The Chemical Space Project

Accounts of Chemical Research
48, 722-730
DOI: 10.1021/ar500432k

Citation Report

#	Article	IF	Citations
1	PDB-Explorer: a web-based interactive map of the protein data bank in shape space. BMC Bioinformatics, 2015, 16, 339.	1.2	31
2	Biomolecular recognition of antagonists by Î±7 nicotinic acetylcholine receptor: Antagonistic mechanism and structureâ€“activity relationships studies. European Journal of Pharmaceutical Sciences, 2015, 76, 119-132.	1.9	5
3	In silico design of low molecular weight proteinâ€“protein interaction inhibitors: Overall concept and recent advances. Progress in Biophysics and Molecular Biology, 2015, 119, 20-32.	1.4	56
4	Discovery and characterization of a novel non-competitive inhibitor of the divalent metal transporter DMT1/SLC11A2. Biochemical Pharmacology, 2015, 96, 216-224.	2.0	24
5	Epigenetic relevant chemical space: a chemoinformatic characterization of inhibitors of DNA methyltransferases. RSC Advances, 2015, 5, 87465-87476.	1.7	30
6	Visualization of multi-property landscapes for compound selection and optimization. Journal of Computer-Aided Molecular Design, 2015, 29, 695-705.	1.3	2
7	Supramolecular Oligothiophene Microfibers Spontaneously Assembled on Surfaces or Coassembled with Proteins inside Live Cells. Accounts of Chemical Research, 2015, 48, 2230-2241.	7.6	51
8	An efficient green protocol for the preparation of acetoacetamides and application of the methodology to a one-pot synthesis of Biginelli dihydropyrimidines. Expansion of dihydropyrimidine topological chemical space. RSC Advances, 2015, 5, 70915-70928.	1.7	13
9	Similarity Mapplet: Interactive Visualization of the Directory of Useful Decoys and ChEMBL in High Dimensional Chemical Spaces. Journal of Chemical Information and Modeling, 2015, 55, 1509-1516.	2.5	23
10	PASS Targets: Ligand-based multi-target computational system based on a public data and naÃ¯ve Bayes approach. SAR and QSAR in Environmental Research, 2015, 26, 783-793.	1.0	52
11	Going Small: Using Biophysical Screening to Implement Fragment Based Drug Discovery. , 0, , .		1
12	Internet Databases of the Properties, Enzymatic Reactions, and Metabolism of Small Moleculesâ€”Search Options and Applications in Food Science. International Journal of Molecular Sciences, 2016, 17, 2039.	1.8	20
13	Synthetic Strategies for 5- and 6-Membered Ring Azaheterocycles Facilitated by Iminyl Radicals. Molecules, 2016, 21, 660.	1.7	55
14	Extending accessible chemical space for the identification of novel leads. Expert Opinion on Drug Discovery, 2016, 11, 825-829.	2.5	11
15	Chemical philanthropy: a path forward for antibiotic discovery?. Future Medicinal Chemistry, 2016, 8, 925-929.	1.1	23
16	A polymer dataset for accelerated property prediction and design. Scientific Data, 2016, 3, 160012.	2.4	139
17	Enantiopure hydroxymethylated cycloalkenols as privileged small molecular multifunctional scaffolds for the asymmetric synthesis of carbocycles. Tetrahedron: Asymmetry, 2016, 27, 498-512.	1.8	3
18	BIGCHEM: Challenges and Opportunities for Big Data Analysis in Chemistry. Molecular Informatics, 2016, 35, 615-621.	1.4	85

#	Article	IF	Citations
19	In search of novel ligands using a structure-based approach: a case study on the adenosine A2A receptor. Journal of Computer-Aided Molecular Design, 2016, 30, 863-874.	1.3	20
20	Synthesis in the Chemical Space Age. CheM, 2016, 1, 6-9.	5.8	8
21	FSees: Customized Enumeration of Chemical Subspaces with Limited Main Memory Consumption. Journal of Chemical Information and Modeling, 2016, 56, 1641-1653.	2.5	7
22	Study of the Chemical Space of Selected Bacteriostatic Sulfonamides from an Information Theory Point of View. ChemPhysChem, 2016, 17, 4003-4010.	1.0	7
23	Diastereoselective access to substituted 4-aminopiperidines via a pyridine reduction approach. Tetrahedron Letters, 2016, 57, 5588-5591.	0.7	5
24	Faster Algorithms for Isomer Network Generation. Journal of Chemical Information and Modeling, 2016, 56, 2310-2319.	2.5	4
25	Structural database resources for biological macromolecules. Briefings in Bioinformatics, 2017, 18, bbw049.	3.2	13
26	Visible Light Photocatalysis: Applications and New Disconnections in the Synthesis of Pharmaceutical Agents. Organic Process Research and Development, 2016, 20, 1134-1147.	1.3	293
27	Web-based 3D-visualization of the DrugBank chemical space. Journal of Cheminformatics, 2016, 8, 25.	2.8	15
28	Gene-set analysis based on the pharmacological profiles of drugs to identify repurposing opportunities in schizophrenia. Journal of Psychopharmacology, 2016, 30, 826-830.	2.0	26
29	Advanced Multidimensional Separations in Mass Spectrometry: Navigating the Big Data Deluge. Annual Review of Analytical Chemistry, 2016, 9, 387-409.	2.8	70
30	Combining bioinformatics, chemoinformatics and experimental approaches to design chemical probes: Applications in the field of blood coagulation. Annales Pharmaceutiques Francaises, 2016, 74, 253-266.	0.4	2
31	A graph-based approach to construct target-focused libraries for virtual screening. Journal of Cheminformatics, 2016, 8, 14.	2.8	23
32	ComputergestÃ¼tzte Syntheseplanung: Das Ende vom Anfang. Angewandte Chemie, 2016, 128, 6004-6040.	1.6	35
33	Computerâ€Assisted Synthetic Planning: The End of the Beginning. Angewandte Chemie - International Edition, 2016, 55, 5904-5937.	7.2	395
34	De Novo Design at the Edge of Chaos. Journal of Medicinal Chemistry, 2016, 59, 4077-4086.	2.9	124
35	Filtering promiscuous compounds in early drug discovery: is it a good idea?. Drug Discovery Today, 2016, 21, 868-872.	3.2	73
36	Systematic design of analogs of active compounds covering more than 1000 targets. MedChemComm, 2016, 7, 859-863.	3.5	2

