

CITATION REPORT

List of articles citing

Virtual screeningan overview

DOI: 10.1016/s1359-6446(97)01163-x
Drug Discovery Today, 1998, 3, 160-178.

Source: <https://exaly.com/paper-pdf/28975307/citation-report.pdf>

Version: 2024-04-23

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
835	Plant Metabolite Databases: From Herbal Medicines to Modern Drug Discovery.		
834	Chapter 29. Structure-Based Drug Design. 1999 , 34, 297-306		13
833	Method for Including the Dynamic Fluctuations of a Protein in Computer-Aided Drug Design. 1999 , 103, 10213-10219		91
832	Recognizing molecules with drug-like properties. 1999 , 3, 384-7		235
831	NMR screening in drug discovery. 1999 , 10, 54-8		86
830	The SHAPES strategy: an NMR-based approach for lead generation in drug discovery. 1999 , 6, 755-69		230
829	NMR techniques for characterization of ligand binding: utility for lead generation and optimization in drug discovery. 1999 , 51, 221-43		35
828	Dissimilarity-based algorithms for selecting structurally diverse sets of compounds. 1999 , 6, 447-57		40
827	Molecular hashkeys: a novel method for molecular characterization and its application for predicting important pharmaceutical properties of molecules. 1999 , 42, 1739-48		63
826	Designing libraries with CNS activity. 1999 , 42, 4942-51		255
825	Virtual combinatorial syntheses and computational screening of new potential anti-herpes compounds. 1999 , 42, 3308-14		103
824	Phase jumps and interferometric surface plasmon resonance imaging. 1999 , 75, 3917-3919		120
823	Consensus scoring: A method for obtaining improved hit rates from docking databases of three-dimensional structures into proteins. 1999 , 42, 5100-9		612
822	Glossary of Terms Used in Combinatorial Chemistry. 1999 , 71, 2349-2365		46
821	Chapter 28. Recent Developments in Molecular Diversity: Computational Approaches to Combinatorial Chemistry. 1999 , 34, 287-296		16
820	Organic Synthesis and Medicinal Chemistry. 2000 , 1-16		
819	Designing targeted libraries with genetic algorithms. 2000 , 18, 320-34, 525		39

818	Chemoinformatics - similarity and diversity in chemical libraries. 2000 , 11, 85-8		104
817	Extraction of pharmacophore information from high-throughput screens. 2000 , 11, 97-103		28
816	Neural networks are useful tools for drug design. 2000 , 13, 15-6		44
815	High-throughput and virtual screening: core lead discovery technologies move towards integration. <i>Drug Discovery Today</i> , 2000 , 5, 61-69	8.8	36
814	Diversity screening versus focussed screening in drug discovery. <i>Drug Discovery Today</i> , 2000 , 5, 286-293	8.8	125
813	ADME/PK as part of a rational approach to drug discovery. <i>Drug Discovery Today</i> , 2000 , 5, 409-414	8.8	174
812	Chemoinformatics: are we exploiting this new science?. 'We need to make chemoinformatics tools more accessible to the bench chemist.'. <i>Drug Discovery Today</i> , 2000 , 5, 483-485	8.8	5
811	High-throughput and virtual screening: core lead discovery technologies move towards integration. <i>Drug Discovery Today</i> , 2000 , 5, S61-S69	8.8	21
810	Computational methods for the prediction of 'drug-likeness'. <i>Drug Discovery Today</i> , 2000 , 5, 49-58	8.8	475
809	A recursive algorithm for efficient combinatorial library docking. 2000 , 20, 63-81		29
808	Modifications of the scoring function in FlexX for virtual screening applications. 2000 , 20, 83-98		27
807	Preface. 2000 , 20, 7-11		5
806	A knowledge-based scoring function for protein-ligand interactions: Probing the reference state. 2000 , 20, 99-114		105
805	Predicting binding modes, binding affinities and 'hot spots' for protein-ligand complexes using a knowledge-based scoring function. 2000 , 20, 115-144		86
804	Similarity versus docking in 3D virtual screening. 2000 , 20, 191-207		23
803	Reactant- and product-based approaches to the design of combinatorial libraries. 2002 , 5, 245-54		
802	Towards a new age of virtual ADME/TOX and multidimensional drug discovery. 2002 , 5, 255-75		20
801	Recent developments in structure-based drug design. 2000 , 78, 269-81		188

800	. 2000 ,	70
799	On the topological sub-structural molecular design (TOSS-MODE) in QSPR/QSAR and drug design research. 2000 , 11, 55-73	50
798	Knowledge-based scoring function to predict protein-ligand interactions. 2000 , 295, 337-56	871
797	Similarities in Bioanalogous Structural Transformation Patterns. 2000 , 166-179	1
796	Protein-based virtual screening of chemical databases. 1. Evaluation of different docking/scoring combinations. 2000 , 43, 4759-67	648
795	Developing a dynamic pharmacophore model for HIV-1 integrase. 2000 , 43, 2100-14	248
794	A novel approach for the virtual screening and rational design of anticancer compounds. 2000 , 43, 1975-85	152
793	New approach to molecular docking and its application to virtual screening of chemical databases. 2000 , 40, 254-62	71
792	High-Throughput Screening and Virtual Screening: Entry Points to Drug Discovery. 2000 , 1-14	3
791	Library Filtering Systems and Prediction of Drug-Like Properties. 2000 , 15-32	12
790	Structure-Based Library Design. 2000 , 229-264	7
789	Understanding Receptor-Ligand Interactions as a Prerequisite for Virtual Screening. 2000 , 207-227	5
788	Successful virtual screening of a chemical database for farnesyltransferase inhibitor leads. 2000 , 43, 401-8	124
787	Combinatorial library design: maximizing model-fitting compounds within matrix synthesis constraints. 2000 , 40, 701-5	27
786	Diversity measures for enhancing ADME admissibility of combinatorial libraries. 2000 , 40, 314-22	34
785	Bit-string methods for selective compound acquisition. 2000 , 40, 210-4	21
784	Ligand-protein database: linking protein-ligand complex structures to binding data. 2001 , 44, 3592-8	114
783	Are free energy calculations useful in practice? A comparison with rapid scoring functions for the p38 MAP kinase protein system. 2001 , 44, 3417-23	196

782	Large-scale virtual screening for discovering leads in the postgenomic era. 2001 , 40, 360-376	63
781	How does consensus scoring work for virtual library screening? An idealized computer experiment. 2001 , 41, 1422-6	236
780	Improved scoring of ligand-protein interactions using OWFEG free energy grids. 2001 , 44, 502-11	88
779	Simple selection criteria for drug-like chemical matter. 2001 , 44, 1841-6	451
778	Evaluation of docking functions for protein-ligand docking. 2001 , 44, 3768-85	70
777	Virtual screening of combinatorial libraries across a gene family: in search of inhibitors of <i>Giardia lamblia</i> guanine phosphoribosyltransferase. 2001 , 45, 2571-6	34
776	Computational characterization of substrate binding and catalysis in S-adenosylhomocysteine hydrolase. 2001 , 40, 15143-52	14
775	4D-QSAR analysis of a set of ecdysteroids and a comparison to CoMFA modeling. 2001 , 41, 1587-604	56
774	Selected concepts and investigations in compound classification, molecular descriptor analysis, and virtual screening. 2001 , 41, 233-45	184
773	Fingerprint scaling increases the probability of identifying molecules with similar activity in virtual screening calculations. 2001 , 41, 746-53	53
772	A fast algorithm for searching for molecules containing a pharmacophore in very large virtual combinatorial libraries. 2001 , 41, 731-8	15
771	. 2001 ,	3
770	Integrating Virtual Screening Methods to the Quest for Novel Membrane Protein Ligands. 2001 , 1, 99-112	3
769	Sequential Approach for Identifying Lead Compounds in Large Chemical Databases. 2001 , 16, 154	9
768	Screening of Drug Databases. 2001 , 137-170	2
767	Customized versus universal scoring functions: application to class I MHC-peptide binding free energy predictions. 2001 , 11, 675-9	42
766	High-throughput docking for lead generation. 2001 , 5, 375-82	319
765	Chemogenomic approaches to drug discovery. 2001 , 5, 464-70	151

764	Novel local (fragment-based) topological molecular descriptors for QSPr/QSAR and molecular design. 2001 , 20, 54-64		69
763	Design, docking, and evaluation of multiple libraries against multiple targets. 2001 , 42, 296-318		59
762	Massive docking of flexible ligands using environmental niches in parallelized genetic algorithms. 2001 , 22, 1971-1982		19
761	Subnanomolar wirksame Inhibitoren aus dem Computerscreening: eine Modellstudie an der humanen Carboanhydrase II. 2001 , 113, 404-408		4
760	Ein effizientes Cobalt(I)-Katalysatorsystem für die selektive 1,4-Hydrovinylisierung von 1,3-Dienen. 2001 , 113, 408-410		25
759	Subnanomolar Inhibitors from Computer Screening: A Model Study Using Human Carbonic Anhydrase II. 2001 , 40, 389-393		56
758	Thioformaldehyde S-sulfide (Thiosulfine). 2001 , 40, 393-396		36
757	High-throughput structural proteomics using x-rays. 2001 , 19, 67-71		280
756	High-throughput structural proteomics using x-rays. 2001 , 19, S67-71		26
755	Library design for NMR-based screening. <i>Drug Discovery Today</i> , 2001 , 6, 133-140	8.8	76
754	Miniaturized HTS technologies - uHTS. <i>Drug Discovery Today</i> , 2001 , 6, 637-646	8.8	131
753	The impact of informatics and computational chemistry on synthesis and screening. <i>Drug Discovery Today</i> , 2001 , 6, 1101-1110	8.8	65
752	Combinatorial chemistry and high-throughput screening in drug discovery and development. 2001 , 23-56		5
751	High-throughput screening approaches for investigating drug metabolism and pharmacokinetics. 2001 , 31, 557-89		90
750	Support Vector Machines in Combinatorial Chemistry. 2001 , 34, 235-239		41
749	"Holistic" in silico methods to estimate the systemic and CNS bioavailabilities of potential chemotherapeutic agents. 2001 , 1, 257-75		21
748	Molecular Diversity in Drug Design. 2002 ,		1
747	Approaches to library design for combinatorial chemistry. 2002 , 201, 277-95		

746	Chemogenomics: bridging a drug discovery gap. 2002 , 9, 2077-84	36
745	Nuclear magnetic resonance-based approaches for lead generation in drug discovery. 2001 , 338, 202-30	50
744	Trends in virtual combinatorial library design. 2002 , 9, 2095-101	65
743	Ligand-induced changes in the binding sites of proteins. 2002 , 18, 939-48	45
742	Similarity versus docking in 3D virtual screening. 2000 , 191-207	
741	Combinatorial Library. 2002 ,	2
740	The Design of Small- and Medium-sized Focused Combinatorial Libraries. 2002 , 221-248	1
739	Structure-based screening as applied to human FABP4: a highly efficient alternative to HTS for hit generation. 2002 , 124, 11874-80	45
738	Development of a virtual screening method for identification of "frequent hitters" in compound libraries. 2002 , 45, 137-42	258
737	Rational design and evaluation of new lead compound structures for selective betaARK1 inhibitors. 2002 , 45, 2150-9	36
736	4D-QSAR analysis of a set of propofol analogues: mapping binding sites for an anesthetic phenol on the GABA(A) receptor. 2002 , 45, 3210-21	86
735	Chemoinformatics and Drug Discovery. 2002 , 7, 566-600	114
734	A knowledge-based scoring function for protein-ligand interactions: Probing the reference state. 2000 , 99-114	10
733	Selecting screening candidates for kinase and G protein-coupled receptor targets using neural networks. 2002 , 42, 1256-62	58
732	Reactant- and product-based approaches to the design of combinatorial libraries. 2002 , 16, 371-80	12
731	A common mechanism underlying promiscuous inhibitors from virtual and high-throughput screening. 2002 , 45, 1712-22	924
730	Successful virtual screening for novel inhibitors of human carbonic anhydrase: strategy and experimental confirmation. 2002 , 45, 3588-602	159
729	Simple, intuitive calculations of free energy of binding for protein-ligand complexes. 1. Models without explicit constrained water. 2002 , 45, 2469-83	118

