Development and validation of a genetic algorithm for flexible docking

DOI: 10.1006/jmbi.1996.0897
Journal of Molecular Biology, 1997, 267, 727-48.

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2296 .

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2285 Structure-based analysis of the ultraspiracle protein and docking studies of putative ligands. **2002**, 2, 25 10

2284	IsoStar: a library of information about nonbonded interactions. **1997**, 11, 525-37	233
2283	CASP2 molecular docking predictions with the LIGIN software. **1997**, 29, 210-214	15
2282	Recent advances in structure-based ligand design using molecular dynamics and Monte Carlo methods. **1998**, 15, 368-70	6
2281	RigFit: a new approach to superimposing ligand molecules. **1998**, 12, 491-502	30
2280	Chemical Similarity Searching. **1998**, 38, 983-996	1298
2279	Development of filter functions for protein-ligand docking. **1998**, 16, 121-32	63
2278	Virtual screening□n overview. **1998**, 3, 160-178	769
2277	Assessing search strategies for flexible docking. **1998**, 19, 1623-1631	102
2276	Flexible docking allowing induced fit in proteins: Insights from an open to closed conformational isomers. **1998**, 32, 159-174	96
2275	Screening a peptidyl database for potential ligands to proteins with side-chain flexibility. **1998**, 33, 74-87	90
2274	Predicting structural effects in HIV-1 protease mutant complexes with flexible ligand docking and protein side-chain optimization. **1998**, 33, 295-310	56
2273	Flexible docking using tabu search and an empirical estimate of binding affinity. **1998**, 33, 367-382	277
2272	A hierarchical method for generating low-energy conformers of a protein-ligand complex. **1998**, 33, 475-95	23
2271	GENFOLD: a genetic algorithm for folding protein structures using NMR restraints. **1998**, 7, 491-9	20
2270	Flexible ligand docking using conformational ensembles. **1998**, 7, 938-50	217
2269	The Development, Status and Scientific Impact of Crystallographic Databases. **1998**, 54, 758-771	30
2268	Directional preferences of intermolecular contacts to hydrophobic groups. **1998**, 54, 1183-93	6
2267	Fully automated and rapid flexible docking of inhibitors covalently bound to serine proteases. **1998**, 449-461	26

2266	Low-resolution structures of proteins in solution retrieved from X-ray scattering with a genetic algorithm. **1998**, 74, 2760-75	259
2265	FLEXS: a method for fast flexible ligand superposition. **1998**, 41, 4502-20	226
2264	A method for biomolecular structural recognition and docking allowing conformational flexibility. **1998**, 5, 631-54	47
2263	Reaching the global minimum in docking simulations: a Monte Carlo energy minimization approach using Bezier splines. **1998**, 95, 8011-5	69
2262	A survey of recent work on evolutionary approaches to the protein folding problem.	4
2261	Docking of hydrophobic ligands with interaction-based matching algorithms. **1999**, 15, 243-50	81
2260	Exploring the conformational diversity of loops on conserved frameworks. **1999**, 12, 1075-86	11
2259	"RKKH" peptides from the snake venom metalloproteinase of Bothrops jararaca bind near the metal ion-dependent adhesion site of the human integrin alpha(2) I-domain. **1999**, 274, 31493-505	30
2258	Evolutionary Algorithms in Computer-Aided Molecular Design: A Review of Current Applications and a Look to the Future. **1999**, 255-270	6
2257	4-hydroxy-5,6-dihydro-2H-pyran-2-ones.3. Bicyclic and hetero-aromatic ring systems as 3-position scaffolds to bind to S1' and S2' of the HIV-1 protease enzyme. **1999**, 9, 2019-24	10
2256	On the evolution of ligands: did peptides functionally precede metals and small organic molecules?. **1999**, 55, 513-8	7
2255	MCDOCK: a Monte Carlo simulation approach to the molecular docking problem. **1999**, 13, 435-51	117
2254	Comparison of two implementations of the incremental construction algorithm in flexible docking of thrombin inhibitors. **1999**, 13, 167-83	25
2253	The sensitivity of the results of molecular docking to induced fit effects: application to thrombin, thermolysin and neuraminidase. **1999**, 13, 547-62	136
2252	Computational Approaches to Drug Design. **1999**, 25, 347-371	28
2251	Rational screenning in combinatorial peptide libraries of protein functional loop. **1999**, 44, 2150-2154	
2250	Homology modeling and ab initio calculations identify a basis for ligand selectivity for the PPAR□ nuclear hormone receptor. **1999**, 73, 97-111	5
2249	BLEEP□otential of mean force describing protein□gand interactions: I. Generating potential. **1999**, 20, 1165-1176	179

2248	BLEEP potential of mean force describing protein ligand interactions: II. Calculation of binding energies and comparison with experimental data. **1999**, 20, 1177-1185	100
2247	Three variations of genetic algorithm for searching biomolecular conformation space: Comparison of GAP 1.0, 2.0, and 3.0. **1999**, 20, 1329-1342	19
2246	Low-mode conformational search elucidated: Application to C39H80 and flexible docking of 9-deazaguanine inhibitors into PNP. **1999**, 20, 1671-1684	140
2245	A critical evaluation of several global optimization algorithms for the purpose of molecular docking. **1999**, 20, 1740-1751	36
2244	The particle concept: placing discrete water molecules during protein-ligand docking predictions. **1999**, 34, 17-28	176
2243	Ranking ligand binding affinities with avidin: a molecular dynamics-based interaction energy study. **1999**, 34, 69-81	78
2242	Flexible ligand docking: A multistep strategy approach. **1999**, 36, 1-19	119
2241	Exhaustive docking of molecular fragments with electrostatic solvation. **1999**, 37, 88-105	148
2240	Evaluation of the FLEXX incremental construction algorithm for protein-ligand docking. **1999**, 37, 228-41	677
2239	Efficacy and selectivity in flexible database docking. **1999**, 37, 334-45	40
2238	Towards understanding the mechanisms of molecular recognition by computer simulations of ligand-protein interactions. **1999**, 12, 371-89	32
2237	Die Bedeutung der Balance von Wasserstoffbrückenbindungen und hydrophoben Wechselwirkungen im Wirkstoff-Rezeptor-Komplex. **1999**, 111, 778-792	25
2236	Hydrogen Bonding, Hydrophobic Interactions, and Failure of the Rigid Receptor Hypothesis. **1999**, 38, 736-749	257
2235	Reduced Dimensionality in Ligand Protein Structure Prediction: Covalent Inhibitors of Serine Proteases and Design of Site-Directed Combinatorial Libraries. **1999**, 292-311	56
2234	Two-stage method for protein-ligand docking. **1999**, 42, 4422-33	81
2233	Evaluation of PMF scoring in docking weak ligands to the FK506 binding protein. **1999**, 42, 2498-503	124
2232	Consensus scoring: A method for obtaining improved hit rates from docking databases of three-dimensional structures into proteins. **1999**, 42, 5100-9	612
2231	A general and fast scoring function for protein-ligand interactions: a simplified potential approach. **1999**, 42, 791-804	935

2230	The role of waters in docking strategies with incremental flexibility for carbohydrate derivatives: heat-labile enterotoxin, a multivalent test case. **1999**, 42, 1778-88		65
2229	SuperStar: a knowledge-based approach for identifying interaction sites in proteins. *Journal of Molecular Biology*, **1999**, 289, 1093-108	6.5	187
2228	Memetic Algorithms: A Contemporary Introduction. 1-15		2
2227	New 1,4-dihydropyridine derivatives with C4 heterocyclic substituents. **2000**, 215, 122-126		2
2226	Similarity-driven flexible ligand docking. **2000**, 40, 623-36		74
2225	DARWIN: A program for docking flexible molecules. **2000**, 41, 173-191		110
2224	Structure-based library design: molecular modelling merges with combinatorial chemistry. **2000**, 4, 283-6		62
2223	A method for including protein flexibility in protein-ligand docking: improving tools for database mining and virtual screening. **2000**, 18, 247-57, 302-4		63
2222	Morphological similarity: a 3D molecular similarity method correlated with protein-ligand recognition. **2000**, 14, 199-213		93
2221	Evaluation of docking/scoring approaches: a comparative study based on MMP3 inhibitors. **2000**, 14, 435-48		50
2220	Deciphering common failures in molecular docking of ligand-protein complexes. **2000**, 14, 731-51		168
2219	Computer based screening of compound databases: 1. Preselection of benzamidine-based thrombin inhibitors. **2000**, 14, 411-25		13
2218	Multiple molecular superpositioning as an effective tool for virtual database screening. **2000**, 20, 43-62		5
2217	Modifications of the scoring function in FlexX for virtual screening applications. **2000**, 20, 83-98		27
2216	A knowledge-based scoring function for protein-ligand interactions: Probing the reference state. **2000**, 20, 99-114		105
2215	Virtual screening with solvation and ligand-induced complementarity. **2000**, 20, 171-190		120
2214	Predicting binding modes, binding affinities and 'hot spots' for protein-ligand complexes using a knowledge-based scoring function. **2000**, 20, 115-144		86
2213	Hydrophobicity maps and docking of molecular fragments with solvation. **2000**, 20, 145-169		7

2212	Similarity versus docking in 3D virtual screening. **2000**, 20, 191-207		23
2211	New Techniques and Future Directions. **2000**, 241-264		1
2210	. **2000**,		32
2209	. **2000**,		70
2208	Protein Structure Prediction. **2000**,		6
2207	The steroid 17alpha-acetoxy-6-dimethylaminomethyl-21-fluoro-3-ethoxy-pregna-3, 5-dien-20-one (SC17599) is a selective mu-opioid agonist: implications for the mu-opioid pharmacophore. **2000**, 58, 669-76		5
2206	De novo design of peptides targeted to the EF hands of calmodulin. **2000**, 275, 2676-85		48
2205	Knowledge-based scoring function to predict protein-ligand interactions. *Journal of Molecular Biology*, **2000**, 295, 337-56	6.5	871
2204	Automated docking of ligands to antibodies: methods and applications. **2000**, 20, 280-91		60
2203	Protein-based virtual screening of chemical databases. 1. Evaluation of different docking/scoring combinations. **2000**, 43, 4759-67		648
2202	New approach to molecular docking and its application to virtual screening of chemical databases. **2000**, 40, 254-62		71
2201	Structure-Based Library Design. **2000**, 229-264		7
2200	Understanding Receptor-Ligand Interactions as a Prerequisite for Virtual Screening. **2000**, 207-227		5
2199	Protein-Ligand Docking. **2000**, 31-48		16
2198	Efficient Sampling of Ligand Orientations and Conformations in Free Energy Calculations Using the Dynamics Method. **2000**, 104, 6903-6910		37
2197	Application of a Molecular Dynamics Simulation Method with a Generalized Effective Potential to the Flexible Molecular Docking Problems. **2000**, 104, 354-359		57
2196	Novel treatment of conformational flexibility using interval analysis. **2000**, 40, 339-46		5
2195	Mutations in Plasmodium falciparum cytochrome b that are associated with atovaquone resistance are located at a putative drug-binding site. **2000**, 44, 2100-8		285

2194	Geometrical docking algorithms. A practical approach. **2000**, 143, 377-97		4
2193	Ligand-protein database: linking protein-ligand complex structures to binding data. **2001**, 44, 3592-8		114
2192	How does consensus scoring work for virtual library screening? An idealized computer experiment. **2001**, 41, 1422-6		236
2191	A new concept for multidimensional selection of ligand conformations (MultiSelect) and multidimensional scoring (MultiScore) of protein-ligand binding affinities. **2001**, 44, 2333-43		102
2190	Improved scoring of ligand-protein interactions using OWFEG free energy grids. **2001**, 44, 502-11		88
2189	Protein□ligand Docking in Drug Design. **2001**, 315-360		5
2188	Analysis of selective regions in the active sites of human cytochromes P450, 2C8, 2C9, 2C18, and 2C19 homology models using GRID/CPCA. **2001**, 44, 4072-81		79
2187	SuperStar: improved knowledge-based interaction fields for protein binding sites. *Journal of Molecular Biology*, **2001**, 307, 841-59	6.5	96
2186	FlexE: efficient molecular docking considering protein structure variations. *Journal of Molecular Biology*, **2001**, 308, 377-95	6.5	408
2185	SuperStar: comparison of CSD and PDB-based interaction fields as a basis for the prediction of protein-ligand interactions. *Journal of Molecular Biology*, **2001**, 312, 275-87	6.5	34
2184	Binding mode prediction for a flexible ligand in a flexible pocket using multi-conformation simulated annealing pseudo crystallographic refinement. *Journal of Molecular Biology*, **2001**, 314, 607-17	6.5	31
2183	Hydrophobicity and functionality maps of farnesyltransferase. **2001**, 19, 307-17, 380-7		3
2182	Evaluation of docking functions for protein-ligand docking. **2001**, 44, 3768-85		70
2181	Total synthesis and biological evaluation of the nakijiquinones. **2001**, 123, 11586-93		105
2180	Molecular docking: a problem with thousands of degrees of freedom.		11
2179	Isothermal titration calorimetry in drug discovery. **2001**, 38, 309-76		88
2178	. **2001**,		3
2177	Protein□ligand Interactions: Energetic Contributions and Shape Complementarity. **2001**,		3

2176	Engineering the active site of ascorbate peroxidase. **2001**, 268, 78-85	22
2175	Customized versus universal scoring functions: application to class I MHC-peptide binding free energy predictions. **2001**, 11, 675-9	42
2174	Design, synthesis and stability of N-acyloxymethyl- and N-aminocarbonyloxymethyl-2-azetidinones as human leukocyte elastase inhibitors. **2001**, 11, 1065-8	50
2173	Can an optimization/scoring procedure in ligand-protein docking be employed to probe drug-resistant mutations in proteins?. **2001**, 19, 560-70	19
2172	Prediction of potential toxicity and side effect protein targets of a small molecule by a ligand-protein inverse docking approach. **2001**, 20, 199-218	118
2171	Protein docking using a genetic algorithm. **2001**, 44, 44-56	82
2170	High throughput docking for library design and library prioritization. **2001**, 43, 113-24	231
2169	Ligand-protein inverse docking and its potential use in the computer search of protein targets of a small molecule. **2001**, 43, 217-26	297
2168	Evaluation of a knowledge-based potential of mean force for scoring docked protein□gand complexes. **2001**, 22, 673-688	19
2167	Automatic parameterization of force field by systematic search and genetic algorithms. **2001**, 22, 1219-1228	112
2166	EUDOC: a computer program for identification of drug interaction sites in macromolecules and drug leads from chemical databases. **2001**, 22, 1750-1771	95
2165	Massive docking of flexible ligands using environmental niches in parallelized genetic algorithms. **2001**, 22, 1971-1982	19
2164	A comparative docking study and the design of potentially selective MMP inhibitors. **2001**, 15, 873-81	26
2163	DOCK 4.0: search strategies for automated molecular docking of flexible molecule databases. **2001**, 15, 411-28	866
2162	Protein ligand docking based on empirical method for binding affinity estimation. **2001**, 15, 429-46	24
2161	Ligand-receptor docking with the Mining Minima optimizer. **2001**, 15, 157-71	48
2160	NMR-restrained docking of a peptidic inhibitor to the N-terminal domain of the phosphoenolpyruvate:sugar phosphotransferase enzyme I. **2001**, 15, 103-15	7
2159	Molecular docking of □cyclodextrin inclusion complexes by genetic algorithm and empirical binding free energy function. **2001**, 342, 387-396	12

2158	High-throughput structural proteomics using x-rays. **2001**, 19, 67-71	280
2157	High-throughput structural proteomics using x-rays. **2001**, 19, S67-71	26
2156	Neural networks and genetic algorithms in drug design. **2001**, 6, 102-108	55
2155	The broader applications of neural and genetic modelling methods. **2001**, 6, 1198-1199	7
2154	Computational Chemistry in Lead Identification, Library Design and Lead Optimisation. **2001**, 26, 33-49	
2153	Monte Carlo simulations of HIV-1 protease binding dynamics and thermodynamics with ensembles of protein conformations: Incorporating protein flexibility in deciphering mechanisms of molecular recognition. **2001**, 289-340	2
2152	Molecular Modeling: Protein Modeling. 315-341	
2151	Insights from a three-dimensional model into ligand binding to constitutive active receptor. **2002**, 30, 951-6	31
2150	Molecular docking and dynamics simulations in the ligand binding domain of steroid hormone receptors. **2002**, 32, 57-66	1
2149	Amodiaquine clearance and its metabolism to N-desethylamodiaquine is mediated by CYP2C8: a new high affinity and turnover enzyme-specific probe substrate. **2002**, 300, 399-407	221
2148	Similarity versus docking in 3D virtual screening. **2000**, 191-207	
2147	Predicting the structure of protein cavities created by mutation. **2002**, 15, 669-75	11
2146	Rigidity Theory and Applications. **2002**,	5
2145	Combining pharmacophore and protein modeling to predict CYP450 inhibitors and substrates. **2002** , 357, 133-44	11
2144	Docking of flexible molecules using multiscale ligand representations. **2002**, 45, 4639-46	23
2143	Identification of ligand binding sites on proteins using a multi-scale approach. **2002**, 124, 2337-44	47
2142	Combinatorial library design using a multiobjective genetic algorithm. **2002**, 42, 375-85	130
2141	Mutations in cytochrome b resulting in atovaquone resistance are associated with loss of fitness in Plasmodium falciparum. **2002**, 46, 2435-41	48

2140	Crystal structure of yeast acetohydroxyacid synthase: a target for herbicidal inhibitors. *Journal of Molecular Biology*, **2002**, 317, 249-62	6.5	169
2139	Design, synthesis, and tripeptidyl peptidase II inhibitory activity of a novel series of (S)-2,3-dihydro-2-(4-alkyl-1H-imidazol-2-yl)-1H-indoles. **2002**, 45, 5303-10		16
2138	Algorithms in Bioinformatics. **2002**,		3
2137	A knowledge-based scoring function for protein-ligand interactions: Probing the reference state. **2000**, 99-114		10
2136	Structure-based analysis of the ultraspiracle protein and docking studies of putative ligands. **2002**, 2, 1-11		30
2135	The use of computational methods in the discovery and design of kinase inhibitors. **2002**, 8, 1527-45		26
2134	Molecular modeling in cysteine protease inhibitor design. **2002**, 8, 1673-81		11
2133	In silico approaches to mechanistic and predictive toxicology: an introduction to bioinformatics for toxicologists. **2002**, 32, 67-112		26
2132	Crystal structures of two homologous pathogenesis-related proteins from yellow lupine. *Journal of Molecular Biology*, **2002**, 319, 1223-34	6.5	76
2131	A model binding site for testing scoring functions in molecular docking. *Journal of Molecular Biology*, **2002**, 322, 339-55	6.5	178
2130	Identification of a second binding site in the estrogen receptor. **2002**, 45, 584-9		35
2129	Chemoinformatics. **2002**,		
2128	The molecular and enzyme kinetic basis for the diminished activity of the cytochrome P450 2D6.17 (CYP2D6.17) variant. Potential implications for CYP2D6 phenotyping studies and the clinical use of CYP2D6 substrate drugs in some African populations. **2002**, 64, 1387-98		43
2127	Virtual screening and fast automated docking methods. **2002**, 7, 64-70		214
2126	Virtual screening and fast automated docking methods. **2002**, 7, 64-70		228
2125	Structure-based screening of low-affinity compounds. **2002**, 7, 522-7		123
2124	Prediction of protein-protein interactions by docking methods. **2002**, 12, 28-35		380
2123	Complexity and simplicity of ligand-macromolecule interactions: the energy landscape perspective. **2002**, 12, 197-203		99

2122	Matrix metalloproteinases and collagen catabolism. **2002**, 66, 19-32	179
2121	Pattern recognition and massively distributed computing. **2002**, 23, 1544-50	17
2120	Enhanced docking with the mining minima optimizer: acceleration and side-chain flexibility. **2002**, 23, 1656-70	48
2119	Computation of the physio-chemical properties and data mining of large molecular collections. **2002**, 23, 172-83	52
2118	Targeting thrombin and factor VIIa: design, synthesis, and inhibitory activity of functionally relevant indolizidinones. **2002**, 12, 2907-11	46
2117	Consensus scoring for ligand/protein interactions. **2002**, 20, 281-95	334
2116	A genetic algorithm for the identification of conformationally invariant regions in protein molecules. **2002**, 58, 195-208	113
2115	Life-science applications of the Cambridge Structural Database. **2002**, 58, 879-88	59
2114	Principles of docking: An overview of search algorithms and a guide to scoring functions. **2002**, 47, 409-43	954
2113	ConsDock: A new program for the consensus analysis of protein-ligand interactions. **2002**, 47, 521-33	115
2112	Impact of incorporating the 2C5 crystal structure into comparative models of cytochrome P450 2D6. **2002**, 49, 216-31	62
2111	A new test set for validating predictions of protein-ligand interaction. **2002**, 49, 457-71	383
2110	Protein-based virtual screening of chemical databases. II. Are homology models of G-Protein Coupled Receptors suitable targets?. **2003**, 50, 5-25	225
2109	Virtual screening to enrich hit lists from high-throughput screening: a case study on small-molecule inhibitors of angiogenin. **2003**, 50, 81-93	59
2108	CLiBE: a database of computed ligand binding energy for ligand-receptor complexes. **2002**, 26, 661-6	12
2107	Virtual screening using grid computing: the screensaver project. **2002**, 1, 551-5	64
2106	Designing focused libraries using MoSELECT. **2002**, 20, 491-8	59
2105	Three-dimensional molecular descriptors and a novel QSAR method. **2002**, 21, 161-70	15

2104	Structure activity relationship by NMR and by computer: a comparative study. **2002**, 124, 11073-84	27
2103	Molecular docking and high-throughput screening for novel inhibitors of protein tyrosine phosphatase-1B. **2002**, 45, 2213-21	391
2102	Q-fit: a probabilistic method for docking molecular fragments by sampling low energy conformational space. **2002**, 16, 43-57	29
2101	Further development and validation of empirical scoring functions for structure-based binding affinity prediction. **2002**, 16, 11-26	842
2100	Modified AutoDock for accurate docking of protein kinase inhibitors. **2002**, 16, 113-27	38
2099	A review of protein-small molecule docking methods. **2002**, 16, 151-66	463
2098	Sensitivity of molecular docking to induced fit effects in influenza virus neuraminidase. **2002**, 16, 855-69	48
2097	Distilling the essential features of a protein surface for improving protein-ligand docking, scoring, and virtual screening. **2002**, 16, 883-902	76
2096	CoMFA and docking study of novel estrogen receptor subtype selective ligands. **2003**, 17, 313-28	27
2095	Binding of alpha-hydroxy-beta-amino acid inhibitors to methionine aminopeptidase. The performance of two types of scoring functions. **2003**, 17, 383-97	1
2094	3D-QSAR and docking studies on 4-anilinoquinazoline and 4-anilinoquinoline epidermal growth factor receptor (EGFR) tyrosine kinase inhibitors. **2003**, 17, 475-93	45
2093	Computational studies of new potential antimalarial compounds--stereoelectronic complementarity with the receptor. **2003**, 17, 583-95	7
2092	A novel scoring function for molecular docking. **2003**, 17, 597-605	22
2091	Development and testing of a de novo drug-design algorithm. **2003**, 17, 621-41	12
2090	Comparative study of several algorithms for flexible ligand docking. **2003**, 17, 755-63	245
2089	Predicting drug metabolism: a site of metabolism prediction tool applied to the cytochrome P450 2C9. **2003**, 46, 2313-24	145
2088	Molecular shape diversity of combinatorial libraries: a prerequisite for broad bioactivity. **2003**, 43, 987-1003	302
2087	Binding site characteristics in structure-based virtual screening: evaluation of current docking tools. **2003**, 9, 47-57	176

2086	Homology model of human corticosteroid binding globulin: a study of its steroid binding ability and a plausible mechanism of steroid hormone release at the site of inflammation. **2003**, 9, 183-9	6
2085	Information-based methods in the development of antiparasitic drugs. **2003**, 90 Suppl 2, S91-6	6
2084	GPCRs: an update on structural approaches to drug discovery. **2003**, 2, 19-25	29
2083	Virtual high-throughput in silico screening. **2003**, 1, 143-149	47
2082	FDS: flexible ligand and receptor docking with a continuum solvent model and soft-core energy function. **2003**, 24, 1637-56	86
2081	Anwendung und Grenzen kristallographischer Daten im strukturbezogenen Liganden- und Wirkstoff-Design. **2003**, 115, 2822-2841	16
2080	Application and limitations of X-ray crystallographic data in structure-based ligand and drug design. **2003**, 42, 2718-36	285
2079	A new quantum stochastic tunnelling optimisation method for protein□gand docking. **2003**, 369, 257-263	17
2078	Application of the stochastic tunneling method to high throughput database screening. **2003**, 370, 68-73	34
2077	2,4-Diaminopyrimidines as inhibitors of Leishmanial and Trypanosomal dihydrofolate reductase. **2003**, 11, 4693-711	50
2076	A new strategy for molecular modeling and receptor-based design of carborane containing compounds. **2003**, 680, 223-231	26
2075	Flexible ligand docking using evolutionary algorithms: investigating the effects of variation operators and local search hybrids. **2003**, 72, 57-73	45
2074	Pin1 and Par14 peptidyl prolyl isomerase inhibitors block cell proliferation. **2003**, 10, 15-24	139
2073	LigandFit: a novel method for the shape-directed rapid docking of ligands to protein active sites. **2003**, 21, 289-307	732
2072	Analysis and optimization of structure-based virtual screening protocols (1): exploration of ligand conformational sampling techniques. **2003**, 22, 23-30	15
2071	A web-based platform for virtual screening. **2003**, 22, 71-82	27
2070	A convenient method for the computer-aided molecular design of carborane containing compounds. **2003**, 13, 3213-6	19
2069	Design of EGFR kinase inhibitors: a ligand-based approach and its confirmation with structure-based studies. **2003**, 11, 4643-53	24

2068	Description of protein-DNA complexes in terms of electron-density topological features. **2003**, 59, 2150-62	9
2067	Pharmacophore-based molecular docking to account for ligand flexibility. **2003**, 51, 172-88	79
2066	Improved protein-ligand docking using GOLD. **2003**, 52, 609-23	2006
2065	Molecular mechanisms of ligand-receptor interactions in transmembrane domain V of the alpha2A-adrenoceptor. **2003**, 140, 347-58	23
2064	Rational approaches towards reversible inhibition of type B monoamine oxidase. Design and evaluation of a novel 5H-Indeno[1,2-c]pyridazin-5-one derivative. **2003**, 13, 69-73	15
2063	Design, synthesis and structure-activity relationships of benzoxazinone-based factor Xa inhibitors. **2003**, 13, 561-6	17
2062	A priori molecular descriptors in QSAR: a case of HIV-1 protease inhibitors. I. The chemometric approach. **2003**, 21, 435-48	21
2061	A priori molecular descriptors in QSAR: a case of HIV-1 protease inhibitors. II. Molecular graphics and modeling. **2003**, 21, 499-515	8
2060	Nuclear hormone receptor targeted virtual screening. **2003**, 46, 3045-59	155
2059	Molecular recognition and docking algorithms. **2003**, 32, 335-73	543
2058	Molecular fractionation with conjugate caps for full quantum mechanical calculation of protein–molecule interaction energy. **2003**, 119, 3599-3605	426
2057	Receptor-guided alignment-based comparative 3D-QSAR studies of benzylidene malonitrile tyrphostins as EGFR and HER-2 kinase inhibitors. **2003**, 46, 4657-68	51
2056	3'-C-branched-chain-substituted nucleosides and nucleotides as potent inhibitors of Mycobacterium tuberculosis thymidine monophosphate kinase. **2003**, 46, 3811-21	47
2055	Comparative evaluation of 11 scoring functions for molecular docking. **2003**, 46, 2287-303	749
2054	Applications. 487-622	2
2053	Improving structure-based virtual screening by multivariate analysis of scoring data. **2003**, 46, 5781-9	125
2052	BHB: a simple knowledge-based scoring function to improve the efficiency of database screening. **2003**, 43, 1316-27	22
2051	Parallel solid-phase synthesis and evaluation of inhibitors of Streptomyces coelicolor type II dehydroquinase. **2003**, 46, 5735-44	19

2050	Synthesis and evaluation of a novel nonsteroidal-specific endothelial cell proliferation inhibitor. **2003**, 46, 1289-92		57
2049	Shape signatures: a new approach to computer-aided ligand- and receptor-based drug design. **2003**, 46, 5674-90		109
2048	Quantum mechanical/molecular mechanical (QM/MM) docking: an evaluation for known test systems. **2003**, 101, 2469-2480		32
2047	Surflex: fully automatic flexible molecular docking using a molecular similarity-based search engine. **2003**, 46, 499-511		1063
2046	Efficient conformational sampling of local side-chain flexibility. *Journal of Molecular Biology*, **2003**, 326, 1651-65	6.5	52
2045	Ligand-induced conformational changes and a mechanism for domain closure in Aspergillus nidulans dehydroquinate synthase. *Journal of Molecular Biology*, **2003**, 327, 129-44	6.5	19
2044	Receptor-drug association studies in the inhibition of the hematin aggregation process of malaria. **2003**, 547, 217-22		32
2043	Inhibition of carbonic anhydrase II by steroidal and non-steroidal sulphamates. **2003**, 305, 909-14		69
2042	Synthesis and Ca2+-mobilizing activity of purine-modified mimics of adenophostin A: a model for the adenophostin-Ins(1,4,5)P3 receptor interaction. **2003**, 46, 4860-71		36
2041	New amide-bearing benzolactam-based protein kinase C modulators induce enhanced secretion of the amyloid precursor protein metabolite sAPPalpha. **2003**, 46, 364-73		45
2040	The Biophore Concept. **2003**, 73-105		3
2039	Chppter 30. Recent advances in virtual ligand screening. **2003**, 38, 305-314		8
2038	Mechanism of action of the diazabicyclononanone-type kappa-agonists. **2003**, 46, 1383-9		26
2037	Membrane Transporters. **2003**,		2
2036	Design, synthesis and evaluation of bifunctional inhibitors of type II dehydroquinase. **2003**, 1, 2075-83		19
2035	A Gentle Introduction to Memetic Algorithms. **2003**, 105-144		189
2034	Flexible ligand docking using differential evolution.		26
2033	Molecular modeling and metabolic studies of the interaction of catechol-O-methyltransferase and a new nitrocatechol inhibitor. **2003**, 31, 250-8		34

2032	The negative transcriptional regulator NmrA discriminates between oxidized and reduced dinucleotides. **2003**, 278, 32107-14	59
2031	Chemoinformatics Research at the University of Sheffield: A History and Citation Analysis. **2003**, 29, 249-267	14
2030	Residues glutamate 216 and aspartate 301 are key determinants of substrate specificity and product regioselectivity in cytochrome P450 2D6. **2003**, 278, 4021-7	82
2029	Crystal structure of varicella zoster virus thymidine kinase. **2003**, 278, 24680-7	20
2028	Molecular evaluation using in silico protein interaction profiles. **2003**, 19, 1514-23	11
2027	Genetic algorithms in molecular modelling: a review. **2003**, 23, 109-139	2
2026	L/D Protein Ligand Database (PLD): additional understanding of the nature and specificity of protein-ligand complexes. **2003**, 19, 1856-7	91
2025	Identification of the binding sites of the SR49059 nonpeptide antagonist into the V1a vasopressin receptor using sulfydryl-reactive ligands and cysteine mutants as chemical sensors. **2003**, 278, 40010-9	40
2024	Molecular modeling and molecular dynamics simulations of membrane transporter proteins. **2003**, 227, 335-50	2
2023	Structure of a human carcinogen-converting enzyme, SULT1A1. Structural and kinetic implications of substrate inhibition. **2003**, 278, 7655-62	129
2022	Conformational flexibility models for the receptor in structure based drug design. **2003**, 9, 1635-48	114
2021	Virtual screening of virtual libraries. **2003**, 41, 61-97	31
2020	Molecular modelling probes: docking and scoring. **2003**, 31, 980-4	29
2019	Molecular Docking in Structure-Based Design. **2003**, 417-452	
2018	. **2003**,	52
2017	The FlexX database docking environment--rational extraction of receptor based pharmacophores. **2004**, 1, 49-60	22
2016	A genetic algorithm for the ligand-protein docking problem. **2004**, 27, 605-610	28
2015	Biological Ligands. **2004**, 88-100	

2014	The Cambridge Structural Database. **2004**, 161-168	4
2013	Protein classification using comparative molecular interaction profile analysis system. **2004**, 2, 497-510	
2012	Key amino acids located within the transmembrane domains 5 and 7 account for the pharmacological specificity of the human V1b vasopressin receptor. **2004**, 18, 2777-89	20
2011	Recent advances in the investigation of the bioactive conformation of peptides active at the micro-opioid receptor. conformational analysis of endomorphins. **2004**, 4, 105-21	48
2010	4-thiophenoxy-N-(3,4,5-trialkoxyphenyl)pyrimidine-2-amines as potent and selective inhibitors of the T-cell tyrosine kinase p56lck. **2004**, 11, 747-53	4
2009	Virtual screening for kinase targets. **2004**, 11, 693-707	64
2008	Predicting molecular interactions in silico: II. Protein-protein and protein-drug docking. **2004**, 11, 91-107	68
2007	In silico methods for predicting ligand binding determinants of cytochromes P450. **2004**, 4, 1803-24	60
2006	Integration of virtual screening into the drug discovery process. **2004**, 4, 1053-65	13
2005	Study of a highly accurate and fast protein-ligand docking based on molecular dynamics.	1
2004	Active site mutations and substrate inhibition in human sulfotransferase 1A1 and 1A3. **2004**, 279, 18799-805	45
2003	Recent development and application of virtual screening in drug discovery: an overview. **2004**, 10, 1011-33	158
2002	A pharmacophore-based evolutionary approach for screening estrogen receptor antagonists.	1
2001	New lead generation strategies for protein kinase inhibitors - fragment based screening approaches. **2004**, 4, 301-11	31
2000	Differential inhibition of adenylyl cyclase isoforms and soluble guanylyl cyclase by purine and pyrimidine nucleotides. **2004**, 279, 19955-69	87
1999	A three-dimensional model of the neprilysin 2 active site based on the X-ray structure of neprilysin. Identification of residues involved in substrate hydrolysis and inhibitor binding of neprilysin 2. **2004** , 279, 46172-81	16
1998	FULL AB INITIO COMPUTATION OF PROTEIN-WATER INTERACTION ENERGIES. **2004**, 03, 43-49	32
1997	Computational approaches to understand alpha-conotoxin interactions at neuronal nicotinic receptors. **2004**, 271, 2327-34	41

1996	Docking and scoring in virtual screening for drug discovery: methods and applications. **2004**, 3, 935-49	2083
1995	New targets for an old drug. **2004**, 1, 227-234	2
1994	Prediction of drug-like molecular properties: modeling cytochrome p450 interactions. **2004**, 275, 449-520	9
1993	Docking and scoring of metallo-beta-lactamases inhibitors. **2004**, 18, 287-302	26
1992	Multiple active site corrections for docking and virtual screening. **2004**, 47, 80-9	105
1991	Structural interaction fingerprint (SIFt): a novel method for analyzing three-dimensional protein-ligand binding interactions. **2004**, 47, 337-44	428
1990	Scoring functions for protein-ligand interactions: a critical perspective. **2004**, 1, 231-9	76
1989	The many roles of computation in drug discovery. **2004**, 303, 1813-8	1088
1988	New COX-2/5-LOX inhibitors: apoptosis-inducing agents potentially useful in prostate cancer chemotherapy. **2004**, 47, 6195-206	96
1987	Glide: a new approach for rapid, accurate docking and scoring. 1. Method and assessment of docking accuracy. **2004**, 47, 1739-49	5601
1986	Synthesis, biological evaluation, and molecular modeling studies of a novel, peripherally selective inhibitor of catechol-O-methyltransferase. **2004**, 47, 6207-17	34
1985	Modeling the E. coli 4-hydroxybenzoic acid oligoprenyltransferase (ubiA transferase) and characterization of potential active sites. **2004**, 10, 317-27	23
1984	ProPose: a docking engine based on a fully configurable protein-ligand interaction model. **2004**, 10, 342-57	21
1983	GAsDock: a new approach for rapid flexible docking based on an improved multi-population genetic algorithm. **2004**, 14, 4671-6	51
1982	A practical approach to docking of zinc metalloproteinase inhibitors. **2004**, 22, 293-307	82
1981	Unsupervised guided docking of covalently bound ligands. **2004**, 18, 635-50	17
1980	Studies of binding modes of (S)-mephenytoin to wild types and mutants of cytochrome P450 2C19 and 2C9 using homology modeling and computational docking. **2004**, 21, 2270-8	20
1979	GEMDOCK: a generic evolutionary method for molecular docking. **2004**, 55, 288-304	380

