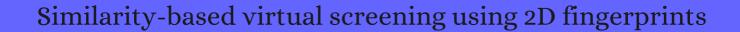
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#	Paper	IF	Citations
684	Advances in virtual screening. 2006, 3, 405-411		87
683	Chemical similarity searches: when is complexity justified?. 2007 , 2, 423-30		43
682	Computer-aided retrometabolic drug design: soft drugs. 2007 , 2, 923-33		5
681	Exploring peptide-likeness of active molecules using 2D fingerprint methods. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 1366-78	6.1	5
680	Introduction of a generally applicable method to estimate retrieval of active molecules for similarity searching using fingerprints. <i>ChemMedChem</i> , 2007 , 2, 1311-20	3.7	20
679	Scaffold composition and biological relevance of screening libraries. 2007 , 3, 442-6		148
678	Chemogenomic approaches to rational drug design. 2007 , 152, 38-52		196
677	Methods for computer-aided chemical biology. Part 2: Evaluation of compound selectivity using 2D molecular fingerprints. 2007 , 70, 195-205		28
676	A similarity-based data-fusion approach to the visual characterization and comparison of compound databases. 2007 , 70, 393-412		65
675	Molecular similarity analysis in virtual screening: foundations, limitations and novel approaches. Drug Discovery Today, 2007 , 12, 225-33	8.8	362
674	A cheminformatic toolkit for mining biomedical knowledge. 2007 , 24, 1791-802		19
673	A successful virtual screening application: prediction of anticonvulsant activity in MES test of widely used pharmaceutical and food preservatives methylparaben and propylparaben. <i>Journal of Computer-Aided Molecular Design</i> , 2007 , 21, 527-38	4.2	24
672	A support vector machines approach for virtual screening of active compounds of single and multiple mechanisms from large libraries at an improved hit-rate and enrichment factor. 2008 , 26, 1276	5-86	66
671	Exploring structure-selectivity relationships of biogenic amine GPCR antagonists using similarity searching and dynamic compound mapping. 2008 , 12, 25-40		17
670	Distribution of randomly generated activity class characteristic substructures in diverse active and database compounds. 2008 , 12, 77-83		4
669	FTree query construction for virtual screening: a statistical analysis. <i>Journal of Computer-Aided Molecular Design</i> , 2008 , 22, 111-8	4.2	4
668	A simple and fuzzy method to align and compare druggable ligand-binding sites. 2008 , 71, 1755-78		83

(2008-2008)

667	Integrating structure- and ligand-based virtual screening: comparison of individual, parallel, and fused molecular docking and similarity search calculations on multiple targets. <i>ChemMedChem</i> , 2008 , 3, 1566-71	3.7	52
666	Strategies for generating less toxic P-selectin inhibitors: pharmacophore modeling, virtual screening and counter pharmacophore screening to remove toxic hits. 2008 , 27, 546-57		11
665	Dissimilarity-based approaches to compound acquisition. 2008 , 12, 366-71		26
664	Random reduction in fingerprint bit density improves compound recall in search calculations using complex reference molecules. 2008 , 71, 511-7		10
663	Support-vector-machine-based ranking significantly improves the effectiveness of similarity searching using 2D fingerprints and multiple reference compounds. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 742-6	6.1	57
662	Fingerprint directed scaffold hopping for identification of CCR2 antagonists. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 1891-902	6.1	21
661	Balancing the influence of molecular complexity on fingerprint similarity searching. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 75-84	6.1	28
660	Evaluation of virtual screening performance of support vector machines trained by sparsely distributed active compounds. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 1227-37	6.1	34
659	NaWe Bayes classification using 2D pharmacophore feature triplet vectors. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 166-78	6.1	59
658	Similarity searching using fingerprints of molecular fragments involved in protein-ligand interactions. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 2308-12	6.1	33
657	Data mining a small molecule drug screening representative subset from NIH PubChem. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 465-75	6.1	60
656	FieldChopper, a new tool for automatic model generation and virtual screening based on molecular fields. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 1131-7	6.1	3
655	Ligand-target interaction-based weighting of substructures for virtual screening. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 1955-64	6.1	29
654	Similarity searching and scaffold hopping in synthetically accessible combinatorial chemistry spaces. 2008 , 51, 2468-80		6 7
653	Structural requirements for drug inhibition of the liver specific human organic cation transport protein 1. 2008 , 51, 5932-42		151
652	Bit silencing in fingerprints enables the derivation of compound class-directed similarity metrics. Journal of Chemical Information and Modeling, 2008, 48, 1754-9	6.1	24
651	Combining pharmacophore fingerprints and PLS-discriminant analysis for virtual screening and SAR elucidation. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 476-88	6.1	11
650	From chemical documentation to chemoinformatics: 50 years of chemical information science. 2008 , 34, 477-499		34

649	Virtual screening and its integration with modern drug design technologies. 2008, 15, 37-46		152
648	Chapter 6:Probabilistic Approaches in Activity Prediction. 2008, 182-216		49
647	Hierarchical Clustering of Large Databases and Classification of Antibiotics at High Noise Levels. 2008 , 1, 183-200		7
646	Comparative analysis of machine learning methods in ligand-based virtual screening of large compound libraries. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2009 , 12, 344-57	1.3	47
645	Current strategies for the discovery of K+ channel modulators. 2009 , 9, 348-61		6
644	Systematic computational analysis of structure-activity relationships: concepts, challenges and recent advances. 2009 , 1, 451-66		42
643	How to recognize and workaround pitfalls in QSAR studies: a critical review. 2009, 16, 4297-313		141
642	Development of decision tree models for substrates, inhibitors, and inducers of p-glycoprotein. 2009 , 10, 339-46		21
641	A mapping of drug space from the viewpoint of small molecule metabolism. 2009 , 5, e1000474		30
640	FINDSITE: a combined evolution/structure-based approach to protein function prediction. <i>Briefings in Bioinformatics</i> , 2009 , 10, 378-91	13.4	79
639	'Metabolite-likeness' as a criterion in the design and selection of pharmaceutical drug libraries. Drug Discovery Today, 2009 , 14, 31-40	8.8	103
638	Improving the search performance of extended connectivity fingerprints through activity-oriented feature filtering and application of a bit-density-dependent similarity function. <i>ChemMedChem</i> , 2009 , 4, 540-8	3.7	34
637	Design, selection, and evaluation of a general kinase-focused library. <i>ChemMedChem</i> , 2009 , 4, 1273-8	3.7	14
636	Molecular fingerprint recombination: generating hybrid fingerprints for similarity searching from different fingerprint types. <i>ChemMedChem</i> , 2009 , 4, 1859-63	3.7	29
635	A virtual screening study of the 18 kDa translocator protein using pharmacophore models combined with 3D-QSAR studies. <i>ChemMedChem</i> , 2009 , 4, 1686-94	3.7	6
634	Distance phenomena in high-dimensional chemical descriptor spaces: consequences for similarity-based approaches. 2009 , 30, 2285-96		20
633	Comparison of structure fingerprint and molecular interaction field based methods in explaining biological similarity of small molecules in cell-based screens. <i>Journal of Computer-Aided Molecular Design</i> , 2009 , 23, 227-39	4.2	9
632	Analysis and use of fragment-occurrence data in similarity-based virtual screening. <i>Journal of Computer-Aided Molecular Design</i> , 2009 , 23, 655-68	4.2	25

(2009-2009)

631	Predicting the similarity search performance of fingerprints and their combination with molecular property descriptors using probabilistic and information theoretic modeling. 2009 , 2, 123-134	ŗ	5
630	Turbo similarity searching: Effect of fingerprint and dataset on virtual-screening performance. 2009 , 2, 103-114	ĵ	30
629	Review of statistical analyses in drug discovery and chemogenomics. 2009 , 2, 88-102		
628	Investigating Enzyme Selectivity and Hit Enrichment by Automatically Interfacing Ligand- and Structure-Based Molecular Design. 2009 , 28, 861-864	2	2
627	Staring off into chemical space. 2009 , 5, 536-7	Ç	9
626	Utilizing target-ligand interaction information in fingerprint searching for ligands of related targets. 2009 , 74, 25-32	:	15
625	Filtering and counting of extended connectivity fingerprint features maximizes compound recall and the structural diversity of hits. 2009 , 74, 92-8	Ç	9
624	Three-dimensional protein-ligand interaction scaling of two-dimensional fingerprints. 2009 , 74, 449-56	Ī	14
623	Clustering files of chemical structures using the Szkely-Rizzo generalization of Ward's method. 2009 , 28, 187-95	3	35
622	LigMatch: a multiple structure-based ligand matching method for 3D virtual screening. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 2056-66	3	33
621	Development of a compound class-directed similarity coefficient that accounts for molecular complexity effects in fingerprint searching. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 1369-76	6 -	15
620	Improving quantitative structure-activity relationships through multiobjective optimization. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 2290-302	4	44
619	Extraction and analysis of chemical modification patterns in drug development. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 1122-9	-	11
618	Effective protocol for database similarity searching of heteronuclear single quantum coherence spectra. 2009 , 81, 9329-35	(5
617	Shannon entropy-based fingerprint similarity search strategy. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 1687-91	-	15
616	Unconventional 2D shape similarity method affords comparable enrichment as a 3D shape method in virtual screening experiments. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 1313-20	-	15
615	A machine learning approach to weighting schemes in the data fusion of similarity coefficients. Journal of Chemical Information and Modeling, 2009 , 49, 185-94	-	14
614	GPU accelerated support vector machines for mining high-throughput screening data. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 2718-25		35

613	Critical comparison of virtual screening methods against the MUV data set. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 2168-78	6.1	38
612	Hit finding: towards 'smarter' approaches. 2009 , 9, 589-93		21
611	Classification of cytochrome p(450) activities using machine learning methods. 2009 , 6, 1920-6		36
610	Searching for target-selective compounds using different combinations of multiclass support vector machine ranking methods, kernel functions, and fingerprint descriptors. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 582-92	6.1	51
609	Chemoinformatic analysis of combinatorial libraries, drugs, natural products, and molecular libraries small molecule repository. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 1010-24	6.1	131
608	Lead Discovery Using Virtual Screening. 2009 , 85-124		
607	Multidentate small-molecule inhibitors of vaccinia H1-related (VHR) phosphatase decrease proliferation of cervix cancer cells. 2009 , 52, 6716-23		45
606	Chemoinformatics-applications in food chemistry. 2009 , 58, 33-56		15
605	Development of a fingerprint reduction approach for Bayesian similarity searching based on Kullback-Leibler divergence analysis. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 1347-58	6.1	27
604	Performance of machine learning methods for ligand-based virtual screening. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2009 , 12, 358-68	1.3	29
603	Exploring novel target space: a need to partner high throughput docking and ligand-based similarity searches?. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2009 , 12, 984-99	1.3	6
602	Virtual screening with support vector machines and structure kernels. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2009 , 12, 409-23	1.3	10
601	Advanced fingerprint methods for similarity searching: balancing molecular complexity effects. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2010 , 13, 220-8	1.3	12
600	In Silico Methods for the Analysis of Metabolites and Drug Molecules. 2010 , 361-381		
599	Predicting the performance of fingerprint similarity searching. 2011 , 672, 159-73		6
598	Some Trends in Chem(o)informatics. 2011 , 672, 1-37		15
597	Similarity searching using 2D structural fingerprints. 2011 , 672, 133-58		81
596	Large-scale systematic analysis of 2D fingerprint methods and parameters to improve virtual screening enrichments. <i>Journal of Chemical Information and Modeling</i> , 2010 , 50, 771-84	6.1	227

(2010-2010)