728	. 2002,			10
727	Virtual Screening in Lead Discovery: A Viewpoint. 2002, 7, 51-62			75
726	Prediction of 'drug-likeness'. 2002, 54, 255-71			307
725	Finding the molecules to fuel chemogenomics. 2002, 1, 125-129			5
724	Virtual screening and fast automated docking methods. <i>Drug Discovery Today</i> , 2002, 7, 64-70	8.8		214
723	Virtual screening and fast automated docking methods. <i>Drug Discovery Today</i> , 2002, 7, 64-70	8.8		228
722	The potential of Internet computing for drug discovery. <i>Drug Discovery Today</i> , 2002, 7, S99-103	8.8		5
721	Structure-based screening and design in drug discovery. <i>Drug Discovery Today</i> , 2002, 7, 471-8	8.8		62
720	Structure-based screening of low-affinity compounds. <i>Drug Discovery Today</i> , 2002, 7, 522-7	8.8		123
719	Grid technologies empowering drug discovery. <i>Drug Discovery Today</i> , 2002, 7, S176-80	8.8		21
718	Chemoproteomics as a basis for post-genomic drug discovery. <i>Drug Discovery Today</i> , 2002, 7, 807-14	8.8		45
717	Why do we need so many chemical similarity search methods?. <i>Drug Discovery Today</i> , 2002, 7, 903-11	8.8		375
716	Leveraging process integration in early drug discovery. <i>Drug Discovery Today</i> , 2002, 7, S181-6	8.8		7
715	Structure-based virtual screening: an overview. <i>Drug Discovery Today</i> , 2002, 7, 1047-55	8.8		469
714	Glossar von Begriffen der Kombinatorischen Chemie. 2002, 114, 893-906			
713	A Method To Identify and Screen Libraries of Guests That Complex to a Synthetic Host. 2002, 114, 1046-1050			4
712	Ansätze zur Beschreibung und Vorhersage der Bindungsaffinität niedermolekularer Liganden an makromolekulare Rezeptoren. 2002, 114, 2764-2798			34
711	A method to identify and screen libraries of guests that complex to a synthetic host. 2002, 41, 1004-8			31

710	Approaches to the description and prediction of the binding affinity of small-molecule ligands to macromolecular receptors. 2002 , 41, 2644-76	595
709	Computation of the physio-chemical properties and data mining of large molecular collections. 2002 , 23, 172-83	52
708	Lead discovery using molecular docking. 2002 , 6, 439-46	355
707	Protein-based virtual screening of chemical databases. II. Are homology models of G-Protein Coupled Receptors suitable targets?. 2003 , 50, 5-25	225
706	High-throughput crystallography for lead discovery in drug design. 2002 , 1, 45-54	432
705	Chemical database techniques in drug discovery. 2002 , 1, 220-7	69
704	Combinatorial informatics in the post-genomics ERA. 2002 , 1, 337-46	92
703	Integration of virtual and high-throughput screening. 2002 , 1, 882-94	615
702	Three-dimensional molecular descriptors and a novel QSAR method. 2002 , 21, 161-70	15
701	Structure activity relationship by NMR and by computer: a comparative study. 2002 , 124, 11073-84	27
700	A review of protein-small molecule docking methods. 2002 , 16, 151-66	463
699	Towards a new age of virtual ADME/TOX and multidimensional drug discovery. 2002 , 16, 381-401	69
698	Mini-fingerprints for virtual screening: design principles and generation of novel prototypes based on information theory. 2003 , 14, 27-40	23
697	Spline-fitting with a genetic algorithm: a method for developing classification structure-activity relationships. 2003 , 43, 1906-15	86
696	A reagent-based strategy for the design of large combinatorial libraries: a preliminary experimental validation. 2003 , 7, 3-14	6
695	Binding site characteristics in structure-based virtual screening: evaluation of current docking tools. 2003 , 9, 47-57	176
694	Markovian chemicals "in silico" design (MARCH-INSIDE), a promising approach for computer-aided molecular design I: discovery of anticancer compounds. 2003 , 9, 395-407	77
693	Information-based methods in the development of antiparasitic drugs. 2003 , 90 Suppl 2, S91-6	6

692	Chemical substructures in drug discovery. <i>Drug Discovery Today</i> , 2003 , 8, 594-602	8.8	64
691	FDS: flexible ligand and receptor docking with a continuum solvent model and soft-core energy function. 2003 , 24, 1637-56		86
690	Selection criteria for drug-like compounds. 2003 , 23, 302-21		288
689	Application of the stochastic tunneling method to high throughput database screening. 2003 , 370, 68-73		34
688	Symmetry considerations in Markovian chemicals 'in silico' design (MARCH-INSIDE) I: central chirality codification, classification of ACE inhibitors and prediction of sigma-receptor antagonist activities. 2003 , 27, 217-27		47
687	Analysis and optimization of structure-based virtual screening protocols (1): exploration of ligand conformational sampling techniques. 2003 , 22, 23-30		15
686	A web-based platform for virtual screening. 2003 , 22, 71-82		27
685	Topological virtual screening: a way to find new anticonvulsant drugs from chemical diversity. 2003 , 13, 2749-54		70
684	Automated generation of MCSS-derived pharmacophoric DOCK site points for searching multiconformation databases. 2003 , 51, 189-202		35
683	SMILIB: Rapid Assembly of Combinatorial Libraries in SMILES Notation. 2003 , 22, 719-721		28
682	Nuclear hormone receptor targeted virtual screening. 2003 , 46, 3045-59		155
681	Molecular recognition and docking algorithms. 2003 , 32, 335-73		543
680	Evaluation of similarity measures for searching the dictionary of natural products database. 2003 , 43, 449-57		45
679	Applications. 487-622		2
678	Pharmacophore features distributions in different classes of compounds. 2003 , 43, 1542-52		19
677	3D-pharmacophores of flavonoid binding at the benzodiazepine GABA(A) receptor site using 4D-QSAR analysis. 2003 , 43, 324-36		44
676	Consideration of molecular weight during compound selection in virtual target-based database screening. 2003 , 43, 267-72		128
675	Rational design of an indolebutanoic acid derivative as a novel aldose reductase inhibitor based on docking and 3D QSAR studies of phenethylamine derivatives. 2003 , 46, 5619-27		28

674	A consensus neural network-based technique for discriminating soluble and poorly soluble compounds. 2003 , 43, 674-9	55
673	Surflex: fully automatic flexible molecular docking using a molecular similarity-based search engine. 2003 , 46, 499-511	1063
672	Tautomerism in computer-aided drug design. 2003 , 23, 361-71	94
671	Overview on High-Throughput Screening. 2003 , 22, 9.4.1	
670	Chapter 30. Recent advances in virtual ligand screening. 2003 , 38, 305-314	8
669	Comparison of MLR, PLS and GA-MLR in QSAR analysis. 2003 , 14, 433-45	73
668	Chapter 1 Role of bioanalysis in pharmaceutical drug development. 2003 , 5, 1-40	
667	In silico tools for drug absorption prediction. 2003 , 1, 133-148	3
666	Comparison of ranking methods for virtual screening in lead-discovery programs. 2003 , 43, 469-74	75
665	High-throughput screening technologies. 2003 , 71-85	5
664	Stochastic optimization methods for structure prediction of biomolecular nanoscale systems. 2003 , 14, 1161-1167	11
663	Theoretical property predictions. 2003 , 3, 1171-92	51
662	Virtual screening of virtual libraries. 2003 , 41, 61-97	31
661	Molecular Docking in Structure-Based Design. 2003 , 417-452	
660	. 2003 ,	5
659	Total and Local Quadratic Indices of the Molecular Pseudograph's Atom Adjacency Matrix: Applications to the Prediction of Physical Properties of Organic Compounds. 2003 , 8, 687-726	68
658	Total and Local Quadratic Indices of the Molecular Pseudograph's Atom Adjacency Matrix: Application to Prediction of Caco-2 Permeability of Drugs. 2003 , 4, 512-536	48
657	STRATEGIES IN THE SEARCH FOR NEW LEAD COMPOUNDS OR ORIGINAL WORKING HYPOTHESES. 2003 , 69-89	2

656	Target Family-Directed Masterkeys in Chemogenomics. 2004 , 5-41	2
655	. 2004 ,	28
654	A Chemical Genomics Approach for Ion Channel Modulators. 2004 , 221-242	3
653	Atom, atom-type, and total linear indices of the "molecular pseudograph's atom adjacency matrix": application to QSPR/QSAR studies of organic compounds. 2004 , 9, 1100-23	52
652	Virtual screening for kinase targets. 2004 , 11, 693-707	64
651	Predicting molecular interactions in silico: I. A guide to pharmacophore identification and its applications to drug design. 2004 , 11, 71-90	114
650	Integration of virtual screening into the drug discovery process. 2004 , 4, 1053-65	13
649	Recent development and application of virtual screening in drug discovery: an overview. 2004 , 10, 1011-33	158
648	RATIONAL DESIGN OF ADVANCED MATERIALS: OPPORTUNITIES IN MATERIALS RESEARCH. 2004 , 43, 481-488	
647	New lead generation strategies for protein kinase inhibitors - fragment based screening approaches. 2004 , 4, 301-11	31
646	Docking and scoring in virtual screening for drug discovery: methods and applications. 2004 , 3, 935-49	2083
645	The many roles of computation in drug discovery. 2004 , 303, 1813-8	1088
644	ESP: a method to predict toxicity and pharmacological properties of chemicals using multiple MCASE databases. 2004 , 44, 704-15	37
643	Similarity searching of chemical databases using atom environment descriptors (MOLPRINT 2D): evaluation of performance. 2004 , 44, 1708-18	265
642	Molecular similarity searching using atom environments, information-based feature selection, and a naïve Bayesian classifier. 2004 , 44, 170-8	226
641	TOMOCOMD-CARDD, a novel approach for computer-aided 'rational' drug design: I. Theoretical and experimental assessment of a promising method for computational screening and in silico design of new anthelmintic compounds. 2004 , 18, 615-34	54
640	Strategies for the design of inhibitors of aldose reductase, an enzyme showing pronounced induced-fit adaptations. 2004 , 61, 783-93	33
639	Virtual screening for inhibitors of human aldose reductase. 2004 , 55, 814-23	43

638	A minimalist approach to fragment-based ligand design using common rings and linkers: application to kinase inhibitors. 2004 , 57, 36-50	21
637	Status of HTS Data Mining Approaches. 2004 , 23, 207-213	29
636	Fluctuation analysis and accuracy of a large-scale in silico screen. 2004 , 25, 1568-75	12
635	The signature molecular descriptor. 3. Inverse-quantitative structure-activity relationship of ICAM-1 inhibitory peptides. 2004 , 22, 263-73	72
634	Ligand identification for G-protein-coupled receptors: a lead generation perspective. 2004 , 8, 287-96	40
633	Impact of receptor conformation on in silico screening performance. 2004 , 390, 500-505	14
632	Reasoning about molecular similarity and properties. 2004 , 266-77	4
631	Drug-like annotation and duplicate analysis of a 23-supplier chemical database totalling 2.7 million compounds. 2004 , 44, 643-51	120
630	Identification of non-phosphate-containing small molecular weight inhibitors of the tyrosine kinase p56 Lck SH2 domain via in silico screening against the pY + 3 binding site. 2004 , 47, 3502-11	57
629	Molecular surface point environments for virtual screening and the elucidation of binding patterns (MOLPRINT 3D). 2004 , 47, 6569-83	46
628	Identification of novel parasitic cysteine protease inhibitors using virtual screening. 1. The ChemBridge database. 2004 , 47, 6609-15	93
627	Characteristic physical properties and structural fragments of marketed oral drugs. 2004 , 47, 224-32	326
626	Predicting protein-ligand binding affinities: a low scoring game?. 2004 , 2, 3267-73	46
625	Drug Discovery, Design, and Development. 2004 , 7-120	4
624	Ligand-based structural hypotheses for virtual screening. 2004 , 47, 947-61	167
623	Virtual screening of human 5-aminoimidazole-4-carboxamide ribonucleotide transformylase against the NCI diversity set by use of AutoDock to identify novel nonfolate inhibitors. 2004 , 47, 6681-90	59
622	Integrating virtual screening in lead discovery. 2004 , 8, 349-58	214
621	High-throughput modeling of human G-protein coupled receptors: amino acid sequence alignment, three-dimensional model building, and receptor library screening. 2004 , 44, 1162-76	76