1978	A detailed comparison of current docking and scoring methods on systems of pharmaceutical relevance. **2004**, 56, 235-49	346
1977	Molecular determinants of thapsigargin binding by SERCA Ca2+-ATPase: a computational docking study. **2004**, 56, 595-606	23
1976	Comparative evaluation of eight docking tools for docking and virtual screening accuracy. **2004**, 57, 225-42	416
1975	Human SARS-coronavirus RNA-dependent RNA polymerase: activity determinants and nucleoside analogue inhibitors. **2004**, 57, 12-4	8
1974	Relative free energy of binding and binding mode calculations of HIV-1 RT inhibitors based on dock-MM-PB/GS. **2004**, 57, 493-503	32
1973	A pharmacophore docking algorithm and its application to the cross-docking of 18 HIV-NNRTI's in their binding pockets. **2004**, 54, 526-33	22
1972	Recovering the true targets of specific ligands by virtual screening of the protein data bank. **2004**, 54, 671-80	92
1971	Simulation-Based Predictions of Binding Affinities of Matrix Metalloproteinase Inhibitors. **2004**, 23, 754-766	8
1970	Design and synthesis of a focused library of novel aryl- and heteroaryl-ketopiperazides. **2004**, 337, 695-703	4
1969	A peptide inhibitor of vascular adhesion protein-1 (VAP-1) blocks leukocyte-endothelium interactions under shear stress. **2004**, 34, 2276-85	37
1968	Development and evaluation of a generic evolutionary method for protein-ligand docking. **2004**, 25, 843-57	40
1967	Ligand-protein docking using a quantum stochastic tunneling optimization method. **2004**, 25, 858-64	24
1966	Fully quantum mechanical energy optimization for protein-ligand structure. **2004**, 25, 1431-7	53
1965	Ribonucleotide activation by enzyme ribonucleotide reductase: understanding the role of the enzyme. **2004**, 25, 2031-7	27
1964	Determination of alpha-conotoxin binding modes on neuronal nicotinic acetylcholine receptors. **2004**, 17, 339-47	36
1963	Synthesis of novel thiazolothiazepine based HIV-1 integrase inhibitors. **2004**, 12, 4459-66	28
1962	Studies of nonnucleoside HIV-1 reverse transcriptase inhibitors. Part 1: Design and synthesis of thiazolidenebenzenesulfonamides. **2004**, 12, 6171-82	16
1961	Active site binding modes of the beta-diketoacids: a multi-active site approach in HIV-1 integrase inhibitor design. **2004**, 12, 6371-81	53

1960	Synthesis and target identification of hymenialdisine analogs. **2004**, 11, 247-59	115
1959	Optimization of virtual screening protocols: FlexX based virtual screening for COX-2 inhibitors reveals the importance of tailoring screen parameters. **2004**, 676, 1-5	2
1958	Characteristics of the Plasmodium falciparum PK5 ATP-binding site: implications for the design of novel antimalarial agents. **2004**, 22, 241-7	12
1957	Use of binding energy in comparative molecular field analysis of isoform selective estrogen receptor ligands. **2004**, 23, 23-38	6
1956	Synthesis, biological activity and molecular modeling studies of novel COX-1 inhibitors. **2004**, 39, 141-51	5
1955	A combination of numeric genetic algorithm and tabu search can be applied to molecular docking. **2004**, 28, 303-312	9
1954	Development of KiBank, a database supporting structure-based drug design. **2004**, 28, 401-7	40
1953	Impact of receptor conformation on in silico screening performance. **2004**, 390, 500-505	14
1952	1-(2-Naphthyl)-1H-pyrazole-5-carboxylamides as potent factor Xa inhibitors. Part 3: Design, synthesis and SAR of orally bioavailable benzamidine-P4 inhibitors. **2004**, 14, 1229-34	42
1951	Computational comparison of microtubule-stabilising agents laulimalide and peloruside with taxol and colchicine. **2004**, 14, 4825-9	63
1950	Evans Blue is an inhibitor of nuclear factor-kappa B (NF-kappaB)-DNA binding. **2004**, 14, 6123-7	13
1949	Combination of a naive Bayes classifier with consensus scoring improves enrichment of high-throughput docking results. **2004**, 47, 4356-9	67
1948	Theoretical analysis of peptidyl alpha-ketoheterocyclic inhibitors of human neutrophil elastase: Insight into the mechanism of inhibition and the application of QM/MM calculations in structure-based drug design. **2004**, 2, 2275-80	18
1947	NMR-based techniques in the hit identification and optimisation processes. **2004**, 8, 597-611	64
1946	Prediction of biological targets using probabilistic neural networks and atom-type descriptors. **2004**, 47, 2645-50	39
1945	HierVLS hierarchical docking protocol for virtual ligand screening of large-molecule databases. **2004**, 47, 56-71	73
1944	Validation of model of cytochrome P450 2D6: an in silico tool for predicting metabolism and inhibition. **2004**, 47, 5340-6	73
1943	Potent and selective farnesyl transferase inhibitors. **2004**, 47, 6812-20	19

1942	Application of machine learning to improve the results of high-throughput docking against the HIV-1 protease. **2004**, 44, 2216-24	49
1941	OptiDock: virtual HTS of combinatorial libraries by efficient sampling of binding modes in product space. **2004**, 6, 530-9	12
1940	Structure-based discovery of nonpeptidic small organic compounds to block the T cell response to myelin basic protein. **2004**, 47, 4989-97	31
1939	Discovery of bicyclic thymidine analogues as selective and high-affinity inhibitors of Mycobacterium tuberculosis thymidine monophosphate kinase. **2004**, 47, 6187-94	40
1938	New fascaplysin-based CDK4-specific inhibitors: design, synthesis and biological activity. **2004**, 1696-7	23
1937	Identification of a minimal subset of receptor conformations for improved multiple conformation docking and two-step scoring. **2004**, 44, 88-96	40
1936	Retrieval of crystallographically-derived molecular geometry information. **2004**, 44, 2133-44	699
1935	Dimers of D-myo-inositol 1,4,5-trisphosphate: design, synthesis, and interaction with Ins(1,4,5)P3 receptors. **2004**, 15, 278-89	28
1934	Ph4Dock: pharmacophore-based protein-ligand docking. **2004**, 47, 6804-11	82
1933	Creating artificial binding pocket boundaries to improve the efficiency of flexible ligand docking. **2004**, 44, 1412-22	6
1932	Accelerated modeling and new ferroelectric materials for naval SONAR. **2004**,	
1931	Design, synthesis, molecular modeling studies, and calpain inhibitory activity of novel alpha-ketoamides incorporating polar residues at the P1'-position. **2004**, 47, 72-9	13
1930	An in silico approach to discovering novel inhibitors of human sirtuin type 2. **2004**, 47, 6292-8	96
1929	Comparing the quality and predictiveness between 3D QSAR models obtained from manual and automated alignment. **2004**, 44, 807-16	32
1928	Virtual screening with flexible docking and COMBINE-based models. Application to a series of factor Xa inhibitors. **2004**, 47, 805-20	50
1927	Combining pharmacophore search, automated docking, and molecular dynamics simulations as a novel strategy for flexible docking. Proof of concept: docking of arginine-glycine-aspartic acid-like compounds into the alphavbeta3 binding site. **2004**, 47, 4178-87	50
1926	Effects of natural flavones and flavonols on the kinase activity of Cdk5. **2004**, 67, 416-20	41
1925	On the modeling of snake venom serine proteinase interactions with benzamidine-based thrombin inhibitors. **2004**, 13, 2355-69	9

1924	Efficient method for high-throughput virtual screening based on flexible docking: discovery of novel acetylcholinesterase inhibitors. **2004**, 47, 4818-28	63
1923	Glide: a new approach for rapid, accurate docking and scoring. 2. Enrichment factors in database screening. **2004**, 47, 1750-9	2943
1922	A quantum mechanics-based scoring function: study of zinc ion-mediated ligand binding. **2004**, 126, 1020-1	142
1921	Structural mining: self-consistent design on flexible protein-peptide docking and transferable binding affinity potential. **2004**, 126, 8515-28	50
1920	Predicting protein-ligand binding affinities: a low scoring game?. **2004**, 2, 3267-73	46
1919	Identification of 1,5-naphthyridine derivatives as a novel series of potent and selective TGF-beta type I receptor inhibitors. **2004**, 47, 4494-506	145
1918	Three-dimensional models of wild-type and mutated forms of cytochrome P450 14alpha-sterol demethylases from Aspergillus fumigatus and Candida albicans provide insights into posaconazole binding. **2004**, 48, 568-74	225
1917	Design and synthesis of novel indole beta-diketo acid derivatives as HIV-1 integrase inhibitors. **2004** , 47, 5298-310	112
1916	A docking score function for estimating ligand-protein interactions: application to acetylcholinesterase inhibition. **2004**, 47, 5492-500	46
1915	Memetic Algorithms. **2004**, 53-85	56
1914	Chemoinformatics. **2004**,	22
1913	Automated protein structure homology modeling: a progress report. **2004**, 5, 405-16	93
1912	CoMFA 3D-QSAR analysis of HIV-1 RT nonnucleoside inhibitors, TIBO derivatives based on docking conformation and alignment. **2004**, 44, 2167-78	43
1911	Sequence divergence of Entamoeba histolytica tubulin is responsible for its altered tertiary structure. **2004**, 319, 1010-6	9
1910	Model structures of the N-methyl-D-aspartate receptor subunit NR1 explain the molecular recognition of agonist and antagonist ligands. **2004**, 145, 205-15	10
1909	Phosphotyrosyl peptides and analogues as substrates and inhibitors of purple acid phosphatases. **2004**, 424, 154-62	50
1908	Evaluation of docking performance: comparative data on docking algorithms. **2004**, 47, 558-65	453
1907	Lessons in molecular recognition: the effects of ligand and protein flexibility on molecular docking accuracy. **2004**, 47, 45-55	315

1906	Conformational analysis of drug-like molecules bound to proteins: an extensive study of ligand reorganization upon binding. **2004**, 47, 2499-510	372
1905	Assessing scoring functions for protein-ligand interactions. **2004**, 47, 3032-47	433
1904	Assessment of docking poses: interactions-based accuracy classification (IBAC) versus crystal structure deviations. **2004**, 44, 871-81	103
1903	Virtual screening using protein-ligand docking: avoiding artificial enrichment. **2004**, 44, 793-806	349
1902	Integrating virtual screening in lead discovery. **2004**, 8, 349-58	214
1901	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
1900	Design and synthesis of potent, orally active, inhibitors of carboxypeptidase U (TAFIa). **2004**, 12, 1151-75	47
1899	An extensive test of 14 scoring functions using the PDBbind refined set of 800 protein-ligand complexes. **2004**, 44, 2114-25	215
1898	New Paradigms in Drug Design and Discovery. **2004**, 1, 663-681	
1897	Molecular modelling of the nucleotide-binding domain of Wilson's disease protein: location of the ATP-binding site, domain dynamics and potential effects of the major disease mutations. **2004**, 382, 293-305	21
1896	Phe120 contributes to the regiospecificity of cytochrome P450 2D6: mutation leads to the formation of a novel dextromethorphan metabolite. **2004**, 380, 353-60	64
1895	Selection-Insertion Schemes in Genetic Algorithms for the Flexible Ligand Docking Problem. **2004**, 368-379	14
1894	Characterization of the CYP2C8 active site by homology modeling. **2004**, 52, 836-41	9
1893	Characterization of the CYP3A4 active site by homology modeling. **2004**, 52, 830-5	26
1892	An Evolutionary Approach with Pharmacophore-Based Scoring Functions for Virtual Database Screening. **2004**, 481-492	1
1891	Informatics (Computational Biology). **2004**,	
1890	Kinetic isotope effects and ligand binding in PQQ-dependent methanol dehydrogenase. **2005**, 388, 123-33	10
1889	Chemoinformatic Tools for Library Design and the Hit-to-Lead Process: A User's Perspective. **2005**, 381-435	1

1888	High-Throughput Flow Cytometry. **2005**, 185-226	
1887	Chapter 12 Structure-Based Lead Optimization. **2005**, 169-183	2
1886	Protein□ligand Docking Virtual Screening with GOLD. **2005**, 379-415	41
1885	Algorithmic Engines in Virtual Screening. **2005**, 59-115	0
1884	An Analysis of Critical Factors Affecting Docking and Scoring. **2005**, 47-85	2
1883	Virtual Screening. **2005**, 3-24	6
1882	Inhibitor-based validation of a homology model of the active-site of tripeptidyl peptidase II. **2005**, 23, 409-18	5
1881	Elucidation of the Na+, K+-ATPase digitalis binding site. **2005**, 23, 465-75	36
1880	Similarities among receptor pockets and among compounds: analysis and application to in silico ligand screening. **2005**, 24, 34-45	69
1879	Structural model of the Plasmodium CDK, Pfmrk, a novel target for malaria therapeutics. **2005**, 24, 72-80	17
1878	Design, synthesis, and evaluation of potent and selective benzoyleneurea-based inhibitors of protein geranylgeranyltransferase-I. **2005**, 13, 677-88	13
1877	Synthesis and biological activity of novel 1,2-disubstituted benzene derivatives as factor Xa inhibitors. **2005**, 13, 1305-23	22
1876	In vitro evaluation of the anti-estrogenic activity of hydroxyl substituted diphenylnaphthyl alkene ligands for the estrogen receptor. **2005**, 13, 1819-28	10
1875	Docking simulation with a purine nucleoside specific homology model of deoxycytidine kinase, a target enzyme for anticancer and antiviral therapy. **2005**, 13, 4160-7	10
1874	Theoretical quantitative structure-activity relationships of flavone ligands interacting with cytochrome P450 1A1 and 1A2 isozymes. **2005**, 13, 4366-74	35
1873	Exploration of a binding mode of indole amide analogues as potent histone deacetylase inhibitors and 3D-QSAR analyses. **2005**, 13, 5424-34	49
1872	Synthetic studies on novel Syk inhibitors. Part 1: Synthesis and structure-activity relationships of pyrimidine-5-carboxamide derivatives. **2005**, 13, 4936-51	51
1871	Amentoflavone and its derivatives as novel natural inhibitors of human Cathepsin B. **2005**, 13, 5819-25	44

1870	Unclassical hydrogen bonds of CH?O and CH?Cl in the crystals of 1,4-diaryl Hantzsch esters. **2005**, 46, 877-879	16
1869	The design and synthesis of novel 3-[2-indol-1-yl-ethyl]-1H-indole derivatives as selective inhibitors of CDK4. **2005**, 46, 1423-1425	38
1868	Functional virtual screening of estrogen receptor modulators by FlexX-Pharm. **2005**, 725, 239-242	3
1867	Computer-aided design of potential anti-HIV-1 non-nucleoside reverse transcriptase inhibitors by contraction of ring in TIBO derivatives. **2005**, 732, 39-45	9
1866	Isoindolinone-based inhibitors of the MDM2-p53 protein-protein interaction. **2005**, 15, 1515-20	80
1865	Structure-based design of protein tyrosine phosphatase-1B inhibitors. **2005**, 15, 2503-7	59
1864	Molecular recognition of 15-deoxy-delta(12,14)-prostaglandin J2 by nuclear factor-kappa B and other cellular proteins. **2005**, 15, 4057-63	37
1863	Identification of coumarin derivatives as a novel class of allosteric MEK1 inhibitors. **2005**, 15, 5467-73	55
1862	Inhibitory activity of polyhydroxycarboxylate chelators against recombinant NF-kappaB p50 protein-DNA binding. **2005**, 33, 67-81	10
1861	Construction of a virtual combinatorial library using SMILES strings to discover potential structure-diverse PPAR modulators. **2005**, 40, 632-40	14
1860	Interaction profiles of protein kinase-inhibitor complexes and their application to virtual screening. **2005**, 48, 121-33	96
1859	Structure-based drug discovery using GPCR homology modeling: successful virtual screening for antagonists of the alpha1A adrenergic receptor. **2005**, 48, 1088-97	243
1858	E-ring modified steroids as novel potent inhibitors of 17beta-hydroxysteroid dehydrogenase type 1. **2005**, 48, 5749-70	70
1857	LigandScout: 3-D pharmacophores derived from protein-bound ligands and their use as virtual screening filters. **2005**, 45, 160-9	1255
1856	Studies on binding free energies and the binding mode by docking and MM-PBSA in gp41-ligand complex. **2005**, 31, 1051-1056	6
1855	Structure, epitope mapping, and docking simulation of a gibberellin mimic peptide as a peptidyl mimotope for a hydrophobic ligand. **2005**, 272, 4938-48	9
1854	The functional role of cysteines adjacent to the NRY motif of the human MT1 melatonin receptor. **2005**, 39, 1-11	21
1853	Computer prediction of drug resistance mutations in proteins. **2005**, 10, 521-9	46

1852	Receptor systems: will mining the receptorome yield novel targets for pharmacotherapy?. **2005**, 108, 59-64	9
1851	The MPSim-Dock hierarchical docking algorithm: application to the eight trypsin inhibitor cocrystals. **2005**, 26, 48-71	27
1850	Evaluation of library ranking efficacy in virtual screening. **2005**, 26, 11-22	98
1849	An efficient molecular docking using conformational space annealing. **2005**, 26, 78-87	26
1848	A scoring function for docking ligands to low-resolution protein structures. **2005**, 26, 374-83	25
1847	New and fast statistical-thermodynamic method for computation of protein-ligand binding entropy substantially improves docking accuracy. **2005**, 26, 1089-95	37
1846	Absolute free energies of binding of peptide analogs to the HIV-1 protease from molecular dynamics simulations. **2005**, 26, 1294-305	7
1845	Study of a highly accurate and fast protein□gand docking method based on molecular dynamics. **2005**, 17, 1627-1641	22
1844	Insights from ab initio quantum chemical calculations into the preferred tautomeric forms and binding affinities to CDK2 of substituted pyrazolopyridines. **2005**, 80, 312-8	6
1843	Yucca: an efficient algorithm for small-molecule docking. **2005**, 2, 1517-24	13
1842	Structurally simple farnesyltransferase inhibitors arrest the growth of malaria parasites. **2005**, 44, 4903-6	34
1841	Structurally Simple Farnesyltransferase Inhibitors Arrest the Growth of Malaria Parasites. **2005**, 117, 4981-4984	1
1840	Model of a specific human histamine H3 receptor (hH3R) binding pocket suitable for virtual drug design. **2005**, 54 Suppl 1, S50-1	8
1839	Binding site of activators of the cystic fibrosis transmembrane conductance regulator in the nucleotide binding domains. **2005**, 62, 446-60	99
1838	In-silico screening using flexible ligand binding pockets: a molecular dynamics-based approach. **2005**, 19, 213-28	30
1837	Asp746 to glycine change may have a greater influence than Cys751 to serine change in accounting for ligand selectivity between EGFR and HER-2 at the ATP site. **2005**, 19, 287-91	1
1836	Evolutionary Algorithms in Drug Design. **2005**, 4, 177-243	31
1835	Knowledge Based Potentials: the Reverse Boltzmann Methodology, Virtual Screening and Molecular Weight Dependence. **2005**, 24, 527-536	10

1834	A pharmacophore-based evolutionary approach for screening selective estrogen receptor modulators. **2005**, 59, 205-20	74
1833	Prediction of binding modes for ligands in the cytochromes P450 and other heme-containing proteins. **2005**, 58, 836-44	84
1832	Molecular modeling of cardiac glycoside binding by the human sequence monoclonal antibody 1B3. **2005**, 60, 382-91	8
1831	Comparing protein-ligand docking programs is difficult. **2005**, 60, 325-32	229
1830	Rational inhibitor design and iterative screening in the identification of selective plasmodial cyclin dependent kinase inhibitors. **2005**, 8, 27-38	24
1829	Why is quinidine an inhibitor of cytochrome P450 2D6? The role of key active-site residues in quinidine binding. **2005**, 280, 38617-24	57
1828	Application of 3D-QSAR techniques in anti-HIV-1 drug design--an overview. **2005**, 11, 3091-110	39
1827	Hierarchical docking of databases of multiple ligand conformations. **2005**, 5, 739-49	120
1826	Strategies for the design of potent and selective kinase inhibitors. **2005**, 11, 1845-63	54
1825	Structure of the Mg-chelatase cofactor GUN4 reveals a novel hand-shaped fold for porphyrin binding. **2005**, 3, e151	69
1824	Structural elucidation of chalcone reductase and implications for deoxychalcone biosynthesis. **2005** , 280, 30496-503	71
1823	From structure to function: methods and applications. **2005**, 6, 171-83	32
1822	Reply to Savarino et al.. **2005**, 191, 1382-1383	7
1821	Use of photoaffinity labeling and site-directed mutagenesis for identification of the key residue responsible for extraordinarily high affinity binding of UCN-01 in human alpha1-acid glycoprotein. **2005**, 280, 1384-91	18
1820	Modeling Polarization in Proteins and Protein-ligand Complexes: Methods and Preliminary Results. **2005**, 72, 79-104	60
1819	Divergent pharmacological activity of novel marine-derived excitatory amino acids on glutamate receptors. **2005**, 314, 1068-78	50
1818	The Design and Docking of Virtual Compound Libraries to Structures of Drug Targets. **2005**, 1, 103-127	15
1817	Chapter 13 Targeting the Kinome with Computational Chemistry. **2005**, 185-202	2

1816	Recent Advances in Docking and Scoring. **2005**, 1, 93-102	115
1815	Consensus scoring criteria in structure-based virtual screening.	3
1814	Intestinal antiinflammatory effect of 5-aminosalicylic acid is dependent on peroxisome proliferator-activated receptor-gamma. **2005**, 201, 1205-15	361
1813	Principles and Methods of Docking and Ligand Design. **2005**, 441-476	2
1812	Structural and kinetic basis for substrate selectivity in Populus tremuloides sinapyl alcohol dehydrogenase. **2005**, 17, 1598-611	66
1811	The structure of human SULT1A1 crystallized with estradiol. An insight into active site plasticity and substrate inhibition with multi-ring substrates. **2005**, 280, 41482-6	85
1810	Beta2 subunit contribution to 4/7 alpha-conotoxin binding to the nicotinic acetylcholine receptor. **2005**, 280, 30460-8	57
1809	Molecular mechanism underlying partial and full agonism mediated by the human cholecystokinin-1 receptor. **2005**, 280, 10664-74	27
1808	Active site driven ligand design: an evolutionary approach. **2005**, 3, 1053-70	5
1807	Flexible protein-ligand docking using particle swarm optimization.	0
1806	Improving conformational searches by geometric screening. **2005**, 21, 624-30	19
1805	Provirus load is lower in human T lymphotropic virus (HTLV)-II carriers than in HTLV-I carriers: a key difference in viral pathogenesis?. **2005**, 191, 1383-5; author reply 1385-6	6
1804	Identification of N10-substituted phenoxazines as potent and specific inhibitors of Akt signaling. **2005**, 280, 31924-35	79
1803	Pharmacological differences between human and guinea pig histamine H1 receptors: Asn84 (2.61) as key residue within an additional binding pocket in the H1 receptor. **2005**, 67, 1045-52	43
1802	Constrained geometric simulation of diffusive motion in proteins. **2005**, 2, S127-36	147
1801	Docking: successes and challenges. **2005**, 11, 323-33	177
1800	Beta-diketo acid pharmacophore hypothesis. 1. Discovery of a novel class of HIV-1 integrase inhibitors. **2005**, 48, 111-20	91
1799	Virtual docking approaches to protein kinase B inhibition. **2005**, 48, 2278-81	48

1798	Virtual screening for beta-secretase (BACE1) inhibitors reveals the importance of protonation states at Asp32 and Asp228. **2005**, 48, 3749-55	79
1797	General and targeted statistical potentials for protein-ligand interactions. **2005**, 61, 272-87	252
1796	Binding mode prediction of cytochrome p450 and thymidine kinase protein-ligand complexes by consideration of water and rescoring in automated docking. **2005**, 48, 2308-18	110
1795	Improved FlexX docking using FlexS-determined base fragment placement. **2005**, 45, 993-1001	23
1794	Optimization and validation of a docking-scoring protocol; application to virtual screening for COX-2 inhibitors. **2005**, 48, 1055-68	36
1793	3D structure and the drug-discovery process. **2005**,	
1792	Crystal structures of a multifunctional triterpene/flavonoid glycosyltransferase from Medicago truncatula. **2005**, 17, 3141-54	263
1791	A Simple Method for Improving Torsion Optimization of Ligand Molecules in Receptor Binding Sites. **2005**, 1, 634-42	2
1790	Searching techniques for databases of two- and three-dimensional chemical structures. **2005**, 48, 4183-99	134
1789	Effects of variable docking conditions and scoring functions on corresponding protein-aligned comparative molecular field analysis models constructed from diverse human protein tyrosine phosphatase 1B inhibitors. **2005**, 48, 8016-34	24
1788	Structure-based virtual screening for plant-based ERbeta-selective ligands as potential preventative therapy against age-related neurodegenerative diseases. **2005**, 48, 3463-6	81
1787	Virtual screening of biogenic amine-binding G-protein coupled receptors: comparative evaluation of protein- and ligand-based virtual screening protocols. **2005**, 48, 5448-65	171
1786	Diketo acid pharmacophore. 2. Discovery of structurally diverse inhibitors of HIV-1 integrase. **2005**, 48, 8009-15	46
1785	A combined STD-NMR/molecular modeling protocol for predicting the binding modes of the glycosidase inhibitors kifunensine and salacinol to Golgi alpha-mannosidase II. **2005**, 44, 6729-37	62
1784	Improving binding mode predictions by docking into protein-specifically adapted potential fields. **2005**, 48, 5466-79	29
1783	PostDOCK: a structural, empirical approach to scoring protein ligand complexes. **2005**, 48, 6821-31	34
1782	Comparative virtual and experimental high-throughput screening for glycogen synthase kinase-3beta inhibitors. **2005**, 48, 7946-59	65
1781	Frontal affinity chromatography with MS detection of EphB2 tyrosine kinase receptor. 2. Identification of small-molecule inhibitors via coupling with virtual screening. **2005**, 48, 3221-30	50

1780	Including tightly-bound water molecules in de novo drug design. Exemplification through the in silico generation of poly(ADP-ribose)polymerase ligands. **2005**, 45, 624-33		48
1779	Metabolic regio- and stereoselectivity of cytochrome P450 2D6 towards 3,4-methylenedioxy-N-alkylamphetamines: in silico predictions and experimental validation. **2005**, 48, 6117-27		56
1778	A flexible docking procedure for the exploration of peptide binding selectivity to known structures and homology models of PDZ domains. **2005**, 127, 14072-9		63
1777	Enrichment of ligands for the serotonin receptor using the Shape Signatures approach. **2005**, 45, 49-57		27
1776	Structure-based design, synthesis, and biological evaluation of inhibitors of Mycobacterium tuberculosis type II dehydroquinase. **2005**, 48, 4871-81		37
1775	3D-QSAR and docking studies of selective GSK-3beta inhibitors. Comparison with a thieno[2,3-b]pyrrolizinone derivative, a new potential lead for GSK-3beta ligands. **2005**, 45, 708-15		25
1774	Receptor flexibility in de novo ligand design and docking. **2005**, 48, 6585-96		57
1773	Fragment-based lead discovery using X-ray crystallography. **2005**, 48, 403-13		379
1772	Multiple Docking for Protein Structure Prediction. **2005**, 24, 131-150		5
1771	Kinetic and molecular analysis of 5-epiaristolochene 1,3-dihydroxylase, a cytochrome P450 enzyme catalyzing successive hydroxylations of sesquiterpenes. **2005**, 280, 3686-96		37
1770	Consensus scoring criteria for improving enrichment in virtual screening. **2005**, 45, 1134-46		182
1769	Enantiomerically pure hexahydropyrazinoquinolines as potent and selective dopamine 3 subtype receptor ligands. **2005**, 48, 3171-81		24
1768	Modeling water molecules in protein-ligand docking using GOLD. **2005**, 48, 6504-15		327
1767	Prediction of multimolecular assemblies by multiple docking. *Journal of Molecular Biology*, **2005**, 349, 435-47	6.5	74
1766	Structures for the potential drug target purine nucleoside phosphorylase from Schistosoma mansoni causal agent of schistosomiasis. *Journal of Molecular Biology*, **2005**, 353, 584-99	6.5	32
1765	Model structures of alpha-2 adrenoceptors in complex with automatically docked antagonist ligands raise the possibility of interactions dissimilar from agonist ligands. **2005**, 150, 126-43		27
1764	Screening of drugs by FRET analysis identifies inhibitors of SARS-CoV 3CL protease. **2005**, 333, 194-9		36
1763	A structural study towards the understanding of the interactions of SoxY, SoxZ, and SoxB, leading to the oxidation of sulfur anions via the novel global sulfur oxidizing (sox) operon. **2005**, 335, 609-15		14

1762	An all atom energy based computational protocol for predicting binding affinities of protein-ligand complexes. **2005**, 579, 6659-66	61
1761	Retrospective docking study of PDE4B ligands and an analysis of the behavior of selected scoring functions. **2005**, 45, 1061-74	19
1760	Rational design of new bifunctional inhibitors of type II dehydroquinase. **2005**, 3, 3102-4	12
1759	Progress in cytochrome P450 active site modeling. **2005**, 433, 361-8	25
1758	Knowledge-based elastic potentials for docking drugs or proteins with nucleic acids. **2005**, 88, 1166-90	20
1757	Structure-based design of potent non-peptide MDM2 inhibitors. **2005**, 127, 10130-1	543
1756	Side-chain flexibility in protein-ligand binding: the minimal rotation hypothesis. **2005**, 14, 1104-14	138
1755	Novel lavendamycin analogues as antitumor agents: synthesis, in vitro cytotoxicity, structure-metabolism, and computational molecular modeling studies with NAD(P)H:quinone oxidoreductase 1. **2005**, 48, 7733-49	67
1754	Design and synthesis of aromatic inhibitors of anthranilate synthase. **2005**, 3, 3629-35	12
1753	Design and synthesis of aromatic inhibitors of anthranilate synthase. **2005**, 3, 2271-81	19
1752	Homology modeling of opioid receptor-ligand complexes using experimental constraints. **2005**, 7, E434-48	71
1751	Computational Intelligence in Bioinformatics. **2005**, 134-152	11
1750	Comparison of automated docking programs as virtual screening tools. **2005**, 48, 962-76	196
1749	Protein/ligand binding free energies calculated with quantum mechanics/molecular mechanics. **2005**, 109, 10474-83	92
1748	In silico footprinting of ligands binding to the minor groove of DNA. **2005**, 45, 1896-907	13
1747	3,6-disubstituted coumarins as mechanism-based inhibitors of thrombin and factor Xa. **2005**, 48, 7592-603	55
1746	Virtual screening and scaffold hopping based on GRID molecular interaction fields. **2005**, 45, 1313-23	53
1745	N-benzylisatin sulfonamide analogues as potent caspase-3 inhibitors: synthesis, in vitro activity, and molecular modeling studies. **2005**, 48, 7637-47	84

1744	Three-dimensional structure-activity relationships of nonsteroidal ligands in complex with androgen receptor ligand-binding domain. **2005**, 48, 917-25	46
1743	Novel and potent 17beta-hydroxysteroid dehydrogenase type 1 inhibitors. **2005**, 48, 2759-62	48
1742	Chapter 9 Calculating Binding Free Energy in Protein□ligand Interaction. **2005**, 1, 113-130	27
1741	A combination of docking, QM/MM methods, and MD simulation for binding affinity estimation of metalloprotein ligands. **2005**, 48, 5437-47	127
1740	Dicarboxylic acid azacycle l-prolyl-pyrrolidine amides as prolyl oligopeptidase inhibitors and three-dimensional quantitative structure-activity relationship of the enzyme-inhibitor interactions. **2005**, 48, 4772-82	12
1739	A knowledge-based energy function for protein-ligand, protein-protein, and protein-DNA complexes. **2005**, 48, 2325-35	236
1738	PatchDock and SymmDock: servers for rigid and symmetric docking. **2005**, 33, W363-7	1963
1737	Chemical Genomics. **2005**,	2
1736	A virtual screening approach for thymidine monophosphate kinase inhibitors as antitubercular agents based on docking and pharmacophore models. **2005**, 45, 1101-8	60
1735	Identification of the molecular mechanisms by which the diterpenoid salvinorin A binds to kappa-opioid receptors. **2005**, 44, 8643-51	77
1734	Bioinformatics and Drug Discovery. **2006**,	1
1733	Identification of ellagic acid as potent inhibitor of protein kinase CK2: a successful example of a virtual screening application. **2006**, 49, 2363-6	119
1732	Structurally simple, potent, Plasmodium selective farnesyltransferase inhibitors that arrest the growth of malaria parasites. **2006**, 49, 5710-27	32
1731	Synthesis and activity of 1,3,5-triphenylimidazolidine-2,4-diones and 1,3,5-triphenyl-2-thioxoimidazolidin-4-ones: characterization of new CB1 cannabinoid receptor inverse agonists/antagonists. **2006**, 49, 872-82	41
1730	PMF scoring revisited. **2006**, 49, 5895-902	233
1729	Discovery of a nanomolar inhibitor of the human murine double minute 2 (MDM2)-p53 interaction through an integrated, virtual database screening strategy. **2006**, 49, 3759-62	117
1728	Binding mode prediction of strand transfer HIV-1 integrase inhibitors using Tn5 transposase as a plausible surrogate model for HIV-1 integrase. **2006**, 49, 3994-7	32
1727	On evaluating molecular-docking methods for pose prediction and enrichment factors. **2006**, 46, 401-15	188

1726	QSAR and Molecular Modeling Studies of HIV Protease Inhibitors. 181-271	5
1725	Prediction of multiple binding modes of the CDK2 inhibitors, anilinopyrazoles, using the automated docking programs GOLD, FlexX, and LigandFit: an evaluation of performance. **2006**, 46, 2552-62	31
1724	Structural insights into monoamine oxidase inhibitory potency and selectivity of 7-substituted coumarins from ligand- and target-based approaches. **2006**, 49, 4912-25	92
1723	Discovery of 4-{4-[3-(pyridin-2-yl)-1H-pyrazol-4-yl]pyridin-2-yl}-N-(tetrahydro-2H-pyran-4-yl)benzamide (GW788388): a potent, selective, and orally active transforming growth factor-beta type I receptor inhibitor. **2006**, 49, 2210-21	81
1722	Docking and three-dimensional quantitative structure-activity relationship (3D QSAR) analyses of nonsteroidal progesterone receptor ligands. **2006**, 49, 4261-8	19
1721	Comparative study of ortho- and meta-nitrated inhibitors of catechol-O-methyltransferase: interactions with the active site and regioselectivity of O-methylation. **2006**, 70, 143-53	40
1720	Guanophostin A: Synthesis and evaluation of a high affinity agonist of the D-myo-inositol 1,4,5-trisphosphate receptor. **2006**, 2015-7	10
1719	Protein Design. **2006**,	
1718	Ant Colony Optimization and Swarm Intelligence. **2006**,	72
1717	Structures of apo- and holo-tyrosine phenol-lyase reveal a catalytically critical closed conformation and suggest a mechanism for activation by K+ ions. **2006**, 45, 7544-52	28
1716	TarFisDock: a web server for identifying drug targets with docking approach. **2006**, 34, W219-24	313
1715	Noise reduction method for molecular interaction energy: application to in silico drug screening and in silico target protein screening. **2006**, 46, 2071-84	24
1714	New insights into the antiviral effects of chloroquine. **2006**, 6, 67-9	384
1713	Postgraduate training in infectious diseases. **2006**, 6, 69	2
1712	Virtual screening of DNA minor groove binders. **2006**, 49, 4232-8	41
1711	An efficient in silico screening method based on the protein-compound affinity matrix and its application to the design of a focused library for cytochrome P450 (CYP) ligands. **2006**, 46, 2610-22	18
1710	Protein-ligand docking: current status and future challenges. **2006**, 65, 15-26	597
1709	Physics-based scoring of protein-ligand complexes: enrichment of known inhibitors in large-scale virtual screening. **2006**, 46, 243-53	127

1708	2-substituted estradiol bis-sulfamates, multitargeted antitumor agents: synthesis, in vitro SAR, protein crystallography, and in vivo activity. **2006**, 49, 7683-96	91
1707	Reverse pharmacognosy: a new concept for accelerating natural drug discovery. **2006**, 1-20	3
1706	Parameter estimation for scoring protein-ligand interactions using negative training data. **2006**, 49, 5856-68	127
1705	Dehydration of ribonucleotides catalyzed by ribonucleotide reductase: the role of the enzyme. **2006**, 90, 2109-19	45
1704	Enantioselective substrate binding in a monooxygenase protein model by molecular dynamics and docking. **2006**, 91, 3206-16	24
1703	Evaluation of the carbohydrate recognition domain of the bacterial adhesin FimH: Design, synthesis and binding properties of mannoside ligands. **2006**, 4, 3913-22	100
1702	Design, synthesis and biological activity of new CDK4-specific inhibitors, based on fascaplysin. **2006**, 4, 787-801	39
1701	Subtype selectivity and flexibility of ionotropic glutamate receptors upon antagonist ligand binding. **2006**, 4, 1058-70	20
1700	Bioinformatics with soft computing. **2006**, 36, 616-635	63
1699	Synthesis and evaluation of potent, highly-selective, 3-aryl-piperazinone inhibitors of protein geranylgeranyltransferase-I. **2006**, 4, 1768-84	43
1698	Are automated molecular dynamics simulations and binding free energy calculations realistic tools in lead optimization? An evaluation of the linear interaction energy (LIE) method. **2006**, 46, 1972-83	56
1697	SLICK--scoring and energy functions for protein-carbohydrate interactions. **2006**, 46, 1635-42	37
1696	Discovery of small molecule integrin alphavbeta3 antagonists as novel anticancer agents. **2006**, 49, 4526-34	100
1695	Protein-ligand binding affinity predictions by implicit solvent simulations: a tool for lead optimization?. **2006**, 49, 7427-39	85
1694	Genetic algorithm-optimized QSPR models for bioavailability, protein binding, and urinary excretion. **2006**, 46, 2674-83	54
1693	Modification of estrone at the 6, 16, and 17 positions: novel potent inhibitors of 17beta-hydroxysteroid dehydrogenase type 1. **2006**, 49, 1325-45	64
1692	Protein-Ligand Interactions: Computational Docking. **2006**,	
1691	Identification of novel parasitic cysteine protease inhibitors by use of virtual screening. 2. The available chemical directory. **2006**, 49, 1576-84	66