595	Molecular graph augmentation with rings and functional groups. <i>Journal of Chemical Information and Modeling</i> , 2010 , 50, 1660-8	6.1	9
594	Exploiting PubChem for Virtual Screening. 2010 , 5, 1205-1220		59
593	New molecular scaffolds for the design of Mycobacterium tuberculosis type II dehydroquinase inhibitors identified using ligand and receptor based virtual screening. 2010 , 16, 693-712		15
592	Spatial chemical distance based on atomic property fields. <i>Journal of Computer-Aided Molecular Design</i> , 2010 , 24, 173-82	4.2	13
591	Screening of benzamidine-based thrombin inhibitors via a linear interaction energy in continuum electrostatics model. <i>Journal of Computer-Aided Molecular Design</i> , 2010 , 24, 117-29	4.2	6
590	KiDoQ: using docking based energy scores to develop ligand based model for predicting antibacterials. 2010 , 11, 125		24
589	Rendering conventional molecular fingerprints for virtual screening independent of molecular complexity and size effects. <i>ChemMedChem</i> , 2010 , 5, 859-68	3.7	9
588	In Silico Screening. 2010 , 73-103		
587	Virtual Activity Profiling of Bioactive Molecules by 1D Fingerprinting. <i>Molecular Informatics</i> , 2010 , 29, 773-9	3.8	1
586	Analysis and comparison of 2D fingerprints: insights into database screening performance using eight fingerprint methods. 2010 , 29, 157-70		275
585	Towards a systematic characterization of the antiprotozoal activity landscape of benzimidazole derivatives. 2010 , 18, 7380-91		54
584	Integration of metabolic databases for the reconstruction of genome-scale metabolic networks. 2010 , 4, 114		67
583	CAESAR models for developmental toxicity. 2010 , 4 Suppl 1, S4		802
582	Estimation of the applicability domain of kernel-based machine learning models for virtual screening. 2010 , 2, 2		33
581	Reduction and recombination of fingerprints of different design increase compound recall and the structural diversity of hits. 2010 , 75, 152-60		20
580	Computational methodologies for compound database searching that utilize experimental protein-ligand interaction information. 2010 , 76, 191-200		19
579	Prediction of adverse drug reactions using decision tree modeling. 2010 , 88, 52-9		60
578	Reducing the algorithmic variability in transcriptome-based inference. 2010 , 26, 1185-91		5

577	Virtual Screening. 2010, 1-46		1
576	Contributions of computational chemistry and biophysical techniques to fragment-based drug discovery. 2010 , 17, 1769-94		36
575	Concepts and applications of "natural computing" techniques in de novo drug and peptide design. 2010 , 16, 1656-65		22
574	Toward the discovery of functional transthyretin amyloid inhibitors: application of virtual screening methods. <i>Journal of Chemical Information and Modeling</i> , 2010 , 50, 1806-20	6.1	13
573	IGERS: inferring Gibbs energy changes of biochemical reactions from reaction similarities. 2010 , 98, 247	8-86	11
572	Identification of Metabotropic Glutamate Receptor Subtype 5 Potentiators Using Virtual High-Throughput Screening. 2010 , 1, 288-305		36
571	A searchable map of PubChem. Journal of Chemical Information and Modeling, 2010, 50, 1924-34	6.1	53
570	Inverse frequency weighting of fragments for similarity-based virtual screening. <i>Journal of Chemical Information and Modeling</i> , 2010 , 50, 1340-9	6.1	13
569	Scaffold hopping using two-dimensional fingerprints: true potential, black magic, or a hopeless endeavor? Guidelines for virtual screening. 2010 , 53, 5707-15		78
568	Atom-centered interacting fragments and similarity search applications. <i>Journal of Chemical Information and Modeling</i> , 2010 , 50, 79-86	6.1	16
567	Chemical space as a source for new drugs. 2010 , 1, 30		200
566	Bioactivity-guided navigation of chemical space. 2010 , 43, 1103-14		202
565	Novel application of 2D and 3D-similarity searches to identify substrates among cytochrome P450 2C9, 2D6, and 3A4. <i>Journal of Chemical Information and Modeling</i> , 2010 , 50, 97-109	6.1	14
564	Modeling liver-related adverse effects of drugs using knearest neighbor quantitative structure-activity relationship method. 2010 , 23, 724-32		88
563	Advances in 2D fingerprint similarity searching. 2010 , 5, 529-42		14
562	Structural basis for computational screening of non-steroidal androgen receptor ligands. 2010 , 5, 5-20		2
561	Synthesis of novel molecular probes inspired by harringtonolide. 2011 , 9, 4570-9		17
560	Scaffold-hopping from aminoglycosides to small synthetic inhibitors of bacterial protein biosynthesis using a pseudoreceptor model. 2011 , 2, 181		1

(2011-2011)

CycloPs: generating virtual libraries of cyclized and constrained peptides including nonnatural amino acids. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 829-36	6.1	22
A Rapid Procedure for Spectral Similarity Matching of Heteronuclear Single Quantum Coherence Spectra. 2011 ,		
Consensus models of activity landscapes with multiple chemical, conformer, and property representations. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 1259-70	6.1	56
Identification of novel functional inhibitors of acid sphingomyelinase. 2011 , 6, e23852		107
Structural Basis and Computational Modeling of Chiral Drugs. 2011 , 297-321		1
Combinatorial QSAR modeling of human intestinal absorption. 2011 , 8, 213-24		28
Graph-based similarity concepts in virtual screening. 2011 , 3, 485-501		5
Computational ligand-based rational design: Role of conformational sampling and force fields in model development. 2011 , 2, 356-370		58
Applied Virtual Screening: Strategies, Recommendations, and Caveats. 2011 , 291-318		10
Comparison of combinatorial clustering methods on pharmacological data sets represented by machine learning-selected real molecular descriptors. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 3036-49	6.1	17
Trends in kinase selectivity: insights for target class-focused library screening. 2011 , 54, 54-66		68
Large-scale similarity search profiling of ChEMBL compound data sets. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 1831-9	6.1	59
New fragment weighting scheme for the Bayesian inference network in ligand-based virtual screening. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 25-32	6.1	32
Chemoinformatics and library design. 2011 , 685, 27-52		8
Chemoinformatics and Computational Chemical Biology. 2011,		6
Rational methods for the selection of diverse screening compounds. 2011 , 6, 208-17		80
Power keys: a novel class of topological descriptors based on exhaustive subgraph enumeration and their application in substructure searching. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2843-51	6.1	10
A binary ant colony optimization classifier for molecular activities. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2690-6	6.1	8
	amino acids. Journal of Chemical Information and Modeling, 2011, 51, 829-36 A Rapid Procedure for Spectral Similarity Matching of Heteronuclear Single Quantum Coherence Spectra. 2011, Consensus models of activity landscapes with multiple chemical, conformer, and property representations. Journal of Chemical Information and Modeling, 2011, 51, 1259-70 Identification of novel functional inhibitors of acid sphingomyelinase. 2011, 6, e23852 Structural Basis and Computational Modeling of Chiral Drugs. 2011, 297-321 Combinatorial QSAR modeling of human intestinal absorption. 2011, 8, 213-24 Graph-based similarity concepts in virtual screening. 2011, 3, 485-501 Computational ligand-based rational design: Role of conformational sampling and force fields in model development. 2011, 2, 356-370 Applied Virtual Screening: Strategies, Recommendations, and Caveats. 2011, 291-318 Comparison of combinatorial clustering methods on pharmacological data sets represented by machine learning-selected real molecular descriptors. Journal of Chemical Information and Modeling, 2011, 51, 3036-49 Trends in kinase selectivity: insights for target class-focused library screening. 2011, 54, 54-66 Large-scale similarity search profiling of ChEMBL compound data sets. Journal of Chemical Information and Modeling, 2011, 51, 1831-9 New fragment weighting scheme for the Bayesian inference network in ligand-based virtual screening. Journal of Chemical Information and Modeling, 2011, 51, 25-32 Chemoinformatics and Computational Chemical Biology. 2011, 51, 25-32 Chemoinformatics and Computational Chemical Biology. 2011, 6, 208-17 Power keys: a novel class of topological descriptors based on exhaustive subgraph enumeration and their application in substructure searching. Journal of Chemical Information and Modeling, 2011, 51, 284-351 A binary and colony optimization classifier for molecular activities. Journal of Chemical Information	A Rapid Procedure for Spectral Similarity Matching of Heteronuclear Single Quantum Coherence Spectra. 2011, Consensus models of activity landscapes with multiple chemical, conformer, and property representations. Journal of Chemical Information and Modeling, 2011, 51, 1259-70 6.1. Consensus models of activity landscapes with multiple chemical, conformer, and property representations. Journal of Chemical Information and Modeling, 2011, 51, 1259-70 6.2. Consensus models of activity landscapes with multiple chemical, conformer, and property representations. Journal of Chemical Information and Modeling, 2011, 51, 1259-70 6.2. Consensus models of activity landscapes with multiple chemical, conformer, and property representations. Journal of Chemical Information and Modeling of Chiral Drugs. 2011, 52, 123-24 Combinatorial QSAR modeling of human intestinal absorption. 2011, 8, 213-24 Companisorial QSAR modeling of human intestinal absorption. 2011, 8, 213-24 Companisorial QSAR modeling of human intestinal absorption. 2011, 8, 213-24 Companisorial QSAR modeling of human intestinal absorption. 2011, 8, 213-24 Companisorial QSAR modeling design: Role of conformational sampling and force fields in model development. 2011, 2, 356-370 Applied Virtual Screening: Strategies, Recommendations, and Caveats. 2011, 291-318 Companisor of combinatorial clustering methods on pharmacological data sets represented by machine learning-selected real molecular descriptors. Journal of Chemical Information and Modeling 2011, 51, 3036-49 Trends in kinase selectivity: insights for target class-focused library screening. 2011, 54, 54-66 Large-scale similarity search profiling of ChEMBL compound data sets. Journal of Chemical Information and Modeling. 2011, 51, 1831-9 New fragment weighting scheme for the Bayesian inference network in ligand-based virtual screening. Journal of Chemical Information and Modeling. 2011, 51, 1831-9 New fragment weighting scheme for the Bayesian inference network in ligand-based virtual screening.

541	How do 2D fingerprints detect structurally diverse active compounds? Revealing compound subset-specific fingerprint features through systematic selection. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2254-65	1	20
540	Multitarget structure-activity relationships characterized by activity-difference maps and consensus similarity measure. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2427-39	1	50
539	Fragment-similarity-based QSAR (FS-QSAR) algorithm for ligand biological activity predictions. 2011 , 22, 385-410		11
538	Applications and Success Stories in Virtual Screening. 2011 , 319-358		17
537	Fragment-based approaches and computer-aided drug discovery. 2012 , 317, 201-22		22
536	Classification of cytochrome P450 inhibitors and noninhibitors using combined classifiers. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 996-1011	1	124
535	In silico prediction of rhabdomyolysis of compounds by self-organizing map and support vector machine. 2011 , 25, 2017-24		4
534	. 2011,		26
533	Integration of virtual and high throughput screening in lead discovery settings. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2011 , 14, 889-97	3	24
532	Exploring and exploiting biologically relevant chemical space. 2011 , 12, 1531-46		32
531	Integrating virtual screening and combinatorial chemistry for accelerated drug discovery. Combinatorial Chemistry and High Throughput Screening, 2011 , 14, 475-87	3	80
530	Combined SVM-based and docking-based virtual screening for retrieving novel inhibitors of c-Met. 2011 , 46, 3675-80		20
529	Effectiveness of 2D fingerprints for scaffold hopping. 2011 , 3, 405-14		49
528	Integrating structure-based and ligand-based approaches for computational drug design. 2011 , 3, 735-50		101
527	Target-Based Virtual Screening to Address Protein Protein Interfaces. 2011, 435-465		
526	Ligand-based approaches to in silico pharmacology. 2011 , 672, 489-502		48
525	Similarity searching. 2011 , 1, 260-282		91
524	Representation of chemical structures. 2011 , 1, 557-579		43