#	Article	IF	Citations
37	Improved fluorescence assays to measure the defects associated with F508delâ€CFTR allow identification of new active compounds. British Journal of Pharmacology, 2017, 174, 525-539.	2.7	17
38	Quantum-chemical insights from deep tensor neural networks. Nature Communications, 2017, 8, 13890.	5.8	884
39	Deep metabolome annotation in natural products research: towards a virtuous cycle in metabolite identification. Current Opinion in Chemical Biology, 2017, 36, 40-49.	2.8	91
40	On the synthesis of machine learning and automated reasoning for an artificial synthetic organic chemist. New Journal of Chemistry, 2017, 41, 1411-1416.	1.4	10
41	Synthesis of Fluorescent Indazoles by Palladium-Catalyzed Benzannulation of Pyrazoles with Alkynes. Organic Letters, 2017, 19, 1450-1453.	2.4	45
42	The impact of in silico screening in the discovery of novel and safer drug candidates. , 2017, 175, 47-66.		85
43	The polypharmacology browser: a web-based multi-fingerprint target prediction tool using ChEMBL bioactivity data. Journal of Cheminformatics, 2017, 9, 11.	2.8	83
44	Quo vadis G protein-coupled receptor ligands? A tool for analysis of the emergence of new groups of compounds over time. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 626-631.	1.0	5
45	Carbonâ€“Nitrogen Bond Formation Through Cross-Dehydrogenative Coupling Reactions. Advances in Organometallic Chemistry, 2017, , 401-481.	0.5	20
46	Fast & easy preparation of 3D scaffolds from methyl benzoate by a diversity oriented synthesis strategy based on Dielsâ€“Alder and ene-reactions. Organic and Biomolecular Chemistry, 2017, 15, 5585-5592.	1.5	2
47	How predictive could alchemical derivatives be?. Physical Chemistry Chemical Physics, 2017, 19, 16003-16012.	1.3	34
48	Fragment Database FDB-17. Journal of Chemical Information and Modeling, 2017, 57, 700-709.	2.5	61
49	Mapping of Drug-like Chemical Universe with Reduced Complexity Molecular Frameworks. Journal of Chemical Information and Modeling, 2017, 57, 680-699.	2.5	16
50	Database fingerprint (DFP): an approach to represent molecular databases. Journal of Cheminformatics, 2017, 9, 9.	2.8	51
51	Identification of acetylcholinesterase inhibitors using homogenous cellâ€based assays in quantitative highâ€throughput screening platforms. Biotechnology Journal, 2017, 12, 1600715.	1.8	10
52	DNA-encoded chemistry: enabling the deeper sampling of chemical space. Nature Reviews Drug Discovery, 2017, 16, 131-147.	21.5	462
53	The chemical space for non-target analysis. TrAC - Trends in Analytical Chemistry, 2017, 97, 179-187.	5.8	57
54	Virtual Exploration of the Ring Systems Chemical Universe. Journal of Chemical Information and Modeling, 2017, 57, 2707-2718.	2.5	27

#	Article	IF	Citations
55	A physicochemical descriptor based method for effective and rapid screening of dual inhibitors against BACE-1 and GSK-3Î² as targets for Alzheimerâ€™s disease. Computational Biology and Chemistry, 2017, 71, 1-9.	1.1	6
56	The octet rule in chemical space: generating virtual molecules. Molecular Diversity, 2017, 21, 769-778.	2.1	0
57	Chemical syntheses of the cochliomycins and certain related resorcylic acid lactones. Tetrahedron Letters, 2017, 58, 4025-4038.	0.7	7
59	Mild Thioâ€Diversification of Bioactive Natural Products. Withaferin A: A Case study.. ChemistrySelect, 2017, 2, 10470-10475.	0.7	2
60	Hit discovery of 4-amino- N -(4-(3-(trifluoromethyl)phenoxy)pyrimidin-5-yl)benzamide: A novel EGFR inhibitor from a designed small library. Bioorganic Chemistry, 2017, 75, 393-405.	2.0	25
61	Chemical space guided discovery of antimicrobial bridged bicyclic peptides against Pseudomonas aeruginosa and its biofilms. Chemical Science, 2017, 8, 6784-6798.	3.7	42
62	Helping to improve the practice of cheminformatics. Journal of Cheminformatics, 2017, 9, 40.	2.8	3
63	Chemical Diversity and Complexity of Scotch Whisky as Revealed by High-Resolution Mass Spectrometry. Journal of the American Society for Mass Spectrometry, 2017, 28, 200-213.	1.2	67
64	Multi-targeting Drug Community Challenge. Cell Chemical Biology, 2017, 24, 1434-1435.	2.5	13
65	ANI-1, A data set of 20 million calculated off-equilibrium conformations for organic molecules. Scientific Data, 2017, 4, 170193.	2.4	178
66	From properties to materials: An efficient and simple approach. Journal of Chemical Physics, 2017, 147, 234105.	1.2	16
67	Molecular Connectivity Predefines Polypharmacology: Aliphatic Rings, Chirality, and sp3 Centers Enhance Target Selectivity. Frontiers in Pharmacology, 2017, 8, 552.	1.6	16
68	Annotation of Peptide Structures Using SMILES and Other Chemical Codesâ€“Practical Solutions. Molecules, 2017, 22, 2075.	1.7	11
69	Drug discovery. , 2017, , 281-420.		1
70	The drug-maker's guide to the galaxy. Nature, 2017, 549, 445-447.	13.7	77
71	Fragment-Based Drug Design by NMR. , 2017, , 741-749.		0
72	A distinctive transformation based diversity oriented synthesis of small ring carbocycles and heterocycles from biocatalytically derived enantiopure Î±-substituted-Î²-hydroxyesters. Organic and Biomolecular Chemistry, 2018, 16, 2549-2575.	1.5	9
73	Chemical compound design using nuclear charge distributions. Journal of Mathematical Chemistry, 2018, 56, 2379-2391.	0.7	2

#	Article	IF	Citations
74	Is artificial intelligence associated with chemistâ€™s creativity represents a threat to humanity?. AI and Society, 2018, 33, 641-643.	3.1	1
76	Nanoscale synthesis and affinity ranking. Nature, 2018, 557, 228-232.	13.7	138
77	An antimicrobial bicyclic peptide from chemical space against multidrug resistant Gram-negative bacteria. Chemical Communications, 2018, 54, 5130-5133.	2.2	25
78	Aptamer chemistry. Advanced Drug Delivery Reviews, 2018, 134, 3-21.	6.6	258
79	Mapping the Efficiency and Physicochemical Trajectories of Successful Optimizations. Journal of Medicinal Chemistry, 2018, 61, 6421-6467.	2.9	79
80	The Alexandria library, a quantum-chemical database of molecular properties for force field development. Scientific Data, 2018, 5, 180062.	2.4	45
81	Chemical probes and drug leads from advances in synthetic planning and methodology. Nature Reviews Drug Discovery, 2018, 17, 333-352.	21.5	182
82	Synthesis of Structurally Diverse Emissive Molecular Rotors with Four-Component Ugi Stators. Journal of Organic Chemistry, 2018, 83, 2570-2581.	1.7	8
83	Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules. ACS Central Science, 2018, 4, 268-276.	5.3	1,761
84	The hitchhikerâ€™s guide to the chemical-biological galaxy. Drug Discovery Today, 2018, 23, 565-574.	3.2	27
85	SchNet â€“ A deep learning architecture for molecules and materials. Journal of Chemical Physics, 2018, 148, 241722.	1.2	1,083
86	Generative Recurrent Networks for De Novo Drug Design. Molecular Informatics, 2018, 37, 1700111.	1.4	305
87	Insights from pharmacological similarity of epigenetic targets in epipolypharmacology. Drug Discovery Today, 2018, 23, 141-150.	3.2	35
88	Harnessing the Properties of Natural Products. Annual Review of Pharmacology and Toxicology, 2018, 58, 451-470.	4.2	64
89	Locked nucleic acid: modality, diversity, and drug discovery. Drug Discovery Today, 2018, 23, 101-114.	3.2	153
90	Chemoinformatics: a perspective from an academic setting in Latin America. Molecular Diversity, 2018, 22, 247-258.	2.1	16
91	Step IIIa: Biological Hit Discovery Through High-Throughput Screening (HTS): Random Approaches and Rational Design. , 2018, , 77-113.		0
92	Step IIIb: The Drug-Like Chemical Diversity Pool: Diverse and Targeted Compound Collections. , 2018, , 115-177.		0