620	New Paradigms in Drug Design and Discovery. 2004 , 1, 663-681	
619	Virtual Compound Libraries and Molecular Modeling. 2004 , 761-783	
618	Theoretical Property Predictions. 2005 , 2, 545-570	
617	High-Throughput Flow Cytometry. 2005 , 185-226	
616	Drug Discovery: Small Molecule Drugs. 2005 , 43-74	
615	Chapter 12 Structure-Based Lead Optimization. 2005 , 169-183	2
614	Virtual Screening. 2005 , 3-24	6
613	Structure-based discovery of human L-xylulose reductase inhibitors from database screening and molecular docking. 2005 , 13, 301-12	18
612	Atom, atom-type and total molecular linear indices as a promising approach for bioorganic and medicinal chemistry: theoretical and experimental assessment of a novel method for virtual screening and rational design of new lead anthelmintic. 2005 , 13, 1005-20	84
611	In silico ADME modelling: prediction models for blood-brain barrier permeation using a systematic variable selection method. 2005 , 13, 3017-28	64
610	A novel non-stochastic quadratic fingerprints-based approach for the 'in silico' discovery of new antitrypanosomal compounds. 2005 , 13, 6264-75	41
609	Quadratic indices of the molecular pseudograph's atom adjacency matrix and their stochastic forms: a novel approach for virtual screening and in silico discovery of new lead paramphistomicide drugs-like compounds. 2005 , 717, 67-79	34
608	Construction of a virtual combinatorial library using SMILES strings to discover potential structure-diverse PPAR modulators. 2005 , 40, 632-40	14
607	LigandScout: 3-D pharmacophores derived from protein-bound ligands and their use as virtual screening filters. 2005 , 45, 160-9	1255
606	Evaluation of library ranking efficacy in virtual screening. 2005 , 26, 11-22	98
605	Water-soluble molecular capsules: self-assembly and binding properties. 2004 , 11, 298-307	75
604	VolSurf analysis of pharmacokinetic properties for several antifungal sesquiterpene lactones isolated from Greek Centaurea sp. 2005 , 19, 617-23	26
603	QSAR Strategy and Experimental Validation for the Development of a GPCR Focused Library. 2005 , 24, 508-516	10

602	Comparison of Three Holographic Fingerprint Descriptors and their Binary Counterparts. 2005 , 24, 961-967	16
601	Future Perspectives. 2005 , 281-303	
600	Components of successful lead generation. 2005 , 5, 421-39	109
599	New methodologies for ligand-based virtual screening. 2005 , 11, 1189-202	118
598	Knowledge-driven lead discovery. 2005 , 5, 1045-52	4
597	Pocketome via comprehensive identification and classification of ligand binding envelopes. 2005 , 4, 752-61	298
596	Prediction methods and databases within chemoinformatics: emphasis on drugs and drug candidates. 2005 , 21, 2145-60	78
595	Drug characteristics prediction.	
594	ALARM NMR: a rapid and robust experimental method to detect reactive false positives in biochemical screens. 2005 , 127, 217-24	184
593	Hit-directed nearest-neighbor searching. 2005 , 48, 240-8	56
592	Development of a quasi-dynamic pharmacophore model for anti-complement peptide analogues. 2005 , 127, 10967-76	20
591	New potential antihistaminic compounds. Virtual combinatorial chemistry, computational screening, real synthesis, and pharmacological evaluation. 2005 , 48, 1260-4	20
590	Evaluating the molecular mechanics poisson-boltzmann surface area free energy method using a congeneric series of ligands to p38 MAP kinase. 2005 , 48, 7796-807	164
589	The discovery of Kv1.5 blockers as a case study for the application of virtual screening approaches. 2005 , 45, 477-85	38
588	Virtual screening workflow development guided by the "receiver operating characteristic" curve approach. Application to high-throughput docking on metabotropic glutamate receptor subtype 4. 2005 , 48, 2534-47	487
587	Bioinformatics and Drug Discovery. 2006 ,	1
586	Grid-enabled high-throughput in silico screening against influenza A neuraminidase. 2006 , 5, 288-95	23
585	Molecular complexity analysis of de novo designed ligands. 2006 , 49, 5869-79	40

584	Physics-based scoring of protein-ligand complexes: enrichment of known inhibitors in large-scale virtual screening. 2006 , 46, 243-53	127
583	Pharmacophore modelling: applications in drug discovery. 2006 , 1, 261-7	40
582	Robust ligand-based modeling of the biological targets of known drugs. 2006 , 49, 2921-38	90
581	Parameter estimation for scoring protein-ligand interactions using negative training data. 2006 , 49, 5856-68	127
580	Bridging chemical and biological space: "target fishing" using 2D and 3D molecular descriptors. 2006 , 49, 6802-10	158
579	Combinatorial Chemistry in the Drug Discovery Process. 2006 , 129-167	2
578	Molecular mechanics methods for predicting protein-ligand binding. 2006 , 8, 5166-77	163
577	Identification of novel parasitic cysteine protease inhibitors by use of virtual screening. 2. The available chemical directory. 2006 , 49, 1576-84	66
576	QSAR Studies on Thiazolidines: A Biologically Privileged Scaffold. 161-249	37
575	Integration of virtual and physical screening. 2006 , 3, 377-385	18
574	Advances in virtual screening. 2006 , 3, 405-411	87
573	Knowledge-based design of target-focused libraries using protein-ligand interaction constraints. 2006 , 49, 490-500	57
572	Virtual screening using binary kernel discrimination: analysis of pesticide data. 2006 , 46, 471-7	43
571	VISCANA: visualized cluster analysis of protein-ligand interaction based on the ab initio fragment molecular orbital method for virtual ligand screening. 2006 , 46, 221-30	112
570	Enhancing specificity and sensitivity of pharmacophore-based virtual screening by incorporating chemical and shape features--a case study of HIV protease inhibitors. 2006 , 46, 1236-44	31
569	Explicit Diversity Index (EDI): a novel measure for assessing the diversity of compound databases. 2006 , 46, 1898-904	3
568	Atomic-Level Rational Drug Design. 2006 , 2, 57-81	4
567	. 2006 ,	56

566	. 2006 ,		6
565	Pharmacophores from Macromolecular Complexes with LigandScout. 2006 , 131-150		20
564	Success Stories of Computer-Aided Design. 2006 , 377-424		41
563	History of Computers in Pharmaceutical Research and Development: A Narrative. 2006 , 1-50		3
562	Application of Pharmacophore Fingerprints to Structure-Based Design and Data Mining. 2006 , 193-206		6
561	The Challenges of Making Useful Protein-Ligand Free Energy Predictions for Drug Discovery. 2006 , 321-351		3
560	Dock around the Clock [Current Status of Small Molecule Docking and Scoring. 2006 , 25, 605-615		37
559	Critical evaluation of methods to incorporate entropy loss upon binding in high-throughput docking. 2007 , 66, 422-35		20
558	Virtual and biomolecular screening converge on a selective agonist for GPR30. 2006 , 2, 207-12		644
557	In silico ADME modelling 2: computational models to predict human serum albumin binding affinity using ant colony systems. 2006 , 14, 4118-29		43
556	Molecular similarity and diversity in chemoinformatics: from theory to applications. 2006 , 10, 39-79		180
555	Reverse fingerprinting, similarity searching by group fusion and fingerprint bit importance. 2006 , 10, 311-32		41
554	Integrating molecular design resources within modern drug discovery research: the Roche experience. <i>Drug Discovery Today</i> , 2006 , 11, 326-33	8.8	60
553	Similarity-based virtual screening using 2D fingerprints. <i>Drug Discovery Today</i> , 2006 , 11, 1046-53	8.8	614
552	FlexNovo: structure-based searching in large fragment spaces. 2006 , 1, 854-68		51
551	Structure-based organic synthesis of drug prototypes: a personal odyssey. 2006 , 1, 1301-30		40
550	Structural Fragments in Marketed Oral Drugs. 2006 , 113-124		2
549	FAF-Drugs: free ADME/tox filtering of compound collections. 2006 , 34, W738-44		96

548	Chemical database preparation for compound acquisition or virtual screening. 2006 , 316, 375-88	13
547	Finding protein kinase hits using structural information. 2006 , 44, 1-63	2
546	Diversity in medicinal chemistry space. 2006 , 6, 3-18	86
545	Structural biology and drug discovery. 2006 , 12, 2087-97	99
544	Molecular descriptors and methods for ligand based virtual high throughput screening in drug discovery. 2006 , 12, 2099-110	45
543	Scoring functions for protein-ligand docking. 2006 , 7, 407-20	168
542	Receptor Targets in Drug Discovery. 2006 ,	
541	High throughput in-silico screening of large ligand databases for rational drug design. 2006 , 179-189	
540	Computational identification of inhibitors of protein-protein interactions. 2007 , 7, 63-82	77
539	In silico three-dimensional pharmacophores for aiding the discovery of the Pfmrk (Plasmodium cyclin-dependent protein kinases) specific inhibitors for the therapeutic treatment of malaria. 2007 , 2, 1115-27	1
538	Pharmacophore modeling in drug discovery and development: an overview. 2007 , 3, 187-97	93
537	From drug target to leads--sketching a physicochemical pathway for lead molecule design in silico. 2007 , 13, 3454-70	52
536	Targeting Amoebiasis: Status and Developments. 2007 , 3, 121-133	23
535	Computer-Aided Drug Design: Integration of Structure-Based and Ligand-Based Approaches in Drug Design. 2007 , 3, 133-148	29
534	Lead Identification by Virtual Screening. 651-704	2
533	Properties Guiding Drug- and Lead-Likeness. 2007 , 439-461	6
532	How Computational Chemistry Became Important in the Pharmaceutical Industry. 2007 , 401-451	7
531	Compound Selection Using Measures of Similarity and Dissimilarity. 2007 , 167-192	4

530	Chemoinformatics Theory. 2007 , 1-49	
529	Molecular properties investigation of a substituted aromatic mannich base: dynamic and static models. 2007 , 47, 818-31	7
528	MolDiA: a novel molecular diversity analysis tool. 1. Principles and architecture. 2007 , 47, 2197-207	2
527	A database of historically-observed chemical replacements. 2007 , 47, 1294-302	46
526	An Introduction To Chemoinformatics. 2007 ,	191
525	Computational Tools for Regulatory Needs. 751-775	8
524	. 2007 ,	6
523	. 2007 ,	1
522	Promiscuous Ligands. 2007 , 737-752	1
521	. 2007 ,	19
520	Focused Library Design Based on Hit and Target Structures: Method and Application in Drug Discovery. 108-124	
519	WinDock: structure-based drug discovery on Windows-based PCs. 2007 , 28, 2347-51	9
518	ANN-QSAR model for selection of anticancer leads from structurally heterogeneous series of compounds. 2007 , 42, 580-5	49
517	The consequences of scoring docked ligand conformations using free energy correlations. 2007 , 42, 921-33	52
516	Structure-based discovery of new small molecule inhibitors of low molecular weight protein tyrosine phosphatase. 2007 , 42, 1102-8	25
515	Accuracy of binding mode prediction with a cascadic stochastic tunneling method. 2007 , 68, 195-204	13
514	Receptor-specific scoring functions derived from quantum chemical models improve affinity estimates for in-silico drug discovery. 2008 , 70, 1264-73	33
513	Scoring functions and enrichment: a case study on Hsp90. 2007 , 8, 27	9