1690	Chapter 15 Structure-Based Design of New Antibacterial Agents. **2006**, 2, 279-295	3
1689	A computer-aided drug discovery system for chemistry teaching. **2006**, 46, 960-70	8
1688	Dual inhibitors of thymidylate synthase and dihydrofolate reductase as antitumor agents: design, synthesis, and biological evaluation of classical and nonclassical pyrrolo[2,3-d]pyrimidine antifolates(1). **2006**, 49, 1055-65	40
1687	A QXP-based multistep docking procedure for accurate prediction of protein-ligand complexes. **2006**, 46, 1174-87	13
1686	Catalytic site prediction and virtual screening of cytochrome P450 2D6 substrates by consideration of water and rescoring in automated docking. **2006**, 49, 2417-30	124
1685	Advances in virtual screening. **2006**, 3, 405-411	87
1684	In silico search of putative adverse drug reaction related proteins as a potential tool for facilitating drug adverse effect prediction. **2006**, 164, 104-12	46
1683	Discovering inhibitors of human sirtuin type 2: novel structural scaffolds. **2006**, 49, 7239-41	48
1682	Molecular evolution of adrenoceptors and dopamine receptors: implications for the binding of catecholamines. **2006**, 49, 1706-19	44
1681	Computational screening of phthalate monoesters for binding to PPARgamma. **2006**, 19, 999-1009	26
1680	In silico prediction of drug binding to CYP2D6: identification of a new metabolite of metoclopramide. **2006**, 34, 1386-92	39
1679	Design of nevirapine derivatives insensitive to the K103N and Y181C HIV-1 reverse transcriptase mutants. **2006**, 17, 183-94	5
1678	Knowledge-based design of target-focused libraries using protein-ligand interaction constraints. **2006**, 49, 490-500	57
1677	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
1676	Protein structures in virtual screening: a case study with CDK2. **2006**, 49, 92-104	45
1675	Structural insights into human 5-lipoxygenase inhibition: combined ligand-based and target-based approach. **2006**, 49, 186-95	40
1674	The influence of variations of ligand protonation and tautomerism on protein-ligand recognition and binding energy landscape. **2006**, 46, 1134-42	14
1673	Comparison of consensus scoring strategies for evaluating computational models of protein-ligand complexes. **2006**, 46, 380-91	119

1672	Finding a needle in a haystack: development of a combinatorial virtual screening approach for identifying high specificity heparin/heparan sulfate sequence(s). **2006**, 49, 3553-62	58
1671	Computational studies of ligand-receptor interactions in bitter taste receptors. **2006**, 26, 611-30	27
1670	A method for induced-fit docking, scoring, and ranking of flexible ligands. Application to peptidic and pseudopeptidic beta-secretase (BACE 1) inhibitors. **2006**, 49, 5885-94	57
1669	In silico-guided target identification of a scaffold-focused library: 1,3,5-triazepan-2,6-diones as novel phospholipase A2 inhibitors. **2006**, 49, 6768-78	62
1668	Bioassay for the identification of natural product-based activators of peroxisome proliferator-activated receptor-gamma (PPARgamma): the marine sponge metabolite psammaplin A activates PPARgamma and induces apoptosis in human breast tumor cells. **2006**, 69, 547-52	39
1667	A novel method to simulate the hydrophobic effect and its application to the ranking of host/guest complexes. **2006**, 46, 2563-73	3
1666	Fatty acid amide hydrolase inhibitors from virtual screening of the endocannabinoid system. **2006**, 49, 4650-6	58
1665	Flexible docking of ligands into synthetic receptors using a two-sided incremental construction algorithm. **2006**, 46, 1695-703	11
1664	Design, synthesis, potency, and cytoselectivity of anticancer agents derived by parallel synthesis from alpha-aminosuberic acid. **2006**, 49, 7611-22	58
1663	N,N'-Bisbenzylidenebenzene-1,4-diamines and N,N'-Bisbenzylidenenaphthalene-1,4-diamines as Sirtuin Type 2 (SIRT2) Inhibitors. **2006**, 49, 7907-11	42
1662	Comparative protein modeling of 1-deoxy-D-xylulose-5-phosphate reductoisomerase enzyme from Plasmodium falciparum: a potential target for antimalarial drug discovery. **2006**, 46, 1360-70	16
1661	Ligand bias of scoring functions in structure-based virtual screening. **2006**, 46, 1334-43	34
1660	The FRB domain of mTOR: NMR solution structure and inhibitor design. **2006**, 45, 10294-302	38
1659	Conformationally constrained analogues of diacylglycerol. 26. Exploring the chemical space surrounding the C1 domain of protein kinase C with DAG-lactones containing aryl groups at the sn-1 and sn-2 positions. **2006**, 49, 3185-203	12
1658	A comparative study on the application of hierarchical-agglomerative clustering approaches to organize outputs of reiterated docking runs. **2006**, 46, 852-62	47
1657	Classification of chemical compounds by protein-compound docking for use in designing a focused library. **2006**, 49, 523-33	35
1656	GFscore: a general nonlinear consensus scoring function for high-throughput docking. **2006**, 46, 1704-12	49
1655	Molecular recognition of an RNA trafficking element by heterogeneous nuclear ribonucleoprotein A2. **2006**, 45, 3943-51	13

1654	Identification of previously unrecognized antiestrogenic chemicals using a novel virtual screening approach. **2006**, 19, 1595-601		36
1653	An Arabidopsis thaliana methyltransferase capable of methylating farnesoic acid. **2006**, 448, 123-32		59
1652	Computational analysis of plasmepsin IV bound to an allophenylnorstatine inhibitor. **2006**, 580, 5910-6		18
1651	A critical assessment of docking programs and scoring functions. **2006**, 49, 5912-31		1258
1650	Extra precision glide: docking and scoring incorporating a model of hydrophobic enclosure for protein-ligand complexes. **2006**, 49, 6177-96		3757
1649	Anthrax lethal factor protease inhibitors: synthesis, SAR, and structure-based 3D QSAR studies. **2006**, 49, 27-30		53
1648	PEARLS: program for energetic analysis of receptor-ligand system. **2006**, 46, 445-50		60
1647	Novel 4-oxo-1,4-dihydroquinoline-3-carboxamide derivatives as new CB2 cannabinoid receptors agonists: synthesis, pharmacological properties and molecular modeling. **2006**, 49, 70-9		71
1646	Structure-based design of spiro-oxindoles as potent, specific small-molecule inhibitors of the MDM2-p53 interaction. **2006**, 49, 3432-5		581
1645	Estrone and estradiol C-16 derivatives as inhibitors of type 1 17beta-hydroxysteroid dehydrogenase. **2006**, 248, 236-8		24
1644	Novel, potent inhibitors of 17beta-hydroxysteroid dehydrogenase type 1. **2006**, 248, 204-7		21
1643	Benzothiazole derivatives as novel inhibitors of human 11beta-hydroxysteroid dehydrogenase type 1. **2006**, 248, 214-7		49
1642	The crystal structure of TrpD, a metabolic enzyme essential for lung colonization by Mycobacterium tuberculosis, in complex with its substrate phosphoribosylpyrophosphate. *Journal of Molecular Biology*, **2006**, 355, 784-97	6.5	37
1641	Interactions in native binding sites cause a large change in protein dynamics. *Journal of Molecular Biology*, **2006**, 358, 213-23	6.5	44
1640	Crystal structure of isoflavone reductase from alfalfa (Medicago sativa L.). *Journal of Molecular Biology*, **2006**, 358, 1341-52	6.5	48
1639	Atomic-Level Rational Drug Design. **2006**, 2, 57-81		4
1638	Studies of Biomacromolecular Structures: Computation and Modeling. **2006**, 249-288		
1637	The Drug Discovery Process. **2006**,		1

1636	Starting point to molecular design: efficient automated 3D model builder Key3D. **2006**, 54, 1680-5	6
1635	Pharmacophores from Macromolecular Complexes with LigandScout. **2006**, 131-150	20
1634	Binding of 7-methoxy-4-(aminomethyl)-coumarin to wild-type and W128F mutant cytochrome P450 2D6 studied by time-resolved fluorescence spectroscopy. **2006**, 393, 635-43	10
1633	The relevance of the Cambridge Structural Database in protein crystallography. **2006**, 558-574	
1632	AClAP, Autonomous hierarchical agglomerative Cluster Analysis based protocol to partition conformational datasets. **2006**, 22, e58-65	37
1631	New cysteine derivatives with antiproliferative activity on melanoma cells. **2006**, 2, 123-32	1
1630	Proteomics. **2006**, 594-654	
1629	Pharmacophore Model Generation Software Tools. **2006**, 15-47	12
1628	Protein□gand docking and structure-based drug design. **2006**,	1
1627	Dock around the Clock □Current Status of Small Molecule Docking and Scoring. **2006**, 25, 605-615	37
1626	Data Pipelines and Virtual Screening: Automating the Process. **2006**, 25, 1181-1191	5
1625	PSI-DOCK: towards highly efficient and accurate flexible ligand docking. **2006**, 62, 934-46	40
1624	De novo ligand design to an ensemble of protein structures. **2006**, 64, 43-59	5
1623	Effective handling of induced-fit motion in flexible docking. **2006**, 63, 878-91	47
1622	ROSETTALIGAND: protein-small molecule docking with full side-chain flexibility. **2006**, 65, 538-48	336
1621	Impact of EGFR point mutations on the sensitivity to gefitinib: insights from comparative structural analyses and molecular dynamics simulations. **2006**, 65, 331-46	49
1620	Complementarity of hydrophobic properties in ATP-protein binding: a new criterion to rank docking solutions. **2007**, 66, 388-98	18
1619	Critical evaluation of methods to incorporate entropy loss upon binding in high-throughput docking. **2007**, 66, 422-35	20

1618	Ligand-supported homology modeling of the human angiotensin II type 1 (AT(1)) receptor: insights into the molecular determinants of telmisartan binding. **2006**, 65, 824-42	24
1617	Characterization of SCP-2 from Euphorbia lagascae reveals that a single Leu/Met exchange enhances sterol transfer activity. **2006**, 273, 5641-55	13
1616	Investigation of potential glycogen synthase kinase 3 inhibitors using pharmacophore mapping and virtual screening. **2006**, 68, 154-65	10
1615	Action mechanisms and structure-activity relationships of PI3Kgamma inhibitors on the enzyme: a molecular modeling study. **2006**, 41, 558-65	8
1614	Solid-phase synthesis and pharmacological evaluation of a library of peptidomimetics as potential farnesyltransferase inhibitors: an approach to new lead compounds. **2006**, 41, 745-55	15
1613	Design, synthesis, and biological evaluation of substituted 2,3-dihydro-1H-cyclopenta[b]quinolin-9-ylamine related compounds as fructose-1,6-bisphosphatase inhibitors. **2006**, 14, 7846-53	7
1612	Investigation of mechanism-based thrombin inhibitors: Implications of a highly conserved water molecule for the binding of coumarins within the S pocket. **2006**, 16, 2017-21	23
1611	Thiazolo[5,4-f]quinazolin-9-ones, inhibitors of glycogen synthase kinase-3. **2006**, 16, 3419-23	51
1610	In silico identification and biochemical characterization of novel inhibitors of NQO1. **2006**, 16, 6246-54	29
1609	Structure-based virtual screening of chemical libraries for drug discovery. **2006**, 10, 194-202	182
1608	Streamlining lead discovery by aligning in silico and high-throughput screening. **2006**, 10, 343-51	74
1607	Binding properties of HABA-type azo derivatives to avidin and avidin-related protein 4. **2006**, 13, 1029-39	32
1606	A monoselective sphingosine-1-phosphate receptor-1 agonist prevents allograft rejection in a stringent rat heart transplantation model. **2006**, 13, 1227-34	110
1605	Tribe-PSO: A novel global optimization algorithm and its application in molecular docking. **2006**, 82, 248-259	41
1604	Structural study of two proteins SigE and ORF1 to predict their roles in the biochemical oxidation of sulfur anions via the global sulfur oxidation operon (sox). **2006**, 30, 227-32	2
1603	Two- and three-dimensional quantitative structure-activity relationships for a series of purine nucleoside phosphorylase inhibitors. **2006**, 14, 516-27	47
1602	Structure-based design of isoquinoline-5-sulfonamide inhibitors of protein kinase B. **2006**, 14, 1255-73	37
1601	An evaluation of automated in silico ligand docking of amino acid ligands to Family C G-protein coupled receptors. **2006**, 14, 2032-9	16

1600	Macrocyclic inhibitors of the malarial aspartic proteases plasmepsin I, II, and IV. **2006**, 14, 2197-208	37
1599	New leads of metallo-beta-lactamase inhibitors from structure-based pharmacophore design. **2006**, 14, 2627-35	45
1598	3D-QSAR and docking studies of aldehyde inhibitors of human cathepsin K. **2006**, 14, 2771-8	15
1597	Mining the NCI antiviral compounds for HIV-1 integrase inhibitors. **2006**, 14, 3785-92	29
1596	Binding mode of new (thio)hydantoin inhibitors of fatty acid amide hydrolase: comparison with two original compounds, OL-92 and JP104. **2006**, 16, 4772-6	13
1595	Tools for building a comprehensive modeling system for virtual screening under real biological conditions: The Computational Titration algorithm. **2006**, 24, 434-9	16
1594	Multiple target screening method for robust and accurate in silico ligand screening. **2006**, 25, 61-70	24
1593	Investigating interactions between HIV-1 gp41 and inhibitors by molecular dynamics simulation and MMPBSA/GBSA calculations. **2006**, 766, 77-82	20
1592	Antitumor activity of ZSTK474, a new phosphatidylinositol 3-kinase inhibitor. **2006**, 98, 545-56	320
1591	Adenosine mimetics as inhibitors of NAD+-dependent histone deacetylases, from kinase to sirtuin inhibition. **2006**, 49, 7307-16	140
1590	MolDock: a new technique for high-accuracy molecular docking. **2006**, 49, 3315-21	1473
1589	Small-molecule inhibitors of the MDM2-p53 protein-protein interaction based on an isoindolinone scaffold. **2006**, 49, 6209-21	124
1588	Knowledge-based interaction fingerprint scoring: a simple method for improving the effectiveness of fast scoring functions. **2006**, 46, 686-98	65
1587	Bioinformatics platform development: from gene to lead compound. **2006**, 316, 389-431	14
1586	Biological evaluation, chelation, and molecular modeling studies of novel metal-chelating inhibitors of NF-kappaB-DNA binding: structure activity relationships. **2006**, 49, 3595-601	17
1585	The design and synthesis of inhibitors of pantothenate synthetase. **2006**, 4, 3598-610	40
1584	Discovery of two novel, small-molecule inhibitors of DNA methylation. **2006**, 49, 678-83	119
1583	A novel, highly selective inhibitor of pestivirus replication that targets the viral RNA-dependent RNA polymerase. **2006**, 80, 149-60	72

1582	New leads for selective GSK-3 inhibition: pharmacophore mapping and virtual screening studies. **2006**, 20, 55-66	18
1581	Comparison of a homology model and the crystallographic structure of human 11beta-hydroxysteroid dehydrogenase type 1 (11betaHSD1) in a structure-based identification of inhibitors. **2006**, 20, 67-81	16
1580	Permuting input for more effective sampling of 3D conformer space. **2006**, 20, 179-90	8
1579	Electrostatic evaluation of isosteric analogues. **2006**, 20, 191-208	7
1578	A virtual active compound produced from the negative image of a ligand-binding pocket, and its application to in-silico drug screening. **2006**, 20, 237-48	8
1577	Development and validation of a modular, extensible docking program: DOCK 5. **2006**, 20, 601-19	325
1576	A combined ligand-based and target-based drug design approach for G-protein coupled receptors: application to salvinorin A, a selective kappa opioid receptor agonist. **2006**, 20, 471-93	34
1575	Investigation of the binding mode of (-)-meptazinol and bis-meptazinol derivatives on acetylcholinesterase using a molecular docking method. **2006**, 12, 390-7	18
1574	Structure-based 3D-QSAR studies on thiazoles as 5-HT3 receptor antagonists. **2007**, 13, 121-31	8
1573	Molecular docking studies on 4-thiazolidinones as HIV-1 RT inhibitors. **2007**, 13, 155-61	17
1572	The estrogen receptor and polyphenols: molecular simulation studies of their interactions, a review. **2006**, 4, 159-174	19
1571	Virtual ligand screening: strategies, perspectives and limitations. **2006**, 11, 580-94	543
1570	Shape Signatures: speeding up computer aided drug discovery. **2006**, 11, 895-904	26
1569	scyllo-inositol pentakisphosphate as an analogue of myo-inositol 1,3,4,5,6-pentakisphosphate: chemical synthesis, physicochemistry and biological applications. **2006**, 7, 1114-22	20
1568	An iterative knowledge-based scoring function to predict protein-ligand interactions: II. Validation of the scoring function. **2006**, 27, 1876-82	122
1567	Discovery and structure-activity relationship studies of a unique class of HIV-1 integrase inhibitors. **2006**, 1, 238-44	12
1566	Focused libraries of 16-substituted estrone derivatives and modified e-ring steroids: inhibitors of 17beta-hydroxysteroid dehydrogenase type 1. **2006**, 1, 464-81	34
1565	Modeling of Cdc25B dual specifity protein phosphatase inhibitors: docking of ligands and enzymatic inhibition mechanism. **2006**, 1, 540-50	54

1564	Automated protein-ligand crystallography for structure-based drug design. **2006**, 1, 827-38	74
1563	Arylthiopyrrole (AThP) derivatives as non-nucleoside HIV-1 reverse transcriptase inhibitors: synthesis, structure-activity relationships, and docking studies (part 1). **2006**, 1, 1367-78	30
1562	Arylthiopyrrole (AThP) derivatives as non-nucleoside HIV-1 reverse transcriptase inhibitors: synthesis, structure-activity relationships, and docking studies (part 2). **2006**, 1, 1379-90	11
1561	Virtual screening for PPAR modulators using a probabilistic neural network. **2006**, 1, 1346-50	17
1560	Combining docking and molecular dynamic simulations in drug design. **2006**, 26, 531-68	453
1559	Chapter 16 Recent Evaluations of High Throughput Docking Methods for Pharmaceutical Lead Finding Consensus and Caveats. **2006**, 2, 297-323	6
1558	Prediction of protein-protein interaction based on structure. **2006**, 340, 207-34	10
1557	Molecular Modeling Studies of Estrogen Receptor Modulators. **2006**, 2, 229-253	1
1556	Multi-objective optimisation of the protein-ligand docking problem in drug discovery. **2006**,	8
1555	Ligand Docking and Virtual Screening in Structure-based Drug Discovery. **2006**,	3
1554	3D structure of Thermus aquaticus single-stranded DNA-binding protein gives insight into the functioning of SSB proteins. **2006**, 34, 6708-17	30
1553	Estrogen receptors: molecular interactions, virtual screening and future prospects. **2006**, 6, 217-43	27
1552	Insights into drug metabolism from modelling studies of cytochrome P450-drug interactions. **2006**, 6, 1619-26	5
1551	Receptor-based computational screening of compound databases: the main docking-scoring engines. **2006**, 7, 369-93	40
1550	A pseudo-ligand approach to virtual screening. **2006**, 9, 359-64	15
1549	Scoring functions for protein-ligand docking. **2006**, 7, 407-20	168
1548	eHiTS: an innovative approach to the docking and scoring function problems. **2006**, 7, 421-35	121
1547	Acetylcholinesterase: molecular modeling with the whole toolkit. **2006**, 6, 57-73	19

1546	Drug binding interactions in the inner cavity of HERG channels: molecular insights from structure-activity relationships of clofilium and ibutilide analogs. **2006**, 69, 509-19	72
1545	Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. **2006**, 1986-1990	
1544	Structure-activity relationships by interligand NOE-based design and synthesis of antiapoptotic compounds targeting Bid. **2006**, 103, 12602-6	81
1543	Chapter 10 Cytochrome P450 Enzymes: Computational Approaches to Substrate Prediction. **2006**, 2, 171-195	3
1542	Determination of binding site residues responsible for the subunit selectivity of novel marine-derived compounds on kainate receptors. **2006**, 69, 1849-60	28
1541	Inhibition of RET tyrosine kinase by SU5416. **2006**, 37, 199-212	62
1540	Function and structure of the molybdenum cofactor carrier protein from Chlamydomonas reinhardtii. **2006**, 281, 30186-94	50
1539	In silico and in vitro screening for inhibition of cytochrome P450 CYP3A4 by comedications commonly used by patients with cancer. **2006**, 34, 534-8	50
1538	Probing the reorganization of the nicotinic acetylcholine receptor during desensitization by time-resolved covalent labeling using [3H]AC5, a photoactivatable agonist. **2006**, 69, 452-61	22
1537	Partial agonism, neutral antagonism, and inverse agonism at the human wild-type and constitutively active cholecystokinin-2 receptors. **2006**, 69, 680-90	19
1536	4SCan/vADME: intelligent library screening as a shortcut from hits to lead compounds. **2006**, 2, 471-84	6
1535	Incorporating protein flexibility into docking and structure-based drug design. **2006**, 1, 335-49	26
1534	Computer-aided molecular design of highly potent HIV-1 RT inhibitors: 3D QSAR and molecular docking studies of efavirenz derivatives. **2006**, 17, 353-70	12
1533	Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. **2006**, 1983-1986	
1532	PLANTS: Application of Ant Colony Optimization to Structure-Based Drug Design. **2006**, 247-258	110
1531	Receptor-binding sites: bioinformatic approaches. **2006**, 316, 291-358	1
1530	Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. **2006**, 1991-1991	
1529	Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. **2006**, 1991-1991	

1528	Homology modelling of the serotoninergic 5-HT2c receptor. **2006**, 21, 285-92	9
1527	Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine. **2006**, 1976-1976	0
1526	High throughput in-silico screening of large ligand databases for rational drug design. **2006**, 179-189	
1525	Structure-Based Drug Discovery. **2007**,	23
1524	An acetylation/deacetylation-SUMOylation switch through a phylogenetically conserved psiKXEP motif in the tumor suppressor HIC1 regulates transcriptional repression activity. **2007**, 27, 2661-75	132
1523	Crystal structure of the heme-IsdC complex, the central conduit of the Isd iron/heme uptake system in Staphylococcus aureus. **2007**, 282, 10625-31	97
1522	Critical role of desolvation in the binding of 20-hydroxyecdysone to the ecdysone receptor. **2007**, 282, 32924-34	60
1521	Differential helical orientations among related G protein-coupled receptors provide a novel mechanism for selectivity. Studies with salvinorin A and the kappa-opioid receptor. **2007**, 282, 3146-56	27
1520	The structure of the R184A mutant of the inositol monophosphatase encoded by suhB and implications for its functional interactions in Escherichia coli. **2007**, 282, 26989-26996	19
1519	Matrix metalloproteinase inhibitors: new challenges in the era of post broad-spectrum inhibitors. **2007**, 13, 2087-100	97
1518	Molecular modeling-guided site-directed mutagenesis of cytochrome P450 2D6. **2007**, 8, 59-77	39
1517	Computational identification of inhibitors of protein-protein interactions. **2007**, 7, 63-82	77
1516	Ab Initio potential grid based docking: From High Performance Computing to In Silico Screening. **2007**,	2
1515	Structure-based approaches in the design of GSK-3 selective inhibitors. **2007**, 8, 352-64	22
1514	Pharmacophore modeling in drug discovery and development: an overview. **2007**, 3, 187-97	93
1513	Ligand docking and structure-based virtual screening in drug discovery. **2007**, 7, 1006-14	203
1512	ParDOCK: an all atom energy based Monte Carlo docking protocol for protein-ligand complexes. **2007**, 14, 632-46	103
1511	From drug target to leads--sketching a physicochemical pathway for lead molecule design in silico. **2007**, 13, 3454-70	52

1510	AmineDB: large scale docking of amines with CYP2D6 and scoring for druglike properties--towards defining the scope of the chemical defense against foreign amines in humans. **2007**, 37, 221-45	9
1509	Classification and Prediction of Tripeptides Inhibiting HIV-1 Tat/TAR-RNA Interaction Using a Self-Organizing Map. **2007**, 4, 410-416	
1508	Structure-based drug design: docking and scoring. **2007**, 8, 312-28	228
1507	Virtual screening in drug discovery -- a computational perspective. **2007**, 8, 329-51	219
1506	Fragment-based drug discovery: what has it achieved so far?. **2007**, 7, 1544-67	62
1505	Molecular modeling and site-directed mutagenesis reveal the benzylisoquinoline binding site of the short-chain dehydrogenase/reductase salutaridine reductase. **2007**, 143, 1493-503	19
1504	The Cambridge Crystallographic Database. **2007**, 389-410	2
1503	IN SILICO DESIGN OF LIGANDS USING PROPERTIES OF TARGET ACTIVE SITES. **2007**, 183-201	
1502	High throughput crystallography of TB drug targets. **2007**, 7, 127-39	42
1501	Structural Information and Computational Methods Used in Design of Neuraminidase Inhibitors. **2007**, 3, 113-132	2
1500	Computer-Aided Drug Design: Integration of Structure-Based and Ligand-Based Approaches in Drug Design. **2007**, 3, 133-148	29
1499	Handbook of Neurochemistry and Molecular Neurobiology. **2007**,	2
1498	Structural features of a cold-adapted Alaskan bacterial lipase. **2007**, 24, 463-70	12
1497	Protein□igand Docking with Evolutionary Algorithms. 167-195	1
1496	A second receptor binding site on human parainfluenza virus type 3 hemagglutinin-neuraminidase contributes to activation of the fusion mechanism. **2007**, 81, 3216-28	78
1495	Structurally unique inhibitors of human mitogen-activated protein kinase phosphatase-1 identified in a pyrrole carboxamide library. **2007**, 322, 940-7	22
1494	Structures of Mycobacterium tuberculosis 1-deoxy-D-xylulose-5-phosphate reductoisomerase provide new insights into catalysis. **2007**, 282, 19905-16	67
1493	Quantum Mechanical Calculations in Medicinal Chemistry: Relevant Method or a Quantum Leap Too Far?. **2007**, 379-420	3

1492	Classification and Learning Using Genetic Algorithms. **2007**,		4
1491	"Plate cherry picking": a novel semi-sequential screening paradigm for cheaper, faster, information-rich compound selection. **2007**, 12, 320-7		33
1490	New Applications for Structure-Based Drug Design. **2007**, 775-806		0
1489	[Docking method for drug discovery]. **2007**, 127, 113-22		4
1488	Computational Studies of HIV-1 Integrase and its Inhibitors. **2007**, 3, 160-190		7
1487	Strategies for developing protein tyrosine phosphatase inhibitors. **2007**, 42, 250-60		42
1486	Dual aromatase-sulfatase inhibitors based on the anastrozole template: synthesis, in vitro SAR, molecular modelling and in vivo activity. **2007**, 5, 2940-52		50
1485	Synthesis and pharmacological characterization of N3-substituted willardiine derivatives: role of the substituent at the 5-position of the uracil ring in the development of highly potent and selective GLUK5 kainate receptor antagonists. **2007**, 50, 1558-70		58
1484	Mechanism-based thrombin inhibitors: design, synthesis, and molecular docking of a new selective 2-oxo-2H-1-benzopyran derivative. **2007**, 50, 3645-50		27
1483	Diverse, high-quality test set for the validation of protein-ligand docking performance. **2007**, 50, 726-41		451
1482	Evaluations of molecular docking programs for virtual screening. **2007**, 47, 1609-18		95
1481	Ensemble modeling of substrate binding to cytochromes P450: analysis of catalytic differences between CYP1A orthologs. **2007**, 46, 2640-54		44
1480	Identification of a novel competitive inhibitor of p38alpha MAPK by a human PBMC screen. **2007**, 352, 656-61		2
1479	Synthesis, biological testing, and binding mode prediction of 6,9-diarylpurin-8-ones as p38 MAP kinase inhibitors. **2007**, 50, 2060-6		23
1478	Study on the binding of Thioflavin T to beta-sheet-rich and non-beta-sheet cavities. **2007**, 158, 358-69		194
1477	Inhibition of human and rat 11beta-hydroxysteroid dehydrogenase type 1 by 18beta-glycyrrhetinic acid derivatives. **2007**, 104, 312-20		21
1476	Novel non-steroidal inhibitors of human 11beta-hydroxysteroid dehydrogenase type 1. **2007**, 104, 123-9		29
1475	A structural comparison of inhibitor binding to PKB, PKA and PKA-PKB chimera. *Journal of Molecular Biology*, **2007**, 367, 882-94	6.5	70

1474	Crystal structure of vestitone reductase from alfalfa (Medicago sativa L.). *Journal of Molecular Biology*, **2007**, 369, 265-76	6.5	27
1473	Crystal structure of Medicago truncatula UGT85H2--insights into the structural basis of a multifunctional (iso)flavonoid glycosyltransferase. *Journal of Molecular Biology*, **2007**, 370, 951-63	6.5	136
1472	A model for how ribosomal release factors induce peptidyl-tRNA cleavage in termination of protein synthesis. **2007**, 27, 758-66		72
1471	Crystal structure of calf spleen purine nucleoside phosphorylase complexed to a novel purine analogue. **2007**, 581, 5082-6		9
1470	X-ray structure of the PHF core C-terminus: insight into the folding of the intrinsically disordered protein tau in Alzheimer's disease. **2007**, 581, 5872-8		17
1469	Enantiomeric separation of 2-aryloxyalkyl- and 2-arylalkyl-2-aryloxyacetic acids on a Penicillin G Acylase-based chiral stationary phase: influence of the chemical structure on retention and enantioselectivity. **2007**, 45, 211-8		11
1468	Multi-target-directed drug design strategy: from a dual binding site acetylcholinesterase inhibitor to a trifunctional compound against Alzheimer's disease. **2007**, 50, 6446-9		225
1467	Fluorescently labeled analogues of dofetilide as high-affinity fluorescence polarization ligands for the human ether-a-go-go-related gene (hERG) channel. **2007**, 50, 2931-41		41
1466	An oxazole-based small-molecule Stat3 inhibitor modulates Stat3 stability and processing and induces antitumor cell effects. **2007**, 2, 787-98		150
1465	Target-based approach to inhibitors of histone arginine methyltransferases. **2007**, 50, 2319-25		124
1464	Improving Docking Accuracy through Molecular Mechanics Generalized Born Optimization and Scoring. **2007**, 3, 1106-19		43
1463	Free Energy Calculations. **2007**,		592
1462	Statistical prediction of protein chemical interactions based on chemical structure and mass spectrometry data. **2007**, 23, 2004-12		73
1461	Alternative to consensus scoring--a new approach toward the qualitative combination of docking algorithms. **2007**, 47, 1036-44		23
1460	Structure-based virtual screening of FGFR inhibitors: cross-decoys and induced-fit effect. **2007**, 21, 31-45		10
1459	Difluoro analogue of UCS15A triggers activation of exogenously expressed c-Src in HCT 116 human colorectal carcinoma cells. **2007**, 22, 638-46		2
1458	Application of fragment screening by X-ray crystallography to beta-secretase. **2007**, 50, 1116-23		139
1457	GlamDock: development and validation of a new docking tool on several thousand protein-ligand complexes. **2007**, 47, 1657-72		53

1456	Analysis of human carbonic anhydrase II: docking reliability and receptor-based 3D-QSAR study. **2007**, 47, 515-25	34
1455	Lessons in molecular recognition. 2. Assessing and improving cross-docking accuracy. **2007**, 47, 2293-302	104
1454	Impact of ligand protonation on virtual screening against beta-secretase (BACE1). **2007**, 47, 2366-73	34
1453	Design of inhibitors of the MurF enzyme of Streptococcus pneumoniae using docking, 3D-QSAR, and de Novo design. **2007**, 47, 1839-46	19
1452	Human pregnane X receptor antagonists and agonists define molecular requirements for different binding sites. **2007**, 72, 592-603	126
1451	Novel, customizable scoring functions, parameterized using N-PLS, for structure-based drug discovery. **2007**, 47, 85-91	21
1450	Docking of ATP to Ca-ATPase: considering protein domain motions. **2007**, 47, 1171-81	8
1449	Comparative performance of several flexible docking programs and scoring functions: enrichment studies for a diverse set of pharmaceutically relevant targets. **2007**, 47, 1599-608	128
1448	Design, synthesis, and characterization of a potent, nonpeptide, cell-permeable, bivalent Smac mimetic that concurrently targets both the BIR2 and BIR3 domains in XIAP. **2007**, 129, 15279-94	175
1447	Homology modeling and receptor-based 3D-QSAR study of carbonic anhydrase IX. **2007**, 47, 2253-62	23
1446	A multivariate approach to investigate docking parameters' effects on docking performance. **2007**, 47, 1673-87	17
1445	Supervised scoring models with docked ligand conformations for structure-based virtual screening. **2007**, 47, 1858-67	9
1444	Validation studies of the site-directed docking program LibDock. **2007**, 47, 2159-71	198
1443	Identification of hot spots within druggable binding regions by computational solvent mapping of proteins. **2007**, 50, 1231-40	118
1442	Active site of epoxide hydrolases revisited: a noncanonical residue in potato StEH1 promotes both formation and breakdown of the alkylenzyme intermediate. **2007**, 46, 2466-79	19
1441	Prediction of the Structure of Complexes Comprised of Proteins and Glycosaminoglycans Using Docking Simulation and Cluster Analysis. **2007**, 3, 2347-56	12
1440	Fast approaches for molecular polarizability calculations. **2007**, 111, 4443-8	56
1439	Conformational study of (8alpha,8'beta)-bis(substituted phenyl)-lignano-9,9'-lactones by means of combined computational, database mining, NMR, and chemometric approaches. **2007**, 111, 6316-33	5

1438	Homology modeling of human Fyn kinase structure: discovery of rosmarinic acid as a new Fyn kinase inhibitor and in silico study of its possible binding modes. **2007**, 50, 1090-100	34
1437	An Introduction To Chemoinformatics. **2007**,	191
1436	Computational Methods for Protein Structure Prediction and Modeling. **2007**,	5
1435	Crystal Structures of Toxicology Targets. 469-519	1
1434	Homology Models Applied to Toxicology. 433-468	
1433	In-Silico docking of HIV-1 integrase inhibitors reveals a novel drug type acting on an enzyme/DNA reaction intermediate. **2007**, 4, 21	59
1432	A flexible approach to induced fit docking. **2007**, 50, 6507-18	142
1431	Supervised consensus scoring for docking and virtual screening. **2007**, 47, 526-34	82
1430	New pyrrole inhibitors of monoamine oxidase: synthesis, biological evaluation, and structural determinants of MAO-A and MAO-B selectivity. **2007**, 50, 922-31	106
1429	Multistructure 3D-QSAR studies on a series of conformationally constrained butyrophenones docked into a new homology model of the 5-HT2A receptor. **2007**, 50, 3242-55	19
1428	Identification of critical residues in novel drug metabolizing mutants of cytochrome P450 BM3 using random mutagenesis. **2007**, 50, 455-61	95
1427	A common reference framework for analyzing/comparing proteins and ligands. Fingerprints for Ligands and Proteins (FLAP): theory and application. **2007**, 47, 279-94	342
1426	GPCR structure-based virtual screening approach for CB2 antagonist search. **2007**, 47, 1626-37	94
1425	Novel class of quinone-bearing polyamines as multi-target-directed ligands to combat Alzheimer's disease. **2007**, 50, 4882-97	113
1424	Extensive SAR and computational studies of 3-{4-[(benzylmethylamino)methyl]phenyl}-6,7-dimethoxy-2H-2-chromenone (AP2238) derivatives. **2007**, 50, 4250-4	72
1423	Docking and Scoring. **2007**, 255-281	
1422	Structural, Energetic, and Dynamic Aspects of Ligand−Receptor Interactions. **2007**, 193-213	5
1421	Virtual Screening. **2007**, 459-494	2

1420	Structure-guided design of β-secretase (BACE-1) inhibitors. **2007**, 2, 1129-38	9
1419	A Fragment-Based Scoring Function to Re-rank ATP Docking Results. **2007**, 8, 1083-1094	5
1418	Chemoinformatics. **2007**, 235-264	1
1417	Computer-Aided Molecular Diversity Analysis and Combinatorial Library Design. **2007**, 1-51	15
1416	. **2007**,	11
1415	Computational Modeling of Receptor-Mediated Toxicity. 315-351	1
1414	. **2007**,	19
1413	Tetrabromocinnamic acid (TBCA) and related compounds represent a new class of specific protein kinase CK2 inhibitors. **2007**, 8, 129-39	104
1412	Scaffold hopping by "fuzzy" pharmacophores and its application to RNA targets. **2007**, 8, 1932-6	41
1411	Improved cyclodextrin-based receptors for camptothecin by inverse virtual screening. **2007**, 13, 6801-9	53
1410	How reliable are current docking approaches for structure-based drug design? Lessons from aldose reductase. **2007**, 46, 3575-8	41
1409	Identification of novel allosteric regulators of human-erythrocyte pyruvate kinase. **2007**, 4, 2603-17	4
1408	Wie verlässlich sind aktuelle Docking-Ansätze für strukturbasiertes Wirkstoffdesign? Fallstudie zur Aldose-Reduktase. **2007**, 119, 3645-3649	
1407	Molecular Docking and Structure-Based Design. 1-23	0
1406	Recent Advances in Drug Discovery Research Using Structure-Based Virtual Screening Techniques: Examples of Success for Diverse Protein Targets. 24-62	
1405	Virtual Screening in Drug Discovery. 63-88	4
1404	Computer-Aided Drug Design. 89-107	3
1403	SODOCK: swarm optimization for highly flexible protein-ligand docking. **2007**, 28, 612-23	96