#	Article	IF	Citations
93	Improved understanding of aqueous solubility modeling through topological data analysis. Journal of Cheminformatics, 2018, 10, 54.	2.8	14
94	Bayesian optimization for accelerated drug discovery. IBM Journal of Research and Development, 2018, 62, 2:1-2:7.	3.2	34
95	Machine Learning and Big-Data in Computational Chemistry. , 2018, , 1-24.		4
97	Cheminformatics in Drug Discovery, an Industrial Perspective. Molecular Informatics, 2018, 37, e1800041.	1.4	32
98	Designing Algorithms To Aid Discovery by Chemical Robots. ACS Central Science, 2018, 4, 793-804.	5.3	64
99	Exploring G Protein-Coupled Receptors (GPCRs) Ligand Space via Cheminformatics Approaches: Impact on Rational Drug Design. Frontiers in Pharmacology, 2018, 9, 128.	1.6	105
100	Inverse molecular design using machine learning: Generative models for matter engineering. Science, 2018, 361, 360-365.	6.0	1,055
101	Virtual Chemical Libraries. Journal of Medicinal Chemistry, 2019, 62, 1116-1124.	2.9	153
102	Exploring Chemical and Biological Space of Terpenoids. Journal of Chemical Information and Modeling, 2019, 59, 3667-3678.	2.5	19
103	A diversity-oriented synthesis of polyheterocycles via the cyclocondensation of azomethine imine. New Journal of Chemistry, 2019, 43, 13721-13724.	1.4	8
104	Using Physicochemical Measurements to Influence Better Compound Design. SLAS Discovery, 2019, 24, 791-801.	1.4	24
105	Finding Constellations in Chemical Space Through Core Analysis. Frontiers in Chemistry, 2019, 7, 510.	1.8	31
106	Pattern Generation and Information Transfer through a Liquid/Liquid Interface in 3D Constitutional Dynamic Networks of Imine Ligands in Response to Metal Cation Effectors. Journal of the American Chemical Society, 2019, 141, 12724-12737.	6.6	26
107	Developing RNA aptamers for potential treatment of neurological diseases. Future Medicinal Chemistry, 2019, 11, 551-565.	1.1	8
109	Automated evaluation of consistency within the PubChem Compound database. Scientific Data, 2019, 6, 190023.	2.4	15
111	Compressing physics with an autoencoder: Creating an atomic species representation to improve machine learning models in the chemical sciences. Journal of Chemical Physics, 2019, 151, 084103.	1.2	16
112	SAR by Space: Enriching Hit Sets from the Chemical Space. Molecules, 2019, 24, 3096.	1.7	24
113	A Mixed Integer Linear Programming Formulation to Artificial Neural Networks. , 2019, , .		7

#	Article	IF	Citations
114	Method for Systematic Analogue Search Using the Mega SAR Matrix Database. Journal of Chemical Information and Modeling, 2019, 59, 3727-3734.	2.5	5
115	Mining large databases to find new leads with low similarity to known actives: application to find new DPP-IV inhibitors. Future Medicinal Chemistry, 2019, 11, 1387-1401.	1.1	1
116	Theoretical studies of conformational analysis and intramolecular dynamic phenomena. Structural Chemistry, 2019, 30, 2029-2055.	1.0	1
117	Reaching for the bright StARs in chemical space. Drug Discovery Today, 2019, 24, 2162-2169.	3.2	25
118	Energy windows for computed compound conformers: covering artefacts or truly large reorganization energies?. Future Medicinal Chemistry, 2019, 11, 97-118.	1.1	10
119	A Million Crystal Structures: The Whole Is Greater than the Sum of Its Parts. Chemical Reviews, 2019, 119, 9427-9477.	23.0	191
120	Current and promising novel drug candidates against visceral leishmaniasis. Pure and Applied Chemistry, 2019, 91, 1385-1404.	0.9	29
121	Predicting Molecular Energy Using Force-Field Optimized Geometries and Atomic Vector Representations Learned from an Improved Deep Tensor Neural Network. Journal of Chemical Theory and Computation, 2019, 15, 4113-4121.	2.3	25
122	Reproducing global potential energy surfaces with continuous-filter convolutional neural networks. Journal of Chemical Physics, 2019, 150, 204104.	1.2	16
123	Acceleration of Inverse Molecular Design by Using Predictive Techniques. Journal of Chemical Information and Modeling, 2019, 59, 2587-2599.	2.5	3
124	Exploring the GDB-13 chemical space using deep generative models. Journal of Cheminformatics, 2019, 11, 20.	2.8	107
125	QligFEP: an automated workflow for small molecule free energy calculations in Q. Journal of Cheminformatics, 2019, 11, 26.	2.8	51
126	Catalysis in medicinal chemistry. Reaction Chemistry and Engineering, 2019, 4, 1530-1535.	1.9	13
127	The chemical space of B, N-substituted polycyclic aromatic hydrocarbons: Combinatorial enumeration and high-throughput first-principles modeling. Journal of Chemical Physics, 2019, 150, 114106.	1.2	16
128	PubChem and ChEMBL beyond Lipinski. Molecular Informatics, 2019, 38, e1900016.	1.4	29
129	Data-Driven Systems Level Approaches for Drug Repurposing: Combating Drug Resistance in Priority Pathogens. , 2019, , 229-253.		3
130	Machine learning-powered antibiotics phenotypic drug discovery. Scientific Reports, 2019, 9, 5013.	1.6	63
131	Fragment Hits: What do They Look Like and How do They Bind?. Journal of Medicinal Chemistry, 2019, 62, 3381-3394.	2.9	53