512	Surflex-Dock 2.1: robust performance from ligand energetic modeling, ring flexibility, and knowledge-based search. 2007 , 21, 281-306	454
511	Virtual screening applications: a study of ligand-based methods and different structure representations in four different scenarios. 2007 , 21, 617-40	29
510	The challenges of developing novel antiparasitic drugs. 2007 , 7, 245-50	26
509	The concept of template-based de novo design from drug-derived molecular fragments and its application to TAR RNA. 2008 , 22, 59-68	17
508	Bond-based linear indices in QSAR: computational discovery of novel anti-trichomonal compounds. 2008 , 22, 523-40	24
507	SHEF: a vHTS geometrical filter using coefficients of spherical harmonic molecular surfaces. 2008 , 14, 393-401	16
506	FURSMASA: a new approach to rapid scoring functions that uses a MD-averaged potential energy grid and a solvent-accessible surface area term with parameters GA fit to experimental data. 2008 , 71, 1519-38	6
505	Virtual screening against Mycobacterium tuberculosis dihydrofolate reductase: suggested workflow for compound prioritization using structure interaction fingerprints. 2008 , 27, 476-88	15
504	Activity of a hydroxybibenzyl bryophyte constituent against Leishmania spp. and Trypanosoma cruzi: in silico, in vitro and in vivo activity studies. 2008 , 43, 1797-807	56
503	Atom-based non-stochastic and stochastic bilinear indices: Application to QSPR/QSAR studies of organic compounds. 2008 , 464, 107-112	20
502	Chemical Descriptors Library (CDL): a generic, open source software library for chemical informatics. 2008 , 48, 1931-42	18
501	Scaffold diversity of natural products: inspiration for combinatorial library design. 2008 , 25, 892-904	178
500	LigEvolutioner, a new strategy for modification and optimization of lead compounds in receptor/ligand complexes. 2008 , 72, 525-32	1
499	Future Perspectives. 359-390	
498	Desirability-based methods of multiobjective optimization and ranking for global QSAR studies. Filtering safe and potent drug candidates from combinatorial libraries. 2008 , 10, 897-913	40
497	Bioactivity and structure of biophenols as mediators of chronic diseases. 2008 , 48, 929-66	25
496	What has virtual screening ever done for drug discovery?. 2008 , 3, 841-51	107
495	Hit Generation. 2008 , 218-279	1

494	MM-GB/SA rescoring of docking poses in structure-based lead optimization. 2008 , 48, 958-70	163
493	Ligand discovery on massively parallel systems. 2008 , 52, 57-67	7
492	Services Oriented Architecture for Managing Workflows of Avian Flu Grid. 2008 ,	11
491	Identification of hits and lead structure candidates with limited resources by adaptive optimization. 2008 , 48, 1473-91	19
490	Systems biology of cyanobacterial secondary metabolite production and its role in drug discovery. 2008 , 3, 903-29	39
489	Virtual screening using PLS discriminant analysis and ROC curve approach: an application study on PDE4 inhibitors. 2008 , 48, 1686-92	39
488	Virtual Screening: A Fast Tool for Drug Design. 2008 , 76, 333-360	45
487	Building a chemical space based on fragment descriptors. 2008 , 11, 661-8	13
486	Molecular recognition and binding free energy calculations in drug development. 2008 , 9, 87-95	13
485	. 2009 ,	236
484	A small-molecule dengue virus entry inhibitor. 2009 , 53, 1823-31	164
483	[Chemoinformatics and virtual screening of molecules for therapeutic use]. 2009 , 25, 871-7	1
482	Scaffold-hopping potential of fragment-based de novo design: the chances and limits of variation. 2009 , 12, 383-96	22
481	Virtual materials design using databases of calculated materials properties. 2009 , 2, 015006	11
480	Drug Discovery. 2009 , 475-560	5
479	Docking, virtual high throughput screening and in silico fragment-based drug design. 2009 , 13, 238-48	103
478	Design of a grid service-based platform for in silico protein-ligand screenings. 2009 , 93, 73-82	8
477	Perspectives. 315-320	1

476	Q-Dock(LHM): Low-resolution refinement for ligand comparative modeling. 2010 , 31, 1093-105	20
475	Similarity methods in chemoinformatics. 2009 , 43, 1-117	51
474	An improved scoring function for suboptimal polar ligand complexes. 2009 , 23, 143-52	3
473	Combinatorial library-based design with Basis Products. 2009 , 23, 725-36	12
472	Comparative virtual screening and novelty detection for NMDA-GlycineB antagonists. 2009 , 23, 869-81	22
471	Emergent strategies for inverse molecular design. 2009 , 52, 1769-1776	9
470	Discovery of Novel Trichomonacids Using LDA-Driven QSAR Models and Bond-Based Bilinear Indices as Molecular Descriptors. 2009 , 28, 9-26	13
469	Pharmacophore-based virtual screening versus docking-based virtual screening: a benchmark comparison against eight targets. 2009 , 30, 1694-708	68
468	The influences of the structure and activity of biologically active compounds on the assessment of inventive step. 2009 , 31, 226-234	3
467	Synthesis and in vitro antitumor activities of novel 4-anilinoquinazoline derivatives. 2009 , 44, 3046-55	98
466	Hydrogen bonding, electrostatic potential, and molecular design. 2009 , 49, 1234-44	118
465	The design of polyvalent scaffolds for targeted delivery. 2009 , 61, 931-9	42
464	Elucidating molecular overlays from pairwise alignments using a genetic algorithm. 2009 , 49, 1847-55	10
463	Searching Fragment Spaces with feature trees. 2009 , 49, 270-9	67
462	Evaluating docking methods for prediction of binding affinities of small molecules to the G protein betagamma subunits. 2009 , 49, 437-43	11
461	Overview of high-throughput screening. 2009 , Chapter 9, Unit 9.4	33
460	Searching New Antiparasitics in Virtual Space. 323-338	1
459	Mining statistically significant molecular substructures for efficient molecular classification. 2009 , 49, 2537-50	16

458	Design, selection, and characterization of thioflavin-based intercalation compounds with metal chelating properties for application in Alzheimer's disease. 2009 , 131, 1436-51	179
457	Bibliography. 2009 , 1-241	1
456	Comparative assessment of scoring functions on a diverse test set. 2009 , 49, 1079-93	373
455	How computational methods try to disclose the estrogen receptor secrecy--modeling the flexibility. 2009 , 16, 2987-3027	14
454	Fragment descriptors in structure-property modeling and virtual screening. 2011 , 672, 213-43	6
453	Large-scale systematic analysis of 2D fingerprint methods and parameters to improve virtual screening enrichments. 2010 , 50, 771-84	227
452	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
451	A knowledge-guided strategy for improving the accuracy of scoring functions in binding affinity prediction. 2010 , 11, 193	16
450	Bioactive conformational generation of small molecules: a comparative analysis between force-field and multiple empirical criteria based methods. 2010 , 11, 545	20
449	Discovery of veterinary antiparasitic agents in the 21st century: a view from industry. 2010 , 40, 1177-81	44
448	In Silico Screening. 2010 , 73-103	
447	ChemInform Abstract: Virtual Screening An Overview. 2010 , 29, no-no	
446	Exhaustive Structure Generation for Inverse-QSPR/QSAR. 2010 , 29, 111-25	36
445	Analysis and comparison of 2D fingerprints: insights into database screening performance using eight fingerprint methods. 2010 , 29, 157-70	275
444	Computational approaches for protein function prediction: a combined strategy from multiple sequence alignment to molecular docking-based virtual screening. 2010 , 1804, 1695-712	68
443	Comparison of structure-based and threading-based approaches to protein functional annotation. 2010 , 78, 118-34	26
442	GPCR 3D modeling. 248-256	
441	Virtual Screening as a Technique for PPAR Modulator Discovery. 2010 , 2010, 861238	23

440	A Comprehensive Task Management system for large-scale Virtual Screening applications. 2010,	
439	A scalable reference-point based algorithm to efficiently search large chemical databases. 2010,	
438	Virtual Screening. 2010, 1-46	1
437	Pharmacophore based drug design approach as a practical process in drug discovery. 2010, 6, 37-49	52
436	Contributions of computational chemistry and biophysical techniques to fragment-based drug discovery. 2010, 17, 1769-94	36
435	Identification of bioactive natural products by pharmacophore-based virtual screening. 2010, 16, 1666-81	49
434	QM/MM approaches in medicinal chemistry research. 2010, 10, 46-54	75
433	Quantitative structure-reactivity modeling of copper-catalyzed atom transfer radical polymerization. 2010, 1, 922	15
432	GAPE: an improved genetic algorithm for pharmacophore elucidation. 2010, 50, 2001-18	16
431	Structural basis for computational screening of non-steroidal androgen receptor ligands. 2010, 5, 5-20	2
430	A Data Management System for Pre-docking in Large-Scale Virtual Screening. 2010,	1
429	StructRank: a new approach for ligand-based virtual screening. 2011, 51, 83-92	26
428	Front Matter. 2011, I-XXX	
427	Ligand-Based Virtual Screening. 2011, 61-85	15
426	Pharmacophore Models for Virtual Screening. 2011, 115-152	5
425	Applied Virtual Screening: Strategies, Recommendations, and Caveats. 2011, 291-318	10
424	Implementing relevance feedback in ligand-based virtual screening using Bayesian inference network. 2011, 16, 1081-8	15
423	Drug Design and Discovery. 2011,	7

422	Chemoinformatics and library design. 2011 , 685, 27-52	8
421	Chemogenomics and Chemical Genetics. 2011 ,	4
420	Chemoinformatics and Computational Chemical Biology. 2011 ,	6
419	Rational methods for the selection of diverse screening compounds. 2011 , 6, 208-17	80
418	Docking methods for structure-based library design. 2011 , 685, 155-74	10
417	. 2011 ,	26
416	Protein Modeling. 2011 ,	
415	Virtual screening strategies in drug design [methods and applications]. 2011 , 3, 249-264	27
414	The design and application of target-focused compound libraries. 2011 , 14, 521-31	82
413	Targeting Catechol-O-Methyl Transferase (COMT) Inhibitors for Schizophrenia:An Approach to Target Validation and Rational Drug Design. 2011 , 8, 246-252	1
412	Integration of virtual and high throughput screening in lead discovery settings. 2011 , 14, 889-97	24
411	Modern Methods & Web Resources in Drug Design & Discovery. 2011 , 8, 469-490	9
410	Simplified receptor based pharmacophore approach to retrieve potent PTP-LAR inhibitors using apoenzyme. 2011 , 7, 159-72	4
409	Computational Approaches for the Discovery of Natural Lead Structures. 2011 , 97-132	
408	Structure tuning of pyrazolopyrrole derivatives as ERK inhibitors utilizing dual tools; 3D-QSAR and side-chain hopping. 2011 , 21, 4900-4	8
407	On various metrics used for validation of predictive QSAR models with applications in virtual screening and focused library design. 2011 , 14, 450-74	159
406	Potential of Complementary and Alternative Medicine in Preventive Management of Novel H1N1 Flu (Swine Flu) Pandemic: Thwarting Potential Disasters in the Bud. 2011 , 2011, 586506	42
405	Chemoinformatics: a history. 2011 , 1, 46-56	37

404	Understanding drug-likeness. 2011 , 1, 760-781	99
403	Drug-drug relationship based on target information: application to drug target identification. 2011 , 5 Suppl 2, S12	5
402	The discovery of potential acetylcholinesterase inhibitors: a combination of pharmacophore modeling, virtual screening, and molecular docking studies. 2011 , 18, 8	92
401	Discrimination of approved drugs from experimental drugs by learning methods. 2011 , 12, 157	2
400	Estimating binding affinities by docking/scoring methods using variable protonation states. 2011 , 79, 304-14	39
399	SwissParam: a fast force field generation tool for small organic molecules. 2011 , 32, 2359-68	1025
398	Discovery of novel SERCA inhibitors by virtual screening of a large compound library. 2011 , 46, 1512-23	14
397	Molecular docking: a powerful approach for structure-based drug discovery. 2011 , 7, 146-57	1083
396	Drug Repositioning on the Cloud. 2011 ,	
395	Recent trends and observations in the design of high-quality screening collections. 2011 , 3, 751-66	47
394	Identification and characterization of novel small-molecule inhibitors against hepatitis delta virus replication by using docking strategies. 2011 , 11, 803-9	6
393	G-quadruplex binding ligands: from naturally occurring to rationally designed molecules. 2012 , 18, 1948-72	79
392	MM-GB/SA rescoring of docking poses. 2012 , 819, 255-68	9
391	Allostery. 2012 ,	4
390	Compound collection preparation for virtual screening. 2012 , 910, 125-43	5
389	Pharmacophore modeling, virtual screening and docking studies to identify novel HNMT inhibitors. 2012 , 43, 493-503	10
388	Structural Bioinformatics and Molecular Dynamics Simulations Studies of Cathepsins as a Potential Target for Drug Discovery. 2012 , 11, 63-74	
387	Structures and biological activity of cinnamoyl derivatives of coumarins and dehydroacetic acid and their boron difluoride complexes. 2012 , 61, 78-90	3