523	Similarity-based data mining in files of two-dimensional chemical structures using fingerprint measures of molecular resemblance. 2011 , 1, 241-251	16
522	Visualisation and subsets of the chemical universe database GDB-13 for virtual screening. <i>Journal of Computer-Aided Molecular Design</i> , 2011 , 25, 637-47	40
521	Visualisation of the chemical space of fragments, lead-like and drug-like molecules in PubChem. <i>Journal of Computer-Aided Molecular Design</i> , 2011 , 25, 649-62 4.2	26
520	Effective feature construction by maximum common subgraph sampling. 2011 , 83, 137-161	14
519	Brainstorming: weighted voting prediction of inhibitors for protein targets. 2011 , 17, 2133-41	15
518	Discovery of potent, novel, non-toxic anti-malarial compounds via quantum modelling, virtual screening and in vitro experimental validation. 2011 , 10, 274	10
517	2D-Qsar for 450 types of amino acid induction peptides with a novel substructure pair descriptor having wider scope. 2011 , 3, 50	3
516	Quantitative measure of structural and geometric similarity of 3D morphologies. 2011 , 16, 40-52	8
515	Molecular similarity and diversity approaches in chemoinformatics. 2011 , 72, 74-84	9
5 1 4	MyMolDB: a micromolecular database solution with open source and free components. 2011 , 32, 2942-8	1
513	Biologie-orientierte Synthese (BIOS). 2011 , 123, 10990-11018	116
512	Biology-oriented synthesis. 2011 , 50, 10800-26	376
511	Molecular path for ligand search. 2011 , 22, 1130-1134	
510	Virtual screening against obesity. 2011 , 18, 2158-73	3
509	bcl::Cluster : A method for clustering biological molecules coupled with visualization in the Pymol Molecular Graphics System. 2011 , 2011, 13-18	114
508	2D autocorrelation modelling of the anti-HIV HEPT analogues using multiple linear regression approaches. 2011 , 37, 72-83	4
507	ChemProt: a disease chemical biology database. 2011 , 39, D367-72	58
506	Enhancing the rate of scaffold discovery with diversity-oriented prioritization. 2011 , 27, 2271-8	7

505	Thematic Analysis Da chemogenomic approach to GPCR drug discovery. 2011 , 11, 1925-43	6
504	Lipoxin A4 is a novel estrogen receptor modulator. 2011 , 25, 4326-37	52
503	Navigating the human metabolome for biomarker identification and design of pharmaceutical molecules. 2011 , 2011,	24
502	Identification and characterization of novel small-molecule inhibitors against hepatitis delta virus replication by using docking strategies. 2011 , 11, 803-9	6
501	The 🛘 -adrenoceptor agonist formoterol stimulates mitochondrial biogenesis. 2012 , 342, 106-18	69
500	Virtual screening methods as tools for drug lead discovery from large chemical libraries. 2012 , 19, 5562-71	21
499	In silico prediction of adverse drug reactions and toxicities based on structural, biological and clinical data. 2012 , 7, 225-37	
498	Significance estimation for sequence-based chemical similarity searching (PhAST) and application to AuroraA kinase inhibitors. 2012 , 4, 1897-906	4
497	Recognizing pitfalls in virtual screening: a critical review. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 867-81	295
496	LYP inhibits T-cell activation when dissociated from CSK. 2012 , 8, 437-46	102
495	Inhibition of hematopoietic protein tyrosine phosphatase augments and prolongs ERK1/2 and p38 activation. 2012 , 7, 367-77	26
494	Assessment of a rule-based virtual screening technology (INDDEx) on a benchmark data set. 2012 , 116, 6732-9	6
493	Shape-based reprofiling of FDA-approved drugs for the Hihistamine receptor. 2012 , 55, 7054-60	29
492	Virtual drug screen schema based on multiview similarity integration and ranking aggregation. Journal of Chemical Information and Modeling, 2012 , 52, 834-43	14
491	QSAR classification model for antibacterial compounds and its use in virtual screening. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 2559-69	33
490	Scanning structure-activity relationships with structure-activity similarity and related maps: from consensus activity cliffs to selectivity switches. <i>Journal of Chemical Information and Modeling</i> , 2012 , 6.1 52, 2485-93	52
489	Locally weighted learning methods for predicting dose-dependent toxicity with application to the human maximum recommended daily dose. 2012 , 25, 2216-26	18
488	GSA: a GPU-accelerated structure similarity algorithm and its application in progressive virtual screening. 2012 , 16, 759-69	13

487	Selecting, Acquiring, and Using Small Molecule Libraries for High-Throughput Screening. 2012, 4, 177-19	91	49
486	Statistical Methods for Predicting Compound Recovery Rates for Ligand-Based Virtual Screening and Assessing the Probability of Activity. 2012 , 229-243		
485	Consensus Models of Activity Landscapes. 2012 , 307-326		14
484	Enantiomeric scaffolding of Eetralone and related scaffolds by EKR (enzymatic kinetic resolution) and stereoselective ketoreduction with ketoreductases. 2012 , 10, 536-47		5
483	Exploring polypharmacology using a ROCS-based target fishing approach. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 492-505	6.1	68
482	Identification, design and biological evaluation of bisaryl quinolones targeting Plasmodium falciparum type II NADH:quinone oxidoreductase (PfNDH2). 2012 , 55, 1831-43		75
481	Shaping a screening file for maximal lead discovery efficiency and effectiveness: elimination of molecular redundancy. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 2937-49	6.1	35
480	Bioactivity landscape modeling: chemoinformatic characterization of structure-activity relationships of compounds tested across multiple targets. 2012 , 20, 5443-52		26
479	Cluster analysis of the DrugBank chemical space using molecular quantum numbers. 2012 , 20, 5372-8		17
478	Fingerprint design and engineering strategies: rationalizing and improving similarity search performance. 2012 , 4, 1945-59		14
477	Identification, design and biological evaluation of heterocyclic quinolones targeting Plasmodium falciparum type II NADH:quinone oxidoreductase (PfNDH2). 2012 , 55, 1844-57		40
476	Improving classical substructure-based virtual screening to handle extrapolation challenges. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 678-85	6.1	8
475	Virtual screening identifies novel sulfonamide inhibitors of ecto-5'-nucleotidase. 2012 , 55, 6576-81		37
474	Identification of novel antimalarial chemotypes via chemoinformatic compound selection methods for a high-throughput screening program against the novel malarial target, PfNDH2: increasing hit rate via virtual screening methods. 2012 , 55, 3144-54		19
473	Computational prediction of blood-brain barrier permeability using decision tree induction. <i>Molecules</i> , 2012 , 17, 10429-45	4.8	54
472	HSQC spectral based similarity matching of compounds using nearest neighbours and a fast discrete genetic algorithm. 2012 , 4, 25		1
471	Enabling large-scale design, synthesis and validation of small molecule protein-protein antagonists. 2012 , 7, e32839		84
47°	Prediction of chemical-protein interactions network with weighted network-based inference method. 2012 , 7, e41064		76

469	Generation of the first structure-based pharmacophore model containing a selective "zinc binding group" feature to identify potential glyoxalase-1 inhibitors. <i>Molecules</i> , 2012 , 17, 13740-58	,	27
468	The enumeration of chemical space. 2012 , 2, 717-733		67
467	Generation of quinolone antimalarials targeting the Plasmodium falciparum mitochondrial respiratory chain for the treatment and prophylaxis of malaria. 2012 , 109, 8298-303		118
466	Chapter 7:Docking and Virtual Screening. <i>RSC Drug Discovery Series</i> , 2012 , 171-194 0.6		
465	Chapter 9:In Silico Lead Generation Approaches in Multi-Target Drug Discovery. <i>RSC Drug Discovery Series</i> , 2012 , 130-140)	2
464	Application of support vector machine to three-dimensional shape-based virtual screening using comprehensive three-dimensional molecular shape overlay with known inhibitors. <i>Journal of 6.1 Chemical Information and Modeling</i> , 2012 , 52, 1015-26		18
463	Contribution of 2D and 3D structural features of drug molecules in the prediction of Drug Profile Matching. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 1733-44		15
462	Combining 2D and 3D in silico methods for rapid selection of potential PDE5 inhibitors from multimillion compounds' repositories: biological evaluation. 2012 , 16, 59-72		11
461	Identification of HIV-1 reverse transcriptase dual inhibitors by a combined shape-, 2D-fingerprint-and pharmacophore-based virtual screening approach. 2012 , 50, 216-29		55
460	Characterization and validation of an in silico toxicology model to predict the mutagenic potential of drug impurities. 2012 , 260, 209-21		38
459	In Silico Models to Discriminate Compounds Inducing and Noninducing Toxic Myopathy. <i>Molecular Informatics</i> , 2012 , 31, 27-39		7
458	New thiazolidinyl analogs containing pyridine ring: synthesis, biological evaluation and QSAR studies. 2013 , 22, 1538-1548		9
457	A Hybrid Structure/Pharmacophore-Based Virtual Screening Approach to Design Potential Leads: A Computer-Aided Design of South African HIV-1 Subtype C Protease Inhibitors. 2013 , 74, 283-295		16
456	The DEER database: a bridge connecting drugs, environmental effects, and regulations. 2013 , 520, 98-105		6
455	Steering target selectivity and potency by fragment-based de novo drug design. 2013, 52, 10006-9		22
454	Comparing neural-network scoring functions and the state of the art: applications to common library screening. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 1726-35		36
453	The Influence of Similarity Measures and Fusion Rules Toward Turbo Similarity Searching. 2013 , 11, 823-833	3	3
452	De novo design of novel DNA-gyrase inhibitors based on 2D molecular fingerprints. 2013 , 23, 4166-71		5

451	Predicting targeted polypharmacology for drug repositioning and multi- target drug discovery. 2013 , 20, 1646-61		54
450	In Silico Drug Discovery and Design. 2013 ,		3
449	PyDPI: freely available python package for chemoinformatics, bioinformatics, and chemogenomics studies. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 3086-96	6.1	61
448	Nonlinear scoring functions for similarity-based ligand docking and binding affinity prediction. Journal of Chemical Information and Modeling, 2013 , 53, 3097-112	6.1	38
447	A polynomial-time maximum common subgraph algorithm for outerplanar graphs and its application to chemoinformatics. 2013 , 69, 343-376		9
446	Cyclic Systems Distribution Along Similarity Measures: Insights for an Application to Activity Landscape Modeling. <i>Molecular Informatics</i> , 2013 , 32, 179-90	3.8	3
445	SMIfp (SMILES fingerprint) chemical space for virtual screening and visualization of large databases of organic molecules. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 1979-89	6.1	45
444	Enhanced ranking of PknB Inhibitors using data fusion methods. 2013 , 5, 2		26
443	Visualization and virtual screening of the chemical universe database GDB-17. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 56-65	6.1	78
442	MQN-mapplet: visualization of chemical space with interactive maps of DrugBank, ChEMBL, PubChem, GDB-11, and GDB-13. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 509-18	6.1	46
441	Big pharma screening collections: more of the same or unique libraries? The AstraZeneca-Bayer Pharma AG case. <i>Drug Discovery Today</i> , 2013 , 18, 1014-24	8.8	52
440	High-throughput respirometric assay identifies predictive toxicophore of mitochondrial injury. 2013 , 272, 490-502		16
439	Similarity-Based Scaffold Hopping Using 2D Fingerprints. 2013 , 105-118		
438	CATS for Scaffold Hopping in Medicinal Chemistry. 2013 , 119-130		
437	Molecular Interaction Fingerprints. 2013 , 215-230		4
436	Encoding protein-ligand interaction patterns in fingerprints and graphs. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 623-37	6.1	106
435	Hit expansion approaches using multiple similarity methods and virtualized query structures. Journal of Chemical Information and Modeling, 2013, 53, 1057-66	6.1	12
434	Carcinogenicity prediction of noncongeneric chemicals by a support vector machine. 2013 , 26, 741-9		16

433	Chemoinformatic Characterization of the Chemical Space and Molecular Diversity of Compound Libraries. 2013 , 325-352		6
432	Prediction of polypharmacological profiles of drugs by the integration of chemical, side effect, and therapeutic space. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 753-62	6.1	77
431	Noncontiguous atom matching structural similarity function. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 2511-24	6.1	9
430	Methods for Similarity-based Virtual Screening. 2013 , 5, e201302009		12
429	CSBB-ConeExclusion, adapting structure based solution virtual screening to libraries on solid support. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 3156-62	6.1	1
428	Integrating structure-and ligand-based approaches for computer-aided drug design. 2013, 190-202		
427	Exploring the ligand-protein networks in traditional chinese medicine: current databases, methods, and applications. 2013 , 2013, 806072		11
426	Chemoinformatics profiling of ionic liquidsautomatic and chemically interpretable cytotoxicity profiling, virtual screening, and cytotoxicophore identification. 2013 , 136, 548-65		19
425	Chemically Advanced Template Search (CATS) for Scaffold-Hopping and Prospective Target Prediction for 'Orphan' Molecules. <i>Molecular Informatics</i> , 2013 , 32, 133-138	3.8	109
424	Steering Target Selectivity and Potency by Fragment-Based De Novo Drug Design. 2013 , 125, 10190-101	93	7
423	. 2013,		12
422	Structure-and-mechanism-based design and discovery of type II Mycobacterium tuberculosis dehydroquinate dehydratase inhibitors. 2014 , 14, 51-63		4
421	Asymmetric clustering index in a case study of 5-HT1A receptor ligands. 2014 , 9, e102069		8
420	Combination of 2D/3D ligand-based similarity search in rapid virtual screening from multimillion compound repositories. Selection and biological evaluation of potential PDE4 and PDE5 inhibitors. Molecules, 2014, 19, 7008-39	4.8	17
419	Computer-Aided Drug Design. 2014 , 01,		1
418	Novel inhibitors of the Plasmodium falciparum electron transport chain. 2014 , 141, 50-65		29
417	Validation and extension of a similarity-based approach for prediction of acute aquatic toxicity towards Daphnia magna. 2014 , 25, 1013-36		13
416	A generalizable definition of chemical similarity for read-across. 2014 , 6, 39		61