#	Article	IF	Citations
132	ISiCLE: A Quantum Chemistry Pipeline for Establishing in Silico Collision Cross Section Libraries. Analytical Chemistry, 2019, 91, 4346-4356.	3.2	74
133	The maximum occupancy condition for the localized property-optimized orbitals. Physical Chemistry Chemical Physics, 2019, 21, 5285-5294.	1.3	7
134	2. SMALL MOLECULES: THE PAST OR THE FUTURE IN DRUG INNOVATION?. , 2019, , 17-48.		5
135	8. DEVELOPING VANADIUM AS AN ANTIDIABETIC OR ANTICANCER DRUG: A CLINICAL AND HISTORICAL PERSPECTIVE. , 2019, 19, 203-230.		24
136	Randomized SMILES strings improve the quality of molecular generative models. Journal of Cheminformatics, 2019, 11, 71.	2.8	162
137	Applications of Deep-Learning in Exploiting Large-Scale and Heterogeneous Compound Data in Industrial Pharmaceutical Research. Frontiers in Pharmacology, 2019, 10, 1303.	1.6	38
138	ACCDB: A collection of chemistry databases for broad computational purposes. Journal of Computational Chemistry, 2019, 40, 839-848.	1.5	42
139	An approach towards enhancement of a screening library: The Next Generation Library Initiative (NGLI) at Bayer â€" against all odds?. Drug Discovery Today, 2019, 24, 668-672.	3.2	43
140	Soft Matter Informatics: Current Progress and Challenges. Advanced Theory and Simulations, 2019, 2, 1800129.	1.3	52
141	OptCAMD: An optimization-based framework and tool for molecular and mixture product design. Computers and Chemical Engineering, 2019, 124, 285-301.	2.0	58
142	The multidimensional brain. Physics of Life Reviews, 2019, 31, 86-103.	1.5	23
143	Virtual Compound Libraries in Computer-Assisted Drug Discovery. Journal of Chemical Information and Modeling, 2019, 59, 644-651.	2.5	55
144	Drug Discovery Maps, a Machine Learning Model That Visualizes and Predicts Kinomeâ€"Inhibitor Interaction Landscapes. Journal of Chemical Information and Modeling, 2019, 59, 1221-1229.	2.5	46
145	Converging a Knowledge-Based Scoring Function: DrugScore²⁰¹⁸. Journal of Chemical Information and Modeling, 2019, 59, 509-521.	2.5	48
146	Synthese enantiomerenangereicherter, vicinaler tertiÃrer und quartÃrer Kohlenstoffâ€Stereozentren innerhalb einer acyclischen Kette. Angewandte Chemie, 2020, 132, 36-49.	1.6	24
147	Synthesis of Enantioenriched Vicinal Tertiary and Quaternary Carbon Stereogenic Centers within an Acyclic Chain. Angewandte Chemie - International Edition, 2020, 59, 36-49.	7.2	93
148	Can artificial intelligency revolutionize drug discovery?. AI and Society, 2020, 35, 501-504.	3.1	4
149	Autonomous Discovery in the Chemical Sciences Partâ€…I: Progress. Angewandte Chemie - International Edition, 2020, 59, 22858-22893.	7.2	180

#	Article	IF	Citations
150	Autonome Entdeckung in den chemischen Wissenschaften, Teilâ€…I: Fortschritt. Angewandte Chemie, 2020, 132, 23054-23091.	1.6	11
151	Recent achievements and current trajectories of diversity-oriented synthesis. Current Opinion in Chemical Biology, 2020, 56, 1-9.	2.8	67
152	The Symbiotic Relationship Between Drug Discovery and Organic Chemistry. Chemistry - A European Journal, 2020, 26, 1196-1237.	1.7	97
153	Focused Library Generator: case of Mdmx inhibitors. Journal of Computer-Aided Molecular Design, 2020, 34, 769-782.	1.3	7
154	DEEPScreen: high performance drugâ€“target interaction prediction with convolutional neural networks using 2-D structural compound representations. Chemical Science, 2020, 11, 2531-2557.	3.7	131
155	Populating Chemical Space with Peptides Using a Genetic Algorithm. Journal of Chemical Information and Modeling, 2020, 60, 121-132.	2.5	18
156	Challenges in the design of formulated products: multiscale process and product design. Current Opinion in Chemical Engineering, 2020, 27, 1-9.	3.8	24
157	Synthesis and biological evaluation of novel pyrazolo[1,5-a]pyrimidines: Discovery of a selective inhibitor of JAK1 JH2 pseudokinase and VPS34. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 126813.	1.0	16
158	Use of QSAR Global Models and Molecular Docking for Developing New Inhibitors of c-src Tyrosine Kinase. International Journal of Molecular Sciences, 2020, 21, 19.	1.8	23
159	The Derivation of a Matched Molecular Pairs Based ADME/Tox Knowledge Base for Compound Optimization. Journal of Chemical Information and Modeling, 2020, 60, 4757-4771.	2.5	9
160	The Advent of Generative Chemistry. ACS Medicinal Chemistry Letters, 2020, 11, 1496-1505.	1.3	64
161	Molecular Sets (MOSES): A Benchmarking Platform for Molecular Generation Models. Frontiers in Pharmacology, 2020, 11, 565644.	1.6	266
162	tmQM Datasetâ€”Quantum Geometries and Properties of 86k Transition Metal Complexes. Journal of Chemical Information and Modeling, 2020, 60, 6135-6146.	2.5	45
163	A Photoaffinityâ€Based Fragmentâ€Screening Platform for Efficient Identification of Protein Ligands. Angewandte Chemie - International Edition, 2020, 59, 21096-21105.	7.2	38
164	A cheminformatic study on chemical space characterization and diversity analysis of 5-LOX inhibitors. Journal of Molecular Graphics and Modelling, 2020, 100, 107699.	1.3	1
165	Hydration free energies from kernel-based machine learning: Compound-database bias. Journal of Chemical Physics, 2020, 153, 014101.	1.2	23
166	Machine learning for chemical discovery. Nature Communications, 2020, 11, 4125.	5.8	117
167	A Photoaffinityâ€Based Fragmentâ€Screening Platform for Efficient Identification of Protein Ligands. Angewandte Chemie, 2020, 132, 21282-21291.	1.6	5