1402	Role of binding entropy in the refinement of protein-ligand docking predictions: analysis based on the use of 11 scoring functions. **2007**, 28, 1364-72	44
1401	Derivatives of Iressa, a specific epidermal growth factor receptor inhibitor, are powerful apoptosis inducers in PC3 prostatic cancer cells. **2007**, 2, 318-32	13
1400	Nanomolar inhibition of type II dehydroquinase based on the enolate reaction mechanism. **2007**, 2, 101-12	23
1399	Nanomolar competitive inhibitors of Mycobacterium tuberculosis and Streptomyces coelicolor type II dehydroquinase. **2007**, 2, 194-207	24
1398	Inhibition of Bcr-Abl phosphorylation and induction of apoptosis by pyrazolo[3,4-d]pyrimidines in human leukemia cells. **2007**, 2, 343-53	25
1397	Structure-activity studies on suramin analogues as inhibitors of NAD+-dependent histone deacetylases (sirtuins). **2007**, 2, 1419-31	163
1396	Rational design, synthesis, and evaluation of nanomolar type II dehydroquinase inhibitors. **2007**, 2, 1015-29	28
1395	Exploration of the binding mode of indanesulfonamides as selective inhibitors of human carbonic anhydrase type VII by targeting Lys 91. **2007**, 2, 1273-80	22
1394	Design, synthesis, and structural studies on potent biaryl inhibitors of type II dehydroquinases. **2007**, 2, 1010-3	21
1393	Chemical medicine: novel 10-substituted cytisine derivatives with increased selectivity for alpha4beta2 nicotinic acetylcholine receptors. **2007**, 2, 1157-61	23
1392	Role of water molecules for binding inhibitors in the SH2 domain of Grb2: A molecular dynamics study. **2007**, 806, 51-66	11
1391	Identification of some novel AHAS inhibitors via molecular docking and virtual screening approach. **2007**, 15, 374-80	31
1390	Prodrug-based design, synthesis, and biological evaluation of N-benzenesulfonylpiperidine derivatives as novel, orally active factor Xa inhibitors. **2007**, 15, 4175-92	11
1389	Explaining cyclodextrin-mycotoxin interactions using a 'natural' force field. **2007**, 15, 4585-94	29
1388	Discovery of structurally diverse HIV-1 integrase inhibitors based on a chalcone pharmacophore. **2007**, 15, 4985-5002	117
1387	The 1,4-naphthoquinone scaffold in the design of cysteine protease inhibitors. **2007**, 15, 5340-50	30
1386	Identification of novel chemical inhibitors for ubiquitin C-terminal hydrolase-L3 by virtual screening. **2007**, 15, 6810-8	41
1385	Virtual screening and bioassay study of novel inhibitors for dengue virus mRNA cap (nucleoside-2'O)-methyltransferase. **2007**, 15, 7795-802	66

1384	Synthesis, biological evaluation and molecular modelling of sulfonohydrazides as selective PI3K p110alpha inhibitors. **2007**, 15, 7677-87	49
1383	Inhibitors of the FEZ-1 metallo-beta-lactamase. **2007**, 17, 964-8	27
1382	Modifications of the GSK3beta substrate sequence to produce substrate-mimetic inhibitors of Akt as potential anti-cancer therapeutics. **2007**, 17, 2068-73	21
1381	Isoform selective inhibition of STAT1 or STAT3 homo-dimerization via peptidomimetic probes: structural recognition of STAT SH2 domains. **2007**, 17, 1875-8	49
1380	Ligand based virtual screening and biological evaluation of inhibitors of chorismate mutase (Rv1885c) from Mycobacterium tuberculosis H37Rv. **2007**, 17, 3053-8	38
1379	N-4-Pyrimidinyl-1H-indazol-4-amine inhibitors of Lck: indazoles as phenol isosteres with improved pharmacokinetics. **2007**, 17, 4363-8	35
1378	Docking-based 3D-QSAR study for selectivity of DPP4, DPP8, and DPP9 inhibitors. **2007**, 17, 3716-21	23
1377	A novel arginine methyltransferase inhibitor with cellular activity. **2007**, 17, 4150-3	93
1376	Evaluation of broad spectrum protein kinase inhibitors to probe the architecture of the malarial cyclin dependent protein kinase Pfmrk. **2007**, 17, 4961-6	20
1375	Identifying common metalloprotease inhibitors by protein fold types using Fourier transform mass spectrometry. **2007**, 17, 6521-4	5
1374	Identification of potential glycogen kinase-3 inhibitors by structure based virtual screening. **2007**, 128, 165-75	19
1373	In-silico drug screening method based on the protein-compound affinity matrix using the factor selection technique. **2007**, 42, 966-76	1
1372	Structure-based 3D-QSAR studies on heteroarylpiperazine derivatives as 5-HT3 receptor antagonists. **2007**, 42, 977-84	4
1371	The consequences of scoring docked ligand conformations using free energy correlations. **2007**, 42, 921-33	52
1370	3D-QSAR and molecular docking study on bisarylmaleimide series as glycogen synthase kinase 3, cyclin dependent kinase 2 and cyclin dependent kinase 4 inhibitors: an insight into the criteria for selectivity. **2007**, 42, 1014-27	36
1369	Fragment-based screening using X-ray crystallography and NMR spectroscopy. **2007**, 11, 485-93	137
1368	Virtual screening strategies in drug discovery. **2007**, 11, 494-502	301
1367	A high-throughput screening approach to anthrax lethal factor inhibition. **2007**, 35, 306-12	26

1366	Discovering new inhibitors of bacterial glucosamine-6P synthase (GlmS) by docking simulations. **2007**, 17, 1966-70	17
1365	Finding ligands for G protein-coupled receptors based on the protein-compound affinity matrix. **2007**, 25, 633-43	6
1364	eHiTS: a new fast, exhaustive flexible ligand docking system. **2007**, 26, 198-212	190
1363	Exploring ligand recognition and ion flow in comparative models of the human GABA type A receptor. **2007**, 26, 760-74	29
1362	A Quantitative Approach to the Estimation of Chemical Space from a Given Geometry by the Combination of Atomic Species. **2007**, 26, 596-607	17
1361	Three-Dimensional Quantitative Structure−Activity Relationship of MT3 Melatonin Binding Site Ligands: A Comparative Molecular Field Analysis. **2007**, 26, 820-827	3
1360	Accounting for ligand-bound metal ions in docking small molecules on adenylyl cyclase toxins. **2007**, 67, 593-605	53
1359	EADock: docking of small molecules into protein active sites with a multiobjective evolutionary optimization. **2007**, 67, 1010-25	131
1358	Accuracy of binding mode prediction with a cascadic stochastic tunneling method. **2007**, 68, 195-204	13
1357	Drug block of the hERG potassium channel: insight from modeling. **2007**, 68, 568-80	87
1356	Structure-based virtual ligand screening with LigandFit: pose prediction and enrichment of compound collections. **2007**, 68, 712-25	41
1355	Protein-inhibitor flexible docking by a multicanonical sampling: native complex structure with the lowest free energy and a free-energy barrier distinguishing the native complex from the others. **2008**, 70, 41-53	40
1354	Evaluation of docking programs for predicting binding of Golgi alpha-mannosidase II inhibitors: a comparison with crystallography. **2007**, 69, 160-76	49
1353	QM/MM linear response method distinguishes ligand affinities for closely related metalloproteins. **2007**, 69, 326-39	23
1352	Modeling of metal interaction geometries for protein-ligand docking. **2008**, 71, 1237-54	50
1351	Crystallographic and computational studies on 4-phenyl-N-(beta-D-glucopyranosyl)-1H-1,2,3-triazole-1-acetamide, an inhibitor of glycogen phosphorylase: comparison with alpha-D-glucose, N-acetyl-beta-D-glucopyranosylamine and N-benzoyl-N'-beta-D-glucopyranosyl urea binding. **2008**, 71, 1307-23	24
1350	ICAM-1 peptide inhibitors of T-cell adhesion bind to the allosteric site of LFA-1. An NMR characterization. **2007**, 70, 347-53	19
1349	Signposts of docking and scoring in drug design. **2007**, 70, 360-5	6

1348	pso@autodock: a fast flexible molecular docking program based on Swarm intelligence. **2007**, 70, 475-84	79
1347	Molecular docking and 3D-QSAR studies of 2-substituted 1-indanone derivatives as acetylcholinesterase inhibitors. **2007**, 28, 2053-63	25
1346	In silico panning for a non-competitive peptide inhibitor. **2007**, 8, 11	21
1345	Scoring functions and enrichment: a case study on Hsp90. **2007**, 8, 27	9
1344	Setting up a large set of protein-ligand PDB complexes for the development and validation of knowledge-based docking algorithms. **2007**, 8, 310	11
1343	Adaptive evolution of multiple-variable exons and structural diversity of drug-metabolizing enzymes. **2007**, 7, 69	31
1342	Coumarin-based inhibitors of human NAD(P)H:quinone oxidoreductase-1. Identification, structure-activity, off-target effects and in vitro human pancreatic cancer toxicity. **2007**, 50, 6316-25	56
1341	Dual aromatase-steroid sulfatase inhibitors. **2007**, 50, 3540-60	72
1340	Nuclear magnetic resonance fragment-based identification of novel FKBP12 inhibitors. **2007**, 50, 6607-17	21
1339	Computational study of glyceraldehyde-3-phosphate dehydrogenase of Entamoeba histolytica: implications for structure-based drug design. **2007**, 25, 25-33	7
1338	3D Structure and the Drug Discovery Process. **2007**, 1-31	1
1337	Combining substrate dynamics, binding statistics, and energy barriers to rationalize regioselective hydroxylation of octane and lauric acid by CYP102A1 and mutants. **2007**, 16, 420-31	33
1336	Pharmacophore modeling for protein tyrosine phosphatase 1B inhibitors. **2007**, 30, 533-42	9
1335	Computational inhibitor design against malaria plasmepsins. **2007**, 64, 2285-305	40
1334	Putrescine N-methyltransferases--a structure-function analysis. **2007**, 63, 787-801	46
1333	Structural differences between the putative carbohydrate-recognition domains of human IL-1 alpha, IL-1 beta and IL-1 receptor antagonist obtained by in silico modeling. **2007**, 24, 183-93	5
1332	Development and application of hybrid structure based method for efficient screening of ligands binding to G-protein coupled receptors. **2006**, 20, 789-802	33
1331	Surflex-Dock 2.1: robust performance from ligand energetic modeling, ring flexibility, and knowledge-based search. **2007**, 21, 281-306	454

1330	Calculations of protein-ligand binding entropy of relative and overall molecular motions. **2007**, 21, 361-70	18
1329	Generation of a homology model of the human histamine H(3) receptor for ligand docking and pharmacophore-based screening. **2007**, 21, 437-53	63
1328	3D-QSAR studies on fluoropyrrolidine amides as dipeptidyl peptidase IV inhibitors by CoMFA and CoMSIA. **2007**, 13, 993-1000	21
1327	An ant colony optimization approach to flexible protein□gand docking. **2007**, 1, 115-134	141
1326	Pharmacophore identification and virtual screening for methionyl-tRNA synthetase inhibitors. **2007** , 25, 813-23	45
1325	3D-QSAR and molecular docking studies on pyrazolopyrimidine derivatives as glycogen synthase kinase-3beta inhibitors. **2007**, 25, 885-95	31
1324	Structural and chemical basis for enhanced affinity and potency for a large series of estrogen receptor ligands: 2D and 3D QSAR studies. **2007**, 26, 434-42	38
1323	Biochemical characterization, homology modeling and docking studies of ornithine delta-aminotransferase--an important enzyme in proline biosynthesis of plants. **2007**, 26, 709-19	28
1322	Analysis of CYP2D6 substrate interactions by computational methods. **2008**, 26, 947-56	39
1321	Selection and flexible optimization of binding modes from conformation ensembles. **2008**, 92, 42-8	4
1320	A fast method of large-scale serial semiempirical calculations of docking complexes. **2008**, 57, 1793-1798	6
1319	Molecular modeling on pyruvate phosphate dikinase of Entamoeba histolytica and in silico virtual screening for novel inhibitors. **2008**, 22, 647-60	13
1318	Bias, reporting, and sharing: computational evaluations of docking methods. **2008**, 22, 201-12	119
1317	Modeling the inhibition of quadruple mutant Plasmodium falciparum dihydrofolate reductase by pyrimethamine derivatives. **2008**, 22, 29-38	14
1316	A knowledge-based approach to generating diverse but energetically representative ensembles of ligand conformers. **2008**, 22, 681-91	15
1315	The concept of template-based de novo design from drug-derived molecular fragments and its application to TAR RNA. **2008**, 22, 59-68	17
1314	Evaluation of the performance of 3D virtual screening protocols: RMSD comparisons, enrichment assessments, and decoy selection--what can we learn from earlier mistakes?. **2008**, 22, 213-28	278
1313	How to do an evaluation: pitfalls and traps. **2008**, 22, 179-90	113

1312	Evaluating docking programs: keeping the playing field level. **2008**, 22, 229-38	22
1311	Customizing scoring functions for docking. **2008**, 22, 269-86	46
1310	Homology modeling of 5-lipoxygenase and hints for better inhibitor design. **2008**, 22, 611-9	29
1309	A new peptide docking strategy using a mean field technique with mutually orthogonal Latin square sampling. **2008**, 22, 815-29	24
1308	Molecular dynamics simulation study of PTP1B with allosteric inhibitor and its application in receptor based pharmacophore modeling. **2008**, 22, 925-33	29
1307	Comparative docking studies of CYP1b1 and its PCG-associated mutant forms. **2008**, 33, 699-713	3
1306	Multiple-step virtual screening using VSM-G: overview and validation of fast geometrical matching enrichment. **2008**, 14, 135-48	15
1305	Exploring the binding pocket for pyridopyrimidine ligands at the CCK1 receptor by molecular docking. **2008**, 14, 303-14	
1304	Molecular docking guided 3D-QSAR CoMFA analysis of N-4-Pyrimidinyl-1H-indazol-4-amine inhibitors of leukocyte-specific protein tyrosine kinase. **2008**, 14, 937-47	7
1303	Fast dynamics perturbation analysis for prediction of protein functional sites. **2008**, 8, 5	25
1302	Carbohydrate-binding modules from family 11: Understanding the binding mode of polysaccharides. **2008**, 108, 2030-2040	20
1301	Molecular determinants of sarco/endoplasmic reticulum calcium ATPase inhibition by hydroquinone-based compounds. **2008**, 70, 639-49	19
1300	Structural rationalization of novel drug metabolizing mutants of cytochrome P450 BM3. **2008**, 71, 336-52	37
1299	Molecular modeling of the second extracellular loop of G-protein coupled receptors and its implication on structure-based virtual screening. **2008**, 71, 599-620	89
1298	Characterization of local geometry of protein surfaces with the visibility criterion. **2008**, 71, 670-83	72
1297	A statistical rescoring scheme for protein-ligand docking: Consideration of entropic effect. **2008**, 70, 1074-83	24
1296	High quality binding modes in docking ligands to proteins. **2008**, 71, 1373-86	33
1295	Three-dimensional model of the human urotensin-II receptor: docking of human urotensin-II and nonpeptide antagonists in the binding site and comparison with an antagonist pharmacophore model. **2008**, 73, 173-84	9

1294	SFCscore: scoring functions for affinity prediction of protein-ligand complexes. **2008**, 73, 395-419	88
1293	Current topics in computer-aided drug design. **2008**, 97, 1089-98	60
1292	A structural model of the membrane-bound aromatic prenyltransferase UbiA from E. coli. **2008**, 9, 982-92	46
1291	Benzene polyphosphates as tools for cell signalling: inhibition of inositol 1,4,5-trisphosphate 5-phosphatase and interaction with the PH domain of protein kinase Balpha. **2008**, 9, 1757-66	15
1290	An indole-binding site is a major determinant of the ligand specificity of the GABA type A receptor-associated protein GABARAP. **2008**, 9, 1767-75	22
1289	Targeting protein-protein interactions: suppression of Stat3 dimerization with rationally designed small-molecule, nonpeptidic SH2 domain binders. **2008**, 9, 2800-3	41
1288	Probing novel 1-aza-9-oxafluorenes as selective GSK-3beta inhibitors. **2008**, 3, 120-6	15
1287	Hyrtiosal, from the marine sponge Hyrtios erectus, inhibits HIV-1 integrase binding to viral DNA by a new inhibitor binding site. **2008**, 3, 173-80	24
1286	Synthesis, biological evaluation, and molecular modeling studies of rebeccamycin analogues modified in the carbohydrate moiety. **2008**, 3, 266-79	16
1285	Non-steroidal aromatase inhibitors based on a biphenyl scaffold: synthesis, in vitro SAR, and molecular modelling. **2008**, 3, 603-18	26
1284	Substituted pyrazolo[3,4-b]pyridines as potent A1 adenosine antagonists: synthesis, biological evaluation, and development of an A1 bovine receptor model. **2008**, 3, 898-913	22
1283	Thiobarbiturates as sirtuin inhibitors: virtual screening, free-energy calculations, and biological testing. **2008**, 3, 1965-76	56
1282	Molecular approaches towards the inhibition of the signal transducer and activator of transcription 3 (Stat3) protein. **2008**, 3, 1159-68	85
1281	Computational studies to discover a new NR2B/NMDA receptor antagonist and evaluation of pharmacological profile. **2008**, 3, 1539-48	33
1280	e-Malaria: the schools Malaria project. **2008**, 20, 225-238	1
1279	17beta-hydroxysteroid dehydrogenase Type 1, and not Type 12, is a target for endocrine therapy of hormone-dependent breast cancer. **2008**, 122, 1931-40	89
1278	Shapelets: possibilities and limitations of shape-based virtual screening. **2008**, 29, 108-14	29
1277	Modeling the hERG potassium channel in a phospholipid bilayer: Molecular dynamics and drug docking studies. **2008**, 29, 795-808	42

1276	Assessment of programs for ligand binding affinity prediction. **2008**, 29, 1316-31	106
1275	Stereoelectronic properties of spiroquinazolinones in differential PDE7 inhibitory activity. **2008**, 29, 1945-54	25
1274	Alpha7 nicotinic acetylcholine receptor agonists: prediction of their binding affinity through a molecular mechanics Poisson-Boltzmann surface area approach. **2008**, 29, 2593-602	34
1273	CYP17 inhibitors. Annulations of additional rings in methylene imidazole substituted biphenyls: synthesis, biological evaluation and molecular modelling. **2008**, 341, 597-609	22
1272	Total synthesis of chondramide C and its binding mode to F-actin. **2008**, 47, 6473-7	62
1271	Stilbene derivatives that are colchicine-site microtubule inhibitors have antileukemic activity and minimal systemic toxicity. **2008**, 83, 390-7	19
1270	Totalsynthese von Chondramid C und Bindung an F-Aktin. **2008**, 120, 6573-6577	20
1269	Molecular modeling of histamine H3 receptor and QSAR studies on arylbenzofuran derived H3 antagonists. **2008**, 26, 834-44	34
1268	An in silico [correction of insilico] approach to bioremediation: laccase as a case study. **2008**, 26, 845-9	46
1267	Prediction of protein-ligand complex structure by docking software guided by other complex structures. **2008**, 26, 1030-3	19
1266	In silico screening against wild-type and mutant Plasmodium falciparum dihydrofolate reductase. **2008**, 26, 1145-52	17
1265	Binding mode analyses and pharmacophore model development for sulfonamide chalcone derivatives, a new class of alpha-glucosidase inhibitors. **2008**, 26, 1202-12	80
1264	Factors affecting nucleolytic efficiency of some ternary metal complexes with DNA binding and recognition domains. Crystal and molecular structure of Zn(phen)(edda). **2008**, 102, 1997-2011	21
1263	3D-QSAR and docking studies of aminopyridine carboxamide inhibitors of c-Jun N-terminal kinase-1. **2008**, 43, 604-13	16
1262	Synthesis of N-aryl-5-amino-4-cyanopyrazole derivatives as potent xanthine oxidase inhibitors. **2008**, 43, 771-80	75
1261	In silico screening of HIV-1 non-nucleoside reverse transcriptase and protease inhibitors. **2008**, 43, 1412-22	7
1260	Novel 9-oxo-thiazolo[5,4-f]quinazoline-2-carbonitrile derivatives as dual cyclin-dependent kinase 1 (CDK1)/glycogen synthase kinase-3 (GSK-3) inhibitors: synthesis, biological evaluation and molecular modeling studies. **2008**, 43, 1469-77	50
1259	An efficient tool for identifying inhibitors based on 3D-QSAR and docking using feature-shape pharmacophore of biologically active conformation--a case study with CDK2/cyclinA. **2008**, 43, 2807-18	30

1258	Homology modeling of MT1 and MT2 receptors. **2008**, 43, 1926-44	20
1257	Synthesis, biological evaluation and docking studies of 4-amino substituted 1H-pyrazolo[3,4-d]pyrimidines. **2008**, 43, 2665-76	66
1256	Synthesis, biological evaluation and molecular modelling studies of methyleneimidazole substituted biaryls as inhibitors of human 17alpha-hydroxylase-17,20-lyase (CYP17). Part I: Heterocyclic modifications of the core structure. **2008**, 16, 1992-2010	73
1255	Docking and hydropathic scoring of polysubstituted pyrrole compounds with antitubulin activity. **2008**, 16, 2235-42	36
1254	Design, synthesis, and evaluation of trifluoromethyl ketones as inhibitors of SARS-CoV 3CL protease. **2008**, 16, 4652-60	55
1253	Synthesis of 3,5-bis(2-indolyl)pyridine and 3-[(2-indolyl)-5-phenyl]pyridine derivatives as CDK inhibitors and cytotoxic agents. **2008**, 16, 4932-53	51
1252	Design, synthesis and biological evaluation of bis(hydroxyphenyl) azoles as potent and selective non-steroidal inhibitors of 17beta-hydroxysteroid dehydrogenase type 1 (17beta-HSD1) for the treatment of estrogen-dependent diseases. **2008**, 16, 6423-35	58
1251	2-N-Methyl modifications and SAR studies of manzamine A. **2008**, 16, 6702-6	24
1250	Novel inhibitors of anthrax edema factor. **2008**, 16, 7225-33	32
1249	QSAR study of imidazoline antihypertensive drugs. **2008**, 16, 7134-40	29
1248	Development of a receptor-based 3D-QSAR study for the analysis of MMP2, MMP3, and MMP9 inhibitors. **2008**, 16, 7749-58	22
1247	Synthesis, biological evaluation, and molecular modeling studies of methylene imidazole substituted biaryls as inhibitors of human 17alpha-hydroxylase-17,20-lyase (CYP17)--part II: Core rigidification and influence of substituents at the methylene bridge. **2008**, 16, 7715-27	50
1246	Characterization of the binding properties of SIRT2 inhibitors with a N-(3-phenylpropenoyl)-glycine tryptamide backbone. **2008**, 16, 8054-62	23
1245	Synthesis, biological active molecular design, and molecular docking study of novel deazaflavin-cholestane hybrid compounds. **2008**, 16, 8685-96	16
1244	Antitumor studies. Part 5: Synthesis, antitumor activity, and molecular docking study of 5-(monosubstituted amino)-2-deoxo-2-phenyl-5-deazaflavins. **2008**, 16, 9161-70	11
1243	Synthesis, biological evaluation, and molecular modeling investigation of chiral 2-(4-chloro-phenoxy)-3-phenyl-propanoic acid derivatives with PPARalpha and PPARgamma agonist activity. **2008**, 16, 9498-510	18
1242	Synthesis, structure-activity relationships and molecular modeling studies of new indole inhibitors of monoamine oxidases A and B. **2008**, 16, 9729-40	27
1241	Multi-target-directed coumarin derivatives: hAChE and BACE1 inhibitors as potential anti-Alzheimer compounds. **2008**, 18, 423-6	171

1240	In silico screening and biological evaluation of inhibitors of Src-SH3 domain interaction with a proline-rich ligand. **2008**, 18, 1217-22	20
1239	Antidiabetic activity of N-(6-substituted-1,3-benzothiazol-2-yl)benzenesulfonamides. **2008**, 18, 2871-7	77
1238	Methoxy-substituted 9-aminomethyl-9,10-dihydroanthracene (AMDA) derivatives exhibit differential binding affinities at the 5-HT(2A) receptor. **2008**, 18, 5268-71	6
1237	Identification of novel protein kinase CK1 delta (CK1delta) inhibitors through structure-based virtual screening. **2008**, 18, 5672-5	34
1236	IRAK-4 inhibitors. Part 1: a series of amides. **2008**, 18, 3211-4	29
1235	Lead finder: an approach to improve accuracy of protein-ligand docking, binding energy estimation, and virtual screening. **2008**, 48, 2371-85	140
1234	Computer-aided discovery of anti-inflammatory thiazolidinones with dual cyclooxygenase/lipoxygenase inhibition. **2008**, 51, 1601-9	136
1233	Chiral aromatase and dual aromatase-steroid sulfatase inhibitors from the letrozole template: synthesis, absolute configuration, and in vitro activity. **2008**, 51, 4226-38	69
1232	Crystal structure of the peroxisome proliferator-activated receptor gamma (PPARgamma) ligand binding domain complexed with a novel partial agonist: a new region of the hydrophobic pocket could be exploited for drug design. **2008**, 51, 7768-76	80
1231	2-Thiazolylimino/heteroarylimino-5-arylidene-4-thiazolidinones as new agents with SHP-2 inhibitory action. **2008**, 51, 5221-8	85
1230	Structural basis for the broad-spectrum inhibition of metallo-beta-lactamases by thiols. **2008**, 6, 2282-94	107
1229	Internet resources in GPCR modelling. **2008**, 19, 11-25	7
1228	Hit identification and binding mode predictions by rigorous free energy simulations. **2008**, 51, 6654-64	56
1227	Symmetrical 1-pyrrolidineacetamide showing anti-HIV activity through a new binding site on HIV-1 integrase. **2008**, 29, 1261-7	20
1226	Rhodanine derivatives as selective protease inhibitors against bacterial toxins. **2008**, 71, 131-9	45
1225	Concept of combinatorial de novo design of drug-like molecules by particle swarm optimization. **2008**, 72, 16-26	45
1224	Identification of novel HCV RNA-dependent RNA polymerase inhibitors using pharmacophore-guided virtual screening. **2008**, 72, 585-91	12
1223	Molecular determinants of ligand specificity in family 11 carbohydrate binding modules: an NMR, X-ray crystallography and computational chemistry approach. **2008**, 275, 2524-35	27

1222	Identification of a glycosphingolipid transfer protein GLTP1 in Arabidopsis thaliana. **2008**, 275, 3421-37	30
1221	Towards the development of universal, fast and highly accurate docking/scoring methods: a long way to go. **2008**, 153 Suppl 1, S7-26	349
1220	Ligand discovery and virtual screening using the program LIDAEUS. **2008**, 153 Suppl 1, S55-67	21
1219	Targeting the cannabinoid CB2 receptor: modelling and structural determinants of CB2 selective ligands. **2008**, 153, 335-46	48
1218	Insights into drug metabolism by cytochromes P450 from modelling studies of CYP2D6-drug interactions. **2008**, 153 Suppl 1, S82-9	34
1217	Characterization of inhibitors and substrates of Anopheles gambiae CYP6Z2. **2008**, 17, 125-35	83
1216	Identification and functional analysis of cyclooxygenase-1 as a molecular target of boswellic acids. **2008**, 75, 503-13	73
1215	Fluoxetine mediates G0/G1 arrest by inducing functional inhibition of cyclin dependent kinase subunit (CKS)1. **2008**, 75, 1924-34	50
1214	Characterisation of novel defective thiopurine S-methyltransferase allelic variants. **2008**, 76, 404-15	46
1213	Discovery of substituted sulfonamides and thiazolidin-4-one derivatives as agonists of human constitutive androstane receptor. **2008**, 76, 1288-97	28
1212	Inhibitors of Escherichia coli serine acetyltransferase block proliferation of Entamoeba histolytica trophozoites. **2008**, 38, 137-41	35
1211	Limitations and lessons in the use of X-ray structural information in drug design. **2008**, 13, 831-41	133
1210	Small-molecule CD4 mimics interact with a highly conserved pocket on HIV-1 gp120. **2008**, 16, 1689-701	143
1209	Dual inhibitors of matrix metalloproteinases and carbonic anhydrases: iminodiacetyl-based hydroxamate-benzenesulfonamide conjugates. **2008**, 51, 7968-79	46
1208	Molecular Recognition: Computational Analysis and Modelling. **2008**, 1	
1207	Benzyl ether-linked glucuronide derivative of 10-hydroxycamptothecin designed for selective camptothecin-based anticancer therapy. **2008**, 51, 1740-6	58
1206	Combined ligand and structure based approaches for narrowing on the essential physicochemical characteristics for CDK4 inhibition. **2008**, 48, 1325-36	12
1205	Synthesis, modeling, and RET protein kinase inhibitory activity of 3- and 4-substituted beta-carbolin-1-ones. **2008**, 51, 7777-87	33

1204	Bis-(-)-nor-meptazinols as novel nanomolar cholinesterase inhibitors with high inhibitory potency on amyloid-beta aggregation. **2008**, 51, 2027-36	69
1203	Recent developments in fragment-based drug discovery. **2008**, 51, 3661-80	525
1202	Ligand binding to the voltage-gated Kv1.5 potassium channel in the open state--docking and computer simulations of a homology model. **2008**, 94, 820-31	49
1201	Molecular docking. **2008**, 443, 365-82	307
1200	Discovery of novel nitrobenzothiazole inhibitors for Mycobacterium tuberculosis ATP phosphoribosyl transferase (HisG) through virtual screening. **2008**, 51, 5984-92	90
1199	Selectins ligand decorated drug carriers for activated endothelial cell targeting. **2008**, 19, 2030-9	30
1198	An alternative method for the evaluation of docking performance: RSR vs RMSD. **2008**, 48, 1411-22	89
1197	Structure based development of phenylimidazole-derived inhibitors of indoleamine 2,3-dioxygenase. **2008**, 51, 4968-77	133
1196	Molecular modeling approaches to study the binding mode on tubulin of microtubule destabilizing and stabilizing agents. **2009**, 286, 279-328	25
1195	Fully automated molecular mechanics based induced fit protein-ligand docking method. **2008**, 48, 1965-73	127
1194	Impact of plasticity and flexibility on docking results for cytochrome P450 2D6: a combined approach of molecular dynamics and ligand docking. **2008**, 51, 7469-77	109
1193	Indoleamine 2,3-dioxygenase is the anticancer target for a novel series of potent naphthoquinone-based inhibitors. **2008**, 51, 1706-18	140
1192	Structure-based design, synthesis, evaluation, and crystallographic studies of conformationally constrained Smac mimetics as inhibitors of the X-linked inhibitor of apoptosis protein (XIAP). **2008**, 51, 7169-80	72
1191	Targets looking for drugs: a multistep computational protocol for the development of structure-based pharmacophores and their applications for hit discovery. **2008**, 48, 2166-79	55
1190	Emerging protein targets for anticancer metallodrugs: inhibition of thioredoxin reductase and cathepsin B by antitumor ruthenium(II)-arene compounds. **2008**, 51, 6773-81	243
1189	Potent antimalarial activity of histone deacetylase inhibitor analogues. **2008**, 52, 1454-61	99
1188	Virtual screening of chemical libraries for drug discovery. **2008**, 3, 1011-26	23
1187	Potent cationic inhibitors of West Nile virus NS2B/NS3 protease with serum stability, cell permeability and antiviral activity. **2008**, 51, 5714-21	68

1186	Potent, Plasmodium-selective farnesyltransferase inhibitors that arrest the growth of malaria parasites: structure-activity relationships of ethylenediamine-analogue scaffolds and homology model validation. **2008**, 51, 5176-97	32
1185	Structure-activity relationships of acetylcholinesterase noncovalent inhibitors based on a polyamine backbone. 4. Further investigation on the inner spacer. **2008**, 51, 7308-12	52
1184	Applied Bioinformatics. **2008**,	5
1183	Modern Genome Annotation. **2008**,	3
1182	Probing the structures of leishmanial farnesyl pyrophosphate synthases: homology modeling and docking studies. **2008**, 48, 1026-40	18
1181	Phosphoinositide-3-kinases (PI3Ks): combined comparative modeling and 3D-QSAR to rationalize the inhibition of p110alpha. **2008**, 48, 629-38	25
1180	Design, synthesis, and biological evaluation of (hydroxyphenyl)naphthalene and -quinoline derivatives: potent and selective nonsteroidal inhibitors of 17beta-hydroxysteroid dehydrogenase type 1 (17beta-HSD1) for the treatment of estrogen-dependent diseases. **2008**, 51, 2158-69	71
1179	BALLDock/SLICK: a new method for protein-carbohydrate docking. **2008**, 48, 1616-25	39
1178	Molecular modelling of phthalates - PPARs interactions. **2008**, 23, 611-6	22
1177	Transition-State Docking of Flunitrazepam and Progesterone in Cytochrome P450. **2008**, 4, 673-81	24
1176	Molecular Modeling of Proteins. **2008**,	27
1175	Discovery of imidazo[1,5-c]imidazol-3-ones: weakly basic, orally active factor Xa inhibitors. **2008**, 51, 3422-36	19
1174	Naïve Bayes classification using 2D pharmacophore feature triplet vectors. **2008**, 48, 166-78	59
1173	Synthesis and evaluation of estrogen agonism of diaryl 4,5-dihydroisoxazoles, 3-hydroxyketones, 3-methoxyketones, and 1,3-diketones: a compound set forming a 4D molecular library. **2008**, 51, 3562-71	28
1172	Vaccines: Structural Approaches. 217-255	
1171	Implication of HMGR in homeostasis of sequestered and de novo produced precursors of the iridoid biosynthesis in leaf beetle larvae. **2008**, 38, 76-88	18
1170	Ligand specificity and evolution of liver X receptors. **2008**, 110, 83-94	54
1169	Structural analysis of PI3-kinase isoforms: identification of residues enabling selective inhibition by small molecule ATP-competitive inhibitors. **2008**, 477, 404-10	25

1168	Synthesis, cannabinoid receptor affinity, and molecular modeling studies of substituted 1-aryl-5-(1H-pyrrol-1-yl)-1H-pyrazole-3-carboxamides. **2008**, 51, 1560-76	61
1167	Binding of serotonin and N1-benzenesulfonyltryptamine-related analogs at human 5-HT6 serotonin receptors: receptor modeling studies. **2008**, 51, 603-11	34
1166	Medicinal chemistry and the molecular operating environment (MOE): application of QSAR and molecular docking to drug discovery. **2008**, 8, 1555-72	510
1165	Inhibition of acetylcholinesterase, beta-amyloid aggregation, and NMDA receptors in Alzheimer's disease: a promising direction for the multi-target-directed ligands gold rush. **2008**, 51, 4381-4	170
1164	Rational design and synthesis of 4-((1R,2R)-2-hydroxycyclohexyl)-2(trifluoromethyl)benzonitrile (PF-998425), a novel, nonsteroidal androgen receptor antagonist devoid of phototoxicity for dermatological indications. **2008**, 51, 7010-4	15
1163	D77, one benzoic acid derivative, functions as a novel anti-HIV-1 inhibitor targeting the interaction between integrase and cellular LEDGF/p75. **2008**, 375, 139-44	68
1162	Potential modes of interaction of 9-aminomethyl-9,10-dihydroanthracene (AMDA) derivatives with the 5-HT2A receptor: a ligand structure-affinity relationship, receptor mutagenesis and receptor modeling investigation. **2008**, 51, 6808-28	27
1161	Ribose-modified purine nucleosides as ribonucleotide reductase inhibitors. Synthesis, antitumor activity, and molecular modeling of N6-substituted 3'-C-methyladenosine derivatives. **2008**, 51, 4260-9	16
1160	Structural basis for selective inhibition of trypanosomatid glyceraldehyde-3-phosphate dehydrogenase: molecular docking and 3D QSAR studies. **2008**, 48, 918-29	38
1159	Protein-ligand docking accounting for receptor side chain and global flexibility in normal modes: evaluation on kinase inhibitor cross docking. **2008**, 51, 3499-506	78
1158	Protein-ligand docking against non-native protein conformers. **2008**, 48, 2214-25	115
1157	MM-GB/SA rescoring of docking poses in structure-based lead optimization. **2008**, 48, 958-70	163
1156	Robust classification of "relevant" water molecules in putative protein binding sites. **2008**, 51, 1063-7	81
1155	Identification of inhibitors of the nicotine metabolising CYP2A6 enzyme--an in silico approach. **2008**, 8, 328-38	21
1154	Lavendamycin antitumor agents: structure-based design, synthesis, and NAD(P)H:quinone oxidoreductase 1 (NQO1) model validation with molecular docking and biological studies. **2008**, 51, 3104-15	36
1153	Machine learning methods and docking for predicting human pregnane X receptor activation. **2008**, 21, 1457-67	61
1152	Novel donepezil-based inhibitors of acetyl- and butyrylcholinesterase and acetylcholinesterase-induced beta-amyloid aggregation. **2008**, 51, 3588-98	163
1151	Synthesis, biological evaluation, and molecular modeling of abiraterone analogues: novel CYP17 inhibitors for the treatment of prostate cancer. **2008**, 51, 5009-18	61