386	High throughput virtual screening with data level parallelism in multi-core processors. 2012,	
385	Virtual drug screen schema based on multiview similarity integration and ranking aggregation. 2012, 52, 834-43	14
384	Going further than Lipinski's rule in drug design. 2012, 7, 99-107	91
383	Drug-likeness analysis of traditional Chinese medicines: prediction of drug-likeness using machine learning approaches. 2012, 9, 2875-86	88
382	Fingerprint design and engineering strategies: rationalizing and improving similarity search performance. 2012, 4, 1945-59	14
381	Virtual compound screening in drug discovery. 2012, 4, 593-602	39
380	Computational Drug Discovery and Design. 2012,	19
379	Ligand and Structure-Based Pharmacophore Modeling for the Discovery of Potential Human HNMT Inhibitors. 2012, 9, 17-29	2
378	Ligand-based virtual screening using Bayesian inference network and reweighted fragments. 2012, 2012, 410914	14
377	Identifying multiple-target ligands via computational chemogenomics approaches. 2012, 12, 1363-75	6
376	Established and emerging trends in computational drug discovery in the structural genomics era. 2012, 19, 29-41	54
375	Generation of receptor structural ensembles for virtual screening using binding site shape analysis and clustering. 2012, 80, 182-93	62
374	Identification of novel, less toxic PTP-LAR inhibitors using in silico strategies: pharmacophore modeling, SADMET-based virtual screening and docking. 2012, 18, 187-201	7
373	An in silico virtual screening study for the design of norovirus inhibitors: fragment-based molecular docking and binding free energy calculations. 2013, 378, 133-8	5
372	Identification of potential bivalent inhibitors from natural compounds for acetylcholinesterase through in silico screening using multiple pharmacophores. 2013, 40, 72-9	7
371	Computational methods for drug design and discovery: focus on China. 2013, 34, 549-59	52
370	Protein Docking Problem as Combinatorial Optimization Using Beta-Complex. 2013, 2685-2740	0
369	Development and evaluation of an integrated virtual screening strategy by combining molecular docking and pharmacophore searching based on multiple protein structures. 2013, 53, 2743-56	53

368	Machine learning based search space optimisation for drug discovery. 2013 ,	5
367	Optimization of molecular docking scores with support vector rank regression. 2013 , 81, 1386-98	11
366	Advanced Technologies for Managing Insect Pests. 2013 ,	1
365	Fragment-Based Design of Focused Compound Libraries. 2013 , 349-371	2
364	Hit and Lead Identification from Fragments. 2013 , 143-200	1
363	Coping with Combinatorial Space in Molecular Design. 2013 , 325-347	3
362	Multiobjective De Novo Design of Synthetically Accessible Compounds. 2013 , 267-285	5
361	Estimation of the size of drug-like chemical space based on GDB-17 data. 2013 , 27, 675-9	184
360	An integrated virtual screening approach for VEGFR-2 inhibitors. 2013 , 53, 3163-77	38
359	Discovery of novel chemoeffectors and rational design of Escherichia coli chemoreceptor specificity. 2013 , 110, 16814-9	34
358	Virtual screening of electron acceptor materials for organic photovoltaic applications. 2013 , 15, 105029	20
357	FPGA-Based Virtual Screening Acceleration of Rigid-Molecule Docking. 2013 , 15, 64-72	
356	Models for the prediction of PPARs agonistic activity of indanylacetic acids. 2013 , 22, 3213-3228	3
355	New molecular scaffolds for the design of Alzheimer's acetylcholinesterase inhibitors identified using ligand- and receptor-based virtual screening. 2013 , 22, 2328-2345	28
354	Recent advances in proteasome inhibitor discovery. 2013 , 8, 537-68	10
353	Advanced Technologies for Managing Insect Pests: An Overview. 2013 , 1-11	1
352	Very large virtual compound spaces: construction, storage and utility in drug discovery. 2013 , 10, e387-94	12
351	Virtual Screening Methods. 2013 , 483-505	

350	Discovery of benzamide analogs as negative allosteric modulators of human neuronal nicotinic receptors: pharmacophore modeling and structure-activity relationship studies. 2013 , 21, 4730-43	6
349	Discovery of Rho-kinase inhibitors by docking-based virtual screening. 2013 , 9, 1511-21	46
348	Bioturbo similarity searching: combining chemical and biological similarity to discover structurally diverse bioactive molecules. 2013 , 53, 692-703	43
347	Automated molecule editing in molecular design. 2013 , 27, 655-64	9
346	Advanced Screening to Identify Novel Pesticides. 2013 , 135-163	2
345	Research on Calculation of Molecular Connectivity Index. 2013 , 303-306, 2671-2674	1
344	Exploration of virtual candidates for human HMG-CoA reductase inhibitors using pharmacophore modeling and molecular dynamics simulations. 2013 , 8, e83496	12
343	A Review of Computational Tools for Designing Drugs Used by General Practitioners. 2014 , 02,	
342	Composing compound libraries for hit discovery--rationality-driven preselection or random choice by structural diversity?. 2014 , 6, 2057-72	14
341	Challenges in Designing Therapeutic Agents for Treating Alzheimer's Disease-from Serendipity to Rationality. 2014 , 40-141	7
340	eMatchSite: sequence order-independent structure alignments of ligand binding pockets in protein models. 2014 , 10, e1003829	23
339	Structural Genomics and Drug Discovery. 2014 ,	3
338	Structure modeling and hybrid virtual screening study of Alzheimer's associated protease kallikrein 8 for the identification of novel inhibitors. 2014 , 23, 3516-3527	3
337	ZINClick: a database of 16 million novel, patentable, and readily synthesizable 1,4-disubstituted triazoles. 2014 , 54, 396-406	17
336	Lead Discovery and Lead Modification. 2014 , 19-122	5
335	Pharmacophore modeling technique applied for the discovery of proteasome inhibitors. 2014 , 9, 931-43	5
334	Potent angiotensin-converting enzyme inhibitory tripeptides identified by a computer-based approach. 2014 , 53, 206-211	6
333	Discovery of novel inhibitors targeting the macrophage migration inhibitory factor via structure-based virtual screening and bioassays. 2014 , 57, 3737-45	61

332	A computational approach to enzyme design: predicting α -aminotransferase catalytic activity using docking and MM-GBSA scoring. 2014 , 54, 2334-46	62
331	Computer based screening for novel inhibitors against <i>Vibrio cholerae</i> using NCI diversity set-II: an alternative approach by targeting transcriptional activator ToxT. 2014 , 6, 108-17	6
330	Assessing an ensemble docking-based virtual screening strategy for kinase targets by considering protein flexibility. 2014 , 54, 2664-79	79
329	Condorcet and borda count fusion method for ligand-based virtual screening. 2014 , 6, 19	13
328	Molpher: a software framework for systematic chemical space exploration. 2014 , 6, 7	24
327	P1 and P1' para-fluoro phenyl groups show enhanced binding and favorable predicted pharmacological properties: structure-based virtual screening of extended lopinavir analogs against multi-drug resistant HIV-1 protease. 2014 , 47, 18-24	3
326	Computer-aided screening of solvents for optimal reaction rates. 2014 , 115, 167-176	8
325	Traditional Chinese herbs as chemical resource library for drug discovery of anti-infective and anti-inflammatory. 2014 , 155, 589-98	20
324	Ring-System-Based Exhaustive Structure Generation for Inverse-QSPR/QSAR. 2014 , 33, 764-78	20
323	. 2015 ,	2
322	- Implicit Solvation Methods in the Study of Ligand-Protein Interactions. 2015 , 266-291	
321	Discovery of Novel ROCK1 Inhibitors via Integrated Virtual Screening Strategy and Bioassays. 2015 , 5, 16749	25
320	A Quantum-Based Similarity Method in Virtual Screening. 2015 , 20, 18107-27	16
319	. 2015 ,	2
318	The application of in silico drug-likeness predictions in pharmaceutical research. 2015 , 86, 2-10	190
317	Molecular dynamics simulations and statistical coupling analysis of GPIIb/IIIa in <i>L. major</i> : functional co-evolution and conservedness reveals potential drug-target sites. 2015 , 11, 958-68	4
316	When drug discovery meets web search: Learning to Rank for ligand-based virtual screening. 2015 , 7, 5	20
315	Structural diversity and potency range distribution of scaffolds from compounds active against current pharmaceutical targets. 2015 , 7, 111-22	3

314	Virtual Screening and Biological Validation of Novel Influenza Virus PA Endonuclease Inhibitors. 2015 , 6, 866-71	25
313	LiSiCA: A Software for Ligand-Based Virtual Screening and Its Application for the Discovery of Butyrylcholinesterase Inhibitors. 2015 , 55, 1521-8	46
312	Multistage virtual screening and identification of novel HIV-1 protease inhibitors by integrating SVM, shape, pharmacophore and docking methods. 2015 , 101, 409-18	20
311	Fragment virtual screening based on Bayesian categorization for discovering novel VEGFR-2 scaffolds. 2015 , 19, 895-913	13
310	A Novel Scoring Based Distributed Protein Docking Application to Improve Enrichment. 2015 , 12, 1464-9	9
309	Drug Discovery and Development. 2015 , 1-34	8
308	Predicting Adsorption Affinities of Small Molecules on Carbon Nanotubes Using Molecular Dynamics Simulation. 2015 , 9, 11761-74	63
307	Network and systems biology: essential steps in virtualising drug discovery and development. 2015 , 15, 33-40	15
306	Structure-Activity Relationships and Anti-inflammatory Activities of N-Carbamothioylformamide Analogues as MIF Tautomerase Inhibitors. 2015 , 55, 1994-2004	5
305	Virtual screening strategies: recent advances in the identification and design of anti-cancer agents. 2015 , 71, 64-70	33
304	Structure based virtual screening to discover putative drug candidates: necessary considerations and successful case studies. 2015 , 71, 135-45	40
303	Protein structure prediction provides comparable performance to crystallographic structures in docking-based virtual screening. 2015 , 71, 77-84	22
302	Molecular Modeling of Proteins. 2015 ,	6
301	Hierarchical virtual screening approaches in small molecule drug discovery. 2015 , 71, 26-37	90
300	In-silico analysis of riboswitch of <i>Nocardia farcinica</i> for design of its inhibitors and pharmacophores. 2016 , 9, 261	2
299	In Silico Prediction of Cytochrome P450-Drug Interaction: QSARs for CYP3A4 and CYP2C9. 2016 , 17,	38
298	Adapting Document Similarity Measures for Ligand-Based Virtual Screening. 2016 , 21, 476	11
297	Structure-Based Virtual Screening for Dopamine D2 Receptor Ligands as Potential Antipsychotics. 2016 , 11, 718-29	33