#	Article	IF	Citations
168	DeepGraphMolGen, a multi-objective, computational strategy for generating molecules with desirable properties: a graph convolution and reinforcement learning approach. Journal of Cheminformatics, 2020, 12, 53.	2.8	42
169	Illuminating elite patches of chemical space. Chemical Science, 2020, 11, 11485-11491.	3.7	12
170	Evaluation of QSAR Equations for Virtual Screening. International Journal of Molecular Sciences, 2020, 21, 7828.	1.8	12
171	Generating Multibillion Chemical Space of Readily Accessible Screening Compounds. IScience, 2020, 23, 101681.	1.9	90
172	Evolution of Novartisâ€™ Small Molecule Screening Deck Design. Journal of Medicinal Chemistry, 2020, 63, 14425-14447.	2.9	31
173	Extending the small-molecule similarity principle to all levels of biology with the Chemical Checker. Nature Biotechnology, 2020, 38, 1087-1096.	9.4	78
174	Evaluation of 3-Dimensionality in Approved and Experimental Drug Space. ACS Medicinal Chemistry Letters, 2020, 11, 1292-1298.	1.3	35
175	Artificial intelligence in chemistry and drug design. Journal of Computer-Aided Molecular Design, 2020, 34, 709-715.	1.3	79
176	A Novel Method for Inference of Chemical Compounds of Cycle Index Two with Desired Properties Based on Artificial Neural Networks and Integer Programming. Algorithms, 2020, 13, 124.	1.2	9
177	Into the latent space. Nature Machine Intelligence, 2020, 2, 151-151.	8.3	3
178	Molecular generation targeting desired electronic properties via deep generative models. Nanoscale, 2020, 12, 6744-6758.	2.8	27
179	Unprecedented Potential for Neural Drug Discovery Based on Self-Organizing hiPSC Platforms. Molecules, 2020, 25, 1150.	1.7	7
180	Complementary Siteâ€Selective Halogenation of Nitrogenâ€Containing (Hetero)Aromatics with Superacids. Chemistry - A European Journal, 2020, 26, 10411-10416.	1.7	16
181	The rise of molecular simulations in fragment-based drug design (FBDD): an overview. Drug Discovery Today, 2020, 25, 1693-1701.	3.2	29
182	Use of Extended-HÃ¼ckel Descriptors for Rapid and Accurate Predictions of Conjugated Torsional Energy Barriers. Journal of Chemical Information and Modeling, 2020, 60, 3534-3545.	2.5	5
183	ChEMBL-Likeness Score and Database GDBChEMBL. Frontiers in Chemistry, 2020, 8, 46.	1.8	33
184	Computer-aided molecular and processes design based on quantum chemistry: current status and future prospects. Current Opinion in Chemical Engineering, 2020, 27, 89-97.	3.8	50
185	Application of Symmetry Functions to Large Chemical Spaces Using a Convolutional Neural Network. Journal of Chemical Information and Modeling, 2020, 60, 1928-1935.	2.5	5

#	Article	IF	Citations
186	Exploring the Multiâ€“Target Neuroprotective Chemical Space of Benzofuran Scaffolds: A New Strategy in Drug Development for Alzheimerâ€™s Disease. Frontiers in Pharmacology, 2019, 10, 1679.	1.6	14
187	Artificial intelligence and machine learning for targeted energy storage solutions. Current Opinion in Electrochemistry, 2020, 21, 160-166.	2.5	33
188	Antitumor activity of new chemical compounds in triple negative mammary adenocarcinoma models. Future Science OA, 2020, 6, FSOA442.	0.9	0
189	Automated in Silico Design of Homogeneous Catalysts. ACS Catalysis, 2020, 10, 2354-2377.	5.5	119
190	A Critical Review of Machine Learning of Energy Materials. Advanced Energy Materials, 2020, 10, 1903242.	10.2	319
192	GEN: highly efficient SMILES explorer using autodidactic generative examination networks. Journal of Cheminformatics, 2020, 12, 22.	2.8	23
193	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
194	Machine learning dihydrogen activation in the chemical space surrounding Vaska's complex. Chemical Science, 2020, 11, 4584-4601.	3.7	93
195	An open-source drug discovery platform enables ultra-large virtual screens. Nature, 2020, 580, 663-668.	13.7	345
196	Predicting Deprotonation Sites Using Alchemical Derivatives. Journal of Physical Chemistry A, 2020, 124, 3754-3760.	1.1	13
197	Machine-learning structural and electronic properties of metal halide perovskites using a hierarchical convolutional neural network. Npj Computational Materials, 2020, 6, .	3.5	93
198	Hydroxylaminâ€abgeleitetes Reagenz als duales Oxidationsmittel und Aminogruppendonor fÃ¼r die eisenkatalysierte Herstellung von ungeschÃ¼tzten Sulfinamiden aus Thiolen. Angewandte Chemie, 2021, 133, 769-776.	1.6	4
199	DrugSpaceX: a large screenable and synthetically tractable database extending drug space. Nucleic Acids Research, 2021, 49, D1170-D1178.	6.5	23
200	Hydroxylamineâ€Derived Reagent as a Dual Oxidant and Amino Group Donor for the Ironâ€Catalyzed Preparation of Unprotected Sulfinamides from Thiols. Angewandte Chemie - International Edition, 2021, 60, 758-765.	7.2	44
201	A Theoretical Exploration of Single-Molecule Mixture Through Combinatorial Method. SSRN Electronic Journal, 0, , .	0.4	0
202	The AI for Scientific Discovery Network+. Patterns, 2021, 2, 100162.	3.1	4
203	The Future of Microbial Drug Resistance. Microbial Drug Resistance, 2021, 27, 1-2.	0.9	2
204	Free Energy Calculations for Proteinâ€“Ligand Binding Prediction. Methods in Molecular Biology, 2021, 2266, 203-226.	0.4	11

#	Article	IF	Citations
205	Natural product-informed exploration of chemical space to enable bioactive molecular discovery. RSC Medicinal Chemistry, 2021, 12, 353-362.	1.7	17
206	An Improved Integer Programming Formulation for Inferring Chemical Compounds with Prescribed Topological Structures. Lecture Notes in Computer Science, 2021, , 197-209.	1.0	0
207	Proposal of the Annotation of Phosphorylated Amino Acids and Peptides Using Biological and Chemical Codes. Molecules, 2021, 26, 712.	1.7	4
208	Systematic optimization of a fragment-based force field against experimental pure-liquid properties considering large compound families: application to oxygen and nitrogen compounds. Physical Chemistry Chemical Physics, 2021, 23, 17774-17793.	1.3	9
209	Virtual Libraries for Docking Methods: Guidelines for the Selection and the Preparation. , 2021, , 99-117.		1
210	Transmol: repurposing a language model for molecular generation. RSC Advances, 2021, 11, 25921-25932.	1.7	4
211	Defining and Exploring Chemical Spaces. Trends in Chemistry, 2021, 3, 133-145.	4.4	60
212	Exploring the Impacts of Conformer Selection Methods on Ion Mobility Collision Cross Section Predictions. Analytical Chemistry, 2021, 93, 3830-3838.	3.2	8
213	Computational compound screening of biomolecules and soft materials by molecular simulations. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 023001.	0.8	15
214	The Playbooks of Medicinal Chemistry Design Moves. Journal of Chemical Information and Modeling, 2021, 61, 729-742.	2.5	11
215	Improved accuracy and transferability of molecular-orbital-based machine learning: Organics, transition-metal complexes, non-covalent interactions, and transition states. Journal of Chemical Physics, 2021, 154, 064108.	1.2	37
216	Accelerated Discovery of Optoelectronic Materials. ACS Photonics, 2021, 8, 699-701.	3.2	1
217	Dataset Construction to Explore Chemical Space with 3D Geometry and Deep Learning. Journal of Chemical Information and Modeling, 2021, 61, 1095-1104.	2.5	11
218	An Inverse QSAR Method Based on a Two-Layered Model and Integer Programming. International Journal of Molecular Sciences, 2021, 22, 2847.	1.8	5
219	One-pot parallel synthesis of 1,3,5-trisubstituted 1,2,4-triazoles. Molecular Diversity, 2022, 26, 993-1004.	2.1	4
220	FragNet, a Contrastive Learning-Based Transformer Model for Clustering, Interpreting, Visualizing, and Navigating Chemical Space. Molecules, 2021, 26, 2065.	1.7	14
221	Prediction of Chromatography Conditions for Purification in Organic Synthesis Using Deep Learning. Molecules, 2021, 26, 2474.	1.7	7
223	Enabling rapid COVID-19 small molecule drug design through scalable deep learning of generative models. International Journal of High Performance Computing Applications, 2021, 35, 469-482.	2.4	21

