep Learning Approach. **2019**,	
775	The Future of Medical Imaging. **2018**, 24, 5487-5488	
774	Quantitative structure-activity relationship models for compounds with anticonvulsant activity. **2019**, 14, 653-665	3
773	Cheminformatics techniques in antimalarial drug discovery and development from natural products 1: basic concepts. **2019**, 4,	1
772	Exploiting machine learning for end-to-end drug discovery and development. **2019**, 18, 435-441	191
771	The significance of artificial intelligence in drug delivery system design. **2019**, 151-152, 169-190	71
770	Search for Catalysts by Inverse Design: Artificial Intelligence, Mountain Climbers, and Alchemists. **2019**, 119, 6595-6612	90
769	Parallel Computing in Deep Learning: Bioinformatics Case Studiesa. **2019**,	
768	Computational advances in combating colloidal aggregation in drug discovery. **2019**, 11, 402-418	35
767	Prediction of Different Classes of Promiscuous and Nonpromiscuous Compounds Using Machine Learning and Nearest Neighbor Analysis. **2019**, 4, 6883-6890	14
766	Analytics and Big Data: Emerging trends and their impact on our lives. **2019**, 19, e1944	1
765	From chemoinformatics to deep learning: an open road to drug discovery. **2019**, 11, 371-374	5
764	Autonomous Molecular Design: Then and Now. **2019**, 11, 24825-24836	48

763	GuacaMol: Benchmarking Models for de Novo Molecular Design. **2019**, 59, 1096-1108	174
762	A new wave of innovation in Semantic web tools for drug discovery. **2019**, 14, 433-444	13
761	Deep learning opens new horizons in personalized medicine. **2019**, 10, 215-217	20
760	PySpark and RDKit: Moving towards Big Data in Cheminformatics. **2019**, 38, e1800082	26
759	Machine Learning Prediction of DNA Charge Transport. **2019**,	
758	Computational Drug Design Methods□Current and Future Perspectives. **2019**, 19-44	29
757	Automated discovery of GPCR bioactive ligands. **2019**, 55, 17-24	5
756	Is one-shot learning a viable option in drug discovery?. **2019**, 14, 601-603	8
755	Machine Learning Prediction of DNA Charge Transport. **2019**, 123, 2801-2811	17
754	Deep-learning-based target screening and similarity search for the predicted inhibitors of the pathways in Parkinson's disease.. **2019**, 9, 10326-10339	20
753	Applications of machine learning in drug discovery and development. **2019**, 18, 463-477	558
752	Approaches for the discovery of metallo-□lactamase inhibitors: A review. **2019**, 94, 1427-1440	12
751	Prediction of Dengue-Human Protein Interaction Using Artificial Neural Network for Anti-Viral Drug Discovery. **2019**,	0
750	Predicting Ion Mobility Collision Cross-Sections Using a Deep Neural Network: DeepCCS. **2019**, 91, 5191-5199	56
749	From personalization to patient centered systems toxicology and pharmacology. **2019**, 11, 14-22	2
748	Automated De Novo Drug Design: Are We Nearly There Yet?. **2019**, 58, 10792-10803	60
747	Roles of computational modelling in understanding p53 structure, biology, and its therapeutic targeting. **2019**, 11, 306-316	11
746	Automated De Novo Drug Design: Are We Nearly There Yet?. **2019**, 131, 10906-10917	9

745	An overview on the mathematical modeling of hydrogels' behavior for drug delivery systems. **2019**, 560, 175-190	43
744	Una guã conceptual para usar y entender Big Data en la investigaciñ clñica. **2019**, 30, 83-94	0
743	Daily Natural Gas Load Forecasting Based on a Hybrid Deep Learning Model. **2019**, 12, 218	19
742	Imputation of Assay Bioactivity Data Using Deep Learning. **2019**, 59, 1197-1204	25
741	GrEDeL: A Knowledge Graph Embedding Based Method for Drug Discovery From Biomedical Literatures. **2019**, 7, 8404-8415	23
740	Editorial for the Special Section "Artificial Intelligence in Drug Discovery". **2019**, 32-33, 1-2	
739	PFDLIS: Privacy-Preserving and Fair Deep Learning Inference Service under Publicly Verifiable Covert Security Setting. **2019**, 8, 1488	1
738	Regression Model for Civil Aero-engine Gas Path Parameter Deviations Based on Res-BP Neural Network. **2019**,	
737	A de novo molecular generation method using latent vector based generative adversarial network. **2019**, 11, 74	78
736	Assisting human experts in the interpretation of their visual process: A case study on assessing copper surface adhesive potency. **2019**,	
735	Attention-based Multi-Input Deep Learning Architecture for Biological Activity Prediction: An Application in EGFR Inhibitors. **2019**,	2
734	Cardiotoxicity Prediction Based on Integreted hERG Database with Molecular Convolution Model. **2019**,	
733	Comparison Study of Computational Prediction Tools for Drug-Target Binding Affinities. **2019**, 7, 782	33
732	Deep Learning for Deep Chemistry: Optimizing the Prediction of Chemical Patterns. **2019**, 7, 809	52
731	Framework for Inverse Mapping Chemistry-Agnostic Coarse-Grained Simulation Models into Chemistry-Specific Models. **2019**, 59, 5045-5056	2
730	The METLIN small molecule dataset for machine learning-based retention time´ prediction. **2019**, 10, 5811	50
729	Autonomous Visual Navigation using Deep Reinforcement Learning: An Overview. **2019**,	1
728	Smart Health. **2019**,	0

727	Randomized SMILES strings improve the quality of molecular generative models. **2019**, 11, 71		74
726	Concepts and Core Principles of Fragment-Based Drug Design. **2019**, 24,		45
725	Applications of Deep-Learning in Exploiting Large-Scale and Heterogeneous Compound Data in Industrial Pharmaceutical Research. **2019**, 10, 1303		26
724	A Graphic Encoding Method for Quantitative Classification of Protein Structure and Representation of Conformational Changes. **2021**, 18, 1336-1349		3
723	Efficient learning of non-autoregressive graph variational autoencoders for molecular graph generation. **2019**, 11, 70		28
722	Opportunities for Artificial Intelligence in Advancing Precision Medicine. **2019**, 7, 208-213		23
721	Development and Validation of a New High-Performance Liquid Chromatography Method for the Simultaneous Quantification of Coenzyme Q10, Phosphatidylserine, and Vitamin C from a Cutting-Edge Liposomal Vehiculization. **2019**, 4, 19710-19715		1
720	Improving the drug discovery process by using multiple classifier systems. **2019**, 121, 292-303		11
719	Exploring Tunable Hyperparameters for Deep Neural Networks with Industrial ADME Data Sets. **2019**, 59, 1005-1016		26
718	Using Drug Expression Profiles and Machine Learning Approach for Drug Repurposing. **2019**, 1903, 219-237		15
717	Formatting biological big data for modern machine learning in drug discovery. **2019**, 9, e1408		6
716	Dissecting Machine-Learning Prediction of Molecular Activity: Is an Applicability Domain Needed for Quantitative Structure-Activity Relationship Models Based on Deep Neural Networks?. **2019**, 59, 117-126		25
715	Application of Bioactivity Profile-Based Fingerprints for Building Machine Learning Models. **2019**, 59, 962-972		14
714	Artificial intelligence in drug development: present status and future prospects. *Drug Discovery Today*, **2019**, 24, 773-780	8.8	202
713	Prediction of higher-selectivity catalysts by computer-driven workflow and machine learning. **2019**, 363,		165
712	Discovery of CDK4´ inhibitors by convolutional neural networks. **2018**,		11
711	Finding the Right Bricks for Molecular Legos: A Data Mining Approach to Organic Semiconductor Design. **2019**, 31, 969-978		30
710	Recent Advancements in Computing Reliable Binding Free Energies in Drug Discovery Projects. **2019**, 221-246		1

709	Advances and challenges in deep generative models for de novo molecule generation. **2019**, 9, e1395	20
708	Deep Confidence: A Computationally Efficient Framework for Calculating Reliable Prediction Errors for Deep Neural Networks. **2019**, 59, 1269-1281	40
707	De Novo Molecule Design by Translating from Reduced Graphs to SMILES. **2019**, 59, 1136-1146	25
706	Models and Machines: How Deep Learning Will Take Clinical Pharmacology to the Next Level. **2019**, 8, 131-134	22
705	Advances with support vector machines for novel drug discovery. **2019**, 14, 23-33	28
704	Practical Model Selection for Prospective Virtual Screening. **2019**, 59, 282-293	27
703	Closed-loop discovery platform integration is needed for artificial intelligence to make an impact in drug discovery. **2019**, 14, 1-4	19
702	Prediction of aqueous solubility of compounds based on neural network. **2020**, 118, e1600754	7
701	The importance of interpretability and visualization in machine learning for applications in medicine and health care. **2020**, 32, 18069-18083	88
700	Automated Machine Learning Diagnostic Support System as a Computational Biomarker for Detecting Drug-Induced Liver Injury Patterns in Whole Slide Liver Pathology Images. **2020**, 18, 1-10	6
699	Graph convolutional networks for computational drug development and discovery. **2020**, 21, 919-935	87
698	Genetic modification to improve disease resistance in crops. **2020**, 225, 70-86	70
697	Deep Learning for Predictive Analytics in Healthcare. **2020**, 32-42	1
696	The impact of artificial intelligence in the diagnosis and management of glaucoma. **2020**, 34, 1-11	27
695	Autonomous Discovery in the Chemical Sciences Part I: Progress. **2020**, 59, 22858-22893	75
694	Autonome Entdeckung in den chemischen Wissenschaften, Teil I: Fortschritt. **2020**, 132, 23054-23091	5
693	Prediction carbon dioxide solubility in ionic liquids based on deep learning. **2020**, 118, e1652367	9
692	From machine learning to deep learning: Advances in scoring functions for protein□gand docking. **2020**, 10, e1429	65

691	Programmable One-Pot Synthesis of Oligosaccharides. **2020**, 59, 3078-3088		14
690	Nanoarchitectonics for Nanocarbon Assembly and Composite. **2020**, 30, 42-55		12
689	A drug-likeness toolbox facilitates ADMET study in drug discovery. *Drug Discovery Today*, **2020**, 25, 248-258		72
688	A hybrid deep learning model for efficient intrusion detection in big data environment. **2020**, 513, 386-396		92
687	Inverse-QSPR for de novo Design: A Review. **2020**, 39, e1900087		17
686	Computational/in silico methods in drug target and lead prediction. **2020**, 21, 1663-1675		40
685	Financial quantitative investment using convolutional neural network and deep learning technology. **2020**, 390, 384-390		11
684	Antidepressant-like effects of Xiaochaihutang in perimenopausal mice. **2020**, 248, 112318		16
683	Undistorted 180´ ° phase reversal of magnetoelectric coupling in bi-layered multiferroic laminate. **2020**, 494, 165802		3
682	Key indicators of phase transition for clinical trials through machine learning. *Drug Discovery Today*, **2020**, 25, 414-421	8.8	11
681	Multiscale modelling of drug mechanism and safety. *Drug Discovery Today*, **2020**, 25, 519-534	8.8	10
680	Less may be more: an informed reflection on molecular descriptors for drug design and discovery. **2020**, 5, 317-329		3
679	Scaffold-based molecular design with a graph generative model. **2019**, 11, 1153-1164		41
678	Deep-learning- and pharmacophore-based prediction of RAGE inhibitors. **2020**, 17, 036003		4
677	Mol-CycleGAN: a generative model for molecular optimization. **2020**, 12, 2		57
676	Exploration of flow reaction conditions using machine-learning for enantioselective organocatalyzed Rauhut-Currier and [3+2] annulation sequence. **2020**, 56, 1259-1262		19
675	Anthelmintics in the future: current trends in the discovery and development of new drugs against gastrointestinal nematodes. *Drug Discovery Today*, **2020**, 25, 430-437	8.8	20
674	Systematic Modeling of log Based on Ensemble Machine Learning, Group Contribution, and Matched Molecular Pair Analysis. **2020**, 60, 63-76		20