296	Rational Hit Generation. 2016 , 159-182	
295	SM-TF: A structural database of small molecule-transcription factor complexes. 2016 , 37, 1559-64	2
294	A pose prediction approach based on ligand 3D shape similarity. 2016 , 30, 457-69	13
293	Constructing and Validating High-Performance MIEC-SVM Models in Virtual Screening for Kinases: A Better Way for Actives Discovery. 2016 , 6, 24817	47
292	Repositioning organohalogen drugs: a case study for identification of potent B-Raf V600E inhibitors via docking and bioassay. 2016 , 6, 31074	20
291	Counting on natural products for drug design. 2016 , 8, 531-41	592
290	Improved pose and affinity predictions using different protocols tailored on the basis of data availability. 2016 , 30, 817-828	3
289	PL-PatchSurfer2: Improved Local Surface Matching-Based Virtual Screening Method That Is Tolerant to Target and Ligand Structure Variation. 2016 , 56, 1676-91	17
288	Prospective evaluation of shape similarity based pose prediction method in D3R Grand Challenge 2015. 2016 , 30, 685-693	10
287	Software and Web Resources for Computer-Aided Molecular Modeling and Drug Discovery. 2016 , 33-99	3
286	[Ring-system-based Chemical Structure Enumeration for de Novo Design]. 2016 , 136, 101-6	1
285	Modeling, molecular docking, probing catalytic binding mode of acetyl-CoA malate synthase G in 16M. 2016 , 8, 192-199	8
284	In search of novel ligands using a structure-based approach: a case study on the adenosine A receptor. 2016 , 30, 863-874	13
283	FSees: Customized Enumeration of Chemical Subspaces with Limited Main Memory Consumption. 2016 , 56, 1641-53	6
282	Norovirus drug candidates that inhibit viral capsid attachment to human histo-blood group antigens. 2016 , 133, 14-22	10
281	Fragment-Based Discovery of 5-Arylisatin-Based Inhibitors of Matrix Metalloproteinases 2 and 13. 2016 , 11, 1892-8	9
280	Boosting Docking-Based Virtual Screening with Deep Learning. 2016 , 56, 2495-2506	175
279	Data Mining in Drug Discovery and Design. 2016 , 181-193	2

278	Modelling the cytotoxic activity of pyrazolo-triazole hybrids using descriptors calculated from the open source tool PaDEL-descriptor Beer review under responsibility of Taibah University. View all notes. 2016 , 10, 896-905	14
277	Combining bioinformatics, chemoinformatics and experimental approaches to design chemical probes: Applications in the field of blood coagulation. 2016 , 74, 253-66	1
276	Investigation on the isoform selectivity of novel kinesin-like protein 1 (KIF11) inhibitor using chemical feature based pharmacophore, molecular docking, and quantum mechanical studies. 2016 , 61, 47-61	6
275	A multilayer screening approach toward the discovery of novel Pf-DHFR inhibitors. 2016 , 62, 36-46	1
274	Identification of small molecules acting against H1N1 influenza A virus. 2016 , 488, 249-58	4
273	An overview of molecular fingerprint similarity search in virtual screening. 2016 , 11, 137-48	99
272	Application of Shape Similarity in Pose Selection and Virtual Screening in CSARdock2014 Exercise. 2016 , 56, 965-73	22
271	An in silico approach towards the identification of novel inhibitors of the TLR-4 signaling pathway. 2016 , 34, 1345-62	2
270	Identification of the Beer Component Hordenine as Food-Derived Dopamine D2 Receptor Agonist by Virtual Screening a 3D Compound Database. 2017 , 7, 44201	20
269	Discovery of Novel and Selective Adenosine A Receptor Antagonists for Treating Parkinson's Disease through Comparative Structure-Based Virtual Screening. 2017 , 57, 1474-1487	35
268	Dry selection and wet evaluation for the rational discovery of new anthelmintics. 2017 , 115, 2300-2313	1
267	Surface area, volume and shape descriptors as a novel tool for polymer lead design and discovery. 2017 , 102, 188-195	6
266	Prediction of new chromene-based inhibitors of tubulin using structure-based virtual screening and molecular dynamics simulation methods. 2017 , 71, 89-97	9
265	Cheminformatics Approaches in Modern Drug Discovery. 2017 , 135-148	3
264	Addressing the Metabolic Stability of Antituberculars through Machine Learning. 2017 , 8, 1099-1104	11
263	Anti-QS/Anti-Biofilm Agents in Controlling Bacterial Disease: An in silico Approach. 2017 , 497-511	
262	In Silico Development of Quorum-Sensing Inhibitors. 2017 , 38, 728-734	5
261	Drug Design: Principles and Applications. 2017 ,	3

260	Shallow Representation Learning via Kernel PCA Improves QSAR Modelability. 2017 , 57, 1859-1867	10
259	Discovery of small molecules binding to the normal conformation of prion by combining virtual screening and multiple biological activity evaluation methods. 2017 , 31, 1053-1062	4
258	Protein-Ligand Blind Docking Using QuickVina-W With Inter-Process Spatio-Temporal Integration. 2017 , 7, 15451	68
257	Anti-HIV-1 Activity Prediction of Novel Gp41 Inhibitors Using Structure-Based Virtual Screening and Molecular Dynamics Simulation. 2017 , 36, 1600060	14
256	Docking into Mycobacterium tuberculosis Thioredoxin Reductase Protein Yields Pyrazolone Lead Molecules for Methicillin-Resistant Staphylococcus aureus. 2017 , 6,	7
255	Research on abnormal data processing and constructing network based on network pharmacology. 2017 ,	
254	Enhance the performance of current scoring functions with the aid of 3D protein-ligand interaction fingerprints. 2017 , 18, 343	11
253	Computational Drug Design and Molecular Dynamic Studies-A Review. 2017 , 06,	5
252	Structural Chemogenomics Databases to Navigate Protein-Ligand Interaction Space. 2017 , 444-471	1
251	Virtual Screening of potential inhibitors from Herbs for the treatment of Breast Cancer. 2017 , 10, 62	1
250	DOCKING ANTIOXIDANT ACTIVITY ON HYDROXY (DIPHENYL) ACETICACID AND ITS DERIVATIVES. 2017 , 10, 263	4
249	Drug Discovery: An Overview. 2018 , 165-194	2
248	Virtual Ligand Screening Using PL-PatchSurfer2, a Molecular Surface-Based Protein-Ligand Docking Method. 2018 , 1762, 105-121	4
247	Computer-Aided Drug Design: An Overview. 2018 , 1762, 1-19	15
246	Predicting Binding Affinity Based on Docking Measures for Spinocerebellar Ataxia: A Study. 2018 , 33-43	
245	FilTer BaSe: A web accessible chemical database for small compound libraries. 2018 , 80, 95-103	6
244	Design, Synthesis, and Preliminary Biological Evaluation of GlcNAc-6P Analogues for the Modulation of Phosphoacetylglucosamine Mutase 1 (AGM1/PGM3). 2018 , 2018, 1946-1952	3
243	Identification of dual kinase inhibitors of CK2 and GSK3 β combined qualitative and quantitative pharmacophore modeling approach. 2018 , 36, 177-194	8

242	Virtual Screening in the Search of New and Potent Anti-Alzheimer Agents. 2018 , 107-137	5
241	Identification of potential isoform-selective histone deacetylase inhibitors for cancer therapy: a combined approach of structure-based virtual screening, ADMET prediction and molecular dynamics simulation assay. 2018 , 36, 3231-3245	20
240	Methods for Virtual Screening of GPCR Targets: Approaches and Challenges. 2018 , 1705, 233-264	2
239	Performance of multiple docking and refinement methods in the pose prediction D3R prospective Grand Challenge 2016. 2018 , 32, 113-127	5
238	The Development of Pharmacophore Modeling: Generation and Recent Applications in Drug Discovery. 2018 , 24, 3424-3439	19
237	Bacteriostatic and Bactericidal Mechanism of Novel Compound Isolated from Ethyl Acetate Stem Bark Extract of <i>Spondias mombin</i> Using Biomarker Repressor LexA gene on <i>Escherichia coli</i> and <i>Bacillus subtilis</i> . 2018 , 09,	1
236	Pranlukast; An Alternative Potential Leptin Stimulator: Structure-Based Virtual Screening Study. 2018 , 04,	
235	Comparative Study Of Complex Network Community Structure Algorithms In network Pharmacology Analysis. 2018 , 232, 01021	
234	Screening Library Design. 2018 , 610, 73-96	2
233	Risk Management in Early Discovery Medicinal Chemistry. 2018 , 610, 1-25	1
232	Fly ash supported NiO as an efficient catalyst for the synthesis of xanthene and its molecular docking study against plasmodium glutathione reductase. 2018 , 44, 7459-7478	4
231	Design, synthesis and molecular modeling of new 4-phenylcoumarin derivatives as tubulin polymerization inhibitors targeting MCF-7 breast cancer cells. 2018 , 26, 3474-3490	22
230	Discovery of potent and novel smoothed antagonists via structure-based virtual screening and biological assays. 2018 , 155, 34-48	18
229	QSAR Modeling of ToxCast Assays Relevant to the Molecular Initiating Events of AOPs Leading to Hepatic Steatosis. 2018 , 58, 1501-1517	38
228	Computational Toxicology Methods in Chemical Library Design and High-Throughput Screening Hit Validation. 2018 , 1800, 275-285	7
227	Transfer and Multi-task Learning in QSAR Modeling: Advances and Challenges. <i>Frontiers in Pharmacology</i> , 2018 , 9, 74	5.6 41
226	Identification of new promising Plasmodium falciparum superoxide dismutase allosteric inhibitors through hierarchical pharmacophore-based virtual screening and molecular dynamics. 2018 , 24, 220	7
225	Docking techniques in pharmacology: How much promising?. 2018 , 76, 210-217	63

224	Investigating the Behavior of Published PAINS Alerts Using a Pharmaceutical Company Data Set. 2018 , 9, 792-796	17
223	In silico design of novel proton-pump inhibitors with reduced adverse effects. 2019 , 13, 277-284	1
222	Small Molecule Drug Design. 2019 , 741-760	6
221	Efficient multi-objective molecular optimization in a continuous latent space. 2019 , 10, 8016-8024	63
220	Development of Predictive Models for Identifying Potential S100A9 Inhibitors Based on Machine Learning Methods. 2019 , 7, 779	8
219	SAnDReS: A Computational Tool for Docking. 2019 , 2053, 51-65	6
218	Docking with AutoDock4. 2019 , 2053, 125-148	20
217	Discovery of novel natural compound inhibitors targeting estrogen receptor β by an integrated virtual screening strategy. 2019 , 25, 278	6
216	Docking Screens for Drug Discovery. 2019 ,	2
215	New Trends in Virtual Screening. 2019 , 59, 3603-3604	6
214	Deep Reinforcement Learning for Multiparameter Optimization in Drug Design. 2019 , 59, 3166-3176	55
213	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
212	Identification of Novel Allosteric Modulators of Metabotropic Glutamate Receptor Subtype 5 Acting at Site Distinct from 2-Methyl-6-(phenylethynyl)-pyridine Binding. 2019 , 10, 3427-3436	3
211	Rescoring Virtual Screening Results with the MM-PBSA Methods: Beware of Internal Dielectric Constants. 2019 , 59, 2714-2728	9
210	Insights into an alternative benzofuran binding mode and novel scaffolds of polyketide synthase 13 inhibitors. 2019 , 25, 130	4
209	Computational advances in combating colloidal aggregation in drug discovery. 2019 , 11, 402-418	35
208	Autonomous Molecular Design: Then and Now. 2019 , 11, 24825-24836	48
207	Structural optimization on a virtual screening hit of smoothed receptor. 2019 , 172, 1-15	5

206	Applications of Ensemble Docking in Potential Inhibitor Screening for Mycobacterium tuberculosis Isocitrate Lyase Using a Local Plant Database. 2019 , 59, 2487-2495	9
205	Bioinformatics and Drug Discovery. 2019 ,	1
204	How to Prepare a Compound Collection Prior to Virtual Screening. 2019 , 1939, 119-138	2
203	Inhibition of Oncogenic Kinases: An In Vitro Validated Computational Approach Identified Potential Multi-Target Anticancer Compounds. 2019 , 9,	20
202	Bromodomains: Promising Targets for Drug Discovery. 2019 , 347-381	1
201	A primer on natural product-based virtual screening. 2019 , 4,	4
200	De Novo Molecular Design by Combining Deep Autoencoder Recurrent Neural Networks with Generative Topographic Mapping. 2019 , 59, 1182-1196	56
199	Efficient molecular encoders for virtual screening. 2019 , 32-33, 19-27	
198	. 2019 ,	1
197	An Overview, Advantages and Therapeutic Potential of Nonpeptide Positive Allosteric Modulators of Glucagon-Like Peptide-1 Receptor. 2019 , 14, 514-521	8
196	Structural bioinformatics-based identification of putative plant based lead compounds for Alzheimer Disease Therapy. 2019 , 78, 359-366	8
195	Structure-Based Drug Design with a Special Emphasis on Herbal Extracts. 2019 , 271-305	
194	In silico identification of inhibitors targeting N-Terminal domain of human Replication Protein A. 2019 , 86, 149-159	4
193	Converging a Knowledge-Based Scoring Function: DrugScore. 2019 , 59, 509-521	28
192	Application of portfolio optimization to drug discovery. 2019 , 475, 29-43	7
191	Dynamic structure based pharmacophore modeling of the Acetylcholinesterase reveals several potential inhibitors. 2019 , 37, 1800-1812	26
190	The Symbiotic Relationship Between Drug Discovery and Organic Chemistry. 2020 , 26, 1196-1237	60
189	Computational basis for the design of PLK-2 inhibitors. 2020 , 31, 275-292	1