415	Efficient ring perception for the Chemistry Development Kit. 2014 , 6, 3		20
414	Integrated approach to structure-based enzymatic drug design: molecular modeling, spectroscopy, and experimental bioactivity. 2014 , 114, 493-537		81
413	Target-Bound Generated Pharmacophore Model to Improve the Pharmacophore-Based Virtual Screening: Identification of G-Protein Coupled Human CCR2 Receptors Inhibitors as Anti-Inflammatory Drugs. 2014 , 7, 45-57		11
412	An efficient multistep ligand-based virtual screening approach for GPR40 agonists. 2014 , 18, 183-93		9
411	Molecular similarity in medicinal chemistry. 2014 , 57, 3186-204		326
410	An unbiased method to build benchmarking sets for ligand-based virtual screening and its application to GPCRs. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 1433-50	6.1	36
409	Rapid in silico selection of an MCHR1 antagonists Focused library from multi-million compounds repositories: biological evaluation. 2014 , 23, 1234-1247		2
408	Machine learning-based prediction of drug-drug interactions by integrating drug phenotypic, therapeutic, chemical, and genomic properties. 2014 , 21, e278-86		163
407	How diverse are diversity assessment methods? A comparative analysis and benchmarking of molecular descriptor space. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 230-42	6.1	53
406	Computational methods in drug discovery. 2014 , 66, 334-95		953
406	Computational methods in drug discovery. 2014 , 66, 334-95 Lead Discovery and Lead Modification. 2014 , 19-122		953
		6.1	
405	Lead Discovery and Lead Modification. 2014 , 19-122 Ligand-based target prediction with signature fingerprints. <i>Journal of Chemical Information and</i>	6.1	5
405 404	Lead Discovery and Lead Modification. 2014, 19-122 Ligand-based target prediction with signature fingerprints. Journal of Chemical Information and Modeling, 2014, 54, 2647-53 SABRE: ligand/structure-based virtual screening approach using consensus molecular-shape		5 35
405 404 403	Lead Discovery and Lead Modification. 2014, 19-122 Ligand-based target prediction with signature fingerprints. Journal of Chemical Information and Modeling, 2014, 54, 2647-53 SABRE: ligand/structure-based virtual screening approach using consensus molecular-shape pattern recognition. Journal of Chemical Information and Modeling, 2014, 54, 338-46 Discovery of novel inhibitors targeting the macrophage migration inhibitory factor via		5 35 13
405 404 403 402	Lead Discovery and Lead Modification. 2014, 19-122 Ligand-based target prediction with signature fingerprints. Journal of Chemical Information and Modeling, 2014, 54, 2647-53 SABRE: ligand/structure-based virtual screening approach using consensus molecular-shape pattern recognition. Journal of Chemical Information and Modeling, 2014, 54, 338-46 Discovery of novel inhibitors targeting the macrophage migration inhibitory factor via structure-based virtual screening and bioassays. 2014, 57, 3737-45 A rotation-translation invariant molecular descriptor of partial charges and its use in ligand-based		5 35 13 61
405 404 403 402 401	Lead Discovery and Lead Modification. 2014, 19-122 Ligand-based target prediction with signature fingerprints. Journal of Chemical Information and Modeling, 2014, 54, 2647-53 SABRE: ligand/structure-based virtual screening approach using consensus molecular-shape pattern recognition. Journal of Chemical Information and Modeling, 2014, 54, 338-46 Discovery of novel inhibitors targeting the macrophage migration inhibitory factor via structure-based virtual screening and bioassays. 2014, 57, 3737-45 A rotation-translation invariant molecular descriptor of partial charges and its use in ligand-based virtual screening. 2014, 6, 23		5 35 13 61

397	Expanding the scaffold for bacterial RNA polymerase inhibitors: design, synthesis and structureBctivity relationships of ureido-heterocyclic-carboxylic acids. 2014 , 4, 2177-2194		24
396	Rational Drug Design. 2014 , 4, 59-85		3
395	Library Design, Chemical Space, and Drug Likeness. 2015 , 79-98		
394	PubChem atom environments. 2015 , 7, 41		4
393	Optimization of TRPV6 Calcium Channel Inhibitors Using a 3D Ligand-Based Virtual Screening Method. 2015 , 127, 14961-14965		1
392	Cheminformatics Based Machine Learning Models for AMA1-RON2 Abrogators for Inhibiting Plasmodium falciparum Erythrocyte Invasion. <i>Molecular Informatics</i> , 2015 , 34, 655-64	3.8	4
391	Fragment-based similarity searching with infinite color space. 2015 , 36, 1597-608		3
390	Chemoinformatics at the University of Sheffield 2002-2014. <i>Molecular Informatics</i> , 2015 , 34, 598-607	3.8	3
389	Optimization of TRPV6 Calcium Channel Inhibitors Using a 3D Ligand-Based Virtual Screening Method. 2015 , 54, 14748-52		29
388	Structural and Modeling Studies on ecto-5'-nucleotidase Aiding in Inhibitor Design. 2015 , 15, 34-40		5
387	Storing the Wisdom: Chemical Concepts and Chemoinformatics. 2015 , 2, 50-67		
386	A structural hierarchy matching approach for molecular similarity/substructure searching. <i>Molecules</i> , 2015 , 20, 8791-9	4.8	
385	Discovery of Novel Liver-Stage Antimalarials through Quantum Similarity. 2015 , 10, e0125593		5
384	Computational Structure-Based De Novo Design of Hypothetical Inhibitors against the Anti-Inflammatory Target COX-2. 2015 , 10, e0134691		18
383	A combination of 2D similarity search, pharmacophore, and molecular docking techniques for the identification of vascular endothelial growth factor receptor-2 inhibitors. 2015 , 26, 399-409		8
382	Identification and Preliminary SAR Analysis of Novel Type-I Inhibitors of TIE-2 via Structure-Based Virtual Screening and Biological Evaluation in in vitro Models. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 2693-704	6.1	8
381	ChemDes: an integrated web-based platform for molecular descriptor and fingerprint computation. 2015 , 7, 60		125
380	Genomes to natural products PRediction Informatics for Secondary Metabolomes (PRISM). 2015 , 43, 9645-62		175

379	Ribavirin as a tri-targeted antitumor repositioned drug. 2015 , 33, 2384-92	31
378	Why is Tanimoto index an appropriate choice for fingerprint-based similarity calculations?. 2015 , 7, 20	451
377	A 'rule of 0.5' for the metabolite-likeness of approved pharmaceutical drugs. 2015 , 11, 323-339	60
376	The chemical space project. 2015 , 48, 722-30	289
375	Biasing Potential Replica Exchange Multisite Dynamics for Efficient Free Energy Calculations. 2015 , 11, 1267-77	25
374	Computational prediction of microRNA networks incorporating environmental toxicity and disease etiology. 2014 , 4, 5576	46
373	Exploring the ligand-protein networks in traditional chinese medicine: current databases, methods and applications. 2015 , 827, 227-57	5
372	A virtual screen discovers novel, fragment-sized inhibitors of Mycobacterium tuberculosis InhA. Journal of Chemical Information and Modeling, 2015 , 55, 645-59	30
371	Insight into the binding theme of CA-074Me to cathepsin B: molecular dynamics simulations and scaffold hopping to identify potential analogues as anti-neurodegenerative diseases. 2015 , 24, 701-713	4
370	CFam: a chemical families database based on iterative selection of functional seeds and seed-directed compound clustering. 2015 , 43, D558-65	5
369	Comprehensive prediction of drug-protein interactions and side effects for the human proteome. 2015 , 5, 11090	74
368	Clustered distribution of natural product leads of drugs in the chemical space as influenced by the privileged target-sites. 2015 , 5, 9325	16
367	De novo design of caseinolytic protein proteases inhibitors based on pharmacophore and 2D molecular fingerprints. 2015 , 25, 2345-52	3
366	Stereoselective virtual screening of the ZINC database using atom pair 3D-fingerprints. 2015 , 7, 3	42
365	Heat-shock protein 90 (Hsp90) as anticancer target for drug discovery: an ample computational perspective. 2015 , 86, 1131-60	12
364	Combining label-free cell phenotypic profiling with computational approaches for novel drug discovery. 2015 , 10, 331-43	17
363	Combination of Pharmacophore Matching, 2D Similarity Search, and In Vitro Biological Assays in the Selection of Potential 5-HT6 Antagonists from Large Commercial Repositories. 2015 , 86, 864-80	5
362	Discovery and Development of Lead Compounds from Natural Sources Using Computational Approaches. 2015 , 455-475	8

361	Merging allosteric and active site binding motifs: de novo generation of target selectivity and potency via natural-product-derived fragments. <i>ChemMedChem</i> , 2015 , 10, 451-4	·7	31
360	Searching molecular structure databases with tandem mass spectra using CSI:FingerID. 2015 , 112, 12580-	5	413
359	PoLi: A Virtual Screening Pipeline Based on Template Pocket and Ligand Similarity. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 1757-70	.1	30
358	Discovery of new proteasome inhibitors using a knowledge-based computational screening approach. 2015 , 19, 1003-19		9
357	Structure-Activity Relationships and Anti-inflammatory Activities of N-Carbamothioylformamide Analogues as MIF Tautomerase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 1994-2	र् य04	5
356	Docking and Virtual Screening Strategies for GPCR Drug Discovery. 2015 , 1335, 251-76		14
355	Harmonization of QSAR Best Practices and Molecular Docking Provides an Efficient Virtual Screening Tool for Discovering New G-Quadruplex Ligands. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 2094-110	.1	14
354	Rational design of promiscuous binding modulators of p53 inducing E3(Ub)-ligases (Mdm2 and Pirh2) as anticancer agents: an in silico approach. 2015 , 6, 1959-1968		3
353	Virtual screening strategies: recent advances in the identification and design of anti-cancer agents. 2015 , 71, 64-70		33
352	iDrug-Target: predicting the interactions between drug compounds and target proteins in cellular networking via benchmark dataset optimization approach. 2015 , 33, 2221-33		167
351	High performance virtual drug screening on many-core processors. 2015 , 29, 119-134		61
350	Advance in Structural Bioinformatics. 2015 ,		4
350 349	Machine-learning approaches in drug discovery: methods and applications. <i>Drug Discovery Today</i>	.8	4 37 ²
	Machine-learning approaches in drug discovery: methods and applications. <i>Drug Discovery Today</i> ,	.8	
349	Machine-learning approaches in drug discovery: methods and applications. <i>Drug Discovery Today</i> , 2015 , 20, 318-31	.8	372
349 348	Machine-learning approaches in drug discovery: methods and applications. <i>Drug Discovery Today</i> , 2015 , 20, 318-31 Applicability Domain for QSAR Models. 2016 , 1, 45-63 Discovery of Potential Orthosteric and Allosteric Antagonists of P2Y1R from Chinese Herbs by Molecular Simulation Methods. 2016 , 2016, 4320201	.8	37 ² 83
349 348 347	Machine-learning approaches in drug discovery: methods and applications. <i>Drug Discovery Today</i> , 2015 , 20, 318-31 Applicability Domain for QSAR Models. 2016 , 1, 45-63 Discovery of Potential Orthosteric and Allosteric Antagonists of P2Y1R from Chinese Herbs by Molecular Simulation Methods. 2016 , 2016, 4320201 Virtual Screening Approaches towards the Discovery of Toll-Like Receptor Modulators.		37 ² 83 9