#	Article	IF	Citations
224	Quantum Chemistry Calculations for Metabolomics. Chemical Reviews, 2021, 121, 5633-5670.	23.0	47
225	Taking the leap between analytical chemistry and artificial intelligence: A tutorial review. Analytica Chimica Acta, 2021, 1161, 338403.	2.6	75
226	Artificial Intelligence-Guided De Novo Molecular Design Targeting COVID-19. ACS Omega, 2021, 6, 12557-12566.	1.6	22
227	Progress on open chemoinformatic tools for expanding and exploring the chemical space. Journal of Computer-Aided Molecular Design, 2022, 36, 341-354.	1.3	25
228	Bioactivity descriptors for uncharacterized chemical compounds. Nature Communications, 2021, 12, 3932.	5.8	44
229	Data Science in Chemical Engineering: Applications to Molecular Science. Annual Review of Chemical and Biomolecular Engineering, 2021, 12, 15-37.	3.3	9
230	Learning molecular potentials with neural networks. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1564.	6.2	19
231	Predicting hydrogen storage in MOFs via machine learning. Patterns, 2021, 2, 100291.	3.1	51
232	On application of deep learning to simplified quantum-classical dynamics in electronically excited states. Machine Learning: Science and Technology, 2021, 2, 035039.	2.4	7
233	The Rise of Neural Networks for Materials and Chemical Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6227-6243.	2.1	39
234	A novel method for inference of acyclic chemical compounds with bounded branch-height based on artificial neural networks and integer programming. Algorithms for Molecular Biology, 2021, 16, 18.	0.3	4
235	Computational discovery of energy materials in the era of big data and machine learning: A critical review. Materials Reports Energy, 2021, 1, 100047.	1.7	24
236	Exploring and mapping chemical space with molecular assembly trees. Science Advances, 2021, 7, eabj2465.	4.7	13
237	Applied Machine Learning for Developing Nextâ€Generation Functional Materials. Advanced Functional Materials, 2021, 31, 2104195.	7.8	28
238	Photocatalysis in the Life Science Industry. Chemical Reviews, 2022, 122, 2907-2980.	23.0	183
239	The role of artificial intelligence in the mass adoption of electric vehicles. Joule, 2021, 5, 2296-2322.	11.7	52
240	The machine-learned radii of atoms. Computational and Theoretical Chemistry, 2021, 1204, 113389.	1.1	1
241	CAT-COSMO-CAMPD: Integrated in silico design of catalysts and processes based on quantum chemistry. Computers and Chemical Engineering, 2021, 153, 107438.	2.0	6

#	Article	IF	Citations
242	De novo generation of dual-target ligands using adversarial training and reinforcement learning. Briefings in Bioinformatics, 2021, 22, .	3.2	7
243	A Novel Method for the Inverse QSAR/QSPR to Monocyclic Chemical Compounds Based on Artificial Neural Networks and Integer Programming. Transactions on Computational Science and Computational Intelligence, 2021, , 641-655.	0.3	3
244	Forecasting System of Computational Time of DFT/TDDFT Calculations under the Multiverse Ansatz via Machine Learning and Cheminformatics. ACS Omega, 2021, 6, 2001-2024.	1.6	6
245	A Novel Method for Inferring Chemical Compounds with Prescribed Topological Substructures Based on Integer Programming. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, PP, 1-1.	1.9	1
246	Generative Models for Automatic Chemical Design. Lecture Notes in Physics, 2020, , 445-467.	0.3	42
247	A New Integer Linear Programming Formulation to the Inverse QSAR/QSPR for Acyclic Chemical Compounds Using Skeleton Trees. Lecture Notes in Computer Science, 2020, , 433-444.	1.0	6
248	Machine Learning and Big-Data in Computational Chemistry. , 2020, , 1939-1962.		5
249	Big Data in Structure-Property Studiesâ€"From Definitions to Models. Challenges and Advances in Computational Chemistry and Physics, 2017, , 529-552.	0.6	1
250	Recent progress on cheminformatics approaches to epigenetic drug discovery. Drug Discovery Today, 2020, 25, 2268-2276.	3.2	33
251	CHAPTER 6. Storing and Using Qualitative and Quantitative Structureâ€"Activity Relationships in the Era of Toxicological and Chemical Data Expansion. Issues in Toxicology, 2019, , 185-213.	0.2	8
252	Materials space of solid-state electrolytes: unraveling chemical compositionâ€"structureâ€"ionic conductivity relationships in garnet-type metal oxides using cheminformatics virtual screening approaches. Physical Chemistry Chemical Physics, 2017, 19, 20904-20918.	1.3	38
253	Open chemoinformatic resources to explore the structure, properties and chemical space of molecules. RSC Advances, 2017, 7, 54153-54163.	1.7	45
254	Deep learning and generative methods in cheminformatics and chemical biology: navigating small molecule space intelligently. Biochemical Journal, 2020, 477, 4559-4580.	1.7	29
258	A Method for the Inverse QSAR/QSPR Based on Artificial Neural Networks and Mixed Integer Linear Programming. , 2020, , .		5
259	ChemMaps: Towards an approach for visualizing the chemical space based on adaptive satellite compounds. F1000Research, 2017, 6, 1134.	0.8	16
260	ChemMaps: Towards an approach for visualizing the chemical space based on adaptive satellite compounds. F1000Research, 2017, 6, 1134.	0.8	25
262	Fragment-based design of selective GPCR ligands guided by free energy simulations. Chemical Communications, 2021, 57, 12305-12308.	2.2	11
263	Individual and collective human intelligence in drug design: evaluating the search strategy. Journal of Cheminformatics, 2021, 13, 80.	2.8	2