188	Bidirectional Molecule Generation with Recurrent Neural Networks. 2020 , 60, 1175-1183	39
187	Latest trends in structure based drug design with protein targets. 2020 , 121, 1-23	1
186	Ligand-based pharmacophore filtering, atom based 3D-QSAR, virtual screening and ADME studies for the discovery of potential ck2 inhibitors. 2020 , 1205, 127670	5
185	Virtual screening identification and chemical optimization of substituted 2-arylbenzimidazoles as new non-zinc-binding MMP-2 inhibitors. 2020 , 28, 115257	2
184	Inhibition of Zea mays coniferyl aldehyde dehydrogenase by daidzin: A potential approach for the investigation of lignocellulose recalcitrance. 2020 , 90, 131-138	9
183	Pharmacophore-driven identification of N-methyl-D-receptor antagonists as potent neuroprotective agents validated using studies. 2020 , 5, bpa013	2
182	Machine Learning Platform to Discover Novel Growth Inhibitors of Neisseria gonorrhoeae. 2020 , 37, 141	4
181	Guidelines for Recurrent Neural Network Transfer Learning-Based Molecular Generation of Focused Libraries. 2020 , 60, 5699-5713	17
180	Flexi-pharma: a molecule-ranking strategy for virtual screening using pharmacophores from ligand-free conformational ensembles. 2020 , 34, 1063-1077	7
179	Structure-Activity relationship of Quercetin and its Tumor Necrosis Factor Alpha inhibition activity by computational and machine learning methods. <i>Materials Today: Proceedings</i> , 2020 , 1.4	2
178	Fast Rescoring Protocols to Improve the Performance of Structure-Based Virtual Screening Performed on Protein-Protein Interfaces. 2020 , 60, 3910-3934	6
177	Cheminformatics in Natural Product-based Drug Discovery. 2020 , 39, e2000171	33
176	Surveying FDA-approved drugs as new potential inhibitors of N-cadherin protein: a virtual screening approach. 2020 , 31, 2355-2369	1
175	In silico discovery and biological validation of ligands of FAD synthase, a promising new antimicrobial target. 2020 , 16, e1007898	8
174	Ensemble Docking Coupled to Linear Interaction Energy Calculations for Identification of Coronavirus Main Protease (3CL) Non-Covalent Small-Molecule Inhibitors. 2020 , 25,	20
173	Druggability and drug-likeness concepts in drug design: are biomodelling and predictive tools having their say?. 2020 , 26, 120	18
172	In silico development of quorum sensing inhibitors. 2020 , 329-357	
171	Rigorous Free Energy Simulations in Virtual Screening. 2020 , 60, 4153-4169	54

170	Virtual screening of small-molecule libraries. 2020 , 103-125	1
169	The power of deep learning to ligand-based novel drug discovery. 2020 , 15, 755-764	24
168	10. A primer on natural product-based virtual screening. 2020 , 251-290	
167	Discovery of novel and potent P2YR antagonists structure-based virtual screening for the treatment of acute gouty arthritis. 2020 , 23, 133-142	7
166	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
165	Development of Natural Compound Molecular Fingerprint (NC-MFP) with the Dictionary of Natural Products (DNP) for natural product-based drug development. 2020 , 12, 6	18
164	Hops compounds modulatory effects and 6-prenylnaringenin dual mode of action on GABA receptors. 2020 , 873, 172962	5
163	Pharmacophore modeling and virtual screening for the discovery of biologically active natural products. 2020 , 64, 321-364	1
162	Developing an effective polarizable bond method for small molecules with application to optimized molecular docking.. 2020 , 10, 15530-15540	7
161	Targeting phosphatidylinositol 3-kinase gamma (PI3K) γ Discovery and development of its selective inhibitors. 2021 , 41, 1599-1621	6
160	Accelerating the identification of subtype selective inhibitors via Three-Dimensional Biologically Relevant Spectrum (BRS-3D): The monoamine oxidase subtypes as a case study. 2021 , 106, 104503	
159	Scopy: an integrated negative design python library for desirable HTS/VS database design. 2021 , 22,	6
158	BACE1 and cholinesterase inhibitory activities of compounds from and : an in silico study. 2021 , 9, 14	3
157	Molecular docking and dynamics simulations of novel drug targets. 2021 , 79-131	0
156	Evaluation of certain medicinal plants compounds as new potential inhibitors of novel corona virus (COVID-19) using molecular docking analysis. 2021 , 9, 10	12
155	Chem-bioinformatic approach for drug discovery. 2021 , 207-243	0
154	PySmash: Python package and individual executable program for representative substructure generation and application. 2021 , 22,	0
153	Discovery of novel selective PI3K α inhibitors through combining machine learning-based virtual screening with multiple protein structures and bio-evaluation.. 2022 , 36, 1-13	3

152	Deep Learning in Virtual Screening: Recent Applications and Developments. 2021 , 22,		22
151	Identification of Potential Binders of Universal Stress Protein (Rv1636) Through an Approach and Insights Into Compound Selection for Experimental Validation. 2021 , 8, 599221		1
150	Investigation of New Inhibitors of UDP-N-Acetylglucosamine Enolpyruvyl Transferase (MurA) by Virtual Screening with Antibacterial Assessment. 2021 , 17, 214-224		1
149	QSAR analysis of 3-pyrimidin-4-yl-oxazolidin-2-one derivatives isocitrate dehydrogenase inhibitors using Topomer CoMFA and HQSAR methods. 2021 , 1		0
148	Prioritisation of Compounds for 3CL Inhibitor Development on SARS-CoV-2 Variants. 2021 , 26,		11
147	Ubiquitination Regulators Discovered by Virtual Screening for the Treatment of Cancer. 2021 , 9, 665646		3
146	Applications of artificial intelligence to drug design and discovery in the big data era: a comprehensive review. 2021 , 25, 1643-1664		4
145	Structure-based virtual screening for novel potential selective inhibitors of class IIa histone deacetylases for cancer treatment. 2021 , 92, 107491		1
144	Growing Preferences towards Analog-based Drug Discovery. 2021 , 22, 1030-1045		1
143	Overview of Viral Pneumonia Associated With Influenza Virus, Respiratory Syncytial Virus, and Coronavirus, and Therapeutics Based on Natural Products of Medicinal Plants. <i>Frontiers in Pharmacology</i> , 2021 , 12, 630834	5.6	2
142	Comprehensive virtual screening of 4.8k flavonoids reveals novel insights into allosteric inhibition of SARS-CoV-2 M. 2021 , 11, 15452		11
141	Genetic Algorithms Applied to Thermodynamic Rational Design of Mimetic Antibodies Based on the GB1 Domain of Streptococcal Protein G: An Atomistic Simulation Study. 2021 , 125, 7985-7996		
140	Discovery of novel MIF inhibitors that attenuate microglial inflammatory activation by structures-based virtual screening and in vitro bioassays. 2021 ,		1
139	GenUI: interactive and extensible open source software platform for de novo molecular generation and cheminformatics. 2021 , 13, 73		1
138	Targeting of Telomeric Repeat-Containing RNA G-Quadruplexes: From Screening to Biophysical and Biological Characterization of a New Hit Compound. 2021 , 22,		1
137	High-Throughput Screening and Molecular Dynamics Simulation of Natural Product-like Compounds against Alzheimer's Disease through Multitarget Approach. 2021 , 14,		11
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 discovery and development: An overview of modern methods and principles. 2021 , 1-41		

134	Molecular docking analysis: Basic technique to predict drug-receptor interactions. 2021 , 131-155	3
133	Advanced approaches and in silico tools of chemoinformatics in drug designing. 2021 , 173-206	1
132	Identification of novel potential cyclooxygenase-2 inhibitors using ligand- and structure-based virtual screening approaches. 2021 , 1-23	3
131	Recent Trends in Quantitative Structure-Activity Relationships. 2003 , 49-76	22
130	Virtual Screening. 2003 , 243-279	3
129	Docking and Scoring Functions/Virtual Screening. 2003 , 281-331	11
128	Receptor Targets in Drug Discovery and Development. 2003 , 319-355	2
127	Design and Diversity Analysis of Compound Libraries for Lead Discovery. 1999 , 409-439	4
126	Chemoinformatics and the Quest for Leads in Drug Discovery. 1508-1531	4
125	Predicting binding modes, binding affinities and hot spots for protein-ligand complexes using a knowledge-based scoring function. 2000 , 115-144	1
124	Increasing Diversity in In-silico Screening with Target Flexibility. 2005 , 186-197	9
123	Molecular docking to flexible targets. 2015 , 1215, 445-69	15
122	Virtual screening for lead discovery. 2011 , 716, 1-22	19
121	Using active site mapping and receptor-based pharmacophore tools: prelude to docking and de novo/fragment-based ligand design. 2011 , 716, 39-54	6
120	Computational approaches towards the quantification of molecular diversity and design of compound libraries. 2003 , 125-56	1
119	High Throughput in-silico Screening against Flexible Protein Receptors. 2004 , 465-472	6
118	Application of Evolutionary Algorithms to Combinatorial Library Design. 2003 , 1-30	2
117	The Applications of Artificial Neural Networks in the Identification of Quantitative Structure-Activity Relationships for Chemotherapeutic Drug Carcinogenicity. 2010 , 137-146	2

116	Challenges for Computer Simulations in Drug Design. 2010 , 431-463	2
115	Repurposing drugs for treatment of SARS-CoV-2 infection: computational design insights into mechanisms of action. 2020 , 1-15	8
114	Docking and Scoring. 2003 ,	1
113	SWEETLEAD: an in silico database of approved drugs, regulated chemicals, and herbal isolates for computer-aided drug discovery. 2013 , 8, e79568	63
112	The In Silico Drug Discovery Toolbox: Applications in Lead Discovery and Optimization. 2019 , 26, 3838-3873	17
111	Design, Synthesis and Biological Evaluation of Spiro Cyclohexane-1,2- Quinazoline Derivatives as Potent Dipeptidyl Peptidase IV Inhibitors. 2019 , 19, 250-269	4
110	The Research of New Inhibitors of Bacterial Methionine Aminopeptidase by Structure Based Virtual Screening Approach of ZINC DATABASE and In Vitro Validation. 2020 , 16, 389-401	2
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	Improved Deep Learning Based Method for Molecular Similarity Searching Using Stack of Deep Belief Networks. 2020 , 26,	10
107	Computational Approaches for the Discovery of Novel Hepatitis C Virus NS3/4A and NS5B Inhibitors. 2017 , 482-518	1
106	Protein-Ligand Docking Methodologies and Its Application in Drug Discovery. 2017 , 891-914	1
105	Virtual Screening and Its Applications in Drug Discovery Process. 2019 , 101-126	0
104	Virtual Screening Methods Based on Bayesian Statistics. 2011 , 190-211	1
103	Identification and Characterization of Novel Small-Molecule Inhibitors against Hepatitis Delta Virus Replication by Using Docking Strategies. 2011 , 11, 803-809	7
102	Ligand- and Structure-Based Virtual Screening in Drug Discovery. 2021 , 281-339	0
101	Bioinformatics as a Tool in Drug Designing. 2021 , 1-24	
100	Potential Novel Thioether-Amide or Guanidine-Linker Class of SARS-CoV-2 Virus RNA-Dependent RNA Polymerase Inhibitors Identified by High-Throughput Virtual Screening Coupled to Free-Energy Calculations. 2021 , 22,	3
99	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. 2021 , 61, 5256-5268	