1150	Determination of protein-ligand binding modes using complexation-induced changes in (1)h NMR chemical shift. **2008**, 51, 2512-7	32
1149	Assessment of additive/nonadditive effects in structure-activity relationships: implications for iterative drug design. **2008**, 51, 7552-62	48
1148	Structure-activity studies on splitomicin derivatives as sirtuin inhibitors and computational prediction of binding mode. **2008**, 51, 1203-13	147
1147	Ligand discovery on massively parallel systems. **2008**, 52, 57-67	7
1146	Computational Intelligence in Bioinformatics. **2008**,	11
1145	Molecular design of inhibitors against the Mproprotein of the severe acute respiratory syndrome (SARS) virus. **2008**, 32, 452-458	0
1144	Fragment-based design of small molecule X-linked inhibitor of apoptosis protein inhibitors. **2008**, 51, 7111-8	49
1143	An integrated approach to ligand- and structure-based drug design: development and application to a series of serine protease inhibitors. **2008**, 48, 1211-26	43
1142	Impact of benchmark data set topology on the validation of virtual screening methods: exploration and quantification by spatial statistics. **2008**, 48, 704-18	25
1141	2-Position base-modified analogues of adenophostin A as high-affinity agonists of the D-myo-inositol trisphosphate receptor: in vitro evaluation and molecular modeling. **2008**, 73, 1682-92	17
1140	Evaluation of different virtual screening programs for docking in a charged binding pocket. **2008**, 48, 2010-20	27
1139	Identification of MMP-12 inhibitors by using biosensor-based screening of a fragment library. **2008**, 51, 3449-59	49
1138	Hidden active information in a random compound library: extraction using a pseudo-structure-activity relationship model. **2008**, 48, 575-82	8
1137	Assessing the role of polarization in docking. **2008**, 112, 12157-63	36
1136	Novel prostaglandin D synthase inhibitors generated by fragment-based drug design. **2008**, 51, 2178-86	58
1135	Ligand-specific scoring functions: improved ranking of docking solutions. **2008**, 19, 91-9	6
1134	Combining docking, molecular dynamics and the linear interaction energy method to predict binding modes and affinities for non-nucleoside inhibitors to HIV-1 reverse transcriptase. **2008**, 51, 2648-56	75
1133	Cross-docking of inhibitors into CDK2 structures. 2. **2008**, 48, 669-78	14

1132	Computationally identified novel diphenyl- and phenylpyridine androgen receptor antagonist structures. **2008**, 48, 1882-90	13
1131	Systems biology of cyanobacterial secondary metabolite production and its role in drug discovery. **2008**, 3, 903-29	39
1130	Using buriedness to improve discrimination between actives and inactives in docking. **2008**, 48, 1269-78	9
1129	Influence of conformational flexibility on complexation-induced changes in chemical shift in a neocarzinostatin protein-ligand complex. **2008**, 51, 4488-95	9
1128	Predicting binding modes from free energy calculations. **2008**, 51, 2657-67	30
1127	Cross-docking of inhibitors into CDK2 structures. 1. **2008**, 48, 659-68	23
1126	Assessment of scaffold hopping efficiency by use of molecular interaction fingerprints. **2008**, 51, 3222-9	64
1125	An anchor-dependent molecular docking process for docking small flexible molecules into rigid protein receptors. **2008**, 48, 1638-55	6
1124	Rational Design for Crystallization of β-Lactoglobulin and Vitamin D3 Complex: Revealing a Secondary Binding Site **2008**, 8, 4268-4276	25
1123	AIScore chemically diverse empirical scoring function employing quantum chemical binding energies of hydrogen-bonded complexes. **2008**, 48, 1492-510	37
1122	MedusaScore: an accurate force field-based scoring function for virtual drug screening. **2008**, 48, 1656-62	131
1121	ASEDock-docking based on alpha spheres and excluded volumes. **2008**, 48, 583-90	123
1120	Azetidine-2,4-diones (4-oxo-beta-lactams) as scaffolds for designing elastase inhibitors. **2008**, 51, 1783-90	24
1119	Selective structure-based virtual screening for full and partial agonists of the beta2 adrenergic receptor. **2008**, 51, 4978-85	124
1118	Insights into ligand-elicited activation of human constitutive androstane receptor based on novel agonists and three-dimensional quantitative structure-activity relationship. **2008**, 51, 7181-92	32
1117	Substituted 6-phenyl-2-naphthols. Potent and selective nonsteroidal inhibitors of 17beta-hydroxysteroid dehydrogenase type 1 (17beta-HSD1): design, synthesis, biological evaluation, and pharmacokinetics. **2008**, 51, 4685-98	57
1116	Development of paramagnetic probes for molecular recognition studies in protein kinases. **2008**, 51, 3460-5	35
1115	Bootstrap-based consensus scoring method for protein-ligand docking. **2008**, 48, 988-96	11

1114	Hydra: a self regenerating high performance computing grid for drug discovery. **2008**, 48, 811-6	5
1113	Improvement of protein-compound docking scores by using amino-acid sequence similarities of proteins. **2008**, 48, 148-56	3
1112	Hierarchical Structure-Based Virtual Screening for Drug Design. **2008**, 22, 634-638	9
1111	Structural analysis of Golgi alpha-mannosidase II inhibitors identified from a focused glycosidase inhibitor screen. **2008**, 47, 10058-68	35
1110	Binding and hydrolysis of soman by human serum albumin. **2008**, 21, 421-31	94
1109	Factor Xa active site substrate specificity with substrate phage display and computational molecular modeling. **2008**, 283, 12343-53	24
1108	Drug-Drug Interactions, Second Edition. **2008**,	6
1107	Design and validation of specific inhibitors of 17beta-hydroxysteroid dehydrogenases for therapeutic application in breast and prostate cancer, and in endometriosis. **2008**, 15, 665-92	103
1106	Targeted rescue of a destabilized mutant of p53 by an in silico screened drug. **2008**, 105, 10360-5	254
1105	Arabidopsis sterol carrier protein-2 is required for normal development of seeds and seedlings. **2008**, 59, 3485-99	14
1104	A Structural Analysis of the Mode of Action of ORF1 in Pseudaminobacter salicylatoxidans: Prediction of its Role in the Global Sulfur Oxidation Operon (sox). **2008**, 5, 176-180	
1103	Specific inhibitors of the protein tyrosine phosphatase Shp2 identified by high-throughput docking. **2008**, 105, 7275-80	164
1102	Evolution of the bile salt nuclear receptor FXR in vertebrates. **2008**, 49, 1577-87	77
1101	Identification of a new JNK inhibitor targeting the JNK-JIP interaction site. **2008**, 105, 16809-13	151
1100	In Silico Screening. **2008**, 210-227	1
1099	Computational discovery of novel low micromolar human pregnane X receptor antagonists. **2008**, 74, 662-72	62
1098	Design, synthesis and evaluation of new 6-substituted-5-benzyloxy-4-oxo-4H-pyran-2-carboxamides as potential Src inhibitors. **2008**, 23, 629-40	6
1097	Virtual screening and its integration with modern drug design technologies. **2008**, 15, 37-46	152

1096	Novel opportunities for thymidylate metabolism as a therapeutic target. **2008**, 7, 3029-37	44
1095	Kinetic, thermodynamic and X-ray structural insights into the interaction of melatonin and analogues with quinone reductase 2. **2008**, 413, 81-91	74
1094	Novel analogs and stereoisomers of the marine toxin neodysiherbaine with specificity for kainate receptors. **2008**, 324, 484-96	30
1093	Anticancer steroid sulfatase inhibitors: synthesis of a potent fluorinated second-generation agent, in vitro and in vivo activities, molecular modeling, and protein crystallography. **2008**, 7, 2435-44	37
1092	Virtual Screening of Drugs: Score Functions, Docking, and Drug Design. **2008**, 4, 265-272	27
1091	Molecular docking algorithms. **2008**, 9, 1040-7	131
1090	Response of feline immunodeficiency virus (FIV) to tipranavir may provide new clues for development of broad-based inhibitors of retroviral proteases acting on drug-resistant HIV-1. **2008**, 6, 306-17	11
1089	How to Efficiently Include Receptor Flexibility During Computational Docking. **2008**, 4, 143-153	15
1088	Drug Addiction. **2008**,	4
1087	Small Molecule Docking. **2008**, 469-500	1
1086	Bioinformatics based Ligand-Docking and in-silico screening. **2008**, 56, 742-4	18
1085	Virtual Fragment Scanning: Current Trends, Applications and Web-Based Tools. 223-244	1
1084	Virtual Screening: A Fast Tool for Drug Design. **2008**, 76, 333-360	45
1083	Toward a molecular understanding of the interaction of dual specificity phosphatases with substrates: insights from structure-based modeling and high throughput screening. **2008**, 15, 2536-44	31
1082	Molecular recognition and binding free energy calculations in drug development. **2008**, 9, 87-95	13
1081	. **2008**,	27
1080	. **2008**,	21
1079	A method to enhance the hit ratio by a combination of structure-based drug screening and ligand-based screening. **2008**, 1, 19-28	5

1078	Prospective ligand- and target-based 3D QSAR: state of the art 2008. **2009**, 9, 791-810	23
1077	New approaches to structure-based discovery of dengue protease inhibitors. **2009**, 9, 327-43	35
1076	Chemoinformatics□n introduction for computer scientists. **2009**, 41, 1-38	53
1075	Interaction of actinomycin D with promoter element of c-met and its inhibitory effect on the expression of c-Met. **2009**, 26, 625-36	14
1074	Interaction of antithrombin with sulfated, low molecular weight lignins: opportunities for potent, selective modulation of antithrombin function. **2009**, 284, 20897-908	35
1073	A small-molecule dengue virus entry inhibitor. **2009**, 53, 1823-31	164
1072	Hydropathic analysis and biological evaluation of stilbene derivatives as colchicine site microtubule inhibitors with anti-leukemic activity. **2009**, 24, 1237-44	8
1071	Somatic mutations of ErbB4: selective loss-of-function phenotype affecting signal transduction pathways in cancer. **2009**, 284, 5582-91	49
1070	Efficient simulation of ligand-receptor binding processes using the conformation dynamics approach. **2009**, 7, 811-31	12
1069	Evidence for a direct and functional interaction between the regulators of G protein signaling-2 and phosphorylated C terminus of cholecystokinin-2 receptor. **2009**, 75, 502-13	16
1068	High-performance drug discovery: computational screening by combining docking and molecular dynamics simulations. **2009**, 5, e1000528	109
1067	Apogossypol derivatives as antagonists of antiapoptotic Bcl-2 family proteins. **2009**, 8, 904-13	54
1066	Explicit Treatment of Water Molecules in Protein-Ligand Docking. **2009**, 5, 145-154	16
1065	Computational resources for protein modelling and drug discovery applications. **2009**, 9, 557-62	3
1064	Customizing G Protein-coupled receptor models for structure-based virtual screening. **2009**, 15, 4026-48	62
1063	Modeling Reality for Optimal Docking of Small Molecules to Biological Targets. **2009**, 5, 241-263	12
1062	Bioinformatics tools for screening of antiparasitic drugs. **2009**, 10, 232-9	8
1061	Structure-based drug design strategies in medicinal chemistry. **2009**, 9, 771-90	105

1060	Computational Intelligence Methods for Docking Scores. **2009**, 5, 56-68	26
1059	Molecular Mechanics Force Fields and their Applications in Drug Design. **2009**, 8, 128-150	10
1058	Self-organizing maps in drug discovery: compound library design, scaffold-hopping, repurposing. **2009**, 16, 258-66	90
1057	Conformational sampling and energetics of drug-like molecules. **2009**, 16, 3381-413	56
1056	Engineering enzymes for improved catalytic efficiency: a computational study of site mutagenesis in epothilone-B hydroxylase. **2009**, 22, 257-66	12
1055	Integrating statistical predictions and experimental verifications for enhancing protein-chemical interaction predictions in virtual screening. **2009**, 5, e1000397	47
1054	Challenges predicting ligand-receptor interactions of promiscuous proteins: the nuclear receptor PXR. **2009**, 5, e1000594	94
1053	Apogossypol derivatives as pan-active inhibitors of antiapoptotic B-cell lymphoma/leukemia-2 (Bcl-2) family proteins. **2009**, 52, 4511-23	48
1052	Novel piperazine derivative PMS1339 exhibits tri-functional properties and cognitive improvement in mice. **2009**, 12, 1409-19	16
1051	The Arabidopsis CORONATINE INSENSITIVE1 protein is a jasmonate receptor. **2009**, 21, 2220-36	560
1050	Structure-based discovery of beta2-adrenergic receptor ligands. **2009**, 106, 6843-8	265
1049	Interpretation of the binding affinities of PTP1B inhibitors with the MM-GB/SA method and the X-score scoring function. **2009**, 49, 1033-48	29
1048	A mutation in helicase motif IV of herpes simplex virus type 1 UL5 that results in reduced growth in vitro and lower virulence in a murine infection model is related to the predicted helicase structure. **2009**, 90, 1937-1942	26
1047	The structure of the MAP2K MEK6 reveals an autoinhibitory dimer. **2009**, 17, 96-104	23
1046	An effective docking strategy for virtual screening based on multi-objective optimization algorithm. **2009**, 10, 58	29
1045	Computational multiscale modeling in protein--ligand docking. **2009**, 28, 58-69	11
1044	Docking, virtual high throughput screening and in silico fragment-based drug design. **2009**, 13, 238-48	103
1043	Managing protein flexibility in docking and its applications. **2009**, 14, 394-400	198

1042	Aurintricarboxylic acid inhibits influenza virus neuraminidase. **2009**, 81, 123-31	85
1041	Targeting STAT1 by myricetin and delphinidin provides efficient protection of the heart from ischemia/reperfusion-induced injury. **2009**, 583, 531-41	71
1040	Single amino acid mutations of Medicago glycosyltransferase UGT85H2 enhance activity and impart reversibility. **2009**, 583, 2131-5	32
1039	Evolution of putrescine N-methyltransferase from spermidine synthase demanded alterations in substrate binding. **2009**, 583, 3367-74	13
1038	MK-886, an inhibitor of the 5-lipoxygenase-activating protein, inhibits cyclooxygenase-1 activity and suppresses platelet aggregation. **2009**, 608, 84-90	23
1037	Enantioselective interaction with acetylcholinesterase of an organophosphate insecticide fenamiphos. **2010**, 22, 612-7	15
1036	Crystal structure analysis and in silico pKa calculations suggest strong pKa shifts of ligands as driving force for high-affinity binding to TGT. **2009**, 10, 716-27	21
1035	Synthesis and structure-activity correlation of a brunsvicamide-inspired cyclopeptide collection. **2009**, 10, 1153-62	27
1034	Disruption of transcriptionally active Stat3 dimers with non-phosphorylated, salicylic acid-based small molecules: potent in vitro and tumor cell activities. **2009**, 10, 1959-64	74
1033	Virtual screening and biological characterization of novel histone arginine methyltransferase PRMT1 inhibitors. **2009**, 4, 69-77	66
1032	C6-unsubstituted pyrazolo[3,4-d]pyrimidines are dual Src/Abl inhibitors effective against imatinib mesylate resistant chronic myeloid leukemia cell lines. **2009**, 4, 118-26	25
1031	Pharmacophore-based discovery of small-molecule inhibitors of protein-protein interactions between HIV-1 integrase and cellular cofactor LEDGF/p75. **2009**, 4, 1311-6	81
1030	Elastic potential grids: accurate and efficient representation of intermolecular interactions for fully flexible docking. **2009**, 4, 1264-8	26
1029	How to replace the residual solvation shell of polar active site residues to achieve nanomolar inhibition of tRNA-guanine transglycosylase. **2009**, 4, 2012-23	26
1028	Fast prediction of cytochrome P450 mediated drug metabolism. **2009**, 4, 2070-9	45
1027	A novel method for protein-ligand binding affinity prediction and the related descriptors exploration. **2009**, 30, 900-9	22
1026	A new method for the gradient-based optimization of molecular complexes. **2009**, 30, 1371-8	9
1025	Blind docking method combining search of low-resolution binding sites with ligand pose refinement by molecular dynamics-based global optimization. **2010**, 31, 1080-92	12

1024	Q-Dock(LHM): Low-resolution refinement for ligand comparative modeling. **2010**, 31, 1093-105	20
1023	New mathematic model for predicting chiral separation using molecular docking: mechanism of chiral recognition of triadimenol analogues. **2009**, 32, 2401-7	9
1022	Similarity methods in chemoinformatics. **2009**, 43, 1-117	51
1021	Peptidic modulators of protein-protein interactions: progress and challenges in computational design. **2009**, 91, 505-13	83
1020	PostDock: A novel visualization tool for the analysis of molecular docking. **2009**, 12, 1-7	5
1019	Molecular modeling of the three-dimensional structure of GLP-1R and its interactions with several agonists. **2009**, 15, 53-65	44
1018	A butterfly effect: highly insecticidal resistance caused by only a conservative residue mutated of drosophila melanogaster acetylcholinesterase. **2009**, 15, 1229-36	3
1017	Covalent complexes of proteasome model with peptide aldehyde inhibitors MG132 and MG101: docking and molecular dynamics study. **2009**, 15, 1481-90	23
1016	Combining a genetic algorithm with a linear scaling semiempirical method for protein□gand docking. **2009**, 898, 31-41	12
1015	The identification of novel PLC-gamma inhibitors using virtual high throughput screening. **2009**, 17, 3169-76	40
1014	Synthesis and multidrug resistance reversal activity of dihydroptychantol A and its novel derivatives. **2009**, 17, 4981-9	18
1013	Fascaplysin-inspired diindolyls as selective inhibitors of CDK4/cyclin D1. **2009**, 17, 6073-84	33
1012	Synthesis and biological evaluation of the metabolites of 2-(1-{3-[(6-chloronaphthalen-2-yl)sulfonyl]propanoyl}piperidin-4-yl)-5-methyl-1,2-dihydro-3H-imidazo[1,5-c]imidazol-3-on **2009**, 17, 7993-8002	12
1011	Computational analysis of R and S isoforms of 12-lipoxygenases: homology modeling and docking studies. **2009**, 27, 744-50	10
1010	Induced-fit docking studies of the active and inactive states of protein tyrosine kinases. **2009**, 28, 336-46	72
1009	Preferential binding of anti-cancer drug adriamycin to the Sp1 binding site in c-met promoter region: A spectroscopic and molecular modeling study. **2009**, 920, 208-213	6
1008	Chiral 3-(4,5-dihydrooxazol-2-yl)phenyl alkylcarbamates as novel FAAH inhibitors: Insight into FAAH enantioselectivity by molecular docking and interaction fields. **2009**, 44, 4179-91	22
1007	An improved adaptive genetic algorithm for protein-ligand docking. **2009**, 23, 1-12	24

1006	Effects of protein conformation in docking: improved pose prediction through protein pocket adaptation. **2009**, 23, 355-74	81
1005	Hybrid scoring and classification approaches to predict human pregnane X receptor activators. **2009**, 26, 1001-11	48
1004	Predicting inhibitors of acetylcholinesterase by regression and classification machine learning approaches with combinations of molecular descriptors. **2009**, 26, 2216-24	24
1003	Application of screening methods, shape signatures and engineered biosensors in early drug discovery process. **2009**, 26, 2247-58	19
1002	Use of quantitative (1)H NMR chemical shift changes for ligand docking into barnase. **2009**, 43, 11-9	27
1001	Pressure-dependent 13C chemical shifts in proteins: origins and applications. **2009**, 44, 25-33	13
1000	A novel conformation optimization model and algorithm for structure-based drug design. **2009**, 46, 182-198	2
999	Screening and docking studies of natural phenolic inhibitors of carbonic anhydrase II. **2009**, 52, 332-337	5
998	Emergent strategies for inverse molecular design. **2009**, 52, 1769-1776	9
997	Docking and molecular dynamics studies on the stereoselectivity in the enzymatic synthesis of carbohydrates. **2009**, 122, 283-296	15
996	The unique substrate specificity of human AOC2, a semicarbazide-sensitive amine oxidase. **2009**, 66, 2743-57	27
995	MADAMM: a multistaged docking with an automated molecular modeling protocol. **2009**, 74, 192-206	27
994	Docking and scoring with alternative side-chain conformations. **2009**, 74, 712-26	29
993	Molecular insights into substrate specificity of prostate specific antigen through structural modeling. **2009**, 77, 984-93	12
992	Docking Study and Three-Dimensional Quantitative Structure-Activity Relationship (3D-QSAR) Analyses of Transforming Growth Factor-β Type I Receptor Kinase Inhibitors. **2009**, 28, 1300-1308	3
991	Pharmacophore Guided 3D-QSAR CoMFA Analysis of Amino Substituted Nitrogen Heterocycle Ureas as KDR Inhibitors. **2009**, 28, 1524-1536	4
990	Blind docking of pharmaceutically relevant compounds using RosettaLigand. **2009**, 18, 1998-2002	60
989	Crystallographic structure of the tetratricopeptide repeat domain of Plasmodium falciparum FKBP35 and its molecular interaction with Hsp90 C-terminal pentapeptide. **2009**, 18, 2115-24	25

988	Application of the PM6 semi-empirical method to modeling proteins enhances docking accuracy of AutoDock. **2009**, 1, 15	334
987	Shape: automatic conformation prediction of carbohydrates using a genetic algorithm. **2009**, 1, 16	20
986	Combining docking with pharmacophore filtering for improved virtual screening. **2009**, 1, 6	38
985	The CYP3A4*18 genotype in the cytochrome P450 3A4 gene, a rapid metabolizer of sex steroids, is associated with low bone mineral density. **2009**, 85, 312-8	53
984	Pharmacophore-based virtual screening versus docking-based virtual screening: a benchmark comparison against eight targets. **2009**, 30, 1694-708	68
983	Zebrafish chemical screening reveals an inhibitor of Dusp6 that expands cardiac cell lineages. **2009**, 5, 680-7	190
982	Salermide, a Sirtuin inhibitor with a strong cancer-specific proapoptotic effect. **2009**, 28, 781-91	221
981	Comparison of the inward- and outward-open homology models and ligand binding of human P-glycoprotein. **2009**, 276, 7016-26	32
980	AutoGrow: a novel algorithm for protein inhibitor design. **2009**, 73, 168-78	70
979	Discovery and binding studies on a series of novel Pin1 ligands. **2009**, 73, 369-79	9
978	Inhibition of purple acid phosphatase with alpha-alkoxynaphthylmethylphosphonic acids. **2009**, 19, 163-6	28
977	1-Aryl-3,4-dihydroisoquinoline inhibitors of JNK3. **2009**, 19, 2230-4	29
976	Molecular docking: theoretical background, practical applications and perspectives. **2009**, 19, 237-242	16
975	Putrescine N-methyltransferase--the start for alkaloids. **2009**, 70, 1708-18	52
974	Toward the three-dimensional structure and lysophosphatidic acid binding characteristics of the LPA(4)/p2y(9)/GPR23 receptor: a homology modeling study. **2009**, 28, 70-9	7
973	Computer-assisted identification of small-molecule Bcl-2 modulators. **2009**, 33, 451-6	
972	Design, synthesis, and evaluation of benzophenone derivatives as novel acetylcholinesterase inhibitors. **2009**, 44, 1341-8	29
971	Synthesis and biological evaluation of a new family of anti-benzylanilinosulfonamides as CA IX inhibitors. **2009**, 44, 511-8	11

970	Synthesis of new dipyrrolo- and furopyrrolopyrazinones related to tripentones and their biological evaluation as potential kinases (CDKs1-5, GSK-3) inhibitors. **2009**, 44, 708-16	17
969	Fragment and knowledge-based design of selective GSK-3beta inhibitors using virtual screening models. **2009**, 44, 2361-71	24
968	Receptor-based 3D-QSAR studies of checkpoint Wee1 kinase inhibitors. **2009**, 44, 1383-95	14
967	Novel CYP17 inhibitors: synthesis, biological evaluation, structure-activity relationships and modelling of methoxy- and hydroxy-substituted methyleneimidazolyl biphenyls. **2009**, 44, 2765-75	55
966	Discovery of potential new InhA direct inhibitors based on pharmacophore and 3D-QSAR analysis followed by in silico screening. **2009**, 44, 3718-30	21
965	Non-peptidic substrate-mimetic inhibitors of Akt as potential anti-cancer agents. **2009**, 17, 1764-71	23
964	Ligand-based and structure-based virtual screening to identify carbonic anhydrase IX inhibitors. **2009**, 17, 553-7	14
963	Design, synthesis and biological evaluation of novel stilbene-based antitumor agents. **2009**, 17, 512-22	23
962	Structure-based virtual screening for novel inhibitors of the sarco/endoplasmic reticulum calcium ATPase and their experimental evaluation. **2009**, 17, 1353-60	12
961	Novel 6-methanesulfonamide-3,4-methylenedioxyphenyl-N-acylhydrazones: orally effective anti-inflammatory drug candidates. **2009**, 17, 1125-31	29
960	Development of 3-substituted-1H-indole derivatives as NR2B/NMDA receptor antagonists. **2009**, 17, 1640-7	28
959	Discovery of 2-(5-nitrothiazol-2-ylthio)benzo[d]thiazoles as novel c-Jun N-terminal kinase inhibitors. **2009**, 17, 2712-7	19
958	Structure-activity relationship studies of a novel series of anthrax lethal factor inhibitors. **2009**, 17, 3352-68	19
957	Synthesis, cannabinoid receptor affinity, molecular modeling studies and in vivo pharmacological evaluation of new substituted 1-aryl-5-(1H-pyrrol-1-yl)-1H-pyrazole-3-carboxamides. 2. Effect of the 3-carboxamide substituent on the affinity and selectivity profile. **2009**, 17, 5549-64	13
956	The marine natural-derived inhibitors of glycogen synthase kinase-3beta phenylmethylene hydantoins: In vitro and in vivo activities and pharmacophore modeling. **2009**, 17, 6032-9	41
955	alpha-Substituted norstatines as the transition-state mimic in inhibitors of multiple digestive vacuole malaria aspartic proteases. **2009**, 17, 5933-49	32
954	Design, synthesis, and biological evaluation of hydroquinone derivatives as novel inhibitors of the sarco/endoplasmic reticulum calcium ATPase. **2009**, 17, 6613-9	12
953	Synthesis, structure-affinity relationships, and modeling of AMDA analogs at 5-HT2A and H1 receptors: structural factors contributing to selectivity. **2009**, 17, 6496-504	17

952	Computational modeling of novel inhibitors targeting the Akt pleckstrin homology domain. **2009**, 17, 6983-92	27
951	Tetraiodobenzimidazoles are potent inhibitors of protein kinase CK2. **2009**, 17, 7281-9	50
950	Molecular modeling, synthesis, and activity studies of novel biaryl and fused-ring BACE1 inhibitors. **2009**, 19, 264-74	14
949	Combining 3D-QSAR, docking, molecular dynamics and MM/PBSA methods to predict binding modes for nonsteroidal selective modulator to glucocorticoid receptor. **2009**, 19, 393-6	9
948	Discovery of novel inhibitors of Trypanosoma cruzi trans-sialidase from in silico screening. **2009**, 19, 589-96	60
947	Indolyl-pyrrolone as a new scaffold for Pim1 inhibitors. **2009**, 19, 1512-6	27
946	Design, synthesis, and evaluation of peptidomimetics containing Freidinger lactams as STAT3 inhibitors. **2009**, 19, 1733-6	22
945	Discovery of betrixaban (PRT054021), N-(5-chloropyridin-2-yl)-2-(4-(N,N-dimethylcarbamimidoyl)benzamido)-5-methoxybenzamide, a highly potent, selective, and orally efficacious factor Xa inhibitor. **2009**, 19, 2179-85	76
944	Discovery and structure-guided drug design of inhibitors of 11beta-hydroxysteroid-dehydrogenase type I based on a spiro-carboxamide scaffold. **2009**, 19, 3682-5	25
943	Discovery and structure-activity relationships of pentanedioic acid diamides as potent inhibitors of 11beta-hydroxysteroid dehydrogenase type I. **2009**, 19, 2674-8	20
942	Discovery of novel benzene 1,3-dicarboxylic acid inhibitors of bacterial MurD and MurE ligases by structure-based virtual screening approach. **2009**, 19, 2668-73	61
941	Structural and theoretical studies of [6-bromo-1-(4-fluorophenylmethyl)-4(1H)-quinolinon-3-yl)]-4-hydroxy-2-oxo-3-butenoic acid as HIV-1 integrase inhibitor. **2009**, 19, 4806-9	7
940	Discovery of a novel protein kinase B inhibitor by structure-based virtual screening. **2009**, 19, 4634-8	16
939	The first pharmacophore model for potent NF-kappaB inhibitors. **2009**, 19, 5665-9	8
938	Phosphoinositide-3-kinase (PI3K) inhibitors: identification of new scaffolds using virtual screening. **2009**, 19, 5842-7	24
937	Structure-activity relationship (SAR) studies of 3-(2-amino-ethyl)-5-(4-ethoxy-benzylidene)-thiazolidine-2,4-dione: development of potential substrate-specific ERK1/2 inhibitors. **2009**, 19, 6042-6	32
936	Design of novel alpha7-subtype-preferring nicotinic acetylcholine receptor agonists: application of docking and MM-PBSA computational approaches, synthetic and pharmacological studies. **2009**, 19, 6353-7	26
935	Molecular dynamics simulation study of valyl-tRNA synthetase with its pre- and post-transfer editing substrates. **2009**, 143, 34-43	8

934	Design, synthesis, and structure-activity relationship of substrate competitive, selective, and in vivo active triazole and thiadiazole inhibitors of the c-Jun N-terminal kinase. **2009**, 52, 1943-52	62
933	Discovery and development of the covalent hydrates of trifluoromethylated pyrazoles as riboflavin synthase inhibitors with antibiotic activity against Mycobacterium tuberculosis. **2009**, 74, 5297-303	44
932	A Linear-Time Graph Kernel. **2009**,	48
931	Virtual screening and prediction of site of metabolism for cytochrome P450 1A2 ligands. **2009**, 49, 43-52	71
930	Reduced Catalytic Activity of P450 2A6 Mutants with Coumarin: A Computational Investigation. **2009**, 5, 1411-20	22
929	Improving quantitative structure-activity relationships through multiobjective optimization. **2009**, 49, 2290-302	44
928	Steering protein-ligand docking with quantitative NMR chemical shift perturbations. **2009**, 49, 2260-71	32
927	Structure-activity relations of nanolipoblockers with the atherogenic domain of human macrophage scavenger receptor A. **2009**, 10, 1381-91	22
926	Hybrid structure-based virtual screening protocol for the identification of novel BACE1 inhibitors. **2009**, 49, 647-57	24
925	Identification of xenoestrogens in food additives by an integrated in silico and in vitro approach. **2009**, 22, 52-63	64
924	Docking ligands into flexible and solvated macromolecules. 5. Force-field-based prediction of binding affinities of ligands to proteins. **2009**, 49, 2564-71	29
923	Protein-ligand docking using mutually orthogonal Latin squares (MOLSDOCK). **2009**, 49, 2687-94	11
922	Influence of protonation, tautomeric, and stereoisomeric states on protein-ligand docking results. **2009**, 49, 1535-46	106
921	Testing assumptions and hypotheses for rescoring success in protein-ligand docking. **2009**, 49, 1871-8	26
920	Elucidating molecular overlays from pairwise alignments using a genetic algorithm. **2009**, 49, 1847-55	10
919	Structure-based CoMFA as a predictive model - CYP2C9 inhibitors as a test case. **2009**, 49, 853-64	24
918	Comparative docking study of anibamine as the first natural product CCR5 antagonist in CCR5 homology models. **2009**, 49, 120-32	32
917	Importance of ligand reorganization free energy in protein-ligand binding-affinity prediction. **2009**, 131, 13709-21	59

916	Design, synthesis, biological evaluation, and NMR studies of a new series of arylsulfones as selective and potent matrix metalloproteinase-12 inhibitors. **2009**, 52, 6347-61		42
915	Recombinant plasmepsin 1 from the human malaria parasite plasmodium falciparum: enzymatic characterization, active site inhibitor design, and structural analysis. **2009**, 48, 4086-99		18
914	Binding ensemble profiling with photoaffinity labeling (BEProFL) approach: mapping the binding poses of HDAC8 inhibitors. **2009**, 52, 7003-13		39
913	Mechanism of NS2B-mediated activation of NS3pro in dengue virus: molecular dynamics simulations and bioassays. **2009**, 83, 1060-70		41
912	Charges for Large Scale Binding Free Energy Calculations with the Linear Interaction Energy Method. **2009**, 5, 380-95		12
911	Docking of hydroxamic acids into HDAC1 and HDAC8: a rationalization of activity trends and selectivities. **2009**, 49, 2774-85		33
910	A short series of antidiabetic sulfonylureas exhibit multiple ligand PPARgamma-binding patterns. **2009**, 63, 56-62		11
909	Synthesis and evaluation of Apogossypol atropisomers as potential Bcl-xL antagonists. **2009**, 273, 107-13		25
908	The importance of discerning shape in molecular pharmacology. **2009**, 30, 138-47		92
907	Inhibiting the inhibitors: retro-inverso Smac peptides. **2009**, 30, 2374-9		10
906	Identification and characterization of two arginine kinases from the parasitic insect Ctenocephalides felis. **2009**, 39, 634-45		17
905	Specific loops D, E and F of nicotinic acetylcholine receptor beta1 subunit may confer imidacloprid selectivity between Myzus persicae and its predatory enemy Pardosa pseudoannulata. **2009**, 39, 833-41		25
904	The design of novel 17beta-hydroxysteroid dehydrogenase type 3 inhibitors. **2009**, 301, 259-65		22
903	The binding of lignans, flavonoids and coumestrol to CYP450 aromatase: a molecular modelling study. **2009**, 301, 235-44		33
902	Top 100 Most-Cited Articles from JMB. *Journal of Molecular Biology*, **2009**, 385, 8-10	6.5	
901	The regulation mechanism for the auto-inhibition of binding of human filamin A to integrin. *Journal of Molecular Biology*, **2009**, 393, 644-57	6.5	53
900	Understanding the mechanism of drug resistance due to a codon deletion in protoporphyrinogen oxidase through computational modeling. **2009**, 113, 4865-75		43
899	Docking ligands into flexible and solvated macromolecules. 3. Impact of input ligand conformation, protein flexibility, and water molecules on the accuracy of docking programs. **2009**, 49, 997-1009		92

898	Small-molecule inhibitors of the MDM2-p53 protein-protein interaction to reactivate p53 function: a novel approach for cancer therapy. **2009**, 49, 223-41	477
897	Docking studies on a new human immunodeficiency virus integrase-Mg-DNA complex: phenyl ring exploration and synthesis of 1H-benzylindole derivatives through fluorine substitutions. **2009**, 52, 569-73	37
896	Molecular docking of carbohydrate ligands to antibodies: structural validation against crystal structures. **2009**, 49, 2749-60	57
895	Molecular docking studies and anti-tyrosinase activity of Thai mango seed kernel extract. **2009**, 14, 257-65	40
894	Directed discovery of agents targeting the Met tyrosine kinase domain by virtual screening. **2009**, 52, 943-51	54
893	Structure-based design, synthesis, and biological evaluation of a series of novel and reversible inhibitors for the severe acute respiratory syndrome-coronavirus papain-like protease. **2009**, 52, 5228-40	86
892	Fragment-Based Drug Discovery in Academia: Experiences From a Tuberculosis Programme. **2009**, 21-36	3
891	Docking Ligands on Protein Surfaces: The Case Study of Prion Protein. **2009**, 5, 2565-73	30
890	Molecular docking screens using comparative models of proteins. **2009**, 49, 2512-27	116
889	Structure-activity relationships for substrate-based inhibitors of human complement factor B. **2009** , 52, 6042-52	10
888	A docking study using atomistic conformers generated via elastic network model for cyclosporin A/cyclophilin A complex. **2009**, 27, 13-26	40
887	Design, synthesis, and evaluation of N-acyl modified sialic acids as inhibitors of adenoviruses causing epidemic keratoconjunctivitis. **2009**, 52, 3666-78	9
886	Empirical scoring functions for advanced protein-ligand docking with PLANTS. **2009**, 49, 84-96	801
885	Synthesis and biological evaluation of coumarin-based inhibitors of NAD(P)H: quinone oxidoreductase-1 (NQO1). **2009**, 52, 7142-56	70
884	Structure-activity relationship and comparative docking studies for cycloguanil analogs as PfDHFR-TS inhibitors. **2009**, 49, 1787-96	20
883	New insights into the SAR and binding modes of bis(hydroxyphenyl)thiophenes and -benzenes: influence of additional substituents on 17beta-hydroxysteroid dehydrogenase type 1 (17beta-HSD1) inhibitory activity and selectivity. **2009**, 52, 6724-43	68
882	Discovery and characterization of a small molecule inhibitor of the PDZ domain of dishevelled. **2009**, 284, 16256-16263	154
881	How to optimize shape-based virtual screening: choosing the right query and including chemical information. **2009**, 49, 678-92	164

880	Pattern Recognition in Bioinformatics. **2009**,	
879	From Molecules to Medicines. **2009**,	
878	The crystal structure of a complex of acetylcholinesterase with a bis-(-)-nor-meptazinol derivative reveals disruption of the catalytic triad. **2009**, 52, 2543-9	22
877	Molecular docking studies and anti-enzymatic activities of Thai mango seed kernel extract against snake venoms. **2009**, 14, 1404-22	33
876	Predictions of binding for dopamine D2 receptor antagonists by the SIE method. **2009**, 49, 2369-75	22
875	Use of acetylcholine binding protein in the search for novel alpha7 nicotinic receptor ligands. In silico docking, pharmacological screening, and X-ray analysis. **2009**, 52, 2372-83	74
874	Validation of molecular docking programs for virtual screening against dihydropteroate synthase. **2009**, 49, 444-60	237
873	Computational studies of epidermal growth factor receptor: docking reliability, three-dimensional quantitative structure-activity relationship analysis, and virtual screening studies. **2009**, 52, 964-75	30
872	Quinalizarin as a potent, selective and cell-permeable inhibitor of protein kinase CK2. **2009**, 421, 387-95	127
871	New 2-aryloxy-3-phenyl-propanoic acids as peroxisome proliferator-activated receptors alpha/gamma dual agonists with improved potency and reduced adverse effects on skeletal muscle function. **2009**, 52, 6382-93	35
870	Docking scores and QSAR using evolved neural networks for the Pan-inhibition of wild-type and mutant PfDHFR by cycloguanil derivatives. **2009**,	4
869	In silico fragment screening by replica generation (FSRG) method for fragment-based drug design. **2009**, 49, 925-33	16
868	Assessment of QM/MM scoring functions for molecular docking to HIV-1 protease. **2009**, 49, 913-24	41
867	Biophysics and the Challenges of Emerging Threats. **2009**,	
866	Comparative assessment of scoring functions on a diverse test set. **2009**, 49, 1079-93	373
865	Combinatorial library enumeration and lead hopping using comparative interaction fingerprint analysis and classical 2D QSAR methods for seeking novel GABA(A) alpha(3) modulators. **2009**, 49, 2498-511	15
864	Docking and 3D-QSAR studies on isatin sulfonamide analogues as caspase-3 inhibitors. **2009**, 49, 1963-73	36
863	QSAR study of selective I1-imidazoline receptor ligands. **2009**, 20, 133-44	8