#	Article	IF	Citations
264	Novel Reagent Space: Identifying Unorderable but Readily Synthesizable Building Blocks. ACS Medicinal Chemistry Letters, 2021, 12, 1853-1860.	1.3	5
265	DGL-LifeSci: An Open-Source Toolkit for Deep Learning on Graphs in Life Science. ACS Omega, 2021, 6, 27233-27238.	1.6	71
267	Development of Practical Artificial Intelligence System for Drug Discovery and Its Application to Activity Prediction of Small Molecule Protein-Protein Interaction Modulators. Journal of Biological Macromolecules, 2019, 19, 5-10.	0.2	2
268	Extending the Small Molecule Similarity Principle to All Levels of Biology. SSRN Electronic Journal, 0, , .	0.4	0
269	Generation of a Small Library of Natural Products Designed to Cover Chemical Space Inexpensively. , 2019, 1, e190005.		6
270	OBSOLETE: Topical Chemical Space in Relation to Biological Space. , 2019, , .		0
274	Machine Learning-Guided Equations for Super-Fast Prediction of Methane Storage Capacities of COFs. SSRN Electronic Journal, 0, , .	0.4	0
275	Diversity and Chemical Library Networks of Large Data Sets. Journal of Chemical Information and Modeling, 2022, 62, 2186-2201.	2.5	22
276	Towards a systematic analysis of structure-activity relationships of 5-LOX inhibitors through activity landscape and chemotype enrichment. Chemometrics and Intelligent Laboratory Systems, 2020, 207, 104188.	1.8	0
277	Bioactivity characterization of herbal molecules. , 2022, , 145-183.		3
278	Connecting chemistry and biology through molecular descriptors. Current Opinion in Chemical Biology, 2022, 66, 102090.	2.8	24
279	Artificial Intelligence, Machine Learning, and Deep Learning in Real-Life Drug Design Cases. Methods in Molecular Biology, 2022, 2390, 383-407.	0.4	12
280	Multi-objective biofilm algorithm (MOBifi) for de novo drug design with special focus to anti-diabetic drugs. Applied Soft Computing Journal, 2020, 96, 106655.	4.1	3
281	Autonomous Reaction Network Exploration in Homogeneous and Heterogeneous Catalysis. Topics in Catalysis, 2022, 65, 6-39.	1.3	27
282	EViS: An Enhanced Virtual Screening Approach Based on Pocketâ€“Ligand Similarity. Journal of Chemical Information and Modeling, 2022, 62, 498-510.	2.5	4
283	Selecting molecules with diverse structures and properties by maximizing submodular functions of descriptors learned with graph neural networks. Scientific Reports, 2022, 12, 1124.	1.6	4
284	Routescore: Punching the Ticket to More Efficient Materials Development. ACS Central Science, 2022, 8, 122-131.	5.3	8
286	Machine learning and deep learning in data-driven decision making of drug discovery and challenges in high-quality data acquisition in theÂpharmaceutical industry. Future Medicinal Chemistry, 2022, 14, 245-270.	1.1	14

#	Article	IF	Citations
288	Inverse design of 3d molecular structures with conditional generative neural networks. Nature Communications, 2022, 13, 973.	5.8	70
289	Role of the Backbone when Optimizing Functional Groupsâ”€A Theoretical Study Based on an Improved Inverse-Design Approach. Journal of Physical Chemistry A, 2022, 126, 1289-1299.	1.1	1
290	Access to Cyclic N-Trifluoromethyl Ureas through Photocatalytic Activation of Carbamoyl Azides. Journal of the American Chemical Society, 2022, 144, 6100-6106.	6.6	24
291	A new approach to the design of acyclic chemical compounds using skeleton trees and integer linear programming. Applied Intelligence, 0, , .	3.3	0
292	A Data Resource for Prediction of Gas-Phase Thermodynamic Properties of Small Molecules. Data, 2022, 7, 33.	1.2	3
293	MoleGuLAR: Molecule Generation Using Reinforcement Learning with Alternating Rewards. Journal of Chemical Information and Modeling, 2021, 61, 5815-5826.	2.5	22
295	Heuristics and Uncertainty Quantification in Rational and Inverse Compound and Catalyst Design. , 2024, , 485-495.		0
299	Spontaneous Formation of Functional Structures in Messy Environments. Life, 2022, 12, 720.	1.1	4
301	Graph-based molecular Pareto optimisation. Chemical Science, 2022, 13, 7526-7535.	3.7	8
302	Towards universal neural network potential for material discovery applicable to arbitrary combination of 45 elements. Nature Communications, 2022, 13, .	5.8	71
304	Access to high value sp³-rich frameworks using photocatalyzed [2 + 2]-cycloadditions of Î³-alkylideneâ€“Î³-lactams. Chemical Communications, 2022, 58, 8085-8088.	2.2	7
305	Direct Prediction of Physicochemical Properties and Toxicities of Chemicals from Analytical Descriptors by GCâ€“MS. Analytical Chemistry, 2022, 94, 9149-9157.	3.2	4
306	Forty years of combinatorial technology. Drug Discovery Today, 2022, 27, 103308.	3.2	10
307	Organic Chemistry and Synthesis Rely More and More upon Catalysts. Catalysts, 2022, 12, 758.	1.6	2
308	Machine Learning for Electrocatalyst and Photocatalyst Design and Discovery. Chemical Reviews, 2022, 122, 13478-13515.	23.0	120
309	Rapid discovery of stable materials by coordinate-free coarse graining. Science Advances, 2022, 8, .	4.7	15
310	A State-of-the-Art Review on Machine Learning-Based Multiscale Modeling, Simulation, Homogenization and Design of Materials. Archives of Computational Methods in Engineering, 2023, 30, 191-222.	6.0	30
311	Graph-based Automated Macro-Molecule Assembly. Journal of Chemical Information and Modeling, 2022, 62, 3714-3723.	2.5	0