673	Populating Chemical Space with Peptides Using a Genetic Algorithm. **2020**, 60, 121-132	8
672	Artificial Intelligence Steering Molecular Therapy in the Absence of Information on Target Structure and Regulation. **2020**, 60, 460-466	1
671	A novel molecular representation with BiGRU neural networks for learning atom. **2020**, 21, 2099-2111	29
670	Harnessing big 'omics' data and AI for drug discovery in hepatocellular carcinoma. **2020**, 17, 238-251	43
669	Molecular Insights from Conformational Ensembles via Machine Learning. **2020**, 118, 765-780	27
668	Machine learning applications in drug development. **2020**, 18, 241-252	57
667	Applying machine learning to predict the tensile shear strength of bonded beech wood as a function of the composition of polyurethane prepolymers and various pretreatments. **2020**, 54, 19-29	8
666	Detecting bursty terms in computer science research. **2020**, 122, 681-699	9
665	Molecular Generative Model Based on an Adversarially Regularized Autoencoder. **2020**, 60, 29-36	22
664	Deep learning of pharmacogenomics resources: moving towards precision oncology. **2020**, 21, 2066-2083	19
663	Designing phononic crystal with anticipated band gap through a deep learning based data-driven method. **2020**, 361, 112737	50
662	DeepMalaria: Artificial Intelligence Driven Discovery of Potent Antiplasmodials. **2019**, 10, 1526	24
661	Deregulation of Chromosome Segregation and Cancer. **2020**, 4, 257-278	2
660	Chemometrics for QSAR Modeling. **2020**, 599-634	5
659	QN-Docking: An innovative molecular docking methodology based on Q-Networks. **2020**, 96, 106678	1
658	Spectrum of deep learning algorithms in drug discovery. **2020**, 96, 886-901	6
657	IoTPulse: machine learning-based enterprise health information system to predict alcohol addiction in Punjab (India) using IoT and fog computing. **2020**, 1-33	9
656	A Recurrent Neural Network model to predict blood-brain barrier permeability. **2020**, 89, 107377	11

655	FPSC-DTI: drug-target interaction prediction based on feature projection fuzzy classification and super cluster fusion. **2020**, 16, 583-591	3
654	Computer-Aided Drug Design. **2020**,	4
653	Prediction of Energetic Material Properties from Electronic Structure Using 3D Convolutional Neural Networks. **2020**, 60, 4457-4473	14
652	Artificial neural networks for the prediction of solvation energies based on experimental and computational data. **2020**, 22, 24359-24364	8
651	Multitask deep networks with grid featurization achieve improved scoring performance for protein-ligand binding. **2020**, 96, 973-983	4
650	Data-Driven Molecular Dynamics: A Multifaceted Challenge. **2020**, 13,	10
649	SyntaLinker: automatic fragment linking with deep conditional transformer neural networks. **2020**, 11, 8312-8322	22
648	The Advent of Generative Chemistry. **2020**, 11, 1496-1505	30
647	Transfer Learning for Drug Discovery. **2020**, 63, 8683-8694	54
646	SCAM Detective: Accurate Predictor of Small, Colloidally Aggregating Molecules. **2020**, 60, 4056-4063	10
645	Effective Molecular Descriptors for Chemical Accuracy at DFT Cost: Fragmentation, Error-Cancellation, and Machine Learning. **2020**, 16, 4938-4950	8
644	Machine Learning Methods in Drug Discovery. **2020**, 25,	51
643	Memory-assisted reinforcement learning for diverse molecular de novo design. **2020**, 12, 68	20
642	A ligand-based computational drug repurposing pipeline using KNIME and Programmatic Data Access: case studies for rare diseases and COVID-19. **2020**, 12, 71	6
641	Automatic discovery of clinically interpretable imaging biomarkers for Mycobacterium tuberculosis supersusceptibility using deep learning. **2020**, 62, 103094	4
640	Adaptive Optimization of Chemical Reactions with Minimal Experimental Information. **2020**, 1, 100247	16
639	tmQM Dataset-Quantum Geometries and Properties of 86k Transition Metal Complexes. **2020**, 60, 6135-6146	21
638	Applications of machine learning in metal-organic frameworks. **2020**, 423, 213487	51

637	Drug-target interactions prediction using marginalized denoising model on heterogeneous networks. **2020**, 21, 330	1
636	Machine Learning for Polymer Swelling in Liquids. **2020**, 2, 3576-3586	5
635	Allosteric Regulation at the Crossroads of New Technologies: Multiscale Modeling, Networks, and Machine Learning. **2020**, 7, 136	18
634	Relevant Applications of Generative Adversarial Networks in Drug Design and Discovery: Molecular Design, Dimensionality Reduction, and Peptide and Protein Design. **2020**, 25,	23
633	Machine Learning Paradigms. **2020**,	6
632	Generative Model for Proposing Drug Candidates Satisfying Anticancer Properties Using a Conditional Variational Autoencoder. **2020**, 5, 18642-18650	6
631	A review of computational drug repositioning: strategies, approaches, opportunities, challenges, and directions. **2020**, 12, 46	59
630	Digital Pharmaceutical Sciences. **2020**, 21, 206	29
629	Challenge-Enabled Machine Learning to Drug-Response Prediction. **2020**, 22, 106	2
628	. **2020**,	14
627	Rapid, accurate, precise and reproducible ligand-protein binding free energy prediction. **2020**, 10, 20200007	31
626	Machine learning corrected alchemical perturbation density functional theory for catalysis applications. **2020**, 66, e17041	6
625	A Turing Test for Molecular Generators. **2020**, 63, 11964-11971	17
624	Molecular representations in AI-driven drug discovery: a review and practical guide. **2020**, 12, 56	59
623	Drug Design of Targeted Chemical Libraries Based on Artificial Intelligence and Pair-Based Multiobjective Optimization. **2020**, 60, 4582-4593	20
622	ChemGrapher: Optical Graph Recognition of Chemical Compounds by Deep Learning. **2020**, 60, 4506-4517	12
621	Artificial neural networks training acceleration through network science strategies. **2020**, 24, 17787-17795	3
620	Machine Learning in Oncology: What Should Clinicians Know?. **2020**, 4, 799-810	17

619	Internet of things assisted condition-based support for smart manufacturing industry using learning technique. **2020**, 36, 1737-1754	5
618	Artificial Intelligence for COVID-19 Drug Discovery and Vaccine Development. **2020**, 3, 65	80
617	Predicting and Quantifying Antagonistic Effects of Natural Compounds Given with Chemotherapeutic Agents: Applications for High-Throughput Screening. **2020**, 12,	2
616	Deep neural network modeling based virtual screening and prediction of potential inhibitors for renin protein. **2020**, 1-14	1
615	Use of machine learning in geriatric clinical care for chronic diseases: a systematic literature review. **2020**, 3, 459-471	11
614	Tree-Based QSAR Model for Drug Repurposing in the Discovery of New Antibacterial Compounds Against. **2020**, 13,	3
613	Artificial Intelligence-Based Application to Explore Inhibitors of Neurodegenerative Diseases. **2020**, 14, 617327	3
612	Prediction of Compound Bioactivities Using Heat-Diffusion Equation. **2020**, 1, 100140	1
611	Confidence in Inactive and Active Predictions from Structural Alerts. **2020**, 33, 3010-3022	3
610	Transferable MP2-Based Machine Learning for Accurate Coupled-Cluster Energies. **2020**, 16, 7453-7461	5
609	"Ring Breaker": Neural Network Driven Synthesis Prediction of the Ring System Chemical Space. **2020**, 63, 8791-8808	9
608	Deep Docking: A Deep Learning Platform for Augmentation of Structure Based Drug Discovery. **2020**, 6, 939-949	73
607	Direct steering of de novo molecular generation with descriptor conditional recurrent neural networks. **2020**, 2, 254-265	47
606	Feature Extraction Methods in Quantitative Structure–Activity Relationship Modeling: A Comparative Study. **2020**, 8, 78737-78752	8
605	Using Predicted Bioactivity Profiles to Improve Predictive Modeling. **2020**, 60, 2830-2837	7
604	SMILES-based deep generative scaffold decorator for de-novo drug design. **2020**, 12, 38	45
603	Deep Learning Based Drug Screening for Novel Coronavirus 2019-nCov. **2020**, 12, 368-376	72
602	Practical Applications of Deep Learning To Impute Heterogeneous Drug Discovery Data. **2020**, 60, 2848-2857	16

601	PaccMann: a web service for interpretable anticancer compound sensitivity prediction. **2020**, 48, W502-W508		12
600	COVID-19: CADD to the rescue. **2020**, 285, 198022		13
599	Artificial intelligence in chemistry and drug design. **2020**, 34, 709-715		38
598	Chemists: AI Is Here; Unite To Get the Benefits. **2020**, 63, 8695-8704		17
597	Image-based high-content screening in drug discovery. *Drug Discovery Today*, **2020**, 25, 1348-1361	8.8	17
596	Machine learning-based approaches for disease gene prediction. **2020**, 19, 350-363		7
595	15. Cheminformatics techniques in antimalarial drug discovery and development from natural products 1: basic concepts. **2020**, 381-396		
594	Deep Learning-Based Imbalanced Data Classification for Drug Discovery. **2020**, 60, 4180-4190		22
593	SYBA: Bayesian estimation of synthetic accessibility of organic compounds. **2020**, 12, 35		14
592	Combining Cloud-Based Free-Energy Calculations, Synthetically Aware Enumerations, and Goal-Directed Generative Machine Learning for Rapid Large-Scale Chemical Exploration and Optimization. **2020**, 60, 4311-4325		15
591	Diabetic retinopathy and diabetic macular oedema pathways and management: UK Consensus Working Group. **2020**, 34, 1-51		45
590	Generative Adversarial Networks (GANs) Based Synthetic Sampling for Predictive Modeling. **2020**, 39, e2000086		4
589	Leveraging Advances in Artificial Intelligence to Improve the Quality and Timing of Palliative Care. **2020**, 12,		2
588	Missing data imputation with adversarially-trained graph convolutional networks. **2020**, 129, 249-260		19
587	Drug discovery technologies: Caenorhabditis elegans as a model for anthelmintic therapeutics. **2020**, 40, 1715-1753		8
586	Machine learning models for drug-target interactions: current knowledge and future directions. *Drug Discovery Today*, **2020**, 25, 748-756	8.8	40
585	Retrosynthesis with attention-based NMT model and chemical analysis of "wrong" predictions.. **2020**, 10, 1371-1378		11
584	A deep learning-based method for drug-target interaction prediction based on long short-term memory neural network. **2020**, 20, 49		24