343	MetMaxStruct: A Tversky-Similarity-Based Strategy for Analysing the (Sub)Structural Similarities of Drugs and Endogenous Metabolites. 2016 , 7, 266		24
342	. 2016,		18
341	Discovery of a Selective Aurora A Kinase Inhibitor by Virtual Screening. 2016 , 59, 7188-211		38
340	ChemProt-3.0: a global chemical biology diseases mapping. 2016 , 2016,		53
339	In silico identification of anti-cancer compounds and plants from traditional Chinese medicine database. 2016 , 6, 25462		29
338	Using Bayesian modeling on molecular fragments features for virtual screening. 2016,		
337	How Many Fingers Does a Compound Have? Molecular Similarity beyond Chemical Space. 2016 , 331-343		
336	Qualitative consensus of QSAR ready biodegradability predictions. 2016 , 1-24		11
335	Overview of Computer-Aided Drug Design for Epigenetic Targets. 2016 , 21-52		6
334	An Integrated Approach for Fragment-Based Lead Discovery: Virtual, NMR, and High-Throughput Screening Combined with Structure-Guided Design. Application to the Aspartyl Protease Renin 2016 , 447-486		2
333	Computational Discovery and Experimental Confirmation of TLR9 Receptor Antagonist Leads. Journal of Chemical Information and Modeling, 2016 , 56, 1835-46	6.1	16
332	In Silico Exploration for Novel Type-I Inhibitors of Tie-2/TEK: The Performance of Different Selection Strategy in Selecting Virtual Screening Candidates. 2016 , 6, 37628		3
331	Materials design by evolutionary optimization of functional groups in metal-organic frameworks. 2016 , 2, e1600954		55
330	BioTriangle: a web-accessible platform for generating various molecular representations for chemicals, proteins, DNAs/RNAs and their interactions. 2016 , 8, 34		27
329	Enumeration of Chemical Fragment Space. 2016 , 57-74		1
328	Molecular Similarity Approaches in Chemoinformatics: Early History and Literature Status. 2016 , 67-89		3
327	Molecular Mechanism of Action of Antimalarial Benzoisothiazolones: Species-Selective Inhibitors of the Plasmodium spp. MEP Pathway enzyme, IspD. 2016 , 6, 36777		10
326	System Prediction of Drug-Drug Interactions Through the Integration of Drug Phenotypic, Therapeutic, Structural, and Genomic Similarities. <i>Lecture Notes in Computer Science</i> , 2016 , 377-385	0.9	

325	Descriptors and their selection methods in QSAR analysis: paradigm for drug design. <i>Drug Discovery Today</i> , 2016 , 21, 1291-302	147
324	Computationally Guided Identification of Novel Mycobacterium tuberculosis GlmU Inhibitory Leads, Their Optimization, and in Vitro Validation. 2016 , 18, 100-16	23
323	Evaluating enzymatic synthesis of small molecule drugs. 2016 , 33, 138-147	14
322	Compound annotation with real time cellular activity profiles to improve drug discovery. 2016 , 11, 269-80	3
321	Carcinogenicity prediction of noncongeneric chemicals by augmented top priority fragment classification. 2016 , 61, 145-54	1
320	Identification of small molecules acting against H1N1 influenza A virus. 2016 , 488, 249-58	4
319	New design of nucleotide excision repair (NER) inhibitors for combination cancer therapy. 2016 , 65, 71-82	23
318	An overview of molecular fingerprint similarity search in virtual screening. 2016 , 11, 137-48	99
317	Use of similarity scoring in the development of oral solid dosage forms. 2016 , 514, 335-340	6
316	Evaluation of potential flavonoid inhibitors of glyoxalase-I based on virtual screening and in vitro studies. 2016 , 34, 993-1007	19
315	Relational Agreement Measures for Similarity Searching of Cheminformatic Data Sets. 2016 , 13, 158-67	6
314	Ames Test Prediction on High Energy Molecules by On-The-Fly QSAR (OTF-QSAR). 2017 , 42, 24-35	3
313	Identification of CLK1 Inhibitors by a Fragment-linking Based Virtual Screening. <i>Molecular Informatics</i> , 2017 , 36, 1600123	1
312	Investigation of PDE5/PDE6 and PDE5/PDE11 selective potent tadalafil-like PDE5 inhibitors using combination of molecular modeling approaches, molecular fingerprint-based virtual screening protocols and structure-based pharmacophore development. 2017 , 32, 311-330	20
311	Study of Structure-active Relationship for Inhibitors of HIV-1 Integrase LEDGF/p75 Interaction by Machine Learning Methods. <i>Molecular Informatics</i> , 2017 , 36, 1600127	3
310	Towards a chromatographic similarity index to establish localised quantitative structure-retention relationships for retention prediction. II Use of Tanimoto similarity index in ion chromatography. 2017 , 1523, 173-182	9
309	Computational models for the classification of mPGES-1 inhibitors with fingerprint descriptors. 2017 , 21, 661-675	4
308	Computational prediction of drug-drug interactions based on drugs functional similarities. 2017 , 70, 54-64	79

307	Molecular modeling and structure-activity relationships for a series of benzimidazole derivatives as cruzain inhibitors. 2017 , 9, 641-657	15
306	Drug repositioning for enzyme modulator based on human metabolite-likeness. 2017 , 18, 226	9
305	Analysis of drug-endogenous human metabolite similarities in terms of their maximum common substructures. 2017 , 9, 18	19
304	Mapping of Drug-like Chemical Universe with Reduced Complexity Molecular Frameworks. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 680-699	14
303	Integration on Ligand and Structure Based Approaches in GPCRs. 2017, 101-161	O
302	Rational Design, Synthesis, and Biological Evaluation of Heterocyclic Quinolones Targeting the Respiratory Chain of Mycobacterium tuberculosis. 2017 , 60, 3703-3726	28
301	Hybrid Receptor-Bound/MM-GBSA-Per-residue Energy-Based Pharmacophore Modelling: Enhanced Approach for Identification of Selective LTA4H Inhibitors as Potential Anti-inflammatory Drugs. 2017 , 75, 35-48	7
300	Molecular similarity considerations in the licensing of orphan drugs. <i>Drug Discovery Today</i> , 2017 , 22, 377	5
299	Identification of Binding Mode and Prospective Structural Features of Novel Nef Protein Inhibitors as Potential Anti-HIV Drugs. 2017 , 75, 49-64	6
298	Applications of Systematic Molecular Scaffold Enumeration to Enrich Structure-Activity Relationship Information. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 27-35	9
298 297		9
	Relationship Information. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 27-35 Characterizing Chemical Similarity with Vibrational Spectroscopy: New Insights into the Substituent	
297	Relationship Information. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 27-35 Characterizing Chemical Similarity with Vibrational Spectroscopy: New Insights into the Substituent Effects in Monosubstituted Benzenes. 2017 , 121, 8086-8096 Assessing and predicting drug-induced anticholinergic risks: an integrated computational approach.	14
297 296	Characterizing Chemical Similarity with Vibrational Spectroscopy: New Insights into the Substituent Effects in Monosubstituted Benzenes. 2017, 121, 8086-8096 Assessing and predicting drug-induced anticholinergic risks: an integrated computational approach. 2017, 8, 361-370 Predicting novel substrates for enzymes with minimal experimental effort with active learning.	14
297 296 295	Characterizing Chemical Similarity with Vibrational Spectroscopy: New Insights into the Substituent Effects in Monosubstituted Benzenes. 2017, 121, 8086-8096 Assessing and predicting drug-induced anticholinergic risks: an integrated computational approach. 2017, 8, 361-370 Predicting novel substrates for enzymes with minimal experimental effort with active learning. 2017, 44, 171-181	14 10 15
297 296 295	Characterizing Chemical Similarity with Vibrational Spectroscopy: New Insights into the Substituent Effects in Monosubstituted Benzenes. 2017, 121, 8086-8096 Assessing and predicting drug-induced anticholinergic risks: an integrated computational approach. 2017, 8, 361-370 Predicting novel substrates for enzymes with minimal experimental effort with active learning. 2017, 44, 171-181 Overview of Methods and Strategies for Conducting Virtual Small Molecule Screening. 2017, 9, 196-212 The Fragment Network: A Chemistry Recommendation Engine Built Using a Graph Database. 2017,	14 10 15 37
297 296 295 294 293	Characterizing Chemical Similarity with Vibrational Spectroscopy: New Insights into the Substituent Effects in Monosubstituted Benzenes. 2017, 121, 8086-8096 Assessing and predicting drug-induced anticholinergic risks: an integrated computational approach. 2017, 8, 361-370 Predicting novel substrates for enzymes with minimal experimental effort with active learning. 2017, 44, 171-181 Overview of Methods and Strategies for Conducting Virtual Small Molecule Screening. 2017, 9, 196-212 The Fragment Network: A Chemistry Recommendation Engine Built Using a Graph Database. 2017, 60, 6440-6450 Pharmacological relationships and ligand discovery of G protein-coupled receptors revealed by	14 10 15 37

289	MSBIS: A Multi-Step Biomedical Informatics Screening Approach for Identifying Medications that Mitigate the Risks of Metoclopramide-Induced Tardive Dyskinesia. 2017 , 26, 132-137	4
288	Towards a chromatographic similarity index to establish localized quantitative structure-retention models for retention prediction: Use of retention factor ratio. 2017 , 1486, 50-58	28
287	Retrometabolic Drug Design. 2017 , 105-123	
286	Label-Free Screening Technologies. 2017 , 416-433	O
285	Quantum mechanics implementation in drug-design workflows: does it really help?. 2017, 11, 2551-2564	17
284	Discovery of Farnesoid X Receptor Antagonists Based on a Library of Oleanolic Acid 3-O-Esters through Diverse Substituent Design and Molecular Docking Methods. <i>Molecules</i> , 2017 , 22,	2
283	A Systematic Review of Computational Drug Discovery, Development, and Repurposing for Ebola Virus Disease Treatment. <i>Molecules</i> , 2017 , 22,	21
282	Chemical Data Formats, Fingerprints, and Other Molecular Descriptions for Database Analysis and Searching. 2017 , 329-378	11
281	Hit and Lead Generation Strategies. 2017 , 33-63	1
2 80	Practical Approaches to Column Selection for Supercritical Fluid Chromatography. 2017 , 57-101	
279	Consensus queries in ligand-based virtual screening experiments. 2017 , 9, 60	9
278	Molecular structures enumeration and virtual screening in the chemical space with RetroPath2.0. 2017 , 9, 64	10
277	Chemical Identity and Mechanism of Action and Formation of a Cell Growth Inhibitory Compound from Polycarbonate Flasks. 2018 , 90, 4603-4610	3
276	Classification of spatially resolved molecular fingerprints for machine learning applications and development of a codebase for their implementation. 2018 , 3, 431-441	11
275	LS-align: an atom-level, flexible ligand structural alignment algorithm for high-throughput virtual screening. 2018 , 34, 2209-2218	25
274	New Trends in Drug Discovery. 2018 , 1-39	
273	Combining Similarity Searching and Network Analysis for the Identification of Active Compounds. 2018 , 3, 3768-3777	5
272	Representing molecular and materials data for unsupervised machine learning. 2018 , 44, 905-920	14