- 98 Strategies for Molecular Design Beyond the Millennium. **2000**, 3-23
- 97 ELECTRONIC SCREENING: LEAD FINDING FROM DATABASE MINING. **2003**, 131-145
- 96 The impact of combinatorial chemistry on drug discovery. **2003**, 201-20 1
- 95 High-Throughput Screening for Lead Discovery. **2003**, 37-69 2
- 94 Physicochemical concepts in drug design. **2003**, 243-57 0
- 93 Practical database screening with docking tools. **2003**, 127-51 1
- 92 Combinatorial Library Design, Molecular Similarity, and Diversity Applications. **2003**, 187-242 3
- 91 Structure-based design of combinatorial libraries. **2003**, 203-21
- 90 Computational Aspects of Library Design and Combinatorial Chemistry. **2003**,
- 89 The Grid 2 - Pages 675-721. **2004**, 675-721
- 88 Molecular Similarity Methods and QSAR Models As Tools for Virtual Screening. 1
- 87 High-Throughput Flow Cytometry. 1
- 86 In Silico Drug Design Using a Computational Intelligence Technique. 237-256
- 85 Virtual screening by molecular docking. **2011**, 213-224
- 84 QM Scoring Function and its Application to TOP1 Inhibitors. **2011**, 32, 1127-1128
- 83 In silico-screening approaches for lead generation: identification of novel allosteric modulators of human-erythrocyte pyruvate kinase. **2012**, 796, 351-67
- 82 Application of Docking Methods: An Effective In Silico Tool for Drug Design. **2013**, 6, 100-103 3
- 81 CRITICAL ASSESSMENT OF VIRTUAL SCREENING FOR HIT IDENTIFICATION. 113-130

- 80 Combinatorial Chemistry Library Design. 40-63
- 79 Ligand screening using enzymatic assays. **2014**, 1140, 291-304
- 78 Computational Approaches for the Discovery of Novel Hepatitis C Virus NS3/4A and NS5B Inhibitors. **2015**, 318-353
- 77 Iran Virtual Screening (IranVScreen): An Integrated Virtual Screening Interface. **2015**, 3, 1
- 76 Protein-Ligand Docking Methodologies and Its Application in Drug Discovery. **2016**, 196-219
- 75 Accelerating Group Fusion for Ligand-Based Virtual Screening on Multi-core and Many-core Platforms.
- 74 Practical Aspects of Building, Validation and Application of 3D-Pharmacophore Models. **2016**, 159-181
- 73 Cancer and Biotechnology: A Matchup that Should Never Slowdown. **2017**, 73-97 2
- 72 Pharmacophore-driven Identification of N-Methyl-D-Receptor Antagonists as Potent Neuroprotective Agents Validated Using In-Vivo Studies.
- 71 A Novel analog approach for fast evaluation of affinity between ligand and receptor in scaled up molecular models.
- 70 Methods to Improve Ranking Chemical Structures in Ligand-Based Virtual Screening. **2020**, 259-269
- 69 Features Reweighting and Selection in ligand-based Virtual Screening for Molecular Similarity Searching Based on Deep Belief Networks. **2020**, 12, 2050009 1
- 68 Computaci3n heterog3nea de alta performance: aplicaci3n en el dise3o racional de f3rmacos. **2020**,
- 67 Discovery and computational studies of 2-phenyl-benzoxazole acetamide derivatives as promising P2YR antagonists with anti-gout potential. **2022**, 227, 113933 0
- 66 Virtual Screening of Anticancer Drugs Using Deep Learning. **2020**, 1293-1298 0
- 65 Mol2Image: Improved Conditional Flow Models for Molecule to Image Synthesis. **2021**, 4
- 64 In silicodiscovery and biological validation of ligands of FAD synthase, a promising new antimicrobial target.
- 63 Cosolvent and Dynamic Effects in Binding Pocket Search by Docking Simulations. **2021**, 61, 5508-5523 0

62	Subset-Selection Methods For Chemical Databases. 2002 , 115-140	1
61	A recursive algorithm for efficient combinatorial library docking. 2000 , 63-81	
60	Modifications of the scoring function in FlexX for virtual screening applications. 2000 , 83-98	
59	Discovery of novel TrkA allosteric inhibitors: Structure-based virtual screening, biological evaluation and preliminary SAR studies. 2021 , 228, 114022	1
58	Computational Docking Technique for Drug Discovery: A Review. 2021 , 5558-5562	
57	A unified drug-target interaction prediction framework based on knowledge graph and recommendation system. 2021 , 12, 6775	11
56	New biologically dynamic hybrid pharmacophore triazinoindole-based-thiadiazole as potent β -glucosidase inhibitors: In vitro and in silico study.. 2021 ,	1
55	Similarity-Based Virtual Screen Using Enhanced Siamese Deep Learning Methods.. 2022 , 7, 4769-4786	0
54	TEXT MINING OF THE PEOPLE'S PHARMACY RADIO SHOW TRANSCRIPTS CAN IDENTIFY NOVEL DRUG REPURPOSING HYPOTHESES.	
53	Quantum of selectivity testing: detection of isomers and close homologs using an AZO based e-nose without a prior training.	2
52	Nuisance small molecules under a machine-learning lens.	0
51	Discovery of Small-Molecule Inhibitors of the PD-1/PD-L1 Axis That Promote PD-L1 Internalization and Degradation.. 2022 ,	5
50	Personalized Liver Cancer Risk Prediction Using Big Data Analytics Techniques with Image Processing Segmentation.. 2022 , 2022, 8154523	0
49	Redox active or thiol reactive? Optimization of rapid screens to identify less evident nuisance compounds.. <i>Drug Discovery Today</i> , 2022 ,	8.8 2
48	Design, synthesis, docking studies and antibiotic evaluation (in vitro) of some novel (E)-4-(3-(diphenylamino)phenyl)-1-(4-methoxyphenyl)-2-methylbut-3-en-1-one and their analogues. 2022 , 46,	0
47	On the Value of Using 3D Shape and Electrostatic Similarities in Deep Generative Methods.. 2022 ,	0
46	Application of deep metric learning to molecular graph similarity.. 2022 , 14, 11	0
45	Understanding the I/O Impact on the Performance of High-Throughput Molecular Docking. 2021 ,	0

44	Repurposing of Drugs for SARS-CoV-2 Using Inverse Docking Fingerprints.. 2021 , 9, 757826		4
43	Accelerating Molecular Dynamics Enrichments of High-Affinity Ligands for Proteins. 2021 ,		
42	Data_Sheet_1.ZIP. 2019 ,		
41	Table_1.docx. 2019 ,		
40	Machine Learning and Its Applications for Protozoal Pathogens and Protozoal Infectious Diseases.. 2022 , 12, 882995		1
39	Artificial intelligence in virtual screening: Models versus experiments. <i>Drug Discovery Today</i> , 2022 ,	8.8	4
38	Comparative Analyses of Medicinal Chemistry and Cheminformatics Filters with Accessible Implementation in Konstanz Information Miner (KNIME). 2022 , 23, 5727		1
37	Quantum Molecular Unfolding.		1
36	Insights into the Pharmacological Effects of Flavonoids: The Systematic Review of Computer Modeling. 2022 , 23, 6023		2
35	Deep Learning Based-Virtual Screening Using 2D Pharmacophore Fingerprint in Drug Discovery. <i>Neural Processing Letters</i> ,	2.4	
34	Finding a novel electrolyte solution of lithium-ion batteries using an autonomous search system based on ensemble optimization. <i>Journal of Power Sources</i> , 2022 , 541, 231698	8.9	0
33	Review on molecular docking analysis of herbal compounds and their activity against SARS and JEV using In-silico and In vitro approaches. <i>IP International Journal of Medical Microbiology and Tropical Diseases</i> , 2022 , 8, 103-114	0.2	
32	Fundamental considerations in drug design. 2022 , 17-55		0
31	Molecular docking and antibacterial activity of some natural products against cariogenic <i>Staphylococcus aureus</i> . <i>Materials Today: Proceedings</i> , 2022 ,	1.4	1
30	Multi-Objective Drug Design Based on Graph-Fragment Molecular Representation and Deep Evolutionary Learning. <i>Frontiers in Pharmacology</i> , 13,	5.6	0
29	Concepts and applications of chemical fingerprint for hit and lead screening. 2022 , 27, 103356		1
28	General Strategies for Rational Design and Discovery of Multitarget Drugs. 2022 , 677-736		0
27	Library Synthesis: Building Block Selection, Handling, and Tracking. 2022 , 1-11		0

- 26 Experimental, insilico, DFT studies of novel compound 2-{2-[(3,4-dimethoxyphenyl)methylidene]hydrazinecarbonothioyl}-N-methyl-N-phenylhydrazine-1-carbothioamide. **2022**, 4, 100534 ○
- 25 FNN Based-Virtual Screening Using 2D Pharmacophore Fingerprint for Activity Prediction in Drug Discovery. ○
- 24 Machine Learning and Computational Chemistry for the Endocannabinoid System. **2023**, 477-493 ○
- 23 Predicting FDA approvability of small-molecule drugs. ○
- 22 Screening of potential antiplasmodial agents targeting cysteine protease-Falcipain 2: a computational pipeline. 1-44 ○
- 21 Fragment-Sized Thiazoles in Fragment-Based Drug Discovery Campaigns: Friend or Foe?. ○
- 20 Electrochemoinformatics as an Emerging Scientific Field for Designing Materials and Electrochemical Energy Storage and Conversion Devices: An Application in Battery Science and Technology. 2202380 ○
- 19 Structure-based virtual screening to identify potential lipase inhibitors to reduce lipid storage in Wolman disorder. **2022**, ○
- 18 QSAR study, molecular docking and molecular dynamic simulation of Aurora kinase inhibitors derived from imidazo[4,5-b]pyridine derivatives. ○
- 17 A Hybrid Docking and Machine Learning Approach to Enhance the Performance of Virtual Screening Carried out on Protein-Protein Interfaces. **2022**, 23, 14364 ○
- 16 Protein-protein interfaces in molecular glue-induced ternary complexes: classification, characterization, and prediction. ○
- 15 Integration of fingerprint-based similarity searching and kernel-based partial least squares analysis to predict inhibitory activity against CSK, HER2, JAK1, JAK2, and JAK3. ○
- 14 Informatics and databases for phytochemical drug discovery. **2023**, 89-124 ○
- 13 Drug Repurposing: Scopes in Herbal/Natural Products-based Drug Discovery and Role of in silico Techniques. ○
- 12 Trends in modern drug discovery and development: A glance in the present millennium. **2023**, 27-38 ○
- 11 Screening and Analysis for Inhibitors of SHMT2 Enzyme Protein. ○
- 10 A Cloud-based Distributed Computing Approach for Extracting Molecular Descriptors. **2022**, ○
- 9 Machine Learning Scoring Functions for Drug Discovery from Experimental and Computer-Generated Protein-ligand Structures: Towards Per-Target Scoring Functions. **2023**, 28, 1661 ○

- 8 Virtual screening. **2023**, 223-236 ○
- 7 Microbe or cell line quality improvement. **2023**, 101-120 ○
- 6 The Impact of Supervised Learning Methods in Ultralarge High-Throughput Docking. ○
- 5 Molecular Filters in Medicinal Chemistry. **2023**, 3, 501-511 ○
- 4 Multitargeted Virtual Screening and Molecular Simulation of Natural Product-like Compounds against GSK3 β /NMDA-Receptor, and BACE-1 for the Management of Alzheimer's Disease. **2023**, 16, 622 ○
- 3 Discovery of Selective P2Y6R Antagonists with High Affinity and In Vivo Efficacy for Inflammatory Disease Therapy. ○
- 2 Principles of computational drug designing and drug repurposing: An algorithmic approach. **2023**, 129-146 ○
- 1 Uni-Dock: GPU-Accelerated Docking Enables Ultralarge Virtual Screening. ○