583	A self-attention based message passing neural network for predicting molecular lipophilicity and aqueous solubility. **2020**, 12, 15		28
582	Artificial intelligence in oncology. **2020**, 111, 1452-1460		50
581	. **2020**,		2
580	The power of deep learning to ligand-based novel drug discovery. **2020**, 15, 755-764		24
579	Identification of Novel Chemical Entities for Adenosine Receptor Type 2A Using Molecular Modeling Approaches. **2020**, 25,		25
578	Neural networks for protein structure and function prediction and dynamic analysis. **2020**, 12, 569-573		7
577	Predicting or Pretending: Artificial Intelligence for Protein-Ligand Interactions Lack of Sufficiently Large and Unbiased Datasets. **2020**, 11, 69		33
576	Automated De Novo Design in Medicinal Chemistry: Which Types of Chemistry Does a Generative Neural Network Learn?. **2020**, 63, 8809-8823		19
575	Probing the characteristics and biofunctional effects of disease-affected cells and drug response via machine learning applications. **2020**, 40, 951-977		5
574	Advancing computer-aided drug discovery (CADD) by big data and data-driven machine learning modeling. *Drug Discovery Today*, **2020**, 25, 1624-1638	8.8	38
573	Turning genome-wide association study findings into opportunities for drug repositioning. **2020**, 18, 1639-1650		9
572	Optimizing chemical reaction conditions using deep learning: a case study for the Suzuki–Miyaura cross-coupling reaction. **2020**, 7, 2269-2277		6
571	ChEMBL-Likeness Score and Database GDBChEMBL. **2020**, 8, 46		14
570	Identification of DNA N-methyladenine sites by integration of sequence features. **2020**, 13, 8		9
569	Exploring the computational methods for protein-ligand binding site prediction. **2020**, 18, 417-426		33
568	State-of-the-Art Machine Learning Techniques Aiming to Improve Patient Outcomes Pertaining to the Cardiovascular System. **2020**, 9, e013924		43
567	Bioethanol production estimated from volatile compositions in hydrolysates of lignocellulosic biomass by deep learning. **2020**, 129, 723-729		4
566	Machine learning: Accelerating materials development for energy storage and conversion. **2020**, 2, 553-576		86

565	Development of an early-warning system for high-risk patients for suicide attempt using deep learning and electronic health records. **2020**, 10, 72	24
564	Enhancing reaction-based de novo design using a multi-label reaction class recommender. **2020**, 34, 783-803	8
563	Automated, Accelerated Nanoscale Synthesis of Iminopyrrolidines. **2020**, 132, 12523-12527	2
562	Automated, Accelerated Nanoscale Synthesis of Iminopyrrolidines. **2020**, 59, 12423-12427	11
561	Machine-Learning-Assisted De Novo Design of Organic Molecules and Polymers: Opportunities and Challenges. **2020**, 12,	51
560	Image Based Liver Toxicity Prediction. **2020**, 60, 1111-1121	9
559	GEN: highly efficient SMILES explorer using autodidactic generative examination networks. **2020**, 12, 22	12
558	Exploring Novel Biologically-Relevant Chemical Space Through Artificial Intelligence: The NCATS ASPIRE Program. **2019**, 6, 143	2
557	LED-Based Photoacoustic Imaging. **2020**,	3
556	A Structure-Based Platform for Predicting Chemical Reactivity. **2020**, 6, 1379-1390	68
555	Predicting Short-term Survival after Liver Transplantation using Machine Learning. **2020**, 10, 5654	4
554	Machine learning dihydrogen activation in the chemical space surrounding Vaska's complex. **2020**, 11, 4584-4601	47
553	Prediction of Cancer Drug Effectiveness Based on Multi-Fusion Deep Learning Model. **2020**,	1
552	Computational Chemistry on a Budget: Supporting Drug Discovery with Limited Resources. **2020**, 63, 10158-10169	18
551	Industry-scale application and evaluation of deep learning for drug target prediction. **2020**, 12, 26	12
550	Prediction of drug adverse events using deep learning in pharmaceutical discovery. **2021**, 22, 1884-1901	19
549	Virtual screening web servers: designing chemical probes and drug candidates in the cyberspace. **2021**, 22, 1790-1818	36
548	Different molecular enumeration influences in deep learning: an example using aqueous solubility. **2021**, 22,	7

547	Clinical Pharmacology Modeling and Simulation in Drug Development. **2021**, 243-256		
546	Turning liabilities into opportunities: Off-target based drug repurposing in cancer. **2021**, 68, 209-229		11
545	Artificial intelligence and automation in computer aided synthesis planning. **2021**, 6, 27-51		11
544	Current development of integrated web servers for preclinical safety and pharmacokinetics assessments in drug development. **2021**, 22,		5
543	MolAICal: a soft tool for 3D drug design of protein targets by artificial intelligence and classical algorithm. **2021**, 22,		55
542	MDeePred: novel multi-channel protein featurization for deep learning-based binding affinity prediction in drug discovery. **2021**, 37, 693-704		14
541	Current advances in ligand-based target prediction. **2021**, 11, e1504		8
540	Repositioning microbial biotechnology against COVID-19: the case of microbial production of flavonoids. **2021**, 14, 94-110		11
539	Changing the HTS Paradigm: AI-Driven Iterative Screening for Hit Finding. **2021**, 26, 257-262		4
538	Uncertainty quantification in drug design. *Drug Discovery Today*, **2021**, 26, 474-489	8.8	10
537	DeepSIBA: chemical structure-based inference of biological alterations using deep learning. **2021**, 17, 108-120		0
536	Advanced machine-learning techniques in drug discovery. *Drug Discovery Today*, **2021**, 26, 769-777	8.8	36
535	Deep learning in systems medicine. **2021**, 22, 1543-1559		8
534	Artificial intelligence in the early stages of drug discovery. **2021**, 698, 108730		11
533	Image-based profiling for drug discovery: due for a machine-learning upgrade?. **2021**, 20, 145-159		43
532	Drug design targeting active posttranslational modification protein isoforms. **2021**, 41, 1701-1750		7
531	Machine Learning in Predictive Toxicology: Recent Applications and Future Directions for Classification Models. **2021**, 34, 217-239		14
530	The Deep Learning Compiler: A Comprehensive Survey. **2021**, 32, 708-727		18

529	Visualization of Protein-Drug Interactions for the Analysis of Drug Resistance in Lung Cancer. **2021**, 25, 1839-1848	0
528	Artificial Neural Networks. **2021**,	1
527	Research on Classification of Cross-Border E-Commerce Products Based on Image Recognition and Deep Learning. **2021**, 9, 108083-108090	2
526	Decoding regulatory structures and features from epigenomics profiles: A Roadmap-ENCODE Variational Auto-Encoder (RE-VAE) model. **2021**, 189, 44-53	5
525	Covid-19 Containment: Demystifying the Research Challenges and Contributions Leveraging Digital Intelligence Technologies. **2021**, 193-214	
524	Deep Learning-Based Drug Screening for COVID-19 and Case Studies. **2021**, 631	0
523	Applications of deep learning in biomedical engineering. **2021**, 245-270	1
522	Modeling Protein-Ligand Interactions: Are We Ready for Deep Learning?. **2021**, 163-173	
521	Graph Neural Networks in Cheminformatics. **2021**, 823-837	2
520	Artificial intelligence in drug discovery: applications and techniques. **2021**,	1
519	Review of machine learning algorithms' application in pharmaceutical technology. **2021**, 71, 302-317	0
518	AI applications in robotics, diagnostic image analysis and precision medicine: Current limitations, future trends, guidelines on CAD systems for medicine. **2021**, 24, 100596	13
517	Deep Learning Applications for COVID-19 Analysis: A State-of-the-Art Survey. **2021**, 129, 65-98	0
516	State of the Art in Artificial Intelligence and Machine Learning Techniques for Improving Patient Outcomes Pertaining to the Cardiovascular and Respiratory Systems. **2021**, 335-352	2
515	Hypergraph-based persistent cohomology (HPC) for molecular representations in drug design. **2021**, 22,	8
514	Big Data Classification: Applications and Challenges. **2021**, 53-84	1
513	Computational intelligence in healthcare and biosignal processing. **2021**, 31-64	
512	Artificial intelligence-driven drug repurposing and structural biology for SARS-CoV-2. **2021**, 2, 100042	1

511	Trade-off Predictivity and Explainability for Machine-Learning Powered Predictive Toxicology: An in-Depth Investigation with Tox21 Data Sets. **2021**, 34, 541-549	11
510	Android-Based Skin Cancer Recognition System Using Convolutional Neural Network. **2021**, 59-85	
509	Application of Network Pharmacology Based on Artificial Intelligence Algorithms in Drug Development. **2021**, 35-73	1
508	Artificial Intelligence in Precision Medicine: A Perspective in Biomarker and Drug Discovery. **2021**, 71-88	0
507	Transmol: repurposing a language model for molecular generation.. **2021**, 11, 25921-25932	0
506	Computer-Aided Drug Design. **2021**, 137-210	7
505	DenovoProfiling: a webserver for de novo generated molecule library profiling.	
504	Could graph neural networks learn better molecular representation for drug discovery? A comparison study of descriptor-based and graph-based models. **2021**, 13, 12	34
503	Classification models and SAR analysis on CysLT1 receptor antagonists using machine learning algorithms. **2021**, 25, 1597-1616	1
502	Public-Private Partnerships: Compound and Data Sharing in Drug Discovery and Development. **2021**, 26, 604-619	2
501	Using GANs with adaptive training data to search for new molecules. **2021**, 13, 14	5
500	Early Drug Development and Evaluation of Putative Antitubercular Compounds in the -Omics Era. **2020**, 11, 618168	1
499	Computational compound screening of biomolecules and soft materials by molecular simulations. **2021**, 29, 023001	8
498	DTI-SNNFRA: Drug-target interaction prediction by shared nearest neighbors and fuzzy-rough approximation. **2021**, 16, e0246920	1
497	Advances in de Novo Drug Design: From Conventional to Machine Learning Methods. **2021**, 22,	28
496	A survey on deep learning in medicine: Why, how and when?. **2021**, 66, 111-137	65
495	Classification of some chemical drugs by genetic algorithm and deep neural network hybrid method. **2021**, 33, e6242	1
494	Trends in application of advancing computational approaches in GPCR ligand discovery. **2021**, 246, 1011-1024	2