271	Mapping of Activity through Dichotomic Scores (MADS): A new chemoinformatic approach to detect activity-rich structural regions. 2018 , 32, e2994		O
270	Modeling Kinase Inhibition Using Highly Confident Data Sets. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 957-967	6.1	9
269	In-silico guided discovery of novel CCR9 antagonists. <i>Journal of Computer-Aided Molecular Design</i> , 2018 , 32, 573-582	4.2	2
268	Natural products used as a chemical library for protein-protein interaction targeted drug discovery. 2018 , 79, 46-58		9
267	Virtual Screening in the Search of New and Potent Anti-Alzheimer Agents. 2018, 107-137		5
266	Analysing and Navigating Natural Products Space for Generating Small, Diverse, But Representative Chemical Libraries. 2018 , 13, 1700503		18
265	Methods for Virtual Screening of GPCR Targets: Approaches and Challenges. 2018, 1705, 233-264		2
264	Probabilistic frequent subtrees for efficient graph classification and retrieval. 2018 , 107, 1847-1873		2
263	An integrated approach towards the development of novel antifungal agents containing thiadiazole: synthesis and a combined similarity search, homology modelling, molecular dynamics and molecular docking study. 2018 , 12, 121		13
262	A review of ligand-based virtual screening web tools and screening algorithms in large molecular databases in the age of big data. 2018 , 10, 2641-2658		39
261	QSAR Studies of New Pyrido[3,4-]indole Derivatives as Inhibitors of Colon and Pancreatic Cancer Cell Proliferation. 2018 , 27, 2466-2481		6
260	FINDSITE: A New Approach for Virtual Ligand Screening of Proteins and Virtual Target Screening of Biomolecules. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 2343-2354	6.1	19
259	Network-Based Methods for Prediction of Drug-Target Interactions. 2018 , 9, 1134		69
258	Novel Neural Network Approach to Predict Drug-Target Interactions Based on Drug Side Effects and Genome-Wide Association Studies. 2018 , 83, 79-91		
257	The Varieties of the Psychedelic Experience: A Preliminary Study of the Association Between the Reported Subjective Effects and the Binding Affinity Profiles of Substituted Phenethylamines and Tryptamines. 2018 , 12, 54		20
256	Impact of Molecular Descriptors on Computational Models. 2018 , 1825, 171-209		16
255	Experimental models in Chagas disease: a review of the methodologies applied for screening compounds against Trypanosoma cruzi. 2018 , 117, 3367-3380		13
254	Exploring ensembles of bioactive or virtual analogs of X-ray ligands for shape similarity searching. Journal of Computer-Aided Molecular Design, 2018 , 32, 759-767	4.2	2

253	Designing Algorithms To Aid Discovery by Chemical Robots. 2018 , 4, 793-804		45
252	Molecular Descriptors for Structure-Activity Applications: A Hands-On Approach. 2018 , 1800, 3-53		10
251	Development of Matrix Metalloproteinase-2 Inhibitors for Cardioprotection. 2018 , 9, 296		7
250	Artificial intelligence in drug design. 2018 , 61, 1191-1204		72
249	Discovery of Potential Inhibitors of Squalene Synthase from Traditional Chinese Medicine Based on Virtual Screening and In Vitro Evaluation of Lipid-Lowering Effect. <i>Molecules</i> , 2018 , 23,	4.8	9
248	Spectrophores as one-dimensional descriptors calculated from three-dimensional atomic properties: applications ranging from scaffold hopping to multi-target virtual screening. 2018 , 10, 9		8
247	Ligand-Based Approach for In-silico Drug Designing. 2018 , 11-19		0
246	Bioinformatics Techniques for Drug Discovery. 2018 ,		4
245	A mechanistic framework for integrating chemical structure and high-throughput screening results to improve toxicity predictions. 2018 , 8, 1-12		9
244	Recent applications of deep learning and machine intelligence on in silico drug discovery: methods,		
244	tools and databases. <i>Briefings in Bioinformatics</i> , 2019 , 20, 1878-1912	13.4	155
243		13.4	155
	tools and databases. <i>Briefings in Bioinformatics</i> , 2019 , 20, 1878-1912	13.4	
243	tools and databases. <i>Briefings in Bioinformatics</i> , 2019 , 20, 1878-1912 Fingerprints and Pharmacophores. 2019 , 619-627	6.1	
² 43	tools and databases. <i>Briefings in Bioinformatics</i> , 2019 , 20, 1878-1912 Fingerprints and Pharmacophores. 2019 , 619-627 Structure and Function of GPCRs. 2019 , A Quantum-Inspired Method for Three-Dimensional Ligand-Based Virtual Screening. <i>Journal of</i>		1
243 242 241	tools and databases. <i>Briefings in Bioinformatics</i> , 2019 , 20, 1878-1912 Fingerprints and Pharmacophores. 2019 , 619-627 Structure and Function of GPCRs. 2019 , A Quantum-Inspired Method for Three-Dimensional Ligand-Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 4475-4485 Fingerprinting CANDO: Increased Accuracy with Structure- and Ligand-Based Shotgun Drug		5
243 242 241 240	Fingerprints and Pharmacophores. 2019, 619-627 Structure and Function of GPCRs. 2019, A Quantum-Inspired Method for Three-Dimensional Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2019, 59, 4475-4485 Fingerprinting CANDO: Increased Accuracy with Structure- and Ligand-Based Shotgun Drug Repurposing. 2019, 4, 17393-17403 Design and Selection of Novel C1s Inhibitors by In Silico and In Vitro Approaches. Molecules, 2019,	6.1	1 5 10
243 242 241 240 239	Fingerprints and Pharmacophores. 2019, 619-627 Structure and Function of GPCRs. 2019, A Quantum-Inspired Method for Three-Dimensional Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2019, 59, 4475-4485 Fingerprinting CANDO: Increased Accuracy with Structure- and Ligand-Based Shotgun Drug Repurposing. 2019, 4, 17393-17403 Design and Selection of Novel C1s Inhibitors by In Silico and In Vitro Approaches. Molecules, 2019, 24,	6.1	1 5 10 5

235	Identifying Protein Features Responsible for Improved Drug Repurposing Accuracies Using the CANDO Platform: Implications for Drug Design. <i>Molecules</i> , 2019 , 24,	4.8	14
234	Discovering highly selective and diverse PPAR-delta agonists by ligand based machine learning and structural modeling. 2019 , 9, 1106		16
233	Analysis and Comparison of Vector Space and Metric Space Representations in QSAR Modeling. <i>Molecules</i> , 2019 , 24,	4.8	5
232	A HTRF based competitive binding assay for screening specific inhibitors of HIV-1 capsid assembly targeting the C-Terminal domain of capsid. 2019 , 169, 104544		6
231	Ligity: A Non-Superpositional, Knowledge-Based Approach to Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 2600-2616	6.1	8
230	Phenotypic screening of nonsteroidal anti-inflammatory drugs identified mefenamic acid as a drug for the treatment of schistosomiasis. 2019 , 43, 370-379		28
229	In Silico Databases and Tools for Drug Repurposing. 2019 , 703-742		5
228	Stalis: A Computational Method for Template-Based Ab Initio Ligand Design. 2019 , 40, 1622-1632		3
227	Automated discovery of GPCR bioactive ligands. 2019 , 55, 17-24		5
226	RISC: Rapid Inverted-Index Based Search of Chemical Fingerprints. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 2702-2713	6.1	3
225	Identification of a novel scaffold for a small molecule GPR139 receptor agonist. 2019 , 9, 3802		6
224	Network-based prediction of drug combinations. 2019 , 10, 1197		216
223	Accelerating Large-Scale Molecular Similarity Search through Exploiting High Performance Computing. 2019 ,		2
222	Evaluation of Neural Tube Defects (NTDs) After Exposure to Raltegravir During Pregnancy. 2019 , 81, 247-250		9
221	Chemical space of Escherichia coli dihydrofolate reductase inhibitors: New approaches for discovering novel drugs for old bugs. 2019 , 39, 684-705		16
220	Systematic selection of chemical fingerprint features improves the Gibbs energy prediction of biochemical reactions. 2019 , 35, 2634-2643		8
219	Exploring Alternative Strategies for the Identification of Potent Compounds Using Support Vector Machine and Regression Modeling. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 983-992	6.1	6
218	Bifunctional Duocarmycin Analogues as Inhibitors of Protein Tyrosine Kinases. 2019 , 82, 16-26		1

217	CMAUP: a database of collective molecular activities of useful plants. 2019 , 47, D1118-D1127		35
216	Cancer Bioinformatics. 2019 ,		2
215	In Silico Oncology Drug Repositioning and Polypharmacology. 2019 , 1878, 243-261		34
214	Repurposing approach identifies new treatment options for invasive fungal disease. 2019 , 84, 87-97		6
213	Web-based drug repurposing tools: a survey. <i>Briefings in Bioinformatics</i> , 2019 , 20, 299-316	13.4	25
212	Big Data and Artificial Intelligence Modeling for Drug Discovery. 2020 , 60, 573-589		96
211	Autonomous Discovery in the Chemical Sciences Part I: Progress. 2020 , 59, 22858-22893		75
210	Autonome Entdeckung in den chemischen Wissenschaften, Teil I: Fortschritt. 2020 , 132, 23054-23091		5
209	Virtual Screening in the Cloud: How Big Is Big Enough?. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 4274-4282	6.1	22
208	In Silico Identification of Potential Inhibitors of the Wnt Signaling Pathway in Human Breast Cancer. 2020 , 27, 999-1010		2
207	Inverse-QSPR for de novo Design: A Review. <i>Molecular Informatics</i> , 2020 , 39, e1900087	3.8	17
206	Computational network biology: Data, models, and applications. 2020 , 846, 1-66		54
205	Chemometrics for QSAR Modeling. 2020 , 599-634		5
204	Benchmark on Indexing Algorithms for Accelerating Molecular Similarity Search. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 6167-6184	6.1	1
203	Fingerprint-based computational models of 5-lipo-oxygenase activating protein inhibitors: Activity prediction and structure clustering. 2020 , 96, 931-947		1
202	Machine Learning Platform to Discover Novel Growth Inhibitors of Neisseria gonorrhoeae. 2020 , 37, 141		4
201	Next Generation Kinase Inhibitors. 2020,		3
200	LigMate: A Multifeature Integration Algorithm for Ligand-Similarity-Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 6044-6053	6.1	3

(2020-2021)

199	Identification of potential modulator of odorant binding protein 1 by hierarchical virtual screening and molecular dynamics. 2021 , 39, 6031-6043		2
198	Cheminformatics for accelerated design of chemical admixtures. 2020 , 136, 106173		2
197	Semi-supervised Hierarchical Drug Embedding in Hyperbolic Space. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 5647-5657	6.1	2
196	Big Data BigData 2020. Lecture Notes in Computer Science, 2020 ,	0.9	
195	Monomer structure fingerprints: an extension of the monomer composition version for peptide databases. <i>Journal of Computer-Aided Molecular Design</i> , 2020 , 34, 1147-1156	4.2	
194	Similar, or dissimilar, that is the question. How different are methods for comparison of compounds similarity?. 2020 , 88, 107367		2
193	Identification of novel antiplasmodial compound by hierarquical virtual screening and assays. 2021 , 39, 3378-3386		2
192	Structure-Based Virtual Screening: From Classical to Artificial Intelligence. 2020 , 8, 343		100
191	One molecular fingerprint to rule them all: drugs, biomolecules, and the metabolome. 2020 , 12, 43		42
190	Compound collections at KU 19472017: cheminformatic analysis and computational protein target prediction. 2020 , 29, 1211-1222		
189	Computational design of substrate selective inhibition. 2020 , 16, e1007713		3
188	Complexity Reduction in Density Functional Theory Calculations of Large Systems: System Partitioning and Fragment Embedding. 2020 , 16, 2952-2964		10
187	Improved Prediction of Aqueous Solubility of Novel Compounds by Going Deeper With Deep Learning. 2020 , 10, 121		22
186	Advancing computer-aided drug discovery (CADD) by big data and data-driven machine learning modeling. <i>Drug Discovery Today</i> , 2020 , 25, 1624-1638	8.8	38
185	A new paradigm in threshold of toxicological concern based on chemoinformatics analysis of a highly curated database enriched with antimicrobials. 2020 , 143, 111561		13
184	Machine learning and Al-based approaches for bioactive ligand discovery and GPCR-ligand recognition. 2020 , 180, 89-110		18
183	Incorporating Clinical, Chemical and Biological Information for Predicting Small Molecule-microRNA Associations Based on Non-Negative Matrix Factorization. 2021 , 18, 2535-2545		10
182	Target identification among known drugs by deep learning from heterogeneous networks. <i>Chemical Science</i> , 2020 , 11, 1775-1797	9.4	91