#	Article	IF	Citations
312	Chemical Multiverse: An Expanded View of Chemical Space. Molecular Informatics, 2022, 41, .	1.4	20
313	A brief guide to machine learning for antibiotic discovery. Current Opinion in Microbiology, 2022, 69, 102190.	2.3	14
314	On modeling and utilizing chemical compound information with deep learning technologies: A task-oriented approach. Computational and Structural Biotechnology Journal, 2022, 20, 4288-4304.	1.9	3
315	PAC-FragmentDEL â€“ photoactivated covalent capture of DNA-encoded fragments for hit discovery. RSC Medicinal Chemistry, 2022, 13, 1341-1349.	1.7	10
316	Deep learning-based molecular dynamics simulation for structure-based drug design against SARS-CoV-2. Computational and Structural Biotechnology Journal, 2022, 20, 5014-5027.	1.9	6
317	Chemistry must respond to the crisis of transgression of planetary boundaries. Chemical Science, 2022, 13, 11710-11720.	3.7	10
318	De novo functional groups designed to enhance neuronal integrin Î±5Î²1 binding using deep reinforcement learning. MRS Bulletin, 0, , .	1.7	1
319	Why big data and compute are not necessarily the path to big materials science. Communications Materials, 2022, 3, .	2.9	9
320	On drug discovery against infectious diseases and academic medicinal chemistry contributions. Beilstein Journal of Organic Chemistry, 0, 18, 1355-1378.	1.3	0
321	Physics-based representations for machine learning properties of chemical reactions. Machine Learning: Science and Technology, 2022, 3, 045005.	2.4	6
322	Language models for the prediction of SARS-CoV-2 inhibitors. International Journal of High Performance Computing Applications, 2022, 36, 587-602.	2.4	13
323	OSCAR: an extensive repository of chemically and functionally diverse organocatalysts. Chemical Science, 2022, 13, 13782-13794.	3.7	11
324	Scalable training of graph convolutional neural networks for fast and accurate predictions of HOMO-LUMO gap in molecules. Journal of Cheminformatics, 2022, 14, .	2.8	5
325	The Time and Place for Nature in Drug Discovery. Jacs Au, 2022, 2, 2400-2416.	3.6	34
326	Applications of High Throughput Chemistry to Medicinal Chemistry. ACS Symposium Series, 0, , 3-21.	0.5	0
328	Evolving Progress in Ester Activation Driven by High Throughput Experimentation. ACS Symposium Series, 0, , 147-160.	0.5	0
329	High-Throughput Experimentation for Medicinal Chemistry: State of the Art, Challenges, and Opportunities. ACS Symposium Series, 0, , 37-66.	0.5	0
330	Catalytic, Regioselective 1,4â€Fluorodifunctionalization of Dienes. Angewandte Chemie - International Edition, 2023, 62, .	7.2	13

#	Article	IF	Citations
331	Atomic structure generation from reconstructing structural fingerprints. Machine Learning: Science and Technology, 2022, 3, 045018.	2.4	3
332	Catalytic, Regioselective 1,4â€Fluorodifunctionalization of Dienes. Angewandte Chemie, 0, , .	1.6	0
335	HTE as a Tool in Câ€“H Activation Reaction Discovery and Late-Stage Functionalization of Pharmaceuticals. ACS Symposium Series, 0, , 161-179.	0.5	1
337	High Throughput Experimentation as an Enabler to the Success of Biocatalysis in Industry. ACS Symposium Series, 0, , 67-75.	0.5	0
338	High-Throughput Experimentation for Resource-Efficient Discovery of Methane Functionalization Catalysts. ACS Symposium Series, 0, , 123-145.	0.5	0
339	Applications of High-Throughput Experimentation to Enable Discovery Chemistry. ACS Symposium Series, 0, , 23-36.	0.5	0
340	NeuralNEBâ€”neural networks can find reaction paths fast. Machine Learning: Science and Technology, 2022, 3, 045022.	2.4	10
342	Application of High-Throughput Experimentation in Identification of Conditions for Selective Nitro Group Hydrogenation. ACS Symposium Series, 0, , 79-91.	0.5	0
343	Leveraging HTE in Non-canonical Amino Acid Synthesis and Peptide Ligation. ACS Symposium Series, 0, , 109-120.	0.5	0
344	Leveraging High Throughput Experimentation for Improved Access to Privileged Pharmaceutical Structures. ACS Symposium Series, 0, , 93-108.	0.5	0
345	A Gated Spatial-Channel Transformer Network for the Prediction of Molecular Properties. , 2022, , .		0
346	Fragment screening using biolayer interferometry reveals ligands targeting the SHP-motif binding site of the AAA+ÂATPase p97. Communications Chemistry, 2022, 5, .	2.0	2
347	DNAâ€Encoded Libraries: Towards Harnessing their Full Power with Darwinian Evolution. Angewandte Chemie, 2023, 135, .	1.6	3
348	DNAâ€Encoded Libraries: Towards Harnessing their Full Power with Darwinian Evolution. Angewandte Chemie - International Edition, 2023, 62, .	7.2	16
349	Learning with uncertainty to accelerate the discovery of histone lysine-specific demethylase 1A (KDM1A/LSD1) inhibitors. Briefings in Bioinformatics, 2023, 24, .	3.2	2
350	Autonomous Drug Design with Multi-Armed Bandits. , 2022, , .		1
351	Mapping interaction between big spaces; active space from protein structure and available chemical space. , 2023, , 299-332.		0
352	Drug discovery: Standing on the shoulders of giants. , 2023, , 207-338.		0

#	Article	IF	Citations
353	Deep generative fuel design in low data regimes via multi-objective imitation. Chemical Engineering Science, 2023, 274, 118686.	1.9	0
354	Insecticide discoveryâ€“â€œChance favors the prepared mindâ€• Pesticide Biochemistry and Physiology, 2023, 192, 105412.	1.6	3
355	Computational Approaches to Enzyme Inhibition by Marine Natural Products in the Search for New Drugs. Marine Drugs, 2023, 21, 100.	2.2	4
356	Progress of Artificial Intelligence in Drug Synthesis and Prospect of Its Application in Nitrification of Energetic Materials. Molecules, 2023, 28, 1900.	1.7	0
357	Machine learning-inspired battery material innovation. Energy Advances, 2023, 2, 449-464.	1.4	4
359	De novodrug design by iterative multiobjective deep reinforcement learning with graph-based molecular quality assessment. Bioinformatics, 2023, 39, .	1.8	5
360	Artificial Intelligence for Scientific Discovery at High-Performance Computing Scales. Computer, 2023, 56, 116-122.	1.2	0
361	Fragment-based Ligand Discovery (FBLD). , 2023, , 188-230.		0
364	Exploring chemical space with alchemical derivatives. , 2023, , 15-57.		0
376	The Application of Novel Functional Materials to Machine Learning. , 2023, , 95-115.		0
392	Artificial intelligence for natural product drug discovery. Nature Reviews Drug Discovery, 2023, 22, 895-916.	21.5	16
397	Evolutionary Algorithms and Workflows for De Novo Catalyst Design. , 2024, , 540-561.		0
412	PRACTICAL APPLICATIONS OF MACHINE LEARNING FOR ANTI-INFECTIVE DRUG DISCOVERY. Medicinal Chemistry Reviews, 0, , 345-375.	0.1	0
416	Towards Foundation Models for Materials Science: The Open MatSci ML Toolkit. , 2023, , .		0
419	%V_{Bur} index and steric maps: from predictive catalysis to machine learning. Chemical Society Reviews, 2024, 53, 853-882.	18.7	8
420	De Novo Design ofÂTarget-Specific Ligands Using BERT-Pretrained Transformer. Lecture Notes in Computer Science, 2024, , 311-322.	1.0	0