493	Evaluation of multi-target deep neural network models for compound potency prediction under increasingly challenging test conditions. **2021**, 35, 285-295	2
492	An Analysis of QSAR Research Based on Machine Learning Concepts. **2021**, 18, 17-30	9
491	Co-attention fusion based deep neural network for Chinese medical answer selection. **2021**, 51, 6633-6646	1
490	Ollivier Persistent Ricci Curvature-Based Machine Learning for the Protein-Ligand Binding Affinity Prediction. **2021**, 61, 1617-1626	10
489	SMILES Pair Encoding: A Data-Driven Substructure Tokenization Algorithm for Deep Learning. **2021** , 61, 1560-1569	8
488	Target2DeNovoDrug: a novel programmatic tool for -deep learning based drug design for any target of interest. **2021**, 1-6	1
487	Balancing Data on Deep Learning-Based Proteochemometric Activity Classification. **2021**, 61, 1657-1669	1
486	Effects of Pooling Operations on Prediction of Ligand Rotation-Dependent Protein□igand Binding in 3D Graph Convolutional Network. **2021**, 42, 744-747	3
485	A Hybrid Clustering Based Approach To Extract Drug Elements Which Causes Side Effects. **2021**, 1110, 012015	
484	Hyperparameter Optimization for COVID-19 Pneumonia Diagnosis Based on Chest CT. **2021**, 21,	6
483	Review of deep learning: concepts, CNN architectures, challenges, applications, future directions. **2021**, 8, 53	348
482	Potential for Chemistry in Multidisciplinary, Interdisciplinary, and Transdisciplinary Teaching Activities in Higher Education. **2021**, 98, 1124-1145	5
481	A Novel Graph Neural Network Methodology to Investigate Dihydroorotate Dehydrogenase Inhibitors in Small Cell Lung Cancer. **2021**, 11,	1
480	iResponse: An AI and IoT-Enabled Framework for Autonomous COVID-19 Pandemic Management. **2021**, 13, 3797	16
479	Collaborative Innovation of Online Ideological Education Platform with Data Mining and Text Recognition Algorithms. **2021**,	1
478	Computational Screening of Potential Inhibitors of for Pyrite Scale Prevention in Oil and Gas Wells. **2021**, 6, 10607-10617	0
477	Discovering Relationships between OSDAs and Zeolites through Data Mining and Generative Neural Networks. **2021**, 7, 858-867	21
476	Pervasive Intelligent Models to Predict the Outcome of COVID-19 Patients. **2021**, 13, 102	3

475	Artificial intelligence in oncology: From bench to clinic. **2021**,	3
474	A Perspective on Synthetic Biology in Drug Discovery and Development-Current Impact and Future Opportunities. **2021**, 26, 581-603	5
473	Artificial Intelligence in Medicinal Chemistry. 1-19	
472	Artificial intelligence in drug discovery: recent advances and future perspectives. **2021**, 16, 949-959	27
471	PaccMann: De novo generation of hit-like anticancer molecules from transcriptomic data via reinforcement learning. **2021**, 24, 102269	15
470	Docking, Scoring, and Virtual Screening in Drug Discovery. 1-102	1
469	Deep Learning-Based Ligand Design Using Shared Latent Implicit Fingerprints from Collaborative Filtering. **2021**, 61, 2159-2174	1
468	Targeting SARS-CoV-2 Spike Protein/ACE2 Protein-Protein Interactions: a Computational Study. **2021**, 40, e2060080	4
467	Application of deep learning and molecular modeling to identify small drug-like compounds as potential HIV-1 entry inhibitors. **2021**, 1-19	4
466	Deep-learning based repurposing of FDA-approved drugs against dihydrofolate reductase and molecular dynamics study. **2021**, 1-17	2
465	Use of artificial intelligence to enhance phenotypic drug discovery. *Drug Discovery Today*, **2021**, 26, 887-908	7
464	Multi-PLI: interpretable multi-task deep learning model for unifying protein-ligand interaction datasets. **2021**, 13, 30	2
463	Two-step machine learning enables optimized nanoparticle synthesis. **2021**, 7,	27
462	Artificial intelligence to deep learning: machine intelligence approach for drug discovery. **2021**, 25, 1315-1360	65
461	GPCR_LigandClassify.py; a rigorous machine learning classifier for GPCR targeting compounds. **2021**, 11, 9510	4
460	Microfluidics for Drug Development: From Synthesis to Evaluation. **2021**, 121, 7468-7529	22
459	ProtCHOIR: a tool for proteome-scale generation of homo-oligomers. **2021**, 22,	1
458	Translational Applications of Artificial Intelligence and Machine Learning for Diagnostic Pathology in Lymphoid Neoplasms: A Comprehensive and Evolutive Analysis. **2021**, 11,	0

457	Programmable Logic in Metal-Organic Frameworks for Catalysis. **2021**, 33, e2007442		22
456	Multi-Criteria Evaluation of Publication Impacts: Deep Learning in Autonomous Vehicles. **2021**,		
455	A merged molecular representation learning for molecular properties prediction with a web-based service. **2021**, 11, 11028		1
454	A Large-Scale Observational Study on the Temporal Trends and Risk Factors of Opioid Overdose: Real-World Evidence for Better Opioids. **2021**, 8, 393-406		0
453	LAKEVE GELTRLMESNDE YAPAY ZEK17-17		
452	An artificial neural network-pharmacokinetic model and its interpretation using Shapley additive explanations. **2021**, 10, 760-768		5
451	Current and future deep learning algorithms for tandem mass spectrometry (MS/MS)-based small molecule structure elucidation. **2021**, e9120		5
450	Machine learning research towards combating COVID-19: Virus detection, spread prevention, and medical assistance. **2021**, 117, 103751		20
449	Drug Repurposing: A Strategy for Discovering Inhibitors against Emerging Viral Infections. **2021**, 28, 2887-2942		5
448	Deep Learning-Based Conformal Prediction of Toxicity. **2021**, 61, 2648-2657		7
447	Design framework for metasurface optics-based convolutional neural networks. **2021**, 60, 4356-4365		6
446	Big Techs and startups in pharmaceutical R&D - A 2020 perspective on artificial intelligence. *Drug Discovery Today*, **2021**, 26, 2226-2231	8.8	2
445	Predicting Single-Substance Phase Diagrams: A Kernel Approach on Graph Representations of Molecules. **2021**, 125, 4488-4497		2
444	Fine-tuning of a generative neural network for designing multi-target compounds. **2021**, 1		2
443	Machine learning techniques applied to the drug design and discovery of new antivirals: a brief look over the past decade. **2021**, 16, 961-975		4
442	Comparative Study of Deep Generative Models on Chemical Space Coverage. **2021**, 61, 2572-2581		9
441	Artificial Intelligence in Pharmaceutical Field - A Critical Review. **2021**,		0
440	Mathematical Multidimensional Modelling and Structural Artificial Intelligence Pipelines Provide Insights for the Designing of Highly Specific AntiSARS-CoV2 Agents. **2021**, 15, 877		2

439	Graph neural networks for automated de novo drug design. *Drug Discovery Today*, **2021**, 26, 1382-1393	8.8	12
438	Accelerating optical reporting for conformation of tyrosine kinase inhibitors in solutions. **2021**, 121, e26765		3
437	Natural gas consumption forecasting: A discussion on forecasting history and future challenges. **2021**, 90, 103930		14
436	Predicting Polymers' Glass Transition Temperature by a Chemical Language Processing Model. **2021**, 13,		8
435	Backdoor Attacks to Graph Neural Networks. **2021**,		13
434	Convolutional Neural Networks based classification of breast ultrasonography images by hybrid method with respect to benign, malignant, and normal using mRMR. **2021**, 133, 104407		22
433	Recent Progress of Deep Learning in Drug Discovery. **2021**, 27, 2088-2096		1
432	Alkaloids in Contemporary Drug Discovery to Meet Global Disease Needs. **2021**, 26,		4
431	Computational representations of protein-ligand interfaces for structure-based virtual screening. **2021**, 16, 1175-1192		1
430	How can we accelerate COVID-19 vaccine discovery?. **2021**, 16, 1081-1084		1
429	Leveraging Artificial Intelligence (AI) Capabilities for COVID-19 Containment. **2021**, 1-25		5
428	GanDTI: A multi-task neural network for drug-target interaction prediction. **2021**, 92, 107476		1
427	Deep learning prediction of patient response time course from early data via neural-pharmacokinetic/pharmacodynamic modelling. **2021**, 3, 696-704		5
426	Milvus. **2021**,		2
425	A deep learning approach to predict blood-brain barrier permeability. **2021**, 7, e515		2
424	Artificial neural networks in tandem with molecular descriptors as predictive tools for continuous liposome manufacturing. **2021**, 603, 120713		4
423	Machine learning models for classification tasks related to drug safety. **2021**, 25, 1409-1424		9
422	Failure Prediction by Confidence Estimation of Uncertainty-Aware Dirichlet Networks. **2021**,		2

421	A Novel Deep Learning Approach for Anomaly Detection of Time Series Data. **2021**, 2021, 1-11		6
420	Deep Learning for Medical Healthcare: Issues, Challenges, and Opportunities. **2021**, 361-392		
419	Artificial intelligence and the future of life sciences. *Drug Discovery Today*, **2021**, 26, 2515-2526	8.8	1
418	A Machine Learning Model to Predict Drug Transfer Across the Human Placenta Barrier. **2021**, 9, 714678		1
417	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. **2021**, 121, 9816-9872		53
416	Accelerating Optimizing the Design of Carbon-based Electrocatalyst Via Machine Learning.		1
415	How can artificial intelligence be used for peptidomics?. **2021**, 18, 527-556		1
414	Deep Learning Approach for Discovery of In Silico Drugs for Combating COVID-19. **2021**, 2021, 6668985		10
413	Learn and Visually Explain Deep Fair Models: an Application to Face Recognition. **2021**,		
412	Beam Search for Automated Design and Scoring of Novel ROR Ligands with Machine Intelligence*. **2021**, 60, 19477-19482		7
411	Feature importance correlation from machine learning indicates functional relationships between proteins and similar compound binding characteristics. **2021**, 11, 14245		5
410	Development of Machine Learning Models and the Discovery of a New Antiviral Compound against Yellow Fever Virus. **2021**, 61, 3804-3813		2
409	Artificial Intelligence and Cancer Drug Development. **2021**,		1
408	Quantum algorithm for quicker clinical prognostic analysis: an application and experimental study using CT scan images of COVID-19 patients. **2021**, 21, 227		9
407	State-of-the-art of artificial intelligence in medicinal chemistry. **2021**, 7, FSO702		6
406	A Chaotic Neural Network Model for English Machine Translation Based on Big Data Analysis. **2021**, 2021, 3274326		1
405	Prediction of the antimicrobial activity of quaternary ammonium salts against Staphylococcus aureus using artificial neural networks. **2021**, 14, 103233		2
404	Beam-Search zum automatisierten Entwurf und Scoring neuer ROR-Liganden mithilfe maschineller Intelligenz**. **2021**, 133, 19626-19632		