181	Development of a Novel Cell-Permeable Protein-Protein Interaction Inhibitor for the Polo-box Domain of Polo-like Kinase 1. 2020 , 5, 822-831		3
180	Discovery and Characterization of Low-Molecular Weight Inhibitors of. 2020 , 110, 989-998		3
179	A Modified Skip-Gram Algorithm for Extracting Drug-Drug Interactions from AERS Reports. 2020 , 2020, 1747413		3
178	QSAR without borders. 2020 , 49, 3525-3564		196
177	A comprehensive review of computational techniques for the prediction of drug side effects. 2020 , 81, 650-670		4
176	Pharmacophore modeling and virtual screening for the discovery of biologically active natural products. 2020 , 64, 321-364		1
175	Mechanism-Based Rational Discovery and Evaluation of Novel Microtubule Stabilizing Agents with Non-Taxol-Competitive Activity. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 3204-3213	Ĺ	4
174	Virtual screening web servers: designing chemical probes and drug candidates in the cyberspace. Briefings in Bioinformatics, 2021 , 22, 1790-1818	·4	36
173	Current advances in ligand-based target prediction. 2021 , 11, e1504		8
172	Chemically informed analyses of metabolomics mass spectrometry data with Qemistree. 2021 , 17, 146-157	l	29
171	Artificial intelligence and machine learning-aided drug discovery in central nervous system diseases: State-of-the-arts and future directions. 2021 , 41, 1427-1473		26
170	Do Similar Structures Have Similar No Observed Adverse Effect Level (NOAEL) Values? Exploring Chemoinformatics Approaches for Estimating NOAEL Bounds and Uncertainties. 2021 , 34, 616-633		6
169	Simple Method (CHEM-SP) to Predict Solubility from 2-D Chemical Structures. 2021 , 25, 75-81		2
168	Using Domain-Specific Fingerprints Generated Through Neural Networks to Enhance Ligand-Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 664-675	[4
167	Application of In Silico Methods in Pharmacokinetic Studies During Drug Development. 2021 , 499-510		О
166	Molecular Scaffold Hopping via Holistic Molecular Representation. 2021 , 2266, 11-35		3
165	Prediction of Drug Metabolism: Use of Structural Biology and In Silico Tools. 2021 ,		
164	Chemsearch: collaborative compound libraries with structure-aware browsing. 2021, 1,		О

163	Identification of potential antivirals against SARS-CoV-2 using virtual screening method. 2021 , 23, 100	531	8
162	One class classification as a practical approach for accelerating Eco-crystal discovery . <i>Chemical Science</i> , 2020 , 12, 1702-1719	9.4	7
161	A novel antiplasmodial compound: integration of and assays. 2021 , 1-13		
160	PSC-db: A Structured and Searchable 3D-Database for Plant Secondary Compounds. <i>Molecules</i> , 2021 , 26,	4.8	5
159	Analysis of the effects of related fingerprints on molecular similarity using an eigenvalue entropy approach. 2021 , 13, 27		1
158	FRAGSITE: A Fragment-Based Approach for Virtual Ligand Screening. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 2074-2089	6.1	8
157	Analogue discovery of safer alternatives to HCQ and CQ drugs for SAR-CoV-2 by computational design. 2021 , 130, 104222		6
156	Artificial neural network-based quantitative structureEctivity relationships model and molecular docking for virtual screening of novel potent acetylcholinesterase inhibitors. 2021 , 68, 1379-1399		2
155	Chemoinformatics Studies on a Series of Imidazoles as Cruzain Inhibitors. 2021 , 11,		1
154	Docking, Scoring, and Virtual Screening in Drug Discovery. 1-102		1
153	LINGO-DL: a text-based approach for molecular similarity searching. <i>Journal of Computer-Aided Molecular Design</i> , 2021 , 35, 657-665	4.2	
152	Extended similarity indices: the benefits of comparing more than two objects simultaneously. Part 2: speed, consistency, diversity selection. 2021 , 13, 33		9
151	Extended similarity indices: the benefits of comparing more than two objects simultaneously. Part 1: Theory and characteristics. 2021 , 13, 32		7
150	Attacking COVID-19 Progression Using Multi-Drug Therapy for Synergetic Target Engagement. 2021 , 11,		4
149	Atomistic De-novo Inhibitor Generation-Guided Drug Repurposing for SARS-CoV-2 Spike Protein with Free-Energy Validation by Well-Tempered Metadynamics. 2021 , 16, 1634-1642		4
148	Chemical Space Exploration of DprE1 Inhibitors Using Chemoinformatics and Artificial Intelligence. 2021 , 6, 14430-14441		2
147	Systematic comparison of ligand-based and structure-based virtual screening methods on poly (ADP-ribose) polymerase-1 inhibitors. <i>Briefings in Bioinformatics</i> , 2021 , 22,	13.4	1
146	Chemical Space, Scaffolds, and Halogenated Compounds of CMNPD: A Comprehensive Chemoinformatic Analysis. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 3323-3336	6.1	O

145	Statistical Properties of Low-Frequency Signals over FFT-OFDM. 2021 ,	O
144	A comprehensive comparative assessment of 3D molecular similarity tools in ligand-based virtual screening. <i>Briefings in Bioinformatics</i> , 2021 , 22,	2
143	Improving Measures of Chemical Structural Similarity Using Machine Learning on Chemical-Genetic Interactions. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 4156-4172	1
142	Machine Learning in Drug Discovery: A Review. 2021 , 1-53	18
141	Machine learning study of the molecular drivers of natural product prices.	
140	ChemPLAN-Net: A deep learning framework to find novel inhibitor fragments for proteins.	
139	Exploring and mapping chemical space with molecular assembly trees. 2021 , 7, eabj2465	1
138	Rapid Identification of Potential Drug Candidates from Multi-Million Compounds' Repositories. Combination of 2D Similarity Search with 3D Ligand/Structure Based Methods and In Vitro 4.8 Screening. <i>Molecules</i> , 2021 , 26,	O
137	Integrating perspectives in actinomycete research: an ActinoBase review of 2020-21. 2021 , 167,	0
136	Current trends in computer aided drug design and a highlight of drugs discovered via computational techniques: A review. 2021 , 224, 113705	35
135	Drug Screening of Potential Multiple Target Inhibitors for Estrogen Receptor-positive Breast Cancer. 2021 , 35, 761-777	1
134	Extended many-item similarity indices for sets of nucleotide and protein sequences. 2021 , 19, 3628-3639	5
133	Hit discovery. 2021 , 81-102	2
132	Key Aspects for Achieving Hits by Virtual Screening Studies. 2021 , 455-487	2
131	MOLECULAR SIMILARITY ANALYSIS. 343-399	9
130	Interactive Technologies for Leveraging the Known Chemistry of Anchor Residues to Disrupt Protein Interactions. 85-100	1
129	Introduction to Molecular Similarity and Chemical Space. 2014 , 1-81	2
128	Molecular Dynamics and Related Computational Methods with Applications to Drug Discovery. 2018 , 267-285	1

(2021-2008)

127	An Efficiently Computable Graph-Based Metric for the Classification of Small Molecules. <i>Lecture Notes in Computer Science</i> , 2008 , 197-209	0.9	11
126	Evaluating the Jaccard-Tanimoto Index on Multi-core Architectures. <i>Lecture Notes in Computer Science</i> , 2009 , 944-953	0.9	3
125	An Indexing Scheme for Fast and Accurate Chemical Fingerprint Database Searching. <i>Lecture Notes in Computer Science</i> , 2010 , 288-305).9	4
124	Nontest Methods for REACH Legislation. 2017 , 472-490		3
123	Semi-supervised regression trees with application to QSAR modelling. 2020 , 158, 113569		6
122	Structure-Based Discovery of 1H-Indazole-3-carboxamides as a Novel Structural Class of Human GSK-3 Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 2540-51	ó.1	16
121	Chapter 7:In silico Tools for Target Identification and Drug Molecular Docking in Leishmania. <i>RSC Drug Discovery Series</i> , 2017 , 130-152	o.6	1
120	Chapter 12:Developing the Applicability Domain of In Silico Models: Relevance, Importance and Methods. 2010 , 301-333		6
119	Fingerprinting CANDO: Increased Accuracy with Structure and Ligand Based Shotgun Drug Repurposing.		2
118	Activity-relevant similarity values for fingerprints and implications for similarity searching. 2016 , 5,		27
117	Activity-relevant similarity values for fingerprints and implications for similarity searching. 2016 , 5, 591		26
116	Template CoMFA Generates Single 3D-QSAR Models that, for Twelve of Twelve Biological Targets, Predict All ChEMBL-Tabulated Affinities. 2015 , 10, e0129307		13
115	Discovery of indolylpiperazinylpyrimidines with dual-target profiles at adenosine A2A and dopamine D2 receptors for Parkinson's disease treatment. 2018 , 13, e0188212		17
114	Ensemble learning method for the prediction of new bioactive molecules. 2018 , 13, e0189538		16
113	The In Silico Drug Discovery Toolbox: Applications in Lead Discovery and Optimization. 2019 , 26, 3838-38	73	17
112	Five Years of the KNIME Vernalis Cheminformatics Community Contribution. 2020 , 27, 6495-6522		7
111	Chemoinformatics Profiling of the Chromone Nucleus as a MAO-B/A2AAR Dual Binding Scaffold. 2017 , 15, 1117-1135		3
110	Insights into Machine Learning-based Approaches for Virtual Screening in Drug Discovery: Existing Strategies and Streamlining Through FP-CADD. 2021 , 18, 463-472		7

109	Genetic Algorithm-based Feature Selection Approach for Enhancing the Effectiveness of Similarity Searching in Ligand-based Virtual Screening. 2020 , 15, 431-444	5
108	Screening Outside the Catalytic Site: Inhibition of Macromolecular Inter-actions Through Structure-Based Virtual Ligand Screening Experiments. 2008 , 2, 29-37	14
107	Prospective pharmacological effects of psoralen photoxidation products and their cycloadducts with aminothiols: chemoinformatic analysis. 2020 ,	0
106	Graph Applications in Chemoinformatics and Structural Bioinformatics. 1126-1157	1
105	Virtual Screening. 2011 , 28-60	6
104	Virtual Screening Methods Based on Bayesian Statistics. 2011 , 190-211	1
103	Classification with binary gene expressions. 2009 , 02, 390-399	7
102	Identification and Characterization of Novel Small-Molecule Inhibitors against Hepatitis Delta Virus Replication by Using Docking Strategies. 2011 , 11, 803-809	7
101	Pre-docking filter for protein and ligand 3D structures. 2008 , 3, 189-93	3
100	Anti-Oxidation and Anti-Inflammatory Potency Evaluation of Ferulic Acid Derivatives Obtained through Virtual Screening. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	5
99	RealVS: Toward Enhancing the Precision of Top Hits in Ligand-Based Virtual Screening of Drug Leads from Large Compound Databases. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 4924-4939	1
98	A Deep Learning Proteomic Scale Approach for Drug Design.	O
97	Computer-Aided Design and Synthesis of a New Class of PEX14 Inhibitors: Substituted 2,3,4,5-Tetrahydrobenzo[F][1,4]oxazepines as Potential New Trypanocidal Agents. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 5256-5268	
96	The role of machine learning method in the synthesis and biological flvestigation of heterocyclic compounds. 2021 , 1	
95	Novel drug design and bioinformatics: an introduction. 2021,	
94	Exploration of Potential Natural Inhibitors against SARS-Cov-2 nsp10. <i>Molecules</i> , 2021 , 26, 4.8	12
93	Development of Specific Gamma Secretase Inhibitors. 2009 , 423-437	
92	A Simulation Study of the Use of Similarity Fusion for Virtual Screening. 2011 , 46-59	

91	In silico-screening approaches for lead generation: identification of novel allosteric modulators of human-erythrocyte pyruvate kinase. 2012 , 796, 351-67		
90	Integration of Ligand-Based and Structure-Based Approaches for Virtual Screening of Factor Xa Inhibitors. 2012 , 141-154		
89	Interactions Between Weighting Scheme and Similarity Coefficient in Similarity-Based Virtual Screening. 2012 , 2, 28-41		
88	Encyclopedia of Complexity and Systems Science. 2015 , 1-28		
87	Digital Communication and Chemical Structure Codification. 2016 , 1-28		
86	Accelerating Group Fusion for Ligand-Based Virtual Screening on Multi-core and Many-core Platforms.		
85	The Effect of Adding Indirect Relationship to Turbo Similarity Searching. 2016, 3, 99-116		1
84	VIRTUAL SCREENING IN DRUG DESIGN - OVERVIEW OF MOST FREQUENT TECHNIQUES. <i>Military Medical Science Letters (Vojenske Zdravotnicke Listy)</i> , 2016 , 85, 75-79	0.2	
83	Rational Drug Design Rational Drug Design. 2017 , 1144-1174		
82	Improving prediction of compound function from chemical structure using chemical-genetic networks.		2
81	Molecular Similarity Searching with Different Similarity Coefficients and Different Molecular Descriptors. <i>Lecture Notes on Data Engineering and Communications Technologies</i> , 2018 , 39-47	0.4	
80	Molecular structures enumeration and virtual screening in the chemical space with RetroPath2.0.		
79	A big data approach with artificial neural network and molecular similarity for chemical data mining and endocrine disruption prediction. <i>Indian Journal of Pharmacology</i> , 2018 , 50, 169-176	2.5	1
78	Identifying protein subsets and features responsible for improved drug repurposing accuracies using the CANDO platform.		1
77	Target Identification Among Known Drugs by Deep Learning from Heterogeneous Networks. <i>SSRN Electronic Journal</i> ,	1	1
76	Molecular Modeling and Drug Design Techniques in Microbial Drug Discovery. 2019 , 185-231		
75	Screening Technique for Heat Shock Protein 90 Inhibitors from Natural Products. <i>Heat Shock Proteins</i> , 2019 , 411-439	0.2	1
74	Analysis of the effects of related fingerprints on molecular similarity using an eigenvalue entropy approach.		