862 Computational approaches to predict drug metabolism. **2009**, 5, 15-27 36

861 SCDL Applications to Drug Discovery. **2009**, 1

860 . **2009**,

859 Combined Virtual Screening Strategies. **2009**, 5, 23-37 22

858 Novel method for generating structure-based pharmacophores using energetic analysis. **2009**, 49, 2356-68 224

857 Protein-ligand binding free energy calculation by the Smooth Reaction Path Generation (SRPG) Method. **2009**, 49, 1944-51 22

856 Synthesis and evaluation of 2,5-dihydrochorismate analogues as inhibitors of the chorismate-utilising enzymes. **2009**, 7, 2421-9 22

855 SeleX-CS: a new consensus scoring algorithm for hit discovery and lead optimization. **2009**, 49, 623-33 35

854 New pyridinone derivatives as potent HIV-1 nonnucleoside reverse transcriptase inhibitors. **2009**, 52, 3636-43 20

853 Pharmacophore modeling for qualitative prediction of antiestrogenic activity. **2009**, 49, 2489-97 25

852 Automated docking screens: a feasibility study. **2009**, 52, 5712-20 213

851 Exploiting the pyrazolo[3,4-d]pyrimidin-4-one ring system as a useful template to obtain potent adenosine deaminase inhibitors. **2009**, 52, 1681-92 38

850 Quaternary benzyltriethylammonium ion binding to the Na,K-ATPase: a tool to investigate extracellular K+ binding reactions. **2009**, 48, 8105-19 8

849 Molecular docking studies and anti-snake venom metalloproteinase activity of Thai mango seed kernel extract. **2009**, 14, 3198-213 27

848 Bioinformatics Approaches for Analysis of Protein□ligand Interactions. 267-299 2

847 Human Siglec-10 can bind to vascular adhesion protein-1 and serves as its substrate. **2009**, 114, 5385-92 68

846 Predicting multiple binding modes using a kernel method based on a vector space model molecular descriptor. **2009**, 2, 58-80 3

845 QSAR of Carbonic Anhydrase Inhibitors and Their Impact on Drug Design. 375-397

844	Protein-protein interaction inhibition (2P2I): fewer and fewer undruggable targets. **2009**, 12, 968-83	11
843	Steroid hormone binding receptors: application of homology modeling, induced fit docking, and molecular dynamics to study structure-function relationships. **2009**, 9, 844-53	14
842	How computational methods try to disclose the estrogen receptor secrecy--modeling the flexibility. **2009**, 16, 2987-3027	14
841	Protein-drug interaction studies for development of drugs against Plasmodium falciparum. **2009**, 10, 271-8	15
840	Bayesian modeling in virtual high throughput screening. **2009**, 12, 469-83	16
839	G Protein-Coupled Receptors: target-based in silico screening. **2009**, 15, 4049-68	30
838	G protein coupled receptors -in silico drug discovery and design. **2010**, 10, 638-56	23
837	Kinetics and docking studies of a COX-2 inhibitor isolated from Terminalia bellerica fruits. **2010**, 17, 1251-7	23
836	Post processing of protein-compound docking for fragment-based drug discovery (FBDD): in-silico structure-based drug screening and ligand-binding pose prediction. **2010**, 10, 680-94	12
835	GPCR Homology Model Development and Application. **2010**, 279-300	3
834	Protein Flexibility in In Silico Screening. **2010**, 867-887	
833	Three dimensional model for N-terminal A domain of DmpR (2-dimethylphenol) protein based on secondary structure prediction and fold recognition. **2010**, 10, 223-33	5
832	Activity of the multitargeted kinase inhibitor, AT9283, in imatinib-resistant BCR-ABL-positive leukemic cells. **2010**, 116, 2089-95	48
831	Cheminformatics. **2010**, 1	
830	Evaluation of docking calculations on X-ray structures using CONSENSUS-DOCK. **2010**, 58, 1655-7	6
829	[Molecular docking: role of intermolecular contacts in formation of complexes of proteins with nucleotides and peptides]. **2010**, 36, 482-92	11
828	16alpha-Hydroxycleroda-3,13 (14)Z-dien-15,16-olide from Polyalthia longifolia: a safe and orally active antileishmanial agent. **2010**, 159, 1143-50	50
827	Some Trends in Chem(o)informatics. **2011**, 672, 1-37	15

826	Inhibition of chorismate-utilising enzymes by 2-amino-4-carboxypyridine and 4-carboxypyridone and 5-carboxypyridone analogues. **2010**, 8, 3534-42	14
825	Novel alpha-7 nicotinic acetylcholine receptor agonists containing a urea moiety: identification and characterization of the potent, selective, and orally efficacious agonist 1-[6-(4-fluorophenyl)pyridin-3-yl]-3-(4-piperidin-1-ylbutyl) urea (SEN34625/WYE-103914). **2010**, 53, 4379-89	28
824	Tautomer preference in PDB complexes and its impact on structure-based drug discovery. **2010**, 50, 1062-74	51
823	In silico Discovery of Chemotherapeutic Agents. **2010**, 279-304	
822	Addressing limitations with the MM-GB/SA scoring procedure using the WaterMap method and free energy perturbation calculations. **2010**, 50, 547-59	62
821	Gatekeeper mutations mediate resistance to BRAF-targeted therapies. **2010**, 2, 35ra41	127
820	Surface plasmon resonance biosensor based fragment screening using acetylcholine binding protein identifies ligand efficiency hot spots (LE hot spots) by deconstruction of nicotinic acetylcholine receptor β ligands. **2010**, 53, 7192-201	30
819	COVID-19 Outbreak Prediction with Machine Learning.	5
818	Structural basis for active-site probes targeting Staphylococcus aureus serine hydrolase virulence factors.	1
817	Repurposing the antidepressant sertraline as SHMT inhibitor to suppress serine/glycine synthesis addicted breast tumor growth.	1
816	TRAF4 inhibits bladder cancer progression by promoting BMP/SMAD signalling pathway.	1
815	An antibiotic-resistance conferring mutation in a neisserial porin: Structure, ion flux, and ampicillin binding.	1
814	Evaluation of protein-ligand docking methods on peptide-ligand complexes for docking small ligands to peptides.	5
813	Pharmacological Characterisation of Novel Adenosine Receptor A3R Antagonists.	5
812	Why is interoperability between the two fields of chemical crystallography and protein crystallography so difficult?. **2019**, 6, 788-793	5
811	Coordination of a triazine ligand with Cu and Ag investigated by spectral, structural, theoretical and docking studies. **2019**, 75, 1389-1397	4
810	The structure of the Moco carrier protein from Rippkaea orientalis. **2020**, 76, 453-463	3
809	Conformational Analysis, Solvent-Accessible Surface and Geometric Extent of Inhibitors and Substrates. **2006**, 71, 842-858	1

808	Molecular tetris. **2014**,	1
807	Repurposing the Antidepressant Sertraline as SHMT Inhibitor to Suppress Serine/Glycine Synthesis-Addicted Breast Tumor Growth. **2021**, 20, 50-63	12
806	Evidence of multi-functional peptide activity: potential role of KT2 and RT2 for anti-inflammatory, anti-oxidative stress, and anti-apoptosis properties. **2020**, 63,	4
805	Matrix metalloproteinase9 as the protein target in anti-breast cancer drug discovery: an approach by targeting hemopexin domain. **2019**, 5,	10
804	Docking and Scoring. **2003**,	1
803	DNA Drug Interactions. **2011**,	4
802	DOCLASP - Docking ligands to target proteins using spatial and electrostatic congruence extracted from a known holoenzyme and applying simple geometrical transformations. 3, 262	2
801	Combinatorial computational approaches to identify tetracycline derivatives as flavivirus inhibitors. **2007**, 2, e428	72
800	Molecular interaction studies of trimethoxy flavone with human serum albumin. **2010**, 5, e8834	87
799	Elimination of endogenous toxin, creatinine from blood plasma depends on albumin conformation: site specific uremic toxicity & impaired drug binding. **2011**, 6, e17230	84
798	A model of a MAPK substrate complex in an active conformation: a computational and experimental approach. **2011**, 6, e18594	17
797	Exploring DNA topoisomerase I ligand space in search of novel anticancer agents. **2011**, 6, e25150	32
796	Honey bee dopamine and octopamine receptors linked to intracellular calcium signaling have a close phylogenetic and pharmacological relationship. **2011**, 6, e26809	65
795	Application of consensus scoring and principal component analysis for virtual screening against secretase (BACE-1). **2012**, 7, e38086	30
794	An efficient computational method for calculating ligand binding affinities. **2012**, 7, e42846	27
793	Virtual screening as a strategy for the identification of xenobiotics disrupting corticosteroid action. **2012**, 7, e46958	25
792	Conformational transition pathway in the activation process of allosteric glucokinase. **2013**, 8, e55857	11
791	Molecular dynamics reveal binding mode of glutathionylspermidine by trypanothione synthetase. **2013**, 8, e56788	23

790	In silico study on binding specificity of gonadotropins and their receptors: design of a novel and selective peptidomimetic for human follicle stimulating hormone receptor. **2013**, 8, e64475	5
789	CD38 Structure-Based Inhibitor Design Using the N1-Cyclic Inosine 5'-Diphosphate Ribose Template. **2013**, 8, e66247	21
788	In silico mechanistic profiling to probe small molecule binding to sulfotransferases. **2013**, 8, e73587	14
787	Elucidation of substrate specificity in Aspergillus nidulans UDP-galactose-4-epimerase. **2013**, 8, e76803	7
786	Differential effects of genistein on prostate cancer cells depend on mutational status of the androgen receptor. **2013**, 8, e78479	43
785	Synthesis and properties of a selective inhibitor of homeodomain-interacting protein kinase 2 (HIPK2). **2014**, 9, e89176	17
784	Nickel(II) complex of polyhydroxybenzaldehyde N4-thiosemicarbazone exhibits anti-inflammatory activity by inhibiting NF-Β transactivation. **2014**, 9, e100933	42
783	Identification of Small-Molecule Inhibitors against Meso-2, 6-Diaminopimelate Dehydrogenase from Porphyromonas gingivalis. **2015**, 10, e0141126	9
782	Effect of Methamphetamine on Spectral Binding, Ligand Docking and Metabolism of Anti-HIV Drugs with CYP3A4. **2016**, 11, e0146529	7
781	Vinardo: A Scoring Function Based on Autodock Vina Improves Scoring, Docking, and Virtual Screening. **2016**, 11, e0155183	107
780	Discovery of a Series of Acridinones as Mechanism-Based Tubulin Assembly Inhibitors with Anticancer Activity. **2016**, 11, e0160842	6
779	Induction of axial chirality in divanillin by interaction with bovine serum albumin. **2017**, 12, e0178597	9
778	A composite docking approach for the identification and characterization of ectosteric inhibitors of cathepsin K. **2017**, 12, e0186869	5
777	Development of Software Program Predicting the Binding Site and the Binding Mode of Ligands Against a Target Protein. **2008**, 6, 241-245	2
776	Computational methods for calculation of protein-ligand binding affinities in structure-based drug design. **2020**,	1
775	Triterpenoids from exert cytotoxicity and multidrug resistant reversal effect in MCF-7/ADM cells via reactive oxygen species induction and P-glycoprotein inhibition. **2017**, 8, 69465-69476	3
774	Applications of Molecular Simulation in the Discovery of Antituberculosis Drugs: A Review. **2019**, 26, 648-663	5
773	Advances in the Treatment of Explicit Water Molecules in Docking and Binding Free Energy Calculations. **2019**, 26, 7598-7622	5

772	In-Silico Modeling in Drug Metabolism and Interaction: Current Strategies of Lead Discovery. **2019**, 25, 3292-3305	5
771	Synthesis of Eugenol Derivatives and Evaluation of their Antifungal Activity Against f. sp.. **2020**, 26, 1532-1542	2
770	In Silico Studies on Anti-Stress Compounds of Ethanolic Root Extract of Hemidesmus indicus L. **2020**, 21, 502-515	4
769	In Silico Studies against Viral Sexually Transmitted Diseases. **2019**, 20, 1135-1150	0
768	Consensus Analyses in Molecular Docking Studies Applied to Medicinal Chemistry. **2020**, 20, 1322-1340	4
767	Anticholinesterase and Antioxidant Activities of Natural Abietane Diterpenoids with Molecular Docking Studies. **2020**, 17, 269-284	3
766	Virtual Screening Techniques in Drug Discovery: Review and Recent Applications. **2019**, 19, 1751-1767	32
765	Search for Potential Inducible Nitric Oxide Synthase Inhibitors with Favorable ADMET Profiles for the Therapy of Helicobacter pylori Infections. **2019**, 19, 2795-2804	3
764	Antioxidant and Antibacterial Activity of Sulfonamides Derived from Carvacrol: A Structure-Activity Relationship Study. **2020**, 20, 173-181	1
763	Molecular Docking and Quantum Studies of Lawsone Dimers Derivatives: New Investigation of Antioxidant Behavior and Antifungal Activity. **2020**, 20, 182-191	0
762	In Silico Studies in Drug Research Against Neurodegenerative Diseases. **2018**, 16, 664-725	34
761	3D-QSAR and in-silico Studies of Natural Products and Related Derivatives as Monoamine Oxidase Inhibitors. **2018**, 16, 881-900	17
760	In Silico Studies Targeting G-protein Coupled Receptors for Drug Research Against Parkinson's Disease. **2018**, 16, 786-848	10
759	The Development of Tyrosyl-DNA Phosphodyesterase 1 (TDP1) Inhibitors Based on the Amines Combining Aromatic/Heteroaromatic and Monoterpenoid Moieties. **2019**, 16, 597-605	8
758	Relevance of Molecular Docking Studies in Drug Designing. **2020**, 15, 270-278	19
757	Novel Inhibitors of DNA Repair Enzyme TDP1 Combining Monoterpenoid and Adamantane Fragments. **2019**, 19, 463-472	14
756	Alkylamino Phenol Derivative Induces Apoptosis by Inhibiting EGFR Signaling Pathway in Breast Cancer Cells. **2020**, 20, 809-819	2
755	Pyrrolyl Pyrazoline Carbaldehydes as Enoyl-ACP Reductase Inhibitors: Design, Synthesis and Antitubercular Activity. **2017**, 11, 92-108	2

754	Evaluation of Scoring Function Performance on DNA-ligand Complexes. **2019**, 13, 40-49	4
753	Bafilomycin-A1 and ML9 Exert Different Lysosomal Actions to Induce Cell Death. **2019**, 12, 261-271	2
752	Molecular modelling of fentanyl analogs. **2004**, 69, 843-854	6
751	Common structural and pharmacological properties of serotonin 5-HT3 receptors and _7 nicotinic acetylcholine receptors. **2004**, 309-315	1
750	Antidepressant-Like Effect of Terpineol in an Inflammatory Model of Depression: Involvement of the Cannabinoid System and D2 Dopamine Receptor. **2020**, 10,	33
749	Integrated Computational Approaches and Tools forAllosteric Drug Discovery. **2020**, 21,	41
748	Larvicidal Activity of Cinnamic Acid Derivatives: Investigating Alternative Products for L. Control. **2020**, 26,	11
747	First Synthesis of Racemic Propargylamino-Donepezil, a Pleiotrope Agent Able to Both Inhibit AChE and MAO-B, with Potential Interest against Alzheimer's Disease. **2020**, 26,	5
746	Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. **2021**, 9, 71	34
745	Computational enzymology for degradation of chemical warfare agents: promising technologies for remediation processes. **2017**, 3, 108-135	5
744	Computational enzymology for degradation of chemical warfare agents: promising technologies for remediation processes. **2017**, 3, 108-135	4
743	The Comparison of Docking Search Algorithms and Scoring Functions. **2016**, 99-127	4
742	Scoring Functions of Protein-Ligand Interactions. **2016**, 220-245	5
741	Application of Docking Methodologies in QSAR-Based Studies. **2016**, 29-55	2
740	Molecular Docking Challenges and Limitations. **2016**, 56-80	2
739	Computational Approaches for the Discovery of Novel Hepatitis C Virus NS3/4A and NS5B Inhibitors. **2017**, 482-518	1
738	Methods for Docking and Drug Designing. **2017**, 876-890	4
737	Protein-Ligand Docking Methodologies and Its Application in Drug Discovery. **2017**, 891-914	1

736	Molecular Docking Challenges and Limitations. **2017**, 770-794	3
735	Molecular Dynamics Simulations for Biological Systems. **2017**, 1044-1071	1
734	Virtual Screening and Its Applications in Drug Discovery Process. **2019**, 101-126	0
733	The Genetic Algorithm. **2019**, 154-178	2
732	Virtual Screening. **2011**, 28-60	6
731	Binding modes of 2,4-diaminoquinazoline and 2,4-diaminopteridine analogs to P. falciparum dihydrofolate reductase enzyme: Molecular docking studies. **2010**, 72, 324-33	6
730	Generative network complex (GNC) for drug discovery. **2019**, 19, 241-277	8
729	Quantitative Structure-Activity Relationships and Molecular Docking Studies of P56 LCK Inhibitors. **2006**, 27, 266-272	2
728	P56 LCK Inhibitor Identification by Pharmacophore Modelling and Molecular Docking. **2007**, 28, 200-206	5
727	Docking Studies on Formylchromone Derivatives as Protein Tyrosine Phosphatase 1B (PTP1B) Inhibitors. **2007**, 28, 1141-1150	1
726	Pharmacophore Identification for Peroxisome Proliferator-Activated Receptor Gamma Agonists. **2011**, 32, 201-207	8
725	Lipoxygenase Inhibitory Effects of Dibenzylbutane Lignans from the Seeds of Myristica fragrans (Nutmeg). **2014**, 35, 3095-3098	1
724	Docking of phosphonate and trehalose analog inhibitors into M. tuberculosis mycolyltransferase Ag85C: Comparison of the two scoring fitness functions GoldScore and ChemScore, in the GOLD software. **2007**, 1, 339-50	19
723	Modeling of human CCR5 as target for HIV-I and virtual screening with marine therapeutic compounds. **2008**, 3, 89-94	7
722	A utility script for automating and integrating AutoDock and other associated programs for virtual screening. **2009**, 4, 84-6	6
721	Binding of 2CA1P (nocturnal inhibitor) to the active site of RubisCO using genetic algorithm (GA). **2009**, 4, 206-9	2
720	Selection of orlistat as a potential inhibitor for lipase from Candida species. **2011**, 7, 125-9	13
719	Virtual screening of plant derived compounds for aldose reductase inhibition using molecular docking. **2012**, 8, 980-3	2

718	Molecular docking and analgesic studies of Erythrina variegata?s derived phytochemicals with COX enzymes. **2014**, 10, 630-6	4
717	Identification of inhibitors against □sopropylmalate Synthase of Mycobacterium tuberculosis using docking-MM/PBSA hybrid approach. **2017**, 13, 144-148	6
716	Molecular docking and molecular dynamics simulation studies on Thermus thermophilus leucyl-tRNA synthetase complexed with different amino acids and pre-transfer editing substrates. **2016**, 32, 61-69	2
715	Modulating FOXO3 transcriptional activity by small, DBD-binding molecules. **2019**, 8,	5
714	Design and preliminary application of affinity peptide based on the structure of the porcine circovirus type II Capsid (PCV2 Cap). **2019**, 7, e8132	7
713	Discovery of potential targets of Triptolide through inverse docking in ovarian cancer cells. **2020**, 8, e8620	1
712	Coumarins with Xanthine Oxidase Inhibiting and Radical Scavenging Properties: Tools to Combat Oxidative Stress in Cells. **2014**, 4, 234-239	3
711	A Rapid Computational Screening of Millions of Molecules to Identify Sequence-Specific DNA Minor Groove Binders via Physicochemical Descriptors. **2021**, 341-367	1
710	New carvacrol and thymol derivatives as potential insecticides: synthesis, biological activity, computational studies and nanoencapsulation.. **2021**, 11, 34024-34035	3
709	Flavonoid-based inhibitors of the Phi-class glutathione transferase from black-grass to combat multiple herbicide resistance. **2021**, 19, 9211-9222	1
708	Pharmacophore modeling, docking and the integrated use of a ligand- and structure-based virtual screening approach for novel DNA gyrase inhibitors: synthetic and biological evaluation studies.. **2021**, 11, 34462-34478	0
707	A practical guide to large-scale docking. **2021**, 16, 4799-4832	35
706	Synthesis, In Vitro, and In Silico Studies of N-(Substituted-Phenyl)-3-(4-Phenyl-1-Piperazinyl)propanamides as Potent Alkaline Phosphatase Inhibitors. **2021**, 47, 1086-1096	0
705	The inhibitory action of purple tea on in vivo starch digestion compared to other Camellia sinensis teas. **2021**, 150, 110781	1
704	The C2 entity of chitosugars is crucial in molecular selectivity of the Vibrio campbellii chitoporin. **2021**, 297, 101350	0
703	Reverse chemical ecology guides the screening for Grapholita molesta pheromone synergists. **2021** ,	0
702	Prospects of Covalent Approaches in Drug Discovery: An Overview. **2021**, 295-319	0
701	P2Y antagonists: Approved drugs, potential naturally isolated and synthesised compounds, and related in-silico studies. **2022**, 227, 113924	2

700	Serotonin type-3 receptor antagonists selectively kill melanoma cells through classical apoptosis, microtubule depolymerisation, ERK activation, and NF-Β downregulation. **2021**, 1	1
699	Computerized Molecular Modeling for Discovering Promising Glycosaminoglycan Oligosaccharides that Modulate Protein Function. **2022**, 2303, 513-537	1
698	Ligand GA: a genetic algorithm for automated protein inhibitor design.	
697	Discovery of EEDi-5273 as an Exceptionally Potent and Orally Efficacious EED Inhibitor Capable of Achieving Complete and Persistent Tumor Regression. **2021**, 64, 14540-14556	7
696	Beta turn propensity and a model polymer scaling exponent identify intrinsically disordered phase-separating proteins. **2021**, 297, 101343	1
695	Tomatidine and Patchouli Alcohol as Inhibitors of SARS-CoV-2 Enzymes (3CLpro, PLpro and NSP15) by Molecular Docking and Molecular Dynamics Simulations. **2021**, 22,	12
694	Recent Advances in the Prediction of Pharmacokinetics Properties in Drug Design Studies: A Review. **2021**,	1
693	LC-MS Based Analysis and Biological Properties of (Schweinf.) Harms Extracts: A Valuable Source of Antioxidant, Antifungal, and Antibacterial Compounds. **2021**, 10,	6
692	Mangosteen xanthone α-mangostin exerts lowering blood glucose effect with potentiating insulin sensitivity through the mediation of AMPK/PPARγ **2021**, 144, 112333	1
691	Guided rational design with scaffold hopping leading to novel histamine H receptor ligands. **2021**, 117, 105411	0
690	Continuous Sirtuin/HDAC (histone deacetylase) activity assay using thioamides as PET (Photoinduced Electron Transfer)-based fluorescence quencher. **2021**, 117, 105425	2
689	Non-conserved residues dictate dopamine transporter selectivity for the potent synthetic cathinone and psychostimulant MDPV. **2021**, 200, 108820	1
688	Structure-based approaches in modern drug discovery research. **2001**, 123-42	1
687	High-throughput Virtual Chemistry.	
686	ELECTRONIC SCREENING: LEAD FINDING FROM DATABASE MINING. **2003**, 131-145	
685	An Evolutionary Approach for Molecular Docking. **2003**, 2372-2383	1
684	Use of Pharmacophores in Structure-Based Drug Design. **2003**, 453-481	
683	Concepts for Protein Engineering. **2003**,	

682 Computational Aspects of Library Design and Combinatorial Chemistry. **2003**,

681 Structure and Properties of Acetohydroxyacid Synthase. **2003**,

680 The Grid 2 - Pages 675-721. **2004**, 675-721

679 Proteinstrukturen und Structure-Based-Rational-Drug-Design. **2004**, 117-136

678 A Brief History of Glide: A New Paradigm for Docking and Scoring in Virtual Screening. **2005**, 443-478

677 Development of CDK Inhibitors as Anticancer Agents. **2006**, 121-142

676 In Silico Molecular Homology Modeling of Neurotransmitter Receptors. **2007**, 293-304

675 From Inhibitors of Lap to Inhibitors of Pal. **2007**, 365-398

674 Virtual Ligand Screening: A Method to Discover New Drug Leads. **2007**, 251-272

673 ICAM-1 Peptide Inhibitors of T-cell Adhesion bind to the allosteric site of LFA-1. An NMR Characterization. **2007**, 070916035247001-???

672 Protein Structures and Structure-Based Rational Drug Design. **2008**, 117-137

671 Molecular Modeling: Considerations for the Design of Pharmaceuticals and Biopharmaceuticals. **2008**, 267-291

670 Homology Modeling of Opioid Receptor-Ligand Complexes Using Experimental Constraints. **2008**, 559-584

669 Receptor□igand Interactions in Biological Systems. 1 1

668 The Cambridge Structural Database (CSD) of Small Molecule Crystal Structures. 645-666

667 Evolutionary Algorithms and Their Applications in Chemistry. 1239-1280 1

666 Development of Specific Gamma Secretase Inhibitors. **2009**, 423-437

665 Knowledge-Guided Docking of WW Domain Proteins and Flexible Ligands. **2009**, 175-186 1

664	Complementarity of Hydrophobic/Hydrophilic Properties In Protein–Ligand Complexes: A New Tool to Improve Docking Results. **2009**, 21-41	1
663	Molecular Docking Study of Aminoacyl-tRNA Synthetases with Ligand Molecules from Four Different Scaffolds. **2010**, 31, 606-610	1
662	High-Throughput Flow Cytometry. 1	
661	Synthesis and Evaluation of Estradiol Derivatives as Anti-Breast Cancer Agents. **2010**, 7, 389-394	4
660	In silico-screening approaches for lead generation: identification of novel allosteric modulators of human-erythrocyte pyruvate kinase. **2012**, 796, 351-67	
659	Structural Glycobiology of Antibody Recognition in Xenotransplantation and Cancer Immunotherapy. **2012**, 203-228	1
658	Computational Studies of RNA Dynamics and RNA–Ligand Interactions. **2011**,	
657	Entdeckungsstrategien in der Wirkstoffforschung. **2012**, 69-86	
656	System-Specific Scoring Functions: Application to Guanine-Containing Ligands and Thrombin. **2012**, 21-37	
655	Structure based virtual screening of inhibitors for binding at the allosteric site of HCV RNA dependent RNA polymerase. **2012**, 8, 716-9	
654	Method Development for Comparing Scanning Transmission Electron Microscope Images to Theoretical Structures. **2013**, 39-80	
653	Docking of Potent Anticancer Agents; 4-(Pyrazol-4yl)-Pyrimidine Derivatives as Selective Cyclin-Dependent Kinase 4/6 Inhibitors. 419-422	0
652	Combinatorial Chemistry Library Design. 40-63	
651	High throughput screening of tubulin inhibitors from parasitic fungi. 319-322	
650	The Development and Application of Knowledge-Based Approaches to Molecular Design. **1999**, 243-260	
649	A Combined Pharmacophore-Based Virtual Screening, Docking Study and Molecular Dynamics (MD) Simulation Approach to Identify Inhibitors with Novel Scaffolds for Myeloid cell leukemia (Mcl-1). **2014**, 35, 2097-2108	
648	Identifying putative drug targets and potential drug leads: starting points for virtual screening and docking. **2015**, 1215, 425-44	
647	DOCLASP - Docking ligands to target proteins using spatial and electrostatic congruence extracted from a known holoenzyme and applying simple geometrical transformations. **2014**, 3, 262	6

646 Analysis of the Structural Details of DsrO Protein from Allochromatium vinosum to Identify the Role of the Protein in the Redox Transport Process Through the dsr Operon. **2015**, 1-10

645 Integrated in Silico Methods for the Design and Optimization of Novel Drug Candidates. **2015**, 269-317

644 Computational Approaches for the Discovery of Novel Hepatitis C Virus NS3/4A and NS5B Inhibitors. **2015**, 318-353

643 MODELAGEM MOLECULAR APLICADA A NANOBIOSSISTEMAS. **2015**, 219-267

642 Iran Virtual Screening (IranVScreen): An Integrated Virtual Screening Interface. **2015**, 3, 1

641 Protein Ligand Docking Using Simulated Jumping. **2016**, 1-10

640 Molecular Docking at a Glance. **2016**, 1-38 1

639 Memetic Algorithms. **2016**, 1-32 2

638 Protein-Ligand Docking Methodologies and Its Application in Drug Discovery. **2016**, 196-219

637 Structural Fluctuations of Proteins in Folding and Ligand Docking Studied by Replica-Exchange Simulations. **2016**, 183-204

636 Molecular Dynamics Simulations for Biological Systems. **2016**, 286-313 2

635 Protein-Protein Interactions (PPIs) as an Alternative to Targeting the ATP Binding Site of Kinase. **2016**, 249-277

634 Methods for Docking and Drug Designing. **2016**, 39-53 0

633 Applying Computational Scoring Functions to Assess Biomolecular Interactions in Food Science: Applications to the Estrogen Receptors. **2016**, 3,

632 DOCLASP - Docking ligands to target proteins using spatial and electrostatic congruence extracted from a known holoenzyme and applying simple geometrical transformations. **2014**, 3, 262 4

631 Enhanced Solubility and Dissolution Rate of Raloxifene using Cycloencapsulation Technique. **2016**, 2,

630 Application of Docking Methodologies in QSAR-Based Studies. **2017**, 850-876

629 Rational Drug Design Rational Drug Design. **2017**, 1144-1174

628 Protein-Protein Interactions (PPIs) as an Alternative to Targeting the ATP Binding Site of Kinase. **2017**, 1115-1143

627 Scoring Functions of Protein-Ligand Interactions. **2017**, 915-940

626 Integrated in Silico Methods for the Design and Optimization of Novel Drug Candidates. **2017**, 434-481

625 The Comparison of Docking Search Algorithms and Scoring Functions. **2017**, 820-849

624 Molecular Docking at a Glance. **2017**, 764-803

623 Crystal structure of (2)-3-[4-(di-methyl-amino)-phen-yl]-1-(thio-phen-2-yl)prop-2-en-1-one. **2017**, 73, 476-480

622 Computational Modeling of Drugs for Alzheimer□ Disease: Design of Serotonin 5-HT6 Antagonists. **2018**, 419-461

621 Fuzzy Bi-objective Chance-Constrained Programming Model for Timetable Optimization of a Bus Route. **2018**, 312-324

620 Bus Scheduling Timetable Optimization Based on Hybrid Bus Sizes. **2018**, 337-348

619 Chapter 2:Computational Approaches in the Development of Small-molecule Transcription Factor Inhibitors. **2018**, 42-54

618 Protein Docking and Drug Design. **2018**, 207-241

617 HHVSF: A Framework to Accelerate Drug-Based High-Throughput Virtual Screening on High-Performance Computers. **2018**, 3-17

616 Proteinstrukturen und Proteinstruktur-basiertes rationales Wirkstoffdesign. **2018**, 77-93

615 CHAPTER 10:Modeling O2-dependent Heme Enzymes: A Quick Guide for Non-experts. **2018**, 222-248

614 Protein Structures and Structure-Based Rational Drug Design. **2018**, 73-89

613 High-resolution experimental and computational electrophysiology reveals weak □lactam binding events in the porin PorB.

612 New tools for carbohydrate sulphation analysis: Heparan Sulphate 2-O-sulphotranserase (HS2ST) is a target for small molecule protein kinase inhibitors.

611 New tools for evaluating protein tyrosine sulphation: Tyrosyl Protein Sulphotransferases (TPSTs) are novel targets for RAF protein kinase inhibitors.

610 Protein Docking using Constrained Self-adaptive Differential Evolution Algorithm.

609 A high-throughput virtual screening in Grid for new tubulin-targeted inhibitors of plant fungal pathogens. 22, 335-339

608 Refined Molecular Docking with Multi-objective Optimization Method. **2019**, 56-63

607 Anti-inflammatory and Antidote Drug Discovery with Secreted Phospholipase A2. **2019**, 193-211

606 Protein Docking and Drug Design. **2019**, 889-922

605 Molecular Modeling and Drug Design Techniques in Microbial Drug Discovery. **2019**, 185-231

604 Combinatorial Designing of Novel Lead Molecules Towards the Putative Drug Targets of Extreme Drug-Resistant Mycobacterium tuberculosis: A Future Insight for Molecular Medicine. **2019**, 233-281

603 CompScore: boosting structure-based virtual screening performance by incorporating docking scoring functions components into consensus scoring.

602 Computational identification of novel Kir6 channel inhibitors. 1

601 N-(Sulfamoylbenzoyl)-L-proline Derivatives as Potential Non-β-lactam ESBL Inhibitors: Structure-Based Lead Identification, Medicinal Chemistry and Synergistic Antibacterial Activities. **2019**, 15, 196-206

600 Proposed model of the Dictyostelium cAMP receptors bound to cAMP.

599 Design, Synthesis and Pharmacological Evaluation of Novel Antiinflammatory and Analgesic O-Benzyloxime Compounds Derived From Natural Eugenol. **2019**, 16, 1157-1166

598 Molecular modelling and docking analysis of pleurocidin (an antimicrobial peptide) like peptides with enterotoxin H from Klebsilla pneumonia. **2019**, 15, 838-844

597 From the Explored to the Unexplored: Computer-Tailored Drug Design Attempts in the Discovery of Selective Caspase Inhibitors. **2019**, 22, 432-444 1

596 Docking of Glycokinase with Oxo, Sulfo, and Seleno Derivatives of the Carboxamide Activator S41. **2020**, 09, 22-35

595 Integron Gene Cassettes Harboring Novel Variants of D-Alanine-D-Alanine Ligase Confer High-level Resistance to D-Cycloserine.

594 Evaluating Variants of Firefly Algorithm for Ligand Pose Prediction in Protein-ligand Docking Program. **2020**,

593 Evaluation of ExoU inhibitors in a Pseudomonas aeruginosa scratch infection assay.

592	Leveraging non-structural data to predict structures of protein□gand complexes.	1
591	Extracellular alpha/beta-hydrolase from Paenibacillus species shares structural and functional homology to tobacco salicylic acid binding protein 2. **2020**, 210, 107496	1
590	Calix[6]arene diminishes receptor tyrosine kinase lifespan in pancreatic cancer cells and inhibits their migration and invasion efficiency. **2020**, 100, 103881	2
589	Mechanistic Studies of the Stabilization of Insulin Helical Structure by Coomassie Brilliant Blue.	
588	Diaminomaleonitrile derivatives as new potential antichagasic compounds: a study of structure-activity relationships. **2021**, 13, 2167-2183	1
587	Nonantimicrobial Actions of Macrolides: Overview and Perspectives for Future Development. **2021**, 73, 233-262	5
586	Clarifying real receptor binding site between coronavirus HCoV-HKU1 and 9-O-Ac-Sia based on molecular docking.. **2022**, 2150034	
585	Unsymmetrical Trifluoromethyl Methoxyphenyl □Diketones: Effect of the Position of Methoxy Group and Coordination at Cu(II) on Biological Activity. **2021**, 26,	0
584	Inside and Out of the Pore: Comparing Interactions and Molecular Dynamics of Influenza A M2 Viroporin Complexes in Standard Lipid Bilayers. **2021**, 61, 5550-5568	1
583	Improving ligand-ranking of AutoDock Vina by changing the empirical parameters. **2022**, 43, 160-169	6
582	Dibenzofuran Derivatives Inspired from Cercosporamide as Dual Inhibitors of Pim and CLK1 Kinases. **2021**, 26,	
581	Docking and scoring for nucleic acid-ligand interactions: Principles and current status. **2021**,	3
580	Amino Alcohols from Eugenol as Potential Semisynthetic Insecticides: Chemical, Biological, and Computational Insights. **2021**, 26,	3
579	Molecular Docking of SP40 Peptide towards Cellular Receptors for Enterovirus 71 (EV-A71). **2021**, 26,	1
578	System Maintenance Method Based on the Mean Residual Life-Importance Measure. **2022**, 137-148	
577	Cytotoxic and Antifungal Amides Derived from Ferulic Acid: Molecular Docking and Mechanism of Action. **2021**, 2021, 3598000	1
576	Anthrophilia* Algorithm. **2020**, 481-493	
575	Computational Modeling in Virus Infections and Virtual Screening, Docking, and Molecular Dynamics in Drug Design. **2020**, 301-337	

574 LigEGFR: Spatial graph embedding and molecular descriptors assisted bioactivity prediction of ligand molecules for epidermal growth factor receptor on a cell line-based dataset.