403	Compound dataset and custom code for deep generative multi-target compound design. **2021**, 7, FSO715	4
402	Optimizing blood-brain barrier permeation through deep reinforcement learning for de novo drug design. **2021**, 37, i84-i92	1
401	Understanding Software-2.0. **2021**, 30, 1-42	4
400	Prediction of Molecular Properties Using Molecular Topographic Map. **2021**, 26,	2
399	AI-Based Drug Discovery of TKIs Targeting L858R/T790M/C797S-Mutant EGFR in Non-small Cell Lung Cancer. **2021**, 12, 660313	1
398	Deep fair models for complex data: Graphs labeling and explainable face recognition. **2021**,	1
397	Pairing conceptual modeling with machine learning. **2021**, 134, 101909	2
396	Predictive Chromatography of Leaf Extracts Through Encoded Environmental Forcing on Phytochemical Synthesis. **2021**, 12, 613507	
395	Deep Learning for Drug Discovery: A Study of Identifying High Efficacy Drug Compounds Using a Cascade Transfer Learning Approach. **2021**, 11, 7772	1
394	De novo design with deep generative models based on 3D similarity scoring. **2021**, 44, 116308	1
393	Machine Learning in Drug Discovery: A Review. **2021**, 1-53	18
392	LibINVENT: Reaction-based Generative Scaffold Decoration for Library Design. **2021**,	1
391	Artificial Intelligence in Bioinformatics. **2021**, 21-51	0
390	Review of unsupervised pretraining strategies for molecules representation. **2021**, 20, 323-332	6
389	Is there a role for statistics in artificial intelligence?. 1	3
388	Application of an Electrochemical Microflow Reactor for Cyanosilylation: Machine Learning-Assisted Exploration of Suitable Reaction Conditions for Semi-Large-Scale Synthesis. **2021**, 86, 16035-16044	2
387	A primer on applying AI synergistically with domain expertise to oncology. **2021**, 1876, 188548	2
386	Pivotal Role of Quantum Dots in the Advancement of Healthcare Research. **2021**, 2021, 2096208	2

385	A Fragmentation-Based Graph Embedding Framework for QM/ML. **2021**, 125, 6872-6880	1
384	Super-resolution reconstruction algorithm for aerial image data management based on deep learning. 1	
383	Applications of Artificial Intelligence, Machine Learning, Big Data and the Internet of Things to the COVID-19 Pandemic: A Scientometric Review Using Text Mining. **2021**, 18,	11
382	Automatic Identification of Analogue Series from Large Compound Data Sets: Methods and Applications. **2021**, 26,	2
381	Application of deep neural network (DNN) for experimental liquid-liquid equilibrium data of water + butyric acid + 5-methyl-2-hexanone ternary systems. **2021**, 544-545, 113094	1
380	Using molecular embeddings in QSAR modeling: does it make a difference?. **2021**,	1
379	Treasuring the computational approach in medicinal plant research. **2021**, 164, 19-32	7
378	MM-Deacon: Multimodal molecular domain embedding analysis via contrastive learning.	
377	Guided structure-based ligand identification and design via artificial intelligence modeling. **2021**, 1-8	1
376	An Efficient Teaching Model of International Cooperation Based on Artificial Intelligence. **2021**, 2021, 1-7	
375	A general optimization protocol for molecular property prediction using a deep learning network. **2021**,	0
374	Success stories of AI in drug discovery - where do things stand?. **2021**, 1-14	3
373	A roadmap to AI-driven in silico process development: bioprocessing 4.0 in practice. **2021**, 33, 100692	3
372	Efficient Exploration of Chemical Space with Docking and Deep Learning. **2021**, 17, 7106-7119	12
371	The rise of deep learning and transformations in bioactivity prediction power of molecular modeling tools. **2021**, 98, 954-967	3
370	Deep learning in retrosynthesis planning: datasets, models and tools. **2021**,	11
369	Generic and specific recurrent neural network models: Applications for large and small scale biopharmaceutical upstream processes. **2021**, 31, e00640	2
368	Combining Automated Organoid Workflows With Artificial Intelligence-Based Analyses: Opportunities to Build a New Generation of Interdisciplinary High-Throughput Screens for Parkinson's Disease and Beyond. **2021**,	0

367	Application of Deep Neural Network Models in Drug Discovery Programs. **2021**,	0
366	Current trends in computer aided drug design and a highlight of drugs discovered via computational techniques: A review. **2021**, 224, 113705	35
365	Molecular descriptor analysis of approved drugs using unsupervised learning for drug repurposing. **2021**, 138, 104856	1
364	Best Practices for Docking-Based Virtual Screening. **2021**, 75-98	3
363	Application of artificial intelligence in the dental field: A literature review. **2021**,	0
362	The pursuit of mechanism of action: uncovering drug complexity in TB drug discovery. **2021**, 2, 423-440	3
361	WADDAICA: A webserver for aiding protein drug design by artificial intelligence and classical algorithm. **2021**, 19, 3573-3579	8
360	Wide and deep learning for automatic cell type identification. **2021**, 19, 1052-1062	4
359	Pathway-Based Drug-Repurposing Schemes in Cancer: The Role of Translational Bioinformatics. **2020**, 10, 605680	6
358	Machine learning, artificial intelligence, and data science breaking into drug design and neglected diseases. **2021**, 11, e1513	5
357	Deep Learning Techniques and COVID-19 Drug Discovery: Fundamentals, State-of-the-Art and Future Directions. **2021**, 9-31	9
356	Machine learning designs non-hemolytic antimicrobial peptides. **2021**, 12, 9221-9232	12
355	Machine Learning Application in COVID-19 Drug Development. **2021**, 229-244	
354	A critical overview of computational approaches employed for COVID-19 drug discovery. **2021**, 50, 9121-9151	36
353	Practical Applications of Artificial Intelligence for Disease Prognosis and Management. **2021**, 1-36	
352	Using machine learning to minimize delays caused by prior authorization: A brief report. **2021**, 8, 1944961	0
351	Machine-learning Applications to Membrane Active Peptides. **2021**, 198-207	
350	Advanced approaches and in silico tools of chemoinformatics in drug designing. **2021**, 173-206	1

349	Machine learning-integrated omics for the risk and safety assessment of nanomaterials. **2021**, 9, 1598-1608	12
348	Artificial intelligence in process systems engineering. **2021**, 1-10	0
347	A Review on Deep Learning Techniques for the Diagnosis of Novel Coronavirus (COVID-19).. **2021**, 9, 30551-30572	90
346	Application and assessment of deep learning for the generation of potential NMDA receptor antagonists. **2021**, 23, 1197-1214	7
345	Computational Approaches for De Novo Drug Design: Past, Present, and Future. **2021**, 2190, 139-165	5
344	Data Integration Using Advances in Machine Learning in Drug Discovery and Molecular Biology. **2021**, 2190, 167-184	9
343	Mol-CycleGAN - A Generative Model for Molecular Optimization. **2019**, 810-816	2
342	A Transformer Model for Retrosynthesis. **2019**, 817-830	26
341	Augmentation Is What You Need!. **2019**, 831-835	17
340	Generative Models for Automatic Chemical Design. **2020**, 445-467	23
339	Artificial Neural Networks Training Acceleration Through Network Science Strategies. **2020**, 330-336	2
338	Applications of Deep Learning in Drug Discovery. **2020**, 73-91	1
337	Vehicle-Related Scene Understanding Using Deep Learning. **2020**, 61-73	6
336	Deep learning and generative methods in cheminformatics and chemical biology: navigating small molecule space intelligently. **2020**, 477, 4559-4580	16
335	Machine learning assisted hybrid models can improve streamflow simulation in diverse catchments across the conterminous US. **2020**, 15, 104022	19
334	X-MOL: large-scale pre-training for molecular understanding and diverse molecular analysis.	4
333	Practical Model Selection for Prospective Virtual Screening.	1
332	Autoencoder-based Dimensionality Reduction for QSAR Modeling. **2020**,	3

331	AI and IoT Solutions for Tackling COVID-19 Pandemic. **2020**,	8
330	Building attention and edge message passing neural networks for bioactivity and physical-chemical property prediction. **2020**, 12, 1	51
329	In-Silico Modeling in Drug Metabolism and Interaction: Current Strategies of Lead Discovery. **2019**, 25, 3292-3305	5
328	Setting New Routes for Antifungal Drug Discovery Against Pathogenic Fungi. **2020**, 26, 1509-1520	4
327	Outwitting an Old Neglected Nemesis: A Review on Leveraging Integrated Data-Driven Approaches to Aid in Unraveling of Leishmanicides of Therapeutic Potential. **2020**, 20, 349-366	4
326	Virtual Screening Meets Deep Learning. **2019**, 15, 6-28	19
325	A Drug Decision Support System for Developing a Successful Drug Candidate Using Machine Learning Techniques. **2020**, 16, 407-419	4
324	Genetic Algorithm-based Feature Selection Approach for Enhancing the Effectiveness of Similarity Searching in Ligand-based Virtual Screening. **2020**, 15, 431-444	5
323	Role of Artificial Intelligence in Patient Safety Outcomes: Systematic Literature Review. **2020**, 8, e18599	38
322	Multi-Level Comparison of Machine Learning Classifiers and Their Performance Metrics. **2019**, 24,	25
321	Deep Learning. **2019**, 114-130	1
320	A point cloud-based deep learning strategy for protein-ligand binding affinity prediction. **2021**,	3
319	Trust in Artificial Intelligence: Clinicians Are Essential. **2021**, 127-141	0
318	Overcoming barriers to data sharing with medical image generation: a comprehensive evaluation. **2021**, 4, 141	4
317	The Evolution of Data-Driven Modeling in Organic Chemistry. **2021**, 7, 1622-1637	14
316	AI applications in functional genomics. **2021**, 19, 5762-5790	2
315	Bioactive Synthetic Polymers. **2021**, e2105063	11
314	Multi-constraint molecular generation based on conditional transformer, knowledge distillation and reinforcement learning. **2021**, 3, 914-922	9

313	OnionNet-2: A Convolutional Neural Network Model for Predicting Protein-Ligand Binding Affinity Based on Residue-Atom Contacting Shells. **2021**, 9, 753002	13
312	MolGPT: Molecular Generation Using a Transformer-Decoder Model. **2021**,	13
311	The role of machine learning method in the synthesis and biological investigation of heterocyclic compounds. **2021**, 1	
310	Application advances of deep learning methods for de novo drug design and molecular dynamics simulation. e1581	7
309	Generative Deep Learning for Targeted Compound Design. **2021**, 61, 5343-5361	7
308	Development and Implementation of an Early Warning System for High Risk Patients for Suicide Attempt Using Deep Learning and Electronic Health Records (Preprint).	
307	Learning Drug Function from Chemical Structure with Convolutional Neural Networks and Random Forests.	
306	CBSF: A New Empirical Scoring Function for Docking Parameterized by Weights of Neural Network. **2019**, 7, 121-134	
305	Latent cognizance. **2019**,	1
304	Attention and Edge Memory Convolution for Bioactivity Prediction. **2019**, 752-757	1
303	Drug Prediction in Healthcare Using Big Data and Machine Learning. **2019**, 79-92	2
302	Emerging Technologies for Antiviral Drug Discovery. **2019**, 59-71	
301	Drug Development for Hepatitis C Virus Infection: Machine Learning Applications. **2019**, 117-129	1
300	Molecular insights from conformational ensembles via machine learning.	2
299	Healthcare and Applied Artificial Intelligence Systems. **2020**, 109, 974-986	
298	Exploration of Chemical Space with Partial Labeled Noisy Student Self-Training for Improving Deep Learning Performance: Application to Drug Metabolism.	
297	Deep Learning Driven Drug Discovery: Tackling Severe Acute Respiratory Syndrome Coronavirus 2. **2021**, 12, 739684	6
296	A Comparative Study of Amino Acid Encoding Methods for Predicting Drug-Target Interactions in COVID-19 Disease. **2022**, 619-643	