73	Chemical XAI to Discover Probable Compounds paces Based on Mixture of Multiple Mutated Exemplars and Bioassay Existence Ratio. <i>Lecture Notes in Computer Science</i> , 2020 , 177-189	0.9	1
72	An in silico Workflow that Yields Experimentally Comparable Inhibitors for Human Dihydroorotate Dehydrogenase. <i>Current Computer-Aided Drug Design</i> , 2020 , 16, 340-350	1.4	
71	Developing Kinase Inhibitors Using Computer-Aided Drug Design Approaches. 2020, 81-108		
70	Interactions Between Weighting Scheme and Similarity Coefficient in Similarity-Based Virtual Screening. 310-321		
69	Virtual Screening. 229-245		
68	Graph Applications in Chemoinformatics and Structural Bioinformatics. <i>Advances in Data Mining and Database Management Book Series</i> , 386-420	0.6	
67	Cellular Fingerprints: A Novel Concept for the Integration of Experimental Data and Compound-Target-Pathway Relations (Extended Abstract). 2007 , 167-170		
66	Accelerating Drug Discovery and Repurposing by Combining Transcriptional Signature Connectivity with Docking.		
65	Identification of Novel Phyto-chemicals from Ocimum basilicum for the Treatment of Parkinson's Disease using In Silico Approach. <i>Current Computer-Aided Drug Design</i> , 2020 , 16, 420-434	1.4	2
64	Ligand-based drug designing. 2022 , 233-252		1
64	Ligand-based drug designing. 2022, 233-252 Ensemble Machine Learning Approaches in Molecular Fingerprint based Virtual screening. 2021,		1
ĺ		3	3
63	Ensemble Machine Learning Approaches in Molecular Fingerprint based Virtual screening. 2021 , DeepCarc: Deep Learning-Powered Carcinogenicity Prediction Using Model-Level Representation.	3	
6 ₃	Ensemble Machine Learning Approaches in Molecular Fingerprint based Virtual screening. 2021, DeepCarc: Deep Learning-Powered Carcinogenicity Prediction Using Model-Level Representation. Frontiers in Artificial Intelligence, 2021, 4, 757780 SAR study on inhibitors of Hsp90@sing machine learning methods. CCF Transactions on High		
63 62 61	Ensemble Machine Learning Approaches in Molecular Fingerprint based Virtual screening. 2021, DeepCarc: Deep Learning-Powered Carcinogenicity Prediction Using Model-Level Representation. Frontiers in Artificial Intelligence, 2021, 4, 757780 SAR study on inhibitors of Hsp90Husing machine learning methods. CCF Transactions on High Performance Computing, 2021, 3, 353-364 ADENet: a novel network-based inference method for prediction of drug adverse events Briefings	0.7	
63 62 61	Ensemble Machine Learning Approaches in Molecular Fingerprint based Virtual screening. 2021, DeepCarc: Deep Learning-Powered Carcinogenicity Prediction Using Model-Level Representation. Frontiers in Artificial Intelligence, 2021, 4, 757780 SAR study on inhibitors of Hsp90 (using machine learning methods. CCF Transactions on High Performance Computing, 2021, 3, 353-364 ADENet: a novel network-based inference method for prediction of drug adverse events Briefings in Bioinformatics, 2022, wSDTNBI: a novel network-based inference method for virtual screening Chemical Science, 2022,	0.7	3
63 62 61 60	Ensemble Machine Learning Approaches in Molecular Fingerprint based Virtual screening. 2021, DeepCarc: Deep Learning-Powered Carcinogenicity Prediction Using Model-Level Representation. Frontiers in Artificial Intelligence, 2021, 4, 757780 SAR study on inhibitors of Hsp90Husing machine learning methods. CCF Transactions on High Performance Computing, 2021, 3, 353-364 ADENet: a novel network-based inference method for prediction of drug adverse events Briefings in Bioinformatics, 2022, wSDTNBI: a novel network-based inference method for virtual screening Chemical Science, 2022, 13, 1060-1079 Chemicals Informatics: Discover Structural Factors and Optimize Combinations of Compounds for	0.7	3

(2018-2022)

55	Best-Practice Aspects of Quantum-Computer Calculations: A Case Study of the Hydrogen Molecule <i>Molecules</i> , 2022 , 27,	4.8	О
54	Turbo prediction: a new approach for bioactivity prediction <i>Journal of Computer-Aided Molecular Design</i> , 2022 , 36, 77	4.2	1
53	A Novel Network Science and Similarity-Searching-Based Approach for Discovering Potential Tumor-Homing Peptides from Antimicrobials <i>Antibiotics</i> , 2022 , 11,	4.9	O
52	Extended continuous similarity indices: theory and application for QSAR descriptor selection <i>Journal of Computer-Aided Molecular Design</i> , 2022 , 36, 157	4.2	O
51	Introducing a Chemically Intuitive Core-Substituent Fingerprint Designed to Explore Structural Requirements for Effective Similarity Searching and Machine Learning <i>Molecules</i> , 2022 , 27,	4.8	2
50	A Comparison between Enrichment Optimization Algorithm (EOA)-Based and Docking-Based Virtual Screening <i>International Journal of Molecular Sciences</i> , 2021 , 23,	6.3	O
49	Turbo Similarity Searching: Effect of Partial Ranking and Fusion Rules on ChEMBL Database. <i>Molecular Informatics</i> , 2021 , e2100106	3.8	
48	Artificial Intelligence (AI) in Drugs and Pharmaceuticals. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2021 ,	1.3	1
47	A Deep-Learning Proteomic-Scale Approach for Drug Design Pharmaceuticals, 2021, 14,	5.2	O
46	Chemicals Informatics: Explore Structural Factors and Potential Chemicals based on Public Literatures. 2021 ,		
45	Data_Sheet_1.ZIP. 2020 ,		
44	Data_Sheet_1.PDF. 2018 ,		
43	Data_Sheet_2.PDF. 2018 ,		
42	Image1.pdf. 2018 ,		
41	Image2.pdf. 2018 ,		
40	Image3.pdf. 2018 ,		
39	Image4.pdf. 2018 ,		
38	Image5.pdf. 2018 ,		

37 Image6.pdf. **2018**,

36	Efficient Screening of Target-Specific Selected Compounds in Mixtures by 19F NMR Binding Assay with Predicted 19F NMR Chemical Shifts <i>ChemMedChem</i> , 2022 ,	3.7	
35	Improving the Prediction of Potential Kinase Inhibitors with Feature Learning on Multisource Knowledge <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2022 , 1	3.5	О
34	Molar absorption coefficients and acid dissociation constants for fluoroquinolone, sulfonamide, and tetracycline antibiotics of environmental concern <i>Science of the Total Environment</i> , 2022 , 155508	10.2	O
33	Chemicals Informatics: Search Structural Factors and Optimal Composites. <i>Lecture Notes on Data Engineering and Communications Technologies</i> , 2022 , 593-607	0.4	
32	Differential Multimolecule Fingerprint for Similarity Search-Making Use of Active and Inactive Compound Sets in Virtual Screening. <i>Journal of Chemical Information and Modeling</i> ,	6.1	2
31	Towards an Enrichment Optimization Algorithm (EOA)-based target specific docking functions for virtual screening. <i>Molecular Informatics</i> ,	3.8	
30	Emerging Computational Approaches for Antimicrobial Peptide Discovery. <i>Antibiotics</i> , 2022 , 11, 936	4.9	1
29	Combining network-based and matrix factorization to predict novel drug-target interactions: A case study using the Brazilian natural chemical database. 2022 , 17,		
28	Structure-Based Virtual Screening, Docking, ADMET, Molecular Dynamics, and MM-PBSA Calculations for the Discovery of Potential Natural SARS-CoV-2 Helicase Inhibitors from the Traditional Chinese Medicine. 2022 , 2022, 1-23		
27	General Strategies for Rational Design and Discovery of Multitarget Drugs. 2022, 677-736		0
26	Virtual screening techniques in pharmaceutical research. 2022 , 89-128		O
25	Deconstructing Markush: Improving the R&D Efficiency Using Library Selection in Early Drug Discovery. 2022 , 15, 1159		0
24	GCMM: graph convolution network based on multimodal attention mechanism for drug repurposing. 2022 , 23,		O
23	Roughness of Molecular Property Landscapes and Its Impact on Modellability.		1
22	Multi-Task Neural Networks and Molecular Fingerprints to Enhance Compound Identification from LC-MS/MS Data. 2022 , 27, 5827		0
21	Random-forest model for drugEarget interaction prediction via KullbeckEeibler divergence. 2022 , 14,		О
20	Two Distillation Perspectives Based on Tanimoto Coefficient. 2022 ,		O

19	Cachrys spp. from Southern Italy: Phytochemical Characterization and JAK/STAT Signaling Pathway Inhibition. 2022 , 11, 2913	1
18	Convolutional Neural Network Model Based on 2D Fingerprint for Bioactivity Prediction. 2022 , 23, 13230	О
17	The Discovery of Potential SARS-CoV-2 Natural Inhibitors among 4924 African Metabolites Targeting the Papain-like Protease: A Multi-Phase In Silico Approach. 2022 , 12, 1122	0
16	Identification of Active Compounds against Melanoma Growth by Virtual Screening for Non-Classical Human DHFR Inhibitors. 2022 , 23, 13946	О
15	Automated detection of toxicophores and prediction of mutagenicity using PMCSFG algorithm.	O
14	Network Science and Group Fusion Similarity-Based Searching to Explore the Chemical Space of Antiparasitic Peptides. 2022 , 7, 46012-46036	1
13	A parametric approach for molecular encodings using multilevel atomic neighborhoods applied to peptide classification. 2023 , 5,	O
12	Integration of fingerprint-based similarity searching and kernel-based partial least squares analysis to predict inhibitory activity against CSK, HER2, JAK1, JAK2, and JAK3.	Ο
11	On the ability of machine learning methods to discover novel scaffolds. 2023 , 29,	О
10	Artificial Intelligence and Machine Learning Technology Driven Modern Drug Discovery and Development. 2023 , 24, 2026	2
9	Stimulation of natural killer cells with small molecule inhibitors of CD38 for the treatment of neuroblastoma.	О
8	Porous Molecular Materials. 2023 , 251-282	0
7	Quantifying Functional-Group-like Structural Fragments in Molecules and Its Applications in Drug Design. 2023 , 63, 2073-2083	1
6	Prediction of bioactivities of microsomal prostaglandin E 2 synthase-1 inhibitors by machine learning algorithms.	O
5	Computational Chemistry for the Identification of Lead Compounds for Radiotracer Development. 2023 , 16, 317	1
4	Predicting Potent Compounds Using a Conditional Variational Autoencoder Based upon a New Structure B otency Fingerprint. 2023 , 13, 393	O
3	Sunsetting Binding MOAD with its last data update and the addition of 3D-ligand polypharmacology tools. 2023 , 13,	О
2	Partition of topological indices of benzenoid hydrocarbons into ring contributions.	O

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