573 COMPUTER SEARCH OF CHEMICAL COMPOUNDS PROPERTIES ANALOGUES FOR PYRROLIDINOPHENONE DERIVATIVES. 54-60 0

572 Precursor-directed Biosynthesis in Tabernaemontana catharinensis as a New Avenue for Alzheimer's Disease-modifying Agents. **2021**, 87, 136-147 0

571 Structural insights into glycine reuptake inhibition. 1

570 Novel Sigma 1 Receptor Antagonists as Potential Therapeutics for Pain Management. **2021**, 64, 890-904 0

569 The Role of Orthosteric Building Blocks of Bitopic Ligands for Muscarinic M1 Receptors. **2020**, 5, 31706-31715 2

568 A novel chicory fructanase can degrade common microbial fructan product profiles and displays positive cooperativity. **2021**, 7

567 Identification of sources with abnormal radon exhalation rates based on radon concentrations in underground environments. **2021**, 807, 150800 1

566 Bioactive Compounds of Horse Gram (Macrotyloma uniflorum Lam. [Verdc.]). **2020**, 1-39 0

565 Determination of the structural requirements of Opioid receptor ligands with docking. **2020**,

564 Thermodynamics of Protein-Ligand Binding. **2020**, 145-185

563 CHAPTER 3:Computational Methods for the Discovery of Chemical Probes. **2020**, 39-68

562 QM Implementation in Drug Design: Does It Really Help?. **2020**, 2114, 19-35

561 Strategies of Virtual Screening in Medicinal Chemistry. **2020**, 194-225 0

560 The steroidal lactone withaferin A impedes T-cell motility by inhibiting the kinase ZAP70 and subsequent kinome signaling. **2021**, 297, 101377 0

559 Synthesis, In Silico Studies, and Evaluation of Syn and Anti Isomers of -Substituted Indole-3-carbaldehyde Oxime Derivatives as Urease Inhibitors against. **2021**, 26, 1

558 Variability in the response of HBV D-subgenotypes to antiviral therapy: designing pan D-subgenotypic reverse transcriptase inhibitors. **2021**, JVI0180021

557 Antitumor activity of novel POLA1-HDAC11 dual inhibitors. **2021**, 228, 113971 0

556	Binding affinity prediction for protein-ligand complex using deep attention mechanism based on intermolecular interactions. **2021**, 22, 542	4
555	Niazimicin: A thiocarbamate glycoside from Moringa oleifera Lam. seeds with a novel neuroprotective activity. **2021**, 45, e13992	2
554	Beta turn propensity and a model polymer scaling exponent identify disordered proteins that phase separate.	
553	In-Silico Analysis of Secondary Metabolites that Modulates Enzymes of Cholesterol Target.	
552	In silico data mining of large-scale databases for the virtual screening of human interleukin-2 inhibitors. **2021**, 71, 33-56	
551	Computational Techniques in Binding Affinity Prediction of Drugs. 333-347	
550	Multiple molecular superpositioning as an effective tool for virtual database screening. **2000**, 43-62	
549	Modifications of the scoring function in FlexX for virtual screening applications. **2000**, 83-98	
548	Hydrophobicity maps and docking of molecular fragments with solvation. **2000**, 145-169	0
547	Flexibly Screening for Molecules Interacting with Proteins. **2002**, 385-400	
546	Fragment-Based Screening by X-ray Crystallography. **2007**, 99-127	
545	Illustration of Current Challenges in Molecular Docking. **2007**, 201-221	1
544	Entdeckungsstrategien in der Wirkstoffforschung. **2008**, 43-60	
543	The inhibitory effect of KN-93 and KN-62 as a result of CaM-directed blocking animal CaMK2 and plant CDPK activation. 26, 298-304	
542	Conserved interactions required for in vitro inhibition of the main protease of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2).	
541	The Dimensional Synthesis of the Four-Bar Mechanism with a Symbiotic Organisms Search Algorithm. **2021**, 780-791	1
540	Potential Therapeutic Approaches to Alzheimer's Disease By Bioinformatics, Cheminformatics And Predicted Adme-Tox Tools. **2020**, 18, 696-719	2
539	Molecular dynamics, MM/PBSA and in□vitro validation of a novel quinazoline-based EGFR tyrosine kinase inhibitor identified using structure-based in silico screening. **2020**, 99, 107639	1

538	Insight into Mechanism of Action of Anticancer Benzazoles. **2020**, 20, 2056-2069	0
537	The role of stacking interactions in complexes of proteins with adenine and Guanine fragments of ligands. **2009**, 1, 124-7	4
536	Anionic lipids: determinants of binding cytotoxins from snake venom on the surface of cell membranes. **2010**, 2, 88-96	4
535	In Silico Analysis to Compare the Effectiveness of Assorted Drugs Prescribed for Swine flu in Diverse Medicine Systems. **2014**, 76, 10-8	5
534	Computational Investigation of Ginsenoside F1 from Meyer as p38 MAP Kinase Inhibitor: Molecular Docking and Dynamics Simulations, ADMET Analysis, and Drug Likeness Prediction. **2018**, 17, 1318-1327	4
533	Pharmacophore-based virtual screening for the identification of the novel Src inhibitor SJG-136 against lung cancer cell growth and motility. **2020**, 10, 1668-1690	2
532	Investigation of Marine-Derived Natural Products as Raf Kinase Inhibitory Protein (RKIP)-Binding Ligands. **2021**, 19,	1
531	Molecular docking and molecular dynamics simulation. **2022**, 291-304	3
530	Development of isoquinolinone derivatives as immunoproteasome inhibitors. **2021**, 55, 128478	1
529	Investigation of Marine-Derived Natural Products as Raf Kinase Inhibitory Protein (RKIP)-Binding Ligands. **2021**, 19, 581	1
528	Prediction of Binding Free Energy of Protein-Ligand Complexes with a Hybrid Molecular Mechanics/Generalized Born Surface Area and Machine Learning Method.. **2021**, 6, 32938-32947	4
527	Conjugate of meso-carboxysubstituted-BODIPY with thioterpenoid as an effective fluorescent probe: Synthesis, structure, spectral characteristics, and molecular docking. **2021**, 120638	3
526	Role of Cel5H protein surface amino acids in binding with clay minerals and measurements of its forces. **2021**, 51, 17	0
525	Molecular Modeling Strategies of Cancer Multidrug Resistance.. **2021**, 59, 100789	9
524	Kite-Shaped Molecules Block SARS-CoV-2 Cell Entry at a Post-Attachment Step. **2021**, 13,	1
523	Machine Learning Models for the Classification of CK2 Natural Products Inhibitors with Molecular Fingerprint Descriptors. **2021**, 9, 2074	1
522	The discovery of 1, 3-diamino-7H-pyrrol[3, 2-f]quinazoline compounds as potent antimicrobial antifolates. **2021**, 113979	0
521	Challenging Reverse Screening: A Benchmark Study for Comprehensive Evaluation. **2021**, e2100063	

520	Fine tuning for success in structure-based virtual screening. **2021**, 35, 1195-1206	1
519	Molecular docking study of britannin binding to PD-L1 and related anticancer pseudoguaianolide sesquiterpene lactones. **2021**, 1-8	2
518	Repurposing the Trypanosomatidic GSK Kinetobox for the Inhibition of Parasitic Pteridine and Dihydrofolate Reductases.. **2021**, 14,	0
517	Validation of a Field-Based Ligand Screener Using a Novel Benchmarking Data Set for Assessing 3D-Based Virtual Screening Methods. **2021**,	0
516	DockStream: a docking wrapper to enhance de novo molecular design. **2021**, 13, 89	1
515	Powder diffraction. **2021**, 1,	2
514	Structural Determination of Uridine Diphosphate Glycosyltransferases Using X-Ray Crystallography. **2022**, 2396, 227-241	0
513	Synthesis, Crystal Structure, and Biological Evaluation of Novel 5-Hydroxymethylpyrimidines. **2021**, 14,	0
512	Phenotypic and studies for a series of synthetic thiosemicarbazones as New Delhi metallo-beta-lactamase carbapenemase inhibitors. **2021**, 1-13	1
511	Low-dose bisphenol S exposure induces hypospermatogenesis and mitochondrial dysfunction in rats: A possible implication of StAR protein. **2021**,	1
510	Spectroscopic/Computational Characterization and the X-ray Structure of the Adduct of the VO-Picolinato Complex with RNase A. **2021**,	3
509	Molecular modeling in cardiovascular pharmacology: Current state of the art and perspectives. **2021**,	0
508	Preclinical and clinical evaluation of German-sourced ONC201 for the treatment of H3K27M-mutant diffuse intrinsic pontine glioma.. **2021**, 3, vdab169	2
507	Investigating natural compounds against oncogenic RET tyrosine kinase using pharmacoinformatic approaches for cancer therapeutics.. **2021**, 12, 1194-1207	2
506	Structure-Based Drug Discovery of IRE1 Modulators.. **2022**, 2378, 293-315	
505	Computer Modeling Explains the Structural Reasons for the Difference in Reactivity of Amine Transaminases Regarding Prochiral Methylketones.. **2022**, 23,	0
504	Discovery of potent antiproliferative agents from selected oxygen heterocycles as EGFR tyrosine kinase inhibitors from the U.S. National Cancer Institute database by in silico screening and bioactivity evaluation.. **2022**, 58, 128524	1
503	New biologically dynamic hybrid pharmacophore triazinoindole-based-thiadiazole as potent □-glucosidase inhibitors: In vitro and in silico study.. **2021**,	1

502	Polyoxidovanadates' interactions with proteins: An overview. **2022**, 454, 214344	12
501	Virtual screening and in vitro assays of novel hits as promising DPP-4 inhibitors.. **2021**, 194, 43-43	0
500	Sulfonylbis(acylhydrazones) as anticholinesterase inhibitors: Synthesis, in vitro biological evaluation and computational studies. **2022**, 1252, 132215	1
499	DESIGN, SYNTHESIS AND MOLECULAR MECHANISM OF FEW NEURAMINIDASE INHIBITORS IN TREATMENT OF H1N1 BY NMR TECHNIQUES. **2019**, 56, 7-15	
498	SYNTHESIS, BIOLOGICAL EVALUATION AND DOCKING STUDIES OF NON HEPATOTOXIC 5-SUBSTITUTED THIAZOLIDINE-2, 4-DIONES AS ANTIDIABETIC, ANTI-HYPERLIPIDEMIC, ANTI-OXIDANT AND CYTOTOXIC AGENTS. **2020**, 57, 19-37	0
497	Structure-Based Virtual Screening for Ligands of G Protein-Coupled Receptors: What Can Molecular Docking Do for You?. **2021**, 73, 527-565	4
496	Synthesis and Structure-Activity Relationships of Novel Non-Steroidal CYP17A1 Inhibitors as Potential Prostate Cancer Agents.. **2022**, 12,	3
495	Molecular Docking of Phytochemicals against Streptococcus mutans Virulence Targets: A Proteomic Insight into Drug Planning.	
494	Resistor: an algorithm for predicting resistance mutations using Pareto optimization over multistate protein design and mutational signatures.	0
493	Signaling modality within gp130 receptor enhances tissue regeneration.	
492	Multiparameter Optimization of Trypanocidal Cruzain Inhibitors With Activity and Favorable Pharmacokinetics.. **2021**, 12, 774069	1
491	Impact of the ferrocenyl group on cytotoxicity and KSP inhibitory activity of ferrocenyl monastrol conjugates. **2021**,	0
490	Molecular docking-based computational platform for high-throughput virtual screening.. **2022**, 4, 1-12	2
489	Evaluation of Docking Machine Learning and Molecular Dynamics Methodologies for DNA-Ligand Systems.. **2022**, 15,	2
488	Insight investigation of rilpivirine and compounds from mushrooms as feline immunodeficiency virus reverse transcriptase inhibitors using molecular dynamics simulations and quantum chemical calculations. 1-14	
487	Novel Small-Molecule Inhibitors of the SARS-CoV-2 Spike Protein Binding to Neuropilin 1.. **2022**, 15,	7
486	Re-Exploring the Ability of Common Docking Programs to Correctly Reproduce the Binding Modes of Non-Covalent Inhibitors of SARS-CoV-2 Protease M.. **2022**, 15,	4
485	Potential anti-allergic effects of bibenzyl derivatives from liverworts, Radula perrottetii.. **2022**,	0

484	EViS: An Enhanced Virtual Screening Approach Based on Pocket-Ligand Similarity.. **2022**,	0
483	Controlled Uptake of an Iridium Complex inside Engineered apo-Ferritin Nanocages: Study of Structure and Catalysis**.	1
482	Discovery and Characterization of a Cryptic Secondary Binding Site in the Molecular Chaperone HSP70.. **2022**, 27,	0
481	Unraveling the Mechanism of Platelet Aggregation Suppression by Monoterpenoids.. **2022**, 9,	0
480	In silico design and in vitro assessment of anti-Helicobacter pylori compounds as potential small-molecule arginase inhibitors.. **2022**, 1	0
479	Mechanistic Characterization of the Pharmacological Profile of HS-731, a Peripherally Acting Opioid Analgesic, at the □-, □ Opioid and Nociceptin Receptors.. **2022**, 27,	0
478	Molecular docking of brazilin and its analogs to barrier-to-autointegration factor 1 (BAF1).. **2022**,	
477	-Substituted 5-(1-Indol-2-yl)-2-methoxyanilines Are Allosteric Inhibitors of the Linoleate Oxygenase Activity of Selected Mammalian ALOX15 Orthologs: Mechanism of Action.. **2022**,	1
476	Bacterial Indole as a Multifunctional Regulator of Klebsiella oxytoca Complex Enterotoxicity.. **2022**, e0375221	2
475	An molecular modeling approach of halolactone derivatives as potential inhibitors for human immunodeficiency virus type-1 reverse transcriptase enzyme.. **2022**, 1-15	
474	Application of Reverse Docking in the Research of Small Molecule Drugs and Traditional Chinese Medicine. **2021**, 45,	0
473	A unique aromatic cluster near the active site of H. pylori CPA is essential for catalytic function.. **2021**,	0
472	Computational screening of camostat and related compounds against human TMPRSS2: A potential treatment of COVID-19.. **2022**,	2
471	Controlled Uptake of an Iridium Complex inside Engineered apo-Ferritin Nanocages: Study of Structure and Catalysis.. **2022**,	0
470	Histone deacetylase 6 inhibition restores leptin sensitivity and reduces obesity.. **2022**,	1
469	Drug Repurposing Targeting MvfR Using Docking, Virtual Screening, Molecular Dynamics, and Free-Energy Calculations.. **2022**, 11,	1
468	First In Silico Screening of Insect Molecules for Identification of Novel Anti-Parasitic Compounds.. **2022**, 15,	0
467	Structural insights into the discrepant synergistic activity of Codlemone and (Z)-8-dodecenol towards Grapholita molesta pheromones.. **2022**,	0

466	Computational Identification of Possible Allosteric Sites and Modulators of the SARS-CoV-2 Main Protease.. **2022**, 62, 618-626	1
465	Pharmacophore-guided Virtual Screening to Identify New β-Adrenergic Receptor Agonists.. **2021**,	1
464	Reliable Prediction of the Protein-Ligand Binding Affinity Using a Charge Penetration Corrected AMOEBA Force Field: A Case Study of Drug Resistance Mutations in Abl Kinase.. **2022**,	1
463	Highly Antiproliferative Latonduine and Indolo[2,3-]quinoline Derivatives: Complex Formation with Copper(II) Markedly Changes the Kinase Inhibitory Profile.. **2022**, 65, 2238-2261	2
462	Structure-based discovery of small molecules improving stability of human broadly-neutralizing anti-HIV antibody 2F5 in plant suspension cells.. **2022**, e2100266	
461	Putative dual inhibitors of mTOR and RET kinase from natural products: Pharmacophore-based hierarchical virtual screening. **2022**, 350, 118562	0
460	Cinnamic acid derivatives linked to arylpiperazines as novel potent inhibitors of tyrosinase activity and melanin synthesis.. **2022**, 231, 114147	2
459	Dimethoxyindoles based thiosemicarbazones as multi-target agents; synthesis, crystal interactions, biological activity and molecular modeling.. **2022**, 120, 105647	0
458	Carnitine palmitoyl transferase I: Conformational changes induced by long-chain fatty acyl CoA ligands.. **2022**, 112, 108125	0
457	PIGNet: a physics-informed deep learning model toward generalized drug-target interaction predictions.. **2022**, 13, 3661-3673	6
456	Imipridones affect tumor bioenergetics and promote cell lineage differentiation in diffuse midline gliomas.. **2022**,	2
455	Novel Aurora A Kinase Inhibitor Fangchinoline Enhances Cisplatin-DNA Adducts and Cisplatin Therapeutic Efficacy in OVCAR-3 Ovarian Cancer Cells-Derived Xenograft Model.. **2022**, 23,	1
454	Molecular modeling in drug discovery. **2022**, 29, 100880	6
453	Docking Ligands into Flexible and Solvated Macromolecules. 8. Forming New Bonds-Challenges and Opportunities.. **2022**,	2
452	Optimization of Cavity-Based Negative Images to Boost Docking Enrichment in Virtual Screening.. **2022**,	1
451	Virtual high-throughput screening: potential inhibitors for the mycobacterial β-subunit of tryptophan synthase. 1-12	
450	Computational strategies to identify new drug candidates against neuroinflammation.. **2022**,	1
449	Synergistic Behavior of Plant Proteins and Biobased Latexes in Bioplastic Food Packaging Materials: Experimental and Machine Learning Study.. **2022**,	0

448	Propofol inhibits the myeloperoxidase activity by acting as substrate through a redox process.. **2022**, 130100	0
447	Acipimox inhibits human carbonic anhydrases.. **2022**, 37, 672-679	3
446	Using Virtual AChE Homology Screening to Identify Small Molecules With the Ability to Inhibit Marine Biofouling. 8,	1
445	A convenient test system for the identification of CYP4V2 inhibitors. **2021**, 27, 601-607	
444	Sulfonated red and far-red rhodamines to visualize SNAP- and Halo-tagged cell surface proteins.. **2022**,	3
443	Unlocking the computational design of metal-organic cages.. **2022**,	4
442	Gold(Iii) Heteroleptic Complexes with Sns-Thiosemicarbazonate Ligands as Cytotoxic Agents: Experimental and Computational Insights into the Mechanism of Action.	
441	Structural, biological and computational study of oxamide derivative. **2022**, 114-114	
440	In silico studies revealed interaction mechanisms of benzylidene□crylohydrazide derivatives and nsP2 CHIKV. **2022**, 46, 6414-6423	1
439	Covalent cannabinoid receptor ligands □tructural insight and selectivity challenges.	
438	Computational Intelligence-Based Cheminformatics Model as Cancer Therapeutics. **2022**, 251-269	
437	Comparative chemical and biological hydrolytic stability of homologous esters and isosteres.. **2022**, 37, 718-727	0
436	Identification of new putative inhibitors of 3-dehydroshikimate dehydratase from a combination of ligand- and structure-based and deep learning approaches.. **2022**, 1-10	0
435	Mo(VI) Potential Metallodrugs: Explaining the Transport and Cytotoxicity by Chemical Transformations.. **2022**,	3
434	Ligand Binding Path Sampling Based on Parallel Cascade Selection Molecular Dynamics: LB-PaCS-MD.. **2022**, 15,	0
433	A New Study on Optimization of Four-Bar Mechanisms Based on a Hybrid-Combined Differential Evolution and Jaya Algorithm. **2022**, 14, 381	0
432	Potential of the Compounds from Purified Annatto Oil and Its Granules (Chronic) against Dyslipidemia and Inflammatory Diseases: In Silico Studies with Geranylgeraniol and Tocotrienols.. **2022**, 27,	0
431	Trends in coordination of rhenium organometallic complexes in the Protein Data Bank.. **2022**, 9, 180-193	

430	Glutathione -Transferase Genes are Involved in -Cyhalothrin Resistance in via Sequestration.. **2022**,	2
429	FitDock: protein-ligand docking by template fitting.. **2022**,	4
428	Discovery of 3H-pyrrolo[2,3-c]quinolines with activity against Mycobacterium tuberculosis by allosteric inhibition of the glutamate-5-kinase enzyme.. **2022**, 232, 114206	0
427	Protein-Ligand Interaction Graphs: Learning from Ligand-Shaped 3D Interaction Graphs to Improve Binding Affinity Prediction.	0
426	Polymer microspheres modified with pyrazole derivatives as potential agents in anticancer therapy - Preliminary studies.. **2022**, 123, 105765	0
425	In silico identification of small molecule protein-protein interaction inhibitors: targeting hotspot regions at the interface of MXRA8 and CHIKV envelope protein.. **2022**, 1-19	1
424	A Review on In-vivo, In-vitro and In-silico Screening Tools to Investigate the Nephroprotective Effect. 361-378	
423	Cov_DOX: A Method for Structure Prediction of Covalent Protein-Ligand Bindings.. **2022**,	3
422	Sodium or Not Sodium: Should Its Presence Affect the Accuracy of Pose Prediction in Docking GPCR Antagonists?. **2022**, 15,	2
421	Drug design and repurposing with a sequence-to-drug paradigm.	
420	Modelling aptamers with nucleic acid mimics (NAM): From sequence to three-dimensional docking.. **2022**, 17, e0264701	0
419	A novel AMPK activator shows therapeutic potential in hepatocellular carcinoma by suppressing HIF1mediated aerobic glycolysis.. **2022**,	1
418	Effect of Aryl-Cyclohexanones and their Derivatives on Macrophage Polarization In Vitro.. **2022**, 1	1
417	Quantum Key Distribution Over a Channel with Scattering. **2022**, 17,	0
416	Combined Machine Learning and GRID-Independent Molecular Descriptor (GRIND) Models to Probe the Activity Profiles of 5-Lipoxygenase Activating Protein Inhibitors.. **2022**, 13, 825741	1
415	Review of 3D templates for in silico homology models of MATs: improved 3D model of hDAT. **2022**, 31, 643-651	1
414	Collaborative Approach between Explainable Artificial Intelligence and Simplified Chemical Interactions to Explore Active Ligands for Cyclin-Dependent Kinase 2.. **2022**, 7, 10372-10381	0
413	Discovery of a novel inhibitor against urokinase-type plasminogen activator, a potential enzyme with a role in atherosclerotic plaque instability.. **2022**, 1-11	0

412	Pyrazolones as inhibitors of immune checkpoint blocking the PD-1/PD-L1 interaction.. **2022**, 236, 114343	2
411	A Adenosine Receptor Antagonists: Are Triazolotriazine and Purine Scaffolds Interchangeable?. **2022**, 27,	2
410	Quinazoline-based analog of adenine as an antidote against MLL-rearranged leukemia cells: synthesis, inhibition assays and docking studies.. **2022**, 14, 557-570	
409	Insights into the leaves of Ceriscoides campanulata: Natural proanthocyanidins alleviate diabetes, inflammation, and esophageal squamous cell cancer via in vitro and in silico models.. **2022**, 105164	0
408	Dowker complex based machine learning (DCML) models for protein-ligand binding affinity prediction.. **2022**, 18, e1009943	3
407	Computational Analysis and Biological Activities of Oxyresveratrol Analogues, the Putative Cyclooxygenase-2 Inhibitors.. **2022**, 27,	0
406	Mononuclear and polymeric zinc(II) ‖diketonate complexes with aromatic N-donor ligands: Structural, spectral, thermal, theoretical and docking studies. **2022**, 218, 115757	
405	Disclosing the antitumour potential of the marine bromoditerpene sphaerococcenol A on distinct cancer cellular models.. **2022**, 149, 112886	0
404	The inhibitory kinetics of vitamins B9, C, E, and D3 on bovine xanthine oxidase: Gout treatment.. **2022**, 359, 109922	0
403	Gold(III) heteroleptic complexes with SNS-thiosemicarbazonate ligands as cytotoxic agents: Experimental and computational insights into the mechanism of action. **2022**, 219, 115767	
402	Exploration of inhibitors of the bacterial LexA repressor-protease.. **2022**, 65, 128702	0
401	Identification of potent inhibitors against chorismate synthase of Toxoplasma gondii using molecular dynamics simulations.. **2022**, 114, 108183	
400	In vitro studies of a series of synthetic compounds for their anti-acetylcholinesterase activities identified arylpyrano[2,3-f]coumarins as hit compounds. **2022**, 1260, 132799	1
399	Synthesis, anti-cancer activity and molecular docking studies of new nicotinamide containing EP4 antagonists. **2022**, 1260, 132730	
398	Multi-step synthesis of indole-N-ethyltriazole hybrids amalgamated with N-arylated ethanamides: structure-activity relationship and mechanistic explorations through tyrosinase inhibition, kinetics and computational ascriptions. **2022**, 1261, 132953	
397	Computational Tools and Strategies to Develop Peptide-Based Inhibitors of Protein-Protein Interactions.. **2022**, 2405, 205-230	0
396	Evaluation of biological activities of cobalt(II) and copper(II) complexes synthesized from methylcarboxylate and amino alcohol ligand mixtures: spectroscopic, structural and docking studies. 1-9	
395	Dynophore-Based Approach in Virtual Screening: A Case of Human DNA Topoisomerase II‖ **2021**, 22,	2

394	Leveraging nonstructural data to predict structures and affinities of protein-ligand complexes.. **2021**, 118,	2
393	A Comparison between Enrichment Optimization Algorithm (EOA)-Based and Docking-Based Virtual Screening.. **2021**, 23,	0
392	Antifungal Activity of -(4-Halobenzyl)amides against spp. and Molecular Modeling Studies.. **2021**, 23,	5
391	Molecular dynamics investigation of ivermectin bound to importin alpha/beta heterodimer. **2022**, 48, 314-321	1
390	Synthesis and aldose reductase inhibition effects of novel N-benzyl-4-methoxyaniline derivatives. **2021**,	
389	Identification of an ASC oligomerization inhibitor for the treatment of inflammatory diseases.. **2021**, 12, 1155	6
388	Determination of Novel Anti-Cancer Agents by Targeting OGG1 Enzyme Using Integrated Bioinformatics Methods.. **2021**, 18,	0
387	Virtual Screening with Gnina 1.0. **2021**, 26,	3
386	New Deoxycholic Acid Derived Tyrosyl-DNA Phosphodiesterase 1 Inhibitors Also Inhibit Tyrosyl-DNA Phosphodiesterase 2.. **2021**, 27,	4
385	MOLECULAR DOCKING STUDY OF NATURALLY OCCURRING COMPOUNDS AS INHIBITORS OF COVID -19. 69-71	
384	COORDINATION OF AN AMINO ALCOHOLIC SCHIFF BASE LIGAND TOWARD THE ZINC(II) ION: SPECTRAL, STRUCTURAL, THEORETICAL, AND DOCKING STUDIES. **2021**, 62, S8-S19	
383	Multi-Targeted Approaches and Drug Repurposing Reveal Possible SARS-CoV-2 Inhibitors.. **2021**, 10,	0
382	Identification of tripeptides against tyrosine kinase domain of EGFR for lung cancer cell inhibition by in silico and in vitro studies.. **2021**,	0
381	Bioactivities of In Vitro Transepithelial Transported Peptides from Cooked Chicken Breast. **2022**, 28,	
380	Potent but transient immunosuppression of T-cells is a general feature of CD71 erythroid cells. **2021**, 4, 1384	1
379	Molecular docking study of xylogranatins binding to glycogen synthase kinase-3‡**2022**, 5, 9-17	
378	Overcoming multidrug resistance (MDR): design, biological evaluation and molecular modelling studies of‡2,4-substituted quinazoline derivatives.. **2022**,	0
377	TLR8 is activated by 5'-methylthioinosine, a Plasmodium falciparum-derived intermediate of the purine salvage pathway.. **2022**, 39, 110691	1

376	SAMPL7 protein-ligand challenge: A community-wide evaluation of computational methods against fragment screening and pose-prediction.. **2022**,	2
375	4-Heteroaryl Substituted Amino-3,5-Dicyanopyridines as New Adenosine Receptor Ligands: Novel Insights on Structure-Activity Relationships and Perspectives.. **2022**, 15,	
374	New aldo-keto reductase 1C3 (AKR1C3) inhibitors based on the hydroxytriazole scaffold.. **2022**, 237, 114366	0
373	Image_1.pdf. **2019**,	
372	Data_Sheet_1.pdf. **2020**,	
371	DataSheet1.pdf. **2017**,	
370	Data_Sheet_1.PDF. **2018**,	
369	Table_1.docx. **2020**,	
368	Data_Sheet_1.docx. **2020**,	
367	Image_1.TIFF. **2020**,	
366	Presentation_1.pdf. **2018**,	
365	Table_1.docx. **2020**,	
364	DataSheet_1.pdf. **2020**,	
363	Image1.pdf. **2018**,	
362	Image2.pdf. **2018**,	
361	Image3.pdf. **2018**,	
360	Image4.pdf. **2018**,	
359	Image5.pdf. **2018**,	

358	Image6.pdf. **2018**,	
357	datasheet1.docx. **2020**,	
356	Presentation_1.pdf. **2019**,	
355	DataSheet_1.docx. **2019**,	
354	DataSheet_1.pdf. **2019**,	
353	Metabolomic profile and computational analysis for the identification of the potential anti-inflammatory mechanisms of action of the traditional medicinal plants Ocimum basilicum and Ocimum tenuiflorum.. **2022**, 113039	2
352	Investigation of Tumor Cells and Receptor-Ligand Simulation Models for the Development of PET Imaging Probes Targeting PSMA and GRPR and a Possible Crosstalk between the Two Receptors.. **2022**,	2
351	Response Surface Study on Molecular Docking Simulations of Citalopram and Donepezil as Potent CNS Drugs.. **2021**, 20, 560-576	
350	Design and Development of Novel Nutraceuticals: Current Trends and Methodologies. **2022**, 2, 71-90	1
349	Development of Neuropeptide Y and Cell-Penetrating Peptide MAP Adsorbed onto Lipid Nanoparticle Surface.. **2022**, 27,	0
348	Development of an Automatic Pipeline for Participation in the CELPP Challenge.. **2022**, 23,	1
347	Unravelling the binding mode of a methamphetamine aptamer: a spectroscopic and calorimetric investigation.. **2022**,	0
346	Design, Synthesis and Evaluation of Fused Bicyclo[2.2.2]octene as a Potential Core Scaffold for the Non-Covalent Inhibitors of SARS-CoV-2 3CLpro Main Protease. **2022**, 15, 539	0
345	Sequence Analysis and Molecule Docking of Collagenase Inhibitory Peptides from the Peptic Hydrolysate of Flounder Skin. **2022**, 51, 322-333	0
344	Identification of novel off targets of baricitinib and tofacitinib by machine learning with a focus on thrombosis and viral infection.. **2022**, 12, 7843	1
343	Antiproliferative activity of Dioclea violacea lectin in CaCO3 particles on cancer cells after controlled release. **2022**, 57, 8854-8868	0
342	Molecular Mingling: Multimodal Predictions of Ligand Promiscuity in Pentameric Ligand-Gated Ion Channels. **2022**, 9,	1
341	Computational Modeling of Supramolecular Metallo-organic Cages□Challenges and Opportunities. 5806-5826	3

340	The Bradycardic Agent Ivabradine Acts as an Atypical Inhibitor of Voltage-Gated Sodium Channels.. **2022**, 13, 809802	1
339	Development and Validation of a Multi-Level Computational Protocol for Drug Repurposing in the Treatment of Bacterial Infections. **2021**, 8,	
338	Coumarin derivatives: biomedicinal properties and interactions with carrier proteins. **2022**, 173-220	
337	Temporal perturbation of histone deacetylase activity reveals a requirement for HDAC1-3 in mesendoderm cell differentiation.. **2022**, 39, 110818	
336	In Silico Drug Discovery for Treatment of Virus Diseases.. **2022**, 1368, 73-93	
335	Consensus scoring evaluated using the GPCR-Bench dataset: Reconsidering the role of MM/GBSA.. **2022**,	0
334	Ispinesib as an Effective Warhead for the Design of Autophagosome-Tethering Chimeras: Discovery of Potent Degraders of Nicotinamide Phosphoribosyltransferase (NAMPT).. **2022**,	6
333	Metabolism of the antipsychotic drug olanzapine by CYP3A43.. **2022**, 1-29	0
332	Synthesis, molecular docking, and cytotoxicity of quinazolinone and dihydroquinazolinone derivatives as cytotoxic agents.. **2022**, 16, 35	
331	Machine-Learning- and Knowledge-Based Scoring Functions Incorporating Ligand and Protein Fingerprints.	1
330	Adamantane-Monoterpenoid Conjugates Linked via Heterocyclic Linkers Enhance the Cytotoxic Effect of Topotecan. **2022**, 27, 3374	1
329	Organometallic Gold (III) and Platinum (II) Complexes with Thiosemicarbazone: structural behavior, anticancer activity, and molecular docking.	0
328	In Vitro, In Vivo and In Silico Characterization of a Novel Kappa-Opioid Receptor Antagonist. **2022**, 15, 680	1
327	A combined experimental and computational study to discover novel tyrosinase inhibitors. **2022**, 111879	
326	Biocatalytic kinetic resolution to access enantiomerically enriched dihydropyrimidinone/thiones via recognition of a remote stereocentre.	1
325	Site directed mutagenesis of Catharanthus roseus (+)-vincadifformine 19-hydroxylase (CYP71BY3) results in two distinct enzymatic functions. **2022**, 113265	0
324	Itraconazole Reverts ABCB1-Mediated Docetaxel Resistance in Prostate Cancer. 13,	0
323	Synthesis of Coumarin and Homoisoflavonoid Derivatives and Analogs: The Search for New Antifungal Agents. **2022**, 15, 712	1

322	Defined stereoisomers of 2??-amino NAD+ and their activity against human sirtuins and a bacterial (ADP-ribosyl) transferase. **2022**, 116875	0
321	Atomic solution structure of Mycobacterium abscessus F-ATP synthase subunit β and identification of Ep1 Mab F1 as a targeted inhibitor.	0
320	Synthesis and In Silico Evaluation of Potential Insecticide Activity of Benzamides.	
319	Novel benzimidazole-based pseudo-irreversible butyrylcholinesterase inhibitors with neuroprotective activity in an Alzheimer's disease mouse model.	0
318	Protein structural bioinformatics: An overview. **2022**, 105695	0
317	Controlling oncogenic KRAS signaling pathways with a Palladium-responsive peptide. **2022**, 5,	
316	Inversion of hydrogeological parameters based on an adaptive dynamic surrogate model.	
315	Molecular docking study of GSK-3β interaction with nomilin, kihadanin B, and related limonoids and triterpenes with a furyl-β-lactone core.	2
314	Scoring Functions for Protein-Ligand Binding Affinity Prediction Using Structure-based Deep Learning: A Review. 2,	1
313	Design of Novel Enantiopure Dispirooxindolopyrrolidine-Piperidones as Promising Candidates toward COVID-19: Asymmetric Synthesis, Crystal Structure and In Silico Studies. **2022**, 27, 3945	0
312	AI-Based Protein Structure Prediction in Drug Discovery: Impacts and Challenges.	2
311	Structural and Mechanistic Insights into Mycobacterium abscessus Aspartate Decarboxylase PanD and a Pyrazinoic Acid-Derived Inhibitor.	0
310	Application of Artificial intelligence in Drug Discovery. **2022**, 28,	0
309	Crystal structure of BtrK, a decarboxylase involved in the (S)-4-amino-2-hydroxybutyrate (AHBA) formation during butirosin biosynthesis. **2022**, 133576	
308	TRAF4 inhibits bladder cancer progression by promoting BMP/SMAD signalling.	0
307	Possible Charged Residue Switch for Acylglycerol Selectivity of Lipase MAS1.	0
306	Targeting Pseudomonas aeruginosa MvfR in the battle against biofilm formation: a multi-level computational approach.	
305	Basal Mitophagy is Suppressed in Cellular Senescence and Mediates Senescence Phenotypes.	

304	Prediction of drug□arget interaction □ helping hand in drug repurposing. **2022**, 519-536	
303	3D-QSAR-Based Pharmacophore Modeling, Virtual Screening, and Molecular Dynamics Simulations for the Identification of Spleen Tyrosine Kinase Inhibitors. 12,	1
302	Design and Synthesis of Novel PRMT1 Inhibitors and Investigation of Their Effects on the Migration of Cancer Cell. 10,	
301	A Computational Approach Applied to the Study of Potential Allosteric Inhibitors Protease NS2B/NS3 from Dengue Virus. **2022**, 27, 4118	1
300	Novel Rivastigmine Derivatives as Promising Multi-Target Compounds for Potential Treatment of Alzheimer□ Disease. **2022**, 10, 1510	1
299	In-silico discovery of inhibitors against human papillomavirus E1 protein. 1-14	
298	Optimization of Benzoxazinorifamycins to Minimize hPXR Activation for the Treatment of Tuberculosis and HIV Coinfection.	0
297	Optimization of Benzoxazinorifamycins to Improve Mycobacterium tuberculosis RNA Polymerase Inhibition and Treatment of Tuberculosis.	0
296	Docking-Based Virtual Screening Enables Prioritizing Protein Kinase Inhibitors With In Vitro Phenotypic Activity Against Schistosoma mansoni. 12,	0
295	Ligand-Enhanced Negative Images Optimized for Docking Rescoring. **2022**, 23, 7871	1
294	Prediction of novel and potent inhibitors of lanosterol 14-□demethylase. 1-13	2
293	Towards an Enrichment Optimization Algorithm (EOA)-based target specific docking functions for virtual screening.	
292	Binding of sikokianin C and related C-3/C-3?-biflavanones to cystathionine □synthase. A molecular docking study.	0
291	Complete Reaction Phenotyping of Propranolol and 4-Hydroxypropranolol with the 19 Enzymes of the Human UGT1 and UGT2 Families. **2022**, 23, 7476	
290	A Selective Adenylyl Cyclase 1 Inhibitor Relieves Pain Without Causing Tolerance. 13,	
289	Molecular basis for the pheromone-mediated feeding preference of early-instar Mythimna separata larvae.	0
288	Modern drug discovery applications for the identification of novel candidates for COVID-19 infections. **2022**, 104125	1
287	Inactivation Mechanism of the Fatty Acid Amide Hydrolase Inhibitor BIA 10-2474.	