295	Computational Approaches in Drug Development and Phytocompound Analysis. **2020**, 529-548	2
294	Using wavelet transform and dynamic time warping to identify the limitations of the CNN model as an air quality forecasting system. **2020**, 13, 6237-6251	2
293	Drug Administration Route Classification using Machine Learning Models. **2020**,	
292	Target2DeNovoDrugPropMax : a novel programmatic tool incorporating deep learning and in silico methods for automated de novo drug design for any target of interest.	
291	Site2Vec: a reference frame invariant algorithm for vector embedding of protein□gand binding sites. **2021**, 2, 015005	0
290	Drivers of walleye recruitment in Minnesota□ large lakes. **2020**, 77, 1921-1933	1
289	A pilot study of a machine-learning tool to assist in the diagnosis of hand arthritis. **2020**,	3
288	Bioactivity characterization of herbal molecules. **2022**, 145-183	1
287	Artificial Intelligence in Practice □Real-World Examples and Emerging Business Models. **2020**, 77-88	1
286	Machine Learning Approaches to Rational Drug Design. **2020**, 279-306	1
285	Deep Learning Techniques for Geospatial Data Analysis. **2020**, 63-81	2
284	Deep Learning for Image Processing and Reconstruction to Enhance LED-Based Photoacoustic Imaging. **2020**, 203-241	
283	A Peek Into the Reasoning of Neural Networks: Interpreting with Structural Visual Concepts. **2021**,	3
282	Demo of marius. **2021**, 14, 2759-2762	1
281	Role of Artificial Intelligence in Patient Safety Outcomes: Systematic Literature Review (Preprint).	
280	Open Innovation Platform using Cloud-based Applications and Collaborative Space: A Case Study of Solubility Prediction Model Development. **2020**, 20, 5-18	
279	Machine Learning Applied to the Modeling of Pharmacological and ADMET Endpoints. **2022**, 2390, 61-101	1
278	Machine Learning for In Silico ADMET Prediction. **2022**, 2390, 447-460	3

277	Artificial Intelligence in Compound Design. **2022**, 2390, 349-382	0
276	Applications of Artificial Intelligence in Drug Design: Opportunities and Challenges. **2022**, 2390, 1-59	1
275	A Large-Scale Observational Study on the Temporal Trends and Risk Factors of Opioid Overdose: Real-World Evidence for Better Opioids.	
274	Wide and Deep Learning for Automatic Cell Type Identification.	
273	A neural network-based framework to understand the Type 2 Diabetes (T2D)-related alteration of the human gut microbiome.	
272	Deep Learning-based Ligand Design using Shared Latent Implicit Fingerprints from Collaborative Filtering.	
271	Deep learning approaches for de novo drug design: An overview. **2021**, 72, 135-144	5
270	Defining materials using laser signals from long distance via deep learning. **2021**, 13, 101603-101603	
269	Instance Segmentation for Governmental Inspection of Small Touristic Infrastructure in Beach Zones Using Multispectral High-Resolution WorldView-3 Imagery. **2021**, 10, 813	4
268	Deep learning in bioengineering and biofabrication: a powerful technology boosting translation from research to clinics.	1
267	AI Application in Pharmaceutical Industries Being Beneficial to Material Science.	
266	Machine and deep learning amalgamation for feature extraction in Industrial Internet-of-Things. **2021**, 97, 107610	2
265	In silico Methods for Identification of Potential Therapeutic Targets. **2021**, 1	1
264	The Power of Computational Intelligence Methods in the Containment of COVID-19 Pandemic from Detection to Recovery.	
263	Drug Design: Where We Are and Future Prospects. **2021**, 26,	1
262	DrugEx v2: de novo design of drug molecules by Pareto-based multi-objective reinforcement learning in polypharmacology. **2021**, 13, 85	4
261	Drug knowledge discovery via multi-task learning and pre-trained models. **2021**, 21, 251	
260	Deep scaffold hopping with multimodal transformer neural networks. **2021**, 13, 87	3

259	Human Forest vs. Random Forest in Time-Sensitive COVID-19 Clinical Trial Prediction.	0
258	MGraphDTA: deep multiscale graph neural network for explainable drug-target binding affinity prediction.. **2022**, 13, 816-833	6
257	Data construction methodology for convolution neural network based daily runoff prediction and assessment of its applicability. **2022**, 605, 127324	0
256	Prediction of the outflow temperature of large-scale hydropower using theory-guided machine learning surrogate models of a high-fidelity hydrodynamics model. **2022**, 606, 127427	2
255	Exploring a Siamese Neural Network Architecture for One-Shot Drug Discovery. **2020**,	0
254	An auto contrast custom convolutional neural network to identifying Gram-negative bacteria. **2020**,	1
253	Automatic Clarity Threshold Determination of Blurred Images for Computer Vision Tasks Security. **2021**,	
252	Advances in structure-based virtual screening for drug discovery. **2022**, 387-404	
251	Benchmarking Molecular Feature Attribution Methods with Activity Cliffs.. **2022**, 62, 274-283	1
250	Patoloji G tt erinin Derin enme Y temleri le S landEmas	0
249	Network controllability solutions for computational drug repurposing using genetic algorithms.. **2022**, 12, 1437	0
248	Natural product drug discovery in the artificial intelligence era.. **2022**, 13, 1526-1546	11
247	Tutorial on the Use of Deep Learning in Diffuse Optical Tomography. **2022**, 11, 305	5
246	Amelioration of Alzheimer's disease pathology by mitophagy inducers identified via machine learning and a cross-species workflow.. **2022**, 6, 76-93	14
245	Chinese Medicine Prescription Recommendation Using Generative Adversarial Network. **2022**, 10, 12219-12228	0
244	Drug-likeness scoring based on unsupervised learning.. **2022**, 13, 554-565	0
243	High-performance tensor decompositions for compressing and accelerating deep neural networks. **2022**, 293-340	0
242	Interpretation of Structure-Activity Relationships in Real-World Drug Design Data Sets Using Explainable Artificial Intelligence.. **2022**,	0

241	Privacy-Preserving Artificial Intelligence Techniques in Biomedicine.. **2022**,	2
240	Machine learning approaches to optimize small-molecule inhibitors for RNA targeting.. **2022**, 14, 4	0
239	A review of in silico toxicology approaches to support the safety assessment of cosmetics-related materials. **2022**, 21, 100213	1
238	Big Data in Drug Discovery. **2022**, 17-48	1
237	Deep Machine Learning for Computer-Aided Drug Design. **2022**, 2,	1
236	De Novo Peptide and Protein Design Using Generative Adversarial Networks: An Update.. **2022**,	3
235	Ligand-based Modeling of semicarbazones and thiosemicarbazones derivatives as Cathepsin B, H, and L inhibitors: a multi-target approach. **2022**, 132612	1
234	Deep learning for drug repurposing: Methods, databases, and applications.	2
233	Federated Learning of´ Oligonucleotide Drug Molecule Thermodynamics with´ Differentially Private ADMM-Based SVM. **2021**, 459-467	
232	Machine Learning Predicts Electrospray Particle Size.	
231	A Review on Bayesian Deep Learning in Healthcare: Applications and Challenges. **2022**, 1-1	2
230	DLSSAffinity: protein-ligand binding affinity prediction a deep learning model.. **2022**,	2
229	A Deep Convolutional Neural Network for COVID-19 Chest CT-Scan Image Classification. **2022**, 603-612	
228	Identifying Prepubertal Children with Risk for Suicide Using Deep Neural Network Trained on Multimodal Brain Imaging. **2022**, 75-86	1
227	Decoding hexanitrobenzene (HNB) and 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) as two distinctive energetic nitrobenzene compounds by machine learning.. **2022**,	2
226	Perplexity-Based Molecule Ranking and Bias Estimation of Chemical Language Models.. **2022**,	4
225	Proposing a novel deep network for detecting COVID-19 based on chest images.. **2022**, 12, 3116	0
224	USE OF ARTIFICIAL INTELLIGENCE IN IN SILICO DRUG DISCOVERY OF PHARMACEUTICALS. **2022**, 58, 7-15	

223	Deep-Learning-Based Microfluidic Droplet Classification for Multijet Monitoring.. **2022**,	2
222	ARTIFICIAL INTELLIGENCE IN PHARMACY DRUG DESIGN. 21-27	
221	Evolution of Support Vector Machine and Regression Modeling in Chemoinformatics and Drug Discovery.. **2022**, 1	5
220	Statistical distortion of supervised learning predictions in optical microscopy induced by image compression.. **2022**, 12, 3464	
219	Deep Learning for Smart Healthcare-A Survey on Brain Tumor Detection from Medical Imaging.. **2022**, 22,	8
218	Improving Compound Activity Classification via Deep Transfer and Representation Learning.. **2022**, 7, 9465-9483	1
217	MolData, a molecular benchmark for disease and target based machine learning.. **2022**, 14, 10	0
216	On the application of physics informed neural networks (PINN) to solve boundary layer thermal-fluid problems. **2022**, 132, 105890	0
215	A feature transferring workflow between data-poor compounds in various tasks.. **2022**, 17, e0266088	
214	Frequency analysis of extreme flows using an Artificial Neural Network (ANN) model case Western High Atlas - Morocco. 1	
213	Using Structure-guided Fragment-Based Drug Discovery to Target Infections in Cystic Fibrosis.. **2022**, 9, 857000	1
212	Artificial intelligence in interdisciplinary life science and drug discovery research.. **2022**, 8, FSO792	0
211	Deep learning tools for advancing drug discovery and development.. **2022**, 12, 110	2
210	Artificial intelligence techniques for prediction of drug synergy in malignant diseases: Past, present, and future.. **2022**, 144, 105334	0
209	Development of an in silico consensus model for the prediction of the phospholipigenic potential of small molecules. **2022**, 22, 100226	
208	Generative machine learning for de novo drug discovery: A systematic review.. **2022**, 145, 105403	2
207	A survey of deep nonnegative matrix factorization. **2022**, 491, 305-320	2
206	Prediction of inhibitory activities of small molecules against Pantothenate synthetase from Mycobacterium tuberculosis using Machine Learning models.. **2022**, 145, 105453	0

205	Molecular substructure graph attention network for molecular property identification in drug discovery. **2022**, 128, 108659	
204	Network Intrusion Detection by an Approximate Logic Neural Model. **2021**,	
203	An Empirical Comparison of Machine and Deep Learning Algorithms Performance on Chemical Data. **2021**,	
202	Feature Extraction for Class Imbalance Using a Convolutional Autoencoder and Data Sampling. **2021**,	1
201	Screening of 6000 Compounds for Uncoupling Activity: A Comparison Between a Mechanistic Biophysical Model and the Structural Alert Profiler Mitotox. **2021**,	
200	Active Site Sequence Representations of Human Kinases Outperform Full Sequence Representations for Affinity Prediction and Inhibitor Generation: 3D Effects in a 1D Model.. **2021**,	1
199	Network-Based Approaches for Drug Repositioning.. **2021**, e2100200	3
198	Applications of AI and IoT in COVID-19 Vaccine and Its Impact on Social Life. **2022**, 115-127	2
197	Artificial Intelligence (AI) in Drugs and Pharmaceuticals. **2021**,	1
196	Medication Revelation Utilizing Neural Network. **2022**, 37-49	
195	Applying Neuromorphic Computing Simulation in Band Gap Prediction and Chemical Reaction Classification.. **2022**, 7, 168-175	0
194	Topological Distance-Based Electron Interaction Tensor to Apply a Convolutional Neural Network on Drug-like Compounds.. **2021**, 6, 35757-35768	1
193	Explainable Machine Learning for Property Predictions in Compound Optimization.. **2021**, 64, 17744-17752	2
192	Phenotypic drug screening in a human fibrosis model identified a novel class of antifibrotic therapeutics.. **2021**, 7, eabb3673	0
191	Machine Learning in Chemoinformatics and Medicinal Chemistry.. **2022**,	1
190	Deep Learning for Covid-19 Screening Using Chest X-Rays in 2020: A Systematic Review.	2
189	Machine Learning Approaches and their Applications in Drug Discovery and Design.. **2022**,	3
188	Prediction of In Vivo Pharmacokinetic Parameters and Time-Exposure Curves in Rats Using Machine Learning from the Chemical Structure.. **2022**,	1

187	Data-Driven Derivation of Molecular Substructures That Enhance Drug Activity in Gram-Negative Bacteria.. **2022**,	0
186	Deep Evolutionary Learning for Molecular Design. **2022**, 17, 14-28	0
185	Table_1.XLSX. **2019**,	
184	DataSheet_1.docx. **2020**,	
183	DataSheet_2.xlsx. **2020**,	
182	DataSheet_3.csv. **2020**,	
181	DataSheet_4.csv. **2020**,	
180	DataSheet_1.pdf. **2020**,	
179	DataSheet_2.pdf. **2020**,	
178	DataSheet_1.docx. **2019**,	
177	Artificial Intelligence and Machine Learning in Medicinal Chemistry and Validation of Emerging Drug Targets. **2022**, 27-43	4
176	Exploration of chemical space with partial labeled noisy student self-training and self-supervised graph embedding.. **2022**, 23, 158	0
175	The Role of Big Data Analytics in Drug Discovery and Vaccine Development Against COVID-19. **2022** , 232-260	
174	Modeling of the Crystallization Conditions for Organic Synthesis Product Purification Using Deep Learning. **2022**, 11, 1360	
173	A neural network-based framework to understand the type 2 diabetes-related alteration of the human gut microbiome.	1
172	De novo drug design framework based on mathematical programming method and deep learning model.	0
171	DeepAS - Chemical language model for the extension of active analogue series.. **2022**, 66, 116808	0
170	SyntaLinker-Hybrid: A deep learning approach for target specific drug design. **2022**, 2, 100035	0

169	Machine Learning Predicts Electrospray Particle Size. **2022**, 110735	0
168	Drug Discovery Paradigms: Target-Based Drug Discovery. **2022**, 1-24	
167	A Classification Model with Cognitive Reasoning Ability. **2022**, 14, 1034	0
166	History and Present Scenario of Computers in Pharmaceutical Research and Development. **2022**, 1-38	
165	Artificial Intelligence and Its Applications in Drug Discovery, Formulation Development, and Healthcare. **2022**, 309-380	
164	DTIP-TC2A: An analytical framework for drug-target interactions prediction methods. **2022**, 107707	
163	Powerful molecule generation with simple ConvNet.	
162	Attention-wise masked graph contrastive learning for predicting molecular property.	0
161	An Analysis of New Feature Extraction Methods Based on Machine Learning Methods for Classification Radiological Images. **2022**, 2022, 1-13	1
160	Basic Scientific and Clinical Applications. **2022**, 275-303	
159	Validation of Deep Learning-Based DFCNN in Extremely Large-Scale Virtual Screening and Application in Trypsin I Protease Inhibitor Discovery. **2022**, 9,	0
158	Efficient modelling of permanent magnet field distribution for deep learning applications. **2022**, 559, 169521	
157	Research on Intelligent Fault Diagnosis of Rolling Bearing Based on Adaptive Resource Allocation Deep Neural Network. **2022**, 10, 62920-62931	
156	Artificial Intelligence in Oncology: Current Capabilities, Future Opportunities, and Ethical Considerations. **2022**, 1-10	0
155	Contribution of machine learning to tumor growth inhibition modeling for hepatocellular carcinoma patients under Roblitinib (FGF401) drug treatment.	0
154	Generating and screening de novo compounds against given targets using ultrafast deep learning models as core components.	0
153	Learning about allosteric drugs and ways to design them. **2022**, 167692	1
152	Organic Compound Synthetic Accessibility Prediction Based on the Graph Attention Mechanism.	1

151	An adaptive graph learning method for automated molecular interactions and properties predictions.	1
150	Scoring Functions for Protein-Ligand Binding Affinity Prediction Using Structure-based Deep Learning: A Review. 2,	1
149	RELATION: A Deep Generative Model for Structure-Based De Novo Drug Design.	5
148	Exploitation of Emerging Technologies and Advanced Networks for a Smart Healthcare System. **2022**, 12, 5859	3
147	Artificial intelligence methods to repurpose and discover new drugs to fight the Coronavirus disease-2019 pandemic. **2022**, 537-557	
146	A Comparative Evaluation of Deep Learning Methods in Automated Classification of White Blood Cell Images. **2022**,	0
145	How can natural language processing help model informed drug development?: a review. **2022**, 5,	0
144	Drug Prediction in Healthcare Using Big Data and Machine Learning. **2022**, 1062-1071	
143	Artificial Intelligence and Machine Learning for Lead-to-Candidate Decision-Making and Beyond. **2023**, 63,	1
142	Epidemiological challenges in pandemic coronavirus disease (COVID -19): Role of artificial intelligence. **2022**, 12,	1
141	Recent Advances of Graphene and Related Materials in Artificial Intelligence. 2200077	0
140	A Knowledge-Based Discovery Approach Couples Artificial Neural Networks With Weight Engineering to Uncover Immune-Related Processes Underpinning Clinical Traits of Breast Cancer. 13,	
139	Industrializing AI-powered drug discovery: lessons learned from the Patrimony computing platform. 1-10	0
138	A development of a graph-based ensemble machine learning model for skin sensitization hazard and potency assessment.	
137	Application of deep learning methods: From molecular modelling to patient classification. **2022**, 418, 113278	
136	A comprehensive review of artificial intelligence and network based approaches to drug repurposing in Covid-19. **2022**, 153, 113350	2
135	IoMT-Based Mitochondrial and Multifactorial Genetic Inheritance Disorder Prediction Using Machine Learning. **2022**, 2022, 1-8	0
134	Scientific Machine Learning Through Physics–Informed Neural Networks: Where we are and What's Next. **2022**, 92,	15

133	A Survey of Low Rate DDoS Detection Techniques Based on Machine Learning in Software-Defined Networks. **2022**, 14, 1563	2
132	Revealing Retention Mechanisms in Liquid Chromatography: QSRR Approach.	
131	A Generative Approach to Materials Discovery, Design, and Optimization. **2022**, 7, 25958-25973	0
130	Artificial Intelligence-Based Data-Driven Strategy to Accelerate Research, Development, and Clinical Trials of COVID Vaccine. **2022**, 2022, 1-16	0
129	Artificial Intelligence Meets Toxicology. **2022**, 35, 1289-1290	0
128	Attention-wise masked graph contrastive learning for predicting molecular property.	
127	Integrating concept of pharmacophore with graph neural networks for chemical property prediction and interpretation. **2022**, 14,	
126	Deep Learning Promotes the Screening of Natural Products with Potential Microtubule Inhibition Activity. **2022**, 7, 28334-28341	
125	Machine Learning Guided Discovery of Non-Hemolytic Membrane Disruptive Anticancer Peptides.	
124	Towards a comprehensive assessment of QSP models: what would it take?.	1
123	Deep Learning on Site-Specific Drug Delivery System. **2022**, 77-100	0
122	Machine learning and artificial intelligence in physiologically based pharmacokinetic modeling.	1
121	When machine learning meets molecular synthesis. **2022**, 4, 863-885	0
120	A comprehensive review on recent approaches for cancer drug discovery associated with artificial intelligence. **2022**, 150, 106140	1
119	Review on the Change Trend, Attribution Analysis, Retrieval, Simulation, and Prediction of Lake Surface Water Temperature. **2022**, 15, 6324-6355	1
118	Advances in drug development with the application of artificial intelligence. **2022**, 69-88	0
117	DenovoProfiling: A webserver for de novo generated molecule library profiling. **2022**, 20, 4082-4097	0
116	Reformation of the Healthcare Sector With Innovation and Entrepreneurial Approaches. **2022**, 148-157	0

115	CLASSIFICATION OF WHITE BLOOD CELLS USING CNN FOR THE DETECTION OF LEUCOCYTE.	0
114	BindingSiteAugmentedDTA: Enabling A Next-Generation Pipeline for Interpretable Prediction Models in Drug-Repurposing.	0
113	Text Feature Extraction and Representation of Chinese Mental Verbs Based on Deep Learning. **2022**, 2022, 1-9	0
112	AlloMAPS 2: allosteric fingerprints of the AlphaFold and Pfam-trRosetta predicted structures for engineering and design.	2
111	Calculation of exact Shapley values for support vector machines with Tanimoto kernel enables model interpretation. **2022**, 25, 105023	0
110	Deep Learning and Precision Medicine. **2022**, 127-169	0
109	Interpretable Machine Learning Models for Molecular Design of Tyrosine Kinase Inhibitors Using Variational Autoencoders and Perturbation-Based Approach of Chemical Space Exploration. **2022**, 23, 11262	0
108	MolRoPE-BERT: An enhanced molecular representation with Rotary Position Embedding for molecular property prediction. **2022**, 108344	2
107	In Silico Prediction of Human and Rat Liver Microsomal Stability via Machine Learning Methods. **2022**, 35, 1614-1624	0
106	Implementation of deep learning in drug design. **2022**, 1,	0
105	Artificial intelligence and machine learning applications in biopharmaceutical manufacturing. **2022**,	0
104	Deep Learning and Site-Specific Drug Delivery. **2022**, 1-38	0
103	Using Jupyter Tools to Design an Interactive Textbook to Guide Undergraduate Research in Materials Informatics.	0
102	MagicalRsq: Machine-learning-based genotype imputation quality calibration. **2022**,	0
101	iPromoter-Seqvec: identifying promoters using bidirectional long short-term memory and sequence-embedded features. **2022**, 23,	1
100	Artificial Intelligence approaches in drug discovery: Towards the laboratory of the future. **2022**, 22,	1
99	Computational systems biology in disease modeling and control, review and perspectives. **2022**, 8,	1
98	Role of Trust in AI-Driven Healthcare Systems: Discussion from the Perspective of Patient Safety. **2022**, 11, 129-134	1

97	Integrative Multi-Omics Approaches for Identifying Cervical Cancer Therapeutic Targets.	1
96	Leveraging genetic algorithms to maximise the predictive capabilities of the SOAP descriptor.	0
95	De Novo Drug Design Using Reinforcement Learning with Graph-Based Deep Generative Models. **2022**, 62, 4863-4872	2
94	Prediction of drug-likeness using graph convolutional attention network.	0
93	Free energy perturbation calculations of tetrahydroquinolines complexed to the first bromodomain of BRD4.	0
92	Explainable AI and Its Applications in Healthcare. **2023**, 111-133	0
91	A Machine Learning-Based Model for Epidemic Forecasting and Faster Drug Discovery. **2022**, 12, 10766	1
90	KUALA: a machine learning-driven framework for kinase inhibitors repositioning. **2022**, 12,	0
89	A systematic literature review for the prediction of anticancer drug response using various machine learning and deep learning techniques.	0
88	Minimal data requirements for accurate compound activity prediction using machine learning methods of different complexity. **2022**, 101113	0
87	A Multi-Objective Active Learning Platform and Web App for Reaction Optimization. **2022**, 144, 19999-20007	0
86	Not from Scratch: Predicting Thermophysical Properties through Model-Based Transfer Learning Using Graph Convolutional Networks.	0
85	Deep generative molecular design reshapes drug discovery. **2022**, 100794	0
84	MGMAE. **2022**,	0
83	Optimizing interactions to protein binding sites by integrating docking-scoring strategies into generative AI methods. 10,	0
82	Predicting Effectiveness of Antihypertensive Medications for Heart Failure based on Longitudinal Patient Records and Deep Learning.	0
81	MRPO-Deep maxout: Manta ray political optimization based Deep maxout network for big data intrusion detection using spark architecture. **2022**, 174, 103324	0
80	Recent advances and application of generative adversarial networks in drug discovery, development, and targeting. **2022**, 2, 100045	0

79	DNN-PP: A novel Deep Neural Network approach and its applicability in drug-related property prediction. **2023**, 213, 119055	0
78	GCN-Based Structure-Activity Relationship and DFT Studies of Staphylococcus aureus FabI Inhibitors. **2022**, 7, 1-16	0
77	Deep Learning. **2022**, 183-205	0
76	AI-Powered Drug Detection System Utilizing Bioactivity Prediction and Drug Release Tracking. **2022**, 4, 263-273	0
75	Application of Computational Biology and Artificial Intelligence in Drug Design. **2022**, 23, 13568	1
74	Generation of novel Diels□Alder reactions using a generative adversarial network. **2022**, 12, 33801-33807	0
73	Electronic, redox, and optical property prediction of organic □conjugated molecules through a hierarchy of machine learning approaches. **2022**, 14, 203-213	0
72	Identification and classification of exfoliated graphene flakes from microscopy images using a hierarchical deep convolutional neural network. **2023**, 119, 105743	0
71	Specific contributions of artificial intelligence to interdisciplinary life science research □exploring and communicating new opportunities. **2023**, 3, 100052	0
70	DIAGNOSING DISEASES FROM FINGERNAIL IMAGES.	0
69	Multispecies Machine Learning Predictions of In Vitro Intrinsic Clearance with Uncertainty Quantification Analyses.	1
68	Predicting Drug Functions from Adverse Drug Reactions by Multi-label Deep Neural Network. **2023**, 215-226	0
67	Using Artificial Intelligence for Drug Discovery: A Bibliometric Study and Future Research Agenda. **2022**, 15, 1492	2
66	Complementarity Between Investment in Information Technology (IT) and IT Human Resources: Implications for Different Types of Firm Innovation.	0
65	Multi-layer guilt-by-association-based drug repurposing by integrating clinical knowledge on biological heterogeneous networks.	0
64	An Improved Model for Predicting Compound Retrosynthesizability Using Machine Learning. **2022**,	0
63	DRlinker: Deep Reinforcement Learning for Optimization in Fragment Linking Design. **2022**, 62, 5907-5917	1
62	Antibiotic discovery in the artificial intelligence era.	0

61	Toward Pharma 4.0 in Drug Discovery. **2023**, 221-238	0
60	Machine learning methods applied for the prediction of biological activities of triple reuptake inhibitors. 1-10	0
59	Exposing the Limitations of Molecular Machine Learning with Activity Cliffs. **2022**, 62, 5938-5951	0
58	Artificial Neural Network Models Driven Novel Virtual Screening Workflow for the Identification and Biological Evaluation of BACE1 Inhibitors..	0
57	Artificial intelligence systems for the design of magic shotgun drugs. **2022**, 100055	0
56	A multilevel generative framework with hierarchical self-contrasting for bias control and transparency in structure-based ligand design. **2022**, 4, 1130-1142	0
55	Contribution of Deep Learning in the Investigation of Possible Dual LOX-3 Inhibitors/DPPH Scavengers: The Case of Recently Synthesized Compounds. **2022**, 9, 800	0
54	TransG-net: transformer and graph neural network based multi-modal data fusion network for molecular properties prediction.	0
53	Predicting chemical structure using reinforcement learning with a stack-augmented conditional variational autoencoder. **2022**, 14,	0
52	DeepFNN-DTBA: prediction of drug-target binding affinity via feed-forward neural network on drug-protein sequences. **2022**, 32,	0
51	Traditional Machine and Deep Learning for Predicting Toxicity Endpoints. **2023**, 28, 217	0
50	Drug repurposing: Recent advancements, challenges, and future therapeutics for cancer treatment. **2022**, 10, 26-30	0
49	Trends and potential of machine learning and deep learning in drug study at single-cell level.	0
48	Quantitative Mass Spectrometry Imaging Using Multivariate Curve Resolution and Deep Learning: A Case Study.	0
47	AI-Powered Blockchain Technology for Public Health: A Contemporary Review, Open Challenges, and Future Research Directions. **2023**, 11, 81	0
46	Multiple machine learning methods aided virtual screening of Na V 1 .5 inhibitors. **2023**, 27, 266-276	0
45	Human-in-the-loop assisted de novo molecular design. **2022**, 14,	0
44	Electrochemical Carbon-Ferrier Rearrangement Using a Microflow Reactor and Machine Learning-Assisted Exploration of Suitable Conditions.	0

43	An empirical study to accelerate machine learning and artificial intelligence adoption in pharmaceutical manufacturing organizations. 174113432211511	0
42	Computational approaches in COVID-19 vaccine development. **2023**, 339-350	0
41	Introduction to Bioinformatics, AI, and ML for Pharmaceuticals. **2023**, 1-18	0
40	Explainable uncertainty quantifications for deep learning-based molecular property prediction. **2023**, 15,	0
39	Recent Advances of Artificial Intelligence in Drug Discovery Process. **2022**,	0
38	Impact of AI on drug delivery and pharmacokinetics: The present scenario and future prospects. **2023**, 443-465	0
37	Definition and exploration of realistic chemical spaces using the connectivity and cyclic features of ChEMBL and ZINC..	0
36	Computational approaches in drug discovery and design. **2023**, 53-93	0
35	Porous Molecular Materials. **2023**, 251-282	0
34	Generating, Managing, and Mining Big Data in Zeolite Simulations. **2023**, 81-111	0
33	Predicting the toxicity of nanoparticles using artificial intelligence tools: a systematic review. **2023**, 17, 62-77	0
32	Pharma Bio-AI revolution. **2023**, 28, 103515	0
31	NoiseMol: A noise-robusted data augmentation via perturbing noise for molecular property prediction. **2023**, 121, 108454	0
30	GB-score: Minimally designed machine learning scoring function based on distance-weighted interatomic contact features. **2023**, 42, 2200135	0
29	Chemistry42: An AI-Driven Platform for Molecular Design and Optimization. **2023**, 63, 695-701	0
28	Deep Learning-based Identification of Intraocular Pressure-Associated Genes Influencing Trabecular Meshwork Cell and Organelle Morphology.	0
27	Future Prospects and Challenges in the Implementation of AI and ML in Pharma Sector. **2023**, 401-416	0
26	AI, ML and Other Bioinformatics Tools for Preclinical and Clinical Development of Drug Products. **2023**, 255-284	0

25	Comparative Studies on Resampling Techniques in Machine Learning and Deep Learning Models for Drug-Target Interaction Prediction. **2023**, 28, 1663	0
24	Multiscale representation learning for biomedical analysis. **2023**, 9-27	0
23	UnCorrupt SMILES: a novel approach to de novo design. **2023**, 15,	0
22	Latent spaces for antimicrobial peptide design. **2023**, 2, 441-458	0
21	Medication Discovery Using Neural Networks. **2023**, 404-418	0
20	Artificial Intelligence Approaches for Energetic Materials by Design: State of the Art, Challenges, and Future Directions. **2023**, 48,	1
19	Artificial Intelligence, Machine Learning, and Big Data for Ebola Virus Drug Discovery. **2023**, 16, 332	0
18	LuoJiaAI: A cloud-based artificial intelligence platform for remote sensing image interpretation. 1-24	0
17	Nanoinformatics and nanomodeling: Recent developments in computational nanodrug design and delivery systems. **2023**, 297-332	0
16	An approach combining deep learning and molecule docking for drug discovery of cathepsin L. **2023**, 18, 347-356	0
15	HSDL-based intelligent threat detection framework for IoT network. **2023**, 1-16	0
14	Success stories in computer-aided drug design. **2023**, 237-253	0
13	Artificial intelligence (AI) and machine learning in the treatment of various diseases. **2023**, 139-158	0
12	Stacked Deep Learning Framework for Edge-Based Intelligent Threat Detection in IoT Network.	0
11	Improvement of multi-task learning by data enrichment: application for drug discovery. **2023**, 37, 183-200	0
10	Deep learning metal complex properties with natural quantum graphs.	0
9	Machine learning in metastatic cancer research: Potentials, possibilities, and prospects. **2023**, 21, 2454-2470	0
8	A Systematic Review of Deep Learning Methodologies Used in the Drug Discovery Process with Emphasis on In Vivo Validation. **2023**, 24, 6573	0

7	Chemical representation learning for toxicity prediction.	0
6	AI-Guided Discovery of Novel SARS-CoV-2 PLpro Inhibitors: Accelerating Antiviral Drug Development in the Fight Against COVID-19.	0
5	Improving the generalizability of protein-ligand binding predictions with AI-Bind. **2023**, 14,	0
4	The Impact of Supervised Learning Methods in Ultralarge High-Throughput Docking.	0
3	Identification of Black Reef Shipwreck Sites Using AI and Satellite Multispectral Imagery. **2023**, 15, 2030	0
2	Generative Models as an Emerging Paradigm in the Chemical Sciences.	0
1	On QSAR-based cardiotoxicity modeling with the expressiveness-enhanced graph learning model and dual-threshold scheme. 14,	0