286	Comparative Study of Binding Pockets in Human CYP1A2, CYP3A4, CYP3A5, and CYP3A7 with Aflatoxin B1, a Hepato-Carcinogen, by Molecular Dynamics Simulation & Principal Component Analysis. **2022**, 23,	
285	Implementing a Scoring Function Based on Interaction Fingerprint for Autogrow4: Protein Kinase CK1 as a Case Study. 9,	4
284	A fragment-based drug discovery strategy applied to the identification of NDM-1 lactamase inhibitors. **2022**, 240, 114599	3
283	Novel peptidomimetic inhibitors of signal transducer and activator of transcription 3 dimerization and biological activity. **2004**, 3, 261-269	76
282	Eugenol Ester Derivatives: Synthesis, Insecticidal Activity and Computational Studies.	
281	Synthesis and Antitumor Activity of 2,3-Diphenyl-2 H -indazole Derivatives as Potent Antitubulin Agents. **2022**, 7,	
280	Therapeutic targeting of PD-1/PD-L1 blockade by novel small-molecule inhibitors recruits cytotoxic T cells into solid tumor microenvironment. **2022**, 10, e004695	0
279	Consensus combining outcomes of multiple ensemble dockings: examples using dDAT crystalized complexes. **2022**, 101788	
278	Antiviral activity of ouabain against a Brazilian Zika virus strain. **2022**, 12,	
277	Harnessing Protein-Ligand Interaction Fingerprints to Predict New Scaffolds of RIPK1 Inhibitors. **2022**, 27, 4718	
276	Integration of cyclodextrins and associated toxicities: A roadmap for high quality biomedical applications. **2022**, 119880	0
275	Characterization of inulolytic enzymes from the Jerusalem artichoke derived Glutamicibacter mishrai NJAU-1.	
274	Developing New Treatments for COVID-19 through Dual-Action Antiviral/Anti-Inflammatory Small Molecules and Physiologically Based Pharmacokinetic Modeling. **2022**, 23, 8006	1
273	Identification of 2-hydroxybenzoic acid derivatives as selective SIRT5 inhibitors. **2022**, 114623	0
272	Single-chain fragment variable produced by phage display technology: Construction, selection, mutation, expression, and recent applications in food safety.	0
271	Application of InterCriteria Analysis to Assess the Performance of Scoring Functions in Molecular Docking Software Packages. **2022**, 10, 2549	
270	Novel Insights on Human Carbonic Anhydrase Inhibitors Based on Coumalic Acid: Design, Synthesis, Molecular Modeling Investigation, and Biological Studies. **2022**, 23, 7950	1
269	Identification of the Natural Steroid Sapogenin Diosgenin as a Direct Dual-Specific ROR Inverse Agonist. **2022**, 10, 2076	1

268	Identification of potential anti-pneumonia pharmacological components of Glycyrrhizae Radix et Rhizoma after the treatment with Gan An He Ji oral liquid. **2022**,	0
267	Design, Synthesis, and Evaluation of Novel Pyruvate Dehydrogenase Kinase Inhibitors. **2022**, 18,	
266	Design, Synthesis and Pharmacological Evaluation of Novel Conformationally Restricted N-arylpiperazine Derivatives Characterized as D2/D3 Receptor Ligands, Candidates for the Treatment of Neurodegenerative Diseases. **2022**, 12, 1112	
265	Design, synthesis, acetylcholinesterase, butyrylcholinesterase, and amyloid-β aggregation inhibition studies of substituted 4,4?-diimine/4,4?-diazobiphenyl derivatives.	
264	Viral informatics: bioinformatics-based solution for managing viral infections.	1
263	Nanocellulose Composites as Smart Devices With Chassis, Light-Directed DNA Storage, Engineered Electronic Properties, and Chip Integration. 10,	1
262	Covalent docking in CDOCKER.	
261	New Derivatives of 5-((1-Methyl-Pyrrol-2-yl) Methyl)-4-(Naphthalen-1-yl)-1,2,4-Triazoline-3-Thione and Its Coordination Compounds with Anticancer Activity. **2022**, 23, 9162	1
260	Synthesis of 1,2,3-Triazole Tethered Indole Derivatives: Evaluation of Anticancer Activity and Molecular Docking Studies. **2022**, 7,	6
259	Novel effective small-molecule inhibitors of protein kinases related to tau pathology in Alzheimer's disease. **2022**, 14, 1175-1186	
258	Interaction of panduratin A and derivatives with the SARS-CoV-2 main protease (mpro): a molecular docking study. 1-11	1
257	FIBCD1 is an endocytic GAG receptor associated with a novel neurodevelopmental disorder.	0
256	Monomethylsulochrin isolated from biomass extract of Aspergillus sp. against Leishmania amazonensis: In vitro biological evaluation and molecular docking. 12,	
255	New Myrtenal–Adamantane Conjugates Alleviate Alzheimer's-Type Dementia in Rat Model. **2022**, 27, 5456	
254	Anticholinesterase agents for Alzheimer's Disease treatment: an updated overview.. **2022**, 29,	1
253	QM/MM Study of the Reaction Mechanism of Thermophilic Glucuronoyl Esterase for Biomass Treatment.	0
252	Critical Assessment of State-of-the-Art Ligand-Based Virtual Screening Methods. 2200103	1
251	Network Pharmacology-Based Investigation on Therapeutic Mechanisms of the Angelica dahurica Radix and Ligusticum chuanxiong Rhizoma Herb Pair for Anti-Migraine Effect. **2022**, 11, 2196	

250	In Silico Interactions of the Components from the Schinus terebinthifolius Extract with Human Tyrosinase. **2022**, 87,	0
249	Development, Optimization, and In Vivo Validation of New Imidazopyridine Chemotypes as Dual TLR7/TLR9 Antagonists through Activity-Directed Sequential Incorporation of Relevant Structural Subunits.	0
248	Stimulation of platelet P2Y1 receptors by different endogenous nucleotides leads to functional selectivity via biased signalling.	
247	Cupressus sempervirens L. flavonoids as potent inhibitors to xanthine oxidase: in vitro, molecular docking, ADMET and PASS studies. 1-14	
246	Antioxidant and antiglycation activities and inhibitory action of Passiflora cincinnata on collagenase, elastase and tyrosinase: in vitro and in silico study. **2022**, 44, 102464	
245	Monoterpene substituted thiazolidin-4-ones as novel TDP1 inhibitors: Synthesis, biological evaluation and docking. **2022**, 73, 128909	2
244	Exploring enzyme inhibition profiles of novel halogenated chalcone derivatives on some metabolic enzymes: Synthesis, characterization and molecular modeling studies. **2022**, 100, 107748	2
243	Diminishing hERG inhibitory activity of aminopiperidine-naphthyridine linked NBTI antibacterials by structural and physicochemical optimizations. **2022**, 128, 106087	0
242	Graph theory-based simulation tools for protein structure networks. **2022**, 121, 102640	
241	Redesigning and Optimizing UCSF DOCK3.7 on Sunway TaihuLight. **2022**, 33, 4458-4471	
240	An integrated metabolomic and proteomic approach for the identification of covalent inhibitors of the main protease (Mpro) of SARS-COV-2 from crude natural extracts. **2023**, 252, 123824	
239	3,5-Dinitrobenzoate and 3,5-Dinitrobenzamide Derivatives: Mechanistic, Antifungal, and In Silico Studies. **2022**, 2022, 1-17	0
238	Virtual Screening and Bioactivity Modeling for G Protein-Coupled Receptors. **2022**, 388-423	1
237	A reinforcement learning approach for protein□gand binding pose prediction. **2022**, 23,	0
236	6-Formyl Umbelliferone, a Furanocoumarin from Angelica decursiva L., Inhibits Key Diabetes-Related Enzymes and Advanced Glycation End-Product Formation. **2022**, 27, 5720	1
235	Propofol metabolites and derivatives inhibit the oxidant activities of neutrophils and myeloperoxidase. **2022**, 191, 164-175	0
234	Fragment-based design of □cyanoacrylates and □cyanoacrylamides targeting Dengue and Zika NS2B/NS3 proteases.	1
233	Applications of machine learning in computer-aided drug discovery. **2022**, 3,	0

232	Deep eutectic solvents as green and efficient media for biocatalytic processes. **2022**, 161-180	1
231	Lead Optimization in Drug Discovery. **2022**, 481-500	0
230	Switching from ultrafast electron transfer to proton transfer in excited drug–protein complexes upon biotransformation. **2022**, 13, 9644-9654	0
229	Anti-ESBL derivatives of marine endophytic Streptomyces xiamenensis GRG 5 (KY457709) against ESBL producing bacteria. **2022**, 46, 16495-16508	0
228	Self-reporting styrylthiazolium photopharmaceuticals: mitochondrial localisation as well as SAR drive biological activity.	0
227	Computer-Aided Drug Design of Plant-Based Compounds. **2022**, 320-345	0
226	Genetic algorithms and other heuristic techniques in power systems optimization. **2023**, 41-95	0
225	Novel Hits for N-Myristoyltransferase Inhibition Discovered by Docking-Based Screening. **2022**, 27, 5478	0
224	In Vitro Antimicrobial Screening of Benzoylthioureas: Synthesis, Antibacterial Activity toward Streptococcus agalactiae and Molecular Docking Study. **2022**, 7,	0
223	In silico study on the Hepatitis E virus RNA Helicase and its inhibition by silvestrol, rocaglamide and other flavagline compounds. **2022**, 12,	0
222	Potential antifungal activity of novel carbohydrate derivatives validated by POM, molecular docking and molecular dynamic simulations analyses. 1-16	2
221	A high quality, industrial data set for binding affinity prediction: performance comparison in different early drug discovery scenarios.	0
220	Computational Chemistry and Molecular Modeling of Reversible MAO Inhibitors. **2023**, 221-252	0
219	Guttiferone E Displays Antineoplastic Activity Against Melanoma Cells.	0
218	Structural insights into the inhibition of the nsP2 protease from Chikungunya virus by molecular modeling approaches. **2022**, 28,	0
217	Synthesis and structure–activity relationships for some novel diflapolin derivatives with benzimidazole subunit. **2022**, 37, 1752-1764	0
216	Computational discovery of sulfonamide derivatives as potential inhibitors of the cruzain enzyme from T. cruzi by molecular docking, molecular dynamics and MM/GBSA approaches. 1-10	0
215	Gefitinib Inhibits Rifampicin-Induced CYP3A4 Gene Expression in Human Hepatocytes. **2022**, 7, 34034-34044	0

214	Gallic Acid Alkyl Esters: Trypanocidal and Leishmanicidal Activity, and Target Identification via Modeling Studies. **2022**, 27, 5876	0
213	Functional genomics uncovers the transcription factor BNC2 as required for myofibroblastic activation in fibrosis. **2022**, 13,	0
212	Discovery of inhibitors against SARS-CoV-2 associated fungal coinfections via virtual screening, ADMET evaluation, PASS, molecular docking, dynamics and pharmacophore studies. **2022**, 29, 337-350	1
211	Binding of Vialinin A and p-Terphenyl Derivatives to Ubiquitin-Specific Protease 4 (USP4): A Molecular Docking Study. **2022**, 27, 5909	1
210	Novel alpha6 preferring GABA-A receptor ligands based on loreclezole. **2022**, 114780	0
209	In Silico Studies Reveal Peramivir and Zanamivir as an Optimal Drug Treatment Even If H7N9 Avian Type Influenza Virus Acquires Further Resistance. **2022**, 27, 5920	0
208	Structural and Energetic Properties of Weak Noncovalent Interactions in Two Closely Related 3,6-Disubstituted-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole Derivatives: In Vitro Cyclooxygenase Activity, Crystallography, and Computational Investigations. **2022**, 7, 34506-34520	0
207	Novel eIF4A1 inhibitors with anti-tumor activity in lymphoma. **2022**, 28,	0
206	Docking covalent targets for drug discovery: stimulating the computer-aided drug design community of possible pitfalls and erroneous practices.	1
205	Synthesis, Antibacterial, and Antioxidant Activities of Thiazolyl-Pyrazoline Schiff Base Hybrids: A Combined Experimental and Computational Study. **2022**, 2022, 1-19	0
204	Lisaftoclax (APG-2575) is a Novel BCL-2 Inhibitor with Robust Antitumor Activity in Preclinical Models of Hematologic Malignancy.	1
203	Crystal structure of the Rho-associated coiled-coil kinase 2 inhibitor belumosudil bound to CK2. **2022**, 78, 348-353	0
202	Design, Synthesis, Biological Activity, and Structural Analysis of Novel Des-C-Ring and Aromatic-D-Ring Analogues of 1,25-Dihydroxyvitamin D3.	0
201	Design, Synthesis, and in Vitro Evaluation of 4-(4-Hydroxyphenyl)piperazine-Based Compounds Targeting Tyrosinase.	0
200	Dual A1/A3 Adenosine Receptor Antagonists: Binding Kinetics and Structure-Activity Relationship Studies Using Mutagenesis and Alchemical Binding Free Energy Calculations.	0
199	Pharmacophore-Based Virtual Screening and Experimental Validation of Pyrazolone-Derived Inhibitors toward Janus Kinases. **2022**, 7, 33548-33559	0
198	Synthesis, molecular docking and anti-inflammatory evaluation of new trisubstituted pyrazoline derivatives bearing benzenesulfonamide moiety. 1-8	1
197	Machine Learning Approaches to Improve Prediction of Target-Drug Interactions. **2022**, 21-96	0

196	Focusing on C-4 position of Hantzsch 1,4-dihydropyridines: Molecular modifications, enantioseparation, and binding mechanism to L- and T-type calcium channels. **2022**, 244, 114787	0
195	Structural analysis of cannabinoids against EGFR-TK leads a novel target against EGFR-driven cell lines. **2022**, 3, 100132	0
194	Can docking scoring functions guarantee success in virtual screening?. **2022**,	0
193	Pyrazolines as potential anti-alzheimer's agents: DFT, molecular docking, enzyme inhibition and pharmacokinetic studies.	0
192	Docking-Based Virtual Screening for the Discovery of 1,3,4-Oxadiazoles as Aminoacyl-tRNA Synthetase Inhibitors. **2022**, 14, 83-92	0
191	Computational Insights into β-Carboline Inhibition of Monoamine Oxidase A. **2022**, 27, 6711	1
190	From Genome Mining to Protein Engineering: A Structural Bioinformatics Route. **2023**, 79-94	0
189	Molecular insights into the binding of carnosine and anserine to human serum carnosinase 1 (CN1). 4, e25	0
188	Development of machine learning models for the screening of potential HSP90 inhibitors. 9,	0
187	Vutiglabridin improves neurodegeneration in MPTP-induced Parkinson's disease mice by targeting mitochondrial paraoxonase-2.	0
186	Mono-n-butyl Malate-Derived Compounds from Camu-camu (Myrciaria dubia) Malic Acid: The Alkyl-Dependent Antihyperglycemic-Related Activity. **2022**, 7, 39335-39346	0
185	Imaging of KCa3.1 channels in tumor cells with PET and small-molecule fluorescent probes.	0
184	Thioterpenoids as Potential Antithrombotic Drugs: Molecular Docking, Antiaggregant, Anticoagulant and Antioxidant Activities. **2022**, 12, 1599	0
183	Liposomal Formulations Loaded with a Eugenol Derivative for Application as Insecticides: Encapsulation Studies and In Silico Identification of Protein Targets. **2022**, 12, 3583	0
182	Resistor: An algorithm for predicting resistance mutations via Pareto optimization over multistate protein design and mutational signatures. **2022**, 13, 830-843.e3	0
181	Detection of 18-methyl steroids: Case report on a forensic urine sample and corresponding dietary supplements.	0
180	Structural Prediction and Characterization of Canavalia grandiflora (ConGF) Lectin Complexed with MMP1: Unveiling the Antiglioma Potential of Legume Lectins. **2022**, 27, 7089	0
179	In Silico Simulations and Functional Cell Studies Evidence Similar Potency and Distinct Binding of Pacific and Caribbean Ciguatoxins.	0

178	Exploiting ligand binding domain dimerization for development of novel androgen receptor inhibitors.	1
177	Functional Characterization and Synthetic Application of Is2-SDR, a Novel Thermostable and Promiscuous Ketoreductase from a Hot Spring Metagenome. **2022**, 23, 12153	0
176	Prioritizing small sets of molecules for synthesis through in-silico tools: A comparison of common ranking methods..	4
175	Modern computational methods for rational enzyme engineering. **2022**, 2, 2481-2498	1
174	Structure-guided identification of a selective sulfonamide-based inhibitor targeting the human carbonic anhydrase VA isoform.	0
173	In Silico Investigations into the Selectivity of Psychoactive and New Psychoactive Substances in Monoamine Transporters. **2022**, 7, 38311-38321	0
172	From drugs to targets: Reverse engineering the virtual screening process on a proteomic scale. 2,	0
171	Experimental and Computational Studies on the Biotransformation of Pseudopyronines with Human Cytochrome P450 CYP4F2.	0
170	A multilayer dynamic perturbation analysis method for predicting ligand–protein interactions. **2022**, 23,	0
169	Intracellular BAPTA directly inhibits PFKFB3, thereby impeding mTORC1-driven Mcl-1 translation and killing Mcl-1-addicted cancer cells.	0
168	Roles of hybrid donepezil scaffolds as potent human acetylcholinesterase inhibitors using in silico interaction analysis, drug-likeness, and pharmacokinetics prediction. **2022**, 368, 110227	0
167	The molecular basis and enzyme engineering strategies for improvement of coupling efficiency in cytochrome P450s. **2022**, 61, 108051	0
166	Characterizing the ligand-binding affinity to SARS-CoV-2 Mpro via physics and knowledge based approaches.	0
165	Development of Nucleic Acid Targeting Molecules: Molecular Docking Approaches and Recent Advances.	0
164	Generative deep learning enables the discovery of a potent and selective RIPK1 inhibitor. **2022**, 13,	1
163	ToDD: Topological Compound Fingerprinting in Computer-Aided Drug Discovery.	0
162	Application of Computational Biology and Artificial Intelligence in Drug Design. **2022**, 23, 13568	1
161	Singlet oxygen and radical-mediated mechanisms in the oxidative cellular damage photosensitized by the protease inhibitor simeprevir. **2022**,	0

160	FSDscore: An Effective Target-Focused Scoring Criterion for Virtual Screening.	0
159	In silico designed microtubule-stabilizer drugs against tauopathy in Alzheimer disease. 1-21	0
158	Computational drug discovery under RNA times. 1-21	0
157	Structural and Functional Insight into the Mechanism of the Fe-S Cluster-Dependent Dehydratase from Paralcaligenes ureilyticus..	0
156	The protein conformational basis of isoflavone biosynthesis. **2022**, 5,	0
155	CADD, AI and ML in Drug Discovery: A Comprehensive Review. **2022**, 106324	2
154	Molecular Docking and Dynamics Simulation of Several Flavonoids Predict Cyanidin as an Effective Drug Candidate against SARS-CoV-2 Spike Protein. **2022**, 2022, 1-13	0
153	Green synthesis of a new series of pyroglutamides targeting human farnesyltransferase. **2022**, 30, 100894	0
152	The exploration of phytocompounds theoretically combats SARS-CoV-2 pandemic against virus entry, viral replication and immune evasion. **2022**,	0
151	New Insights on Glutathione Supramolecular Arrangement and Its In Silico Analysis as an Angiotensin-Converting Enzyme Inhibitor. **2022**, 27, 7958	1
150	Open Binding Pose Metadynamics: An Effective Approach for the Ranking of Protein igand Binding Poses.	0
149	Advancing the field of computational drug design using multicanonical molecular dynamics-based dynamic docking.	1
148	A Non Exhaustive Search of Exhaustiveness. **2022**, 97-108	0
147	Protein-coding gene interaction network prediction of bioactive plant compound action against SARS-CoV-2: a novel hypothesis using bioinformatics analysis. **2022**, 94,	0
146	Deciphering the biotransformation mechanism of dialkylresorcinols by CYP4F11. **2023**, 131, 106330	0
145	Trends and hotspots for European Journal of Medicinal Chemistry: A bibliometric study. **2023**, 247, 115041	0
144	Tools for protein structure prediction and for molecular docking applied to enzyme active site analysis: A case study using a BAHD hydroxycinnamoyltransferase. **2022**,	0
143	Biocatalytic approach to chiral fluoroaromatic scaffolds. **2022**, 20, 9734-9741	0

142	Hierarchical analysis of the target-based scoring function modification on the example of selected class A GPCRs.	0
141	Molecular modeling of alkaloids bouchardatine and orirenierine binding to sirtuin-1 (SIRT1). **2022**, 5, 276-285	0
140	Perceiver CPI: A nested cross-attention network for compound-protein interaction prediction.	0
139	Computer simulation of molecular recognition in biomolecular system: from in silico screening to generalized ensembles.	1
138	Making Protein Degradation Visible: Discovery of Theranostic PROTACs for Detecting and Degrading NAMPT. **2022**, 65, 15725-15737	1
137	Ligand-Based Discovery of a Small Molecule as Inhibitor of □Synuclein Amyloid Formation. **2022**, 23, 14844	1
136	Integrating model simulation tools and cryo-electron microscopy.	0
135	A Hybrid Docking and Machine Learning Approach to Enhance the Performance of Virtual Screening Carried out on Protein□Protein Interfaces. **2022**, 23, 14364	0
134	Development of QSRR model for hydroxamic acids using PCA-GA-BP algorithm incorporated with molecular interaction-based features. 10,	0
133	Lemon Balm (Melissa officinalis) Essential Oil Moderately Affects Strychnine-Induced and Pentylenetetrazol-Induced Convulsions □n Silico and In Vivo Studies. **2022**, 17, 1934578X2211399	0
132	N-[1,3-Dialkyl(aryl)-2-oxoimidazolidin-4-ylidene]-aryl(alkyl)sulphonamides as Novel Selective Human Cannabinoid Type 2 Receptor (hCB2R) Ligands; Insights into the Mechanism of Receptor Activation/Deactivation. **2022**, 27, 8152	0
131	Changes in Alprazolam Metabolism by CYP3A43 Mutants. **2022**, 10, 3022	1
130	Molecular Modeling, Virtual Screening, and Molecular Dynamics for Leishmania infantum Methionyl-tRNA Synthetase.	0
129	In Vitro and In Silico Studies for the Identification of Potent Metabolites of Some High-Altitude Medicinal Plants from Nepal Inhibiting SARS-CoV-2 Spike Protein. **2022**, 27, 8957	0
128	Investigation into the Use of Encorafenib to Develop Potential PROTACs Directed against BRAFV600E Protein. **2022**, 27, 8513	0
127	Antimelanoma effect of manool in 2D cell cultures and reconstructed human skin models.	0
126	The Anti-Multidrug-Resistant Acinetobacter baumannii Study on 1,3-diamino-7H-pyrrolo[3,2-f]quinazoline Compounds. **2022**, 27, 8609	0
125	Pharmacophore-Oriented Identification of Potential Leads as CCR5 Inhibitors to Block HIV Cellular Entry. **2022**, 23, 16122	0

124	Straightforward Access to a New Class of Dual DYRK1A/CLK1 Inhibitors Possessing a Simple Dihydroquinoline Core. **2023**, 28, 36	0
123	Introducing ligand GA, a genetic algorithm molecular tool for automated protein inhibitor design. **2022**, 12,	0
122	Difference in the Inhibitory Effect of Thiol Compounds and Demetallation Rates from the Zn(II) Active Site of Metallo-β-lactamases (IMP-1 and IMP-6) Associated with a Single Amino Acid Substitution.	0
121	Investigation on Hydrazonobenzenesulfonamides as Human Carbonic Anhydrase I, II, IX and XII Inhibitors. **2023**, 28, 91	0
120	IMIDAZONAPHTHYRIDINE EFFECTS ON CHIKUNGUNYA VIRUS REPLICATION: ANTIVIRAL ACTIVITY BY DEPENDENT AND INDEPENDENT OF INTERFERON TYPE 1 PATHWAYS. **2022**, 199029	0
119	N -Substituted piperidine-3-carbohydrazide-hydrazones against Alzheimer's disease: Synthesis and evaluation of cholinesterase, beta-amyloid inhibitory activity, and antioxidant capacity.	0
118	Synthesis and in vitro assessment of anticholinesterase and antioxidant properties of triazineamide derivatives.	0
117	Caffeic acid N-[3,5-bis(trifluoromethyl)phenyl] amide as a non-steroidal inhibitor for steroid 5α-reductase type 1 using a human keratinocyte cell-based assay and molecular dynamics. **2022**, 12,	0
116	Regioselective Synthesis and Molecular Docking Studies of 1,5-Disubstituted 1,2,3-Triazole Derivatives of Pyrimidine Nucleobases. **2022**, 27, 8467	0
115	Insights into the role of the cobalt(III)-thiosemicarbazone complex as a potential inhibitor of the Chikungunya virus nsP4.	0
114	Improved docking of peptides and small molecules in iMOLSDOCK. **2023**, 29,	1
113	Pesticide informatics expands the opportunity for structure-based molecular design and optimization. **2022**, 1, 139-147	0
112	Intracellular BAPTA directly inhibits PFKFB3, thereby impeding mTORC1-driven Mcl-1 translation and killing Mcl-1-addicted cancer cells.	0
111	Locating Guest Molecules inside Metal–Organic Framework Pores with a Multilevel Computational Approach.	0
110	Investigation of cerebrovascular activity of new GABA-derived short peptides. **2022**, 89-95	0
109	Solving an Old Puzzle: Elucidation and Evaluation of the Binding Mode of Salvinorin A at the Kappa Opioid Receptor. **2023**, 28, 718	0
108	AlteQ: a new complementarity principle-centered method for the evaluation of docking poses. 1-15	0
107	Differential regulation of Cav3.2 and Cav2.2 calcium channels by CB1 receptors and cannabidiol.	0

106	Hydroxylated Coumarin-Based Thiosemicarbazones as Dual Antityrosinase and Antioxidant Agents. **2023**, 24, 1678	0
105	A structure-based virtual high-throughput screening, molecular docking, molecular dynamics and MM/PBSA study identified novel putative drug-like dual inhibitors of trypanosomal cruzain and rhodesain cysteine proteases.	0
104	Latonduine-1-Amino-Hydantoin Hybrid, Triazole-Fused Latonduine Schiff Bases and Their Metal Complexes: Synthesis, X-ray and Electron Diffraction, Molecular Docking Studies and Antiproliferative Activity. **2023**, 11, 30	0
103	Searching for Novel Noncovalent Nuclear Export Inhibitors through a Drug Repurposing Approach.	0
102	Molecular Docking of Cryptoconcatones to Tubulin and Related Pironetin Analogues. **2023**, 12, 296	0
101	Multifunctional organometallic compounds for the treatment of Chagas disease: Re(i) tricarbonyl compounds with two different bioactive ligands.	1
100	Identification of 2-Aryl-Quinolone Inhibitors of Cytochrome bd and Chemical Validation of Combination Strategies for Respiratory Inhibitors against Mycobacterium tuberculosis.	0
99	Neural Networks in the Design of Molecules with Affinity to Selected Protein Domains. **2023**, 24, 1762	0
98	In Vitro and In Silico Studies of Kinase Inhibitor of MAPK3 Protein to Determine Leishmania martiniquensis Treatment.	0
97	Identifying Dopamine D3 Receptor Ligands through Virtual Screening and Exploring the Binding Modes of Hit Compounds. **2023**, 28, 527	1
96	Identification of Natural Products Inhibiting SARS-CoV-2 by Targeting Viral Proteases: A Combined in Silico and in Vitro Approach.	0
95	Experimental heoretical study of laccase as a detoxifier of aflatoxins. **2023**, 13,	2
94	In Silico and In Vitro Study of Janus Kinases Inhibitors from Naphthoquinones. **2023**, 28, 597	0
93	Assessment of AlphaFold structures and optimization methods for virtual screening.	0
92	Fluorescent and theranostic probes for imaging nicotinamide phosphoribosyl transferase (NAMPT). **2023**, 248, 115080	0
91	Design, synthesis, and biological activity studies on benzimidazole derivatives targeting myeloperoxidase. **2023**, 248, 115083	0
90	Synthesis and molecular modeling studies of naphthazarin derivatives as novel selective inhibitors of glucosidase and amylase. **2023**, 1278, 134954	0
89	Chaotic Evolution for Multimodal Optimization Based on Multi-rule Generation Strategy. **2022**,	0

88	An In Vitro and In Silico Investigation about Monteverdia ilicifolia Activity against Helicobacter pylori. **2023**, 12, 46	0
87	Short Lecture Natural products against SARS-CoV-2 or how to catch a butterfly? **2022**,	0
86	A Guide to In Silico Drug Design. **2023**, 15, 49	0
85	ViTRMSE: a three-dimensional RMSE scoring method for protein-ligand docking models based on Vision Transformer. **2022**,	0
84	HCovDock: an efficient docking method for modeling covalent protein ligand interactions. **2023**, 24,	1
83	A Comparative Study of Chamomile Essential Oils and Lipophilic Extracts Obtained by Conventional and Greener Extraction Techniques: Chemometric Approach to Chemical Composition and Biological Activity. **2023**, 10, 18	0
82	Singlet Oxygen and Radical-Mediated Mechanisms in the Oxidative Cellular Damage Photosensitized by the Protease Inhibitor Simeprevir.	0
81	Identification of Activated Cdc42-Associated Kinase Inhibitors as Potential Anticancer Agents Using Pharmacoinformatic Approaches. **2023**, 13, 217	0
80	The Mythimna separata general odorant binding protein 2 (MsepGOBP2) is involved in the larval detection of the sex pheromone (Z)-11-hexadecenal.	0
79	Computational Investigation of a Series of Small Molecules as Potential Compounds for Lysyl Hydroxylase-2 (LH2) Inhibition.	0
78	Interaction of copper potential metallodrugs with TMPRSS2: A comparative study of docking tools and its implications on COVID-19. 11,	0
77	MetalProGNet: a structure-based deep graph model for metalloprotein ligand interaction predictions.	0
76	Synthesis and structure ctivity relationships of pyrazole-based inhibitors of meprin and **2023**, 38,	0
75	Molecular interaction modeling of carbon nanotubes and fullerene toward prioritized targets of SARS-CoV-2 by computer-aided screening and docking studies. **2023**, 157-179	0
74	Identifying Protein igand Interactions via a Novel Distance Self-Feedback Biomolecular Interaction Network. **2023**, 127, 899-911	0
73	MetaDOCK: A Combinatorial Molecular Docking Approach.	0
72	Coumarin-based derivatives targeting Trypanosoma cruzi cruzain and Trypanosoma brucei cathepsin L-like proteases.	0
71	Novel TDP1 Inhibitors: Disubstituted Thiazolidine-2,4-Diones Containing Monoterpene Moieties. **2023**, 24, 3834	0

70	An Arylbenzofuran, Stilbene Dimers, and Prenylated Diels–Alder Adducts as Potent Diabetic Inhibitors from Morus bombycis Leaves. **2023**, 12, 837	0
69	Coumarin-Based Compounds as Inhibitors of Tyrosinase/Tyrosine Hydroxylase: Synthesis, Kinetic Studies, and In Silico Approaches. **2023**, 24, 5216	0
68	Artificial intelligence based virtual screening study for competitive and allosteric inhibitors of the SARS-CoV-2 main protease. 1-19	0
67	A novel molecular docking program based on a multi-swarm competitive algorithm. **2023**, 78, 101292	0
66	Dock-able linear and homodetic di, tri, tetra and pentapeptide library from canonical amino acids: SARS-CoV-2 Mpro as a case study. **2023**,	0
65	Application of computational methods for class A GPCR Ligand discovery. **2023**, 121, 108434	0
64	Structure-based virtual screening for potent inhibitors of GH-20 β-N-acetylglucosaminidase: Classical and machine learning scoring functions, and molecular dynamics simulations. **2023**, 104, 107856	0
63	Synthesis, Insecticidal Activity and Computational Studies of Eugenol-Based Insecticides.	0
62	From Discovery to Production: Challenges and Novel Methodologies for Next Generation Biomanufacturing. **2022**,	0
61	In vitro Analytical Techniques as Screening Tools to investigate the Metal chelate-DNA interactions. **2023**, 8,	1
60	Biosynthesis of silver nanoparticles of Tribulus terrestris food supplement and evaluated antioxidant activity and collagenase, elastase and tyrosinase enzyme inhibition: In vitro and in silico approaches. **2023**, 138, 150-161	0
59	Identification of potential novel inhibitors against glutamine synthetase enzyme of Leishmania major by using computational tools. 1-9	0
58	Computational assessment of the impact of Cu(II) and Al(III) on β-amyloid42 fibrils: Binding sites, structural stability, and possible physiological implications. 17,	0
57	Study of Genotoxicity, Activities on Caspase 8 and on the Stabilization of the Topoisomerase Complex of Isoeleutherin and Analogues. **2023**, 28, 1630	0
56	Bioinformatics and Cheminformatics Tools in Early Drug Discovery. **2023**, 147-181	0
55	Machine Learning Scoring Functions for Drug Discovery from Experimental and Computer-Generated Protein–Ligand Structures: Towards Per-Target Scoring Functions. **2023**, 28, 1661	0
54	Molecular Modeling and In Vitro Evaluation of Piplartine Analogs against Oral Squamous Cell Carcinoma. **2023**, 28, 1675	0
53	Design, synthesis, and biological evaluation of some novel naphthoquinone-glycine / β-alanine anilide derivatives as noncovalent proteasome inhibitors.	0

52	Interaction of Camptothecin Anticancer Drugs with Ribosomal Proteins L15 and L11: A Molecular Docking Study. **2023**, 28, 1828	0
51	Systematic investigation of the mechanism of herbal medicines for the treatment of prostate cancer.	0
50	Synthetic Cinnamides and Cinnamates: Antimicrobial Activity, Mechanism of Action, and In Silico Study. **2023**, 28, 1918	2
49	A new class of peptides from wasp venom: a pathway to antiepileptic/neuroprotective drugs. **2022**, 5,	0
48	Computational Chemistry for the Identification of Lead Compounds for Radiotracer Development. **2023**, 16, 317	1
47	Rationalizing the Binding Modes of PET Radiotracers Targeting the Norepinephrine Transporter. **2023**, 15, 690	0
46	A Critical Study on Acylating and Covalent Reversible Fragment Inhibitors of SARS-CoV-2 Main Protease Targeting the S1 Site with Pyridine.	0
45	Regioselective glucosylation of (+)-catechin using a new variant of sucrose phosphorylase from Bifidobacterium adolescentis. **2023**, 21, 2307-2311	0
44	Comparative Assessment of Docking Programs for Docking and Virtual Screening of Ribosomal Oxazolidinone Antibacterial Agents. **2023**, 12, 463	0
43	Integrating structure-based approaches in generative molecular design. **2023**, 79, 102559	0
42	Virtual screening. **2023**, 223-236	0
41	Alternative biological screening methods. **2023**, 95-137	0
40	Molecular-evaluated and explainable drug repurposing for COVID-19 using ensemble knowledge graph embedding. **2023**, 13,	0
39	SCARdock: A Web Server and Manually Curated Resource for Discovering Covalent Ligands. **2023**, 8, 10397-10402	0
38	Synergistic antifungal interaction of N-(butylcarbamothioyl) benzamide and amphotericin B against Cryptococcus neoformans. 14,	0
37	Dithiocarbazate ligands and their Ni(II) complexes with potential biological activity: Structural, antitumor and molecular docking study. 10,	0
36	Identification and Empiric Evaluation of New Inhibitors of the Multidrug Transporter P-Glycoprotein (ABCB1). **2023**, 24, 5298	0
35	Trypanosoma cruzi Sirtuin 2 as a Relevant Druggable Target: New Inhibitors Developed by Computer-Aided Drug Design. **2023**, 16, 428	0

34	Designed multiple ligands for the treatment of type 2 diabetes mellitus and its complications: Discovery of (5-arylidene-4-oxo-2-thioxothiazolidin-3-yl)alkanoic acids active as novel dual-targeted PTP1B/AKR1B1 inhibitors. **2023**, 252, 115270	0
33	Developing novel indanone-chalcone hybrids bearing ester group with potential anti-Alzheimer effects by combining molecular hybridization and bioisosteric replacement drug design approaches.	0
32	Quorum Quenchers from Reynoutria japonica in the Battle against Methicillin-Resistant Staphylococcus aureus (MRSA). **2023**, 28, 2635	0
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30	Bioinformatics approaches: elucidation of novel sites of action, toxicity prediction tool, and perception of bioactive compounds. **2023**, 309-327	0
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25	Drug repurposing for viral cancers: A paradigm of machine learning, deep learning, and virtual screening-based approaches. **2023**, 95,	0
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21	Exploring and targeting potential druggable antimicrobial resistance targets ArgS, SecY and MurA in Staphylococcus sciuri with TCM inhibitors through subtractive genomics strategy.	0
20	Hydroperoxidation of Docosahexaenoic Acid by Human ALOX12 and pigALOX15-mini-LOX. **2023**, 24, 6064	0
19	Structural Understanding of Fungal Terpene Synthases for the Formation of Linear or Cyclic Terpene Products. **2023**, 13, 4949-4959	0
18	Synthesis, identification and evaluation of molecular docking and experimental anti-cancer and antioxidant activity of new spiro four membered ring derivatives bearing 5-nitro isatin. 1-8	0
17	A computational investigation of galactopyranoside esters as antimicrobial agents through antiviral, molecular docking, molecular dynamics, pharmacokinetics, and bioactivity prediction. 1-16	0

16	Structure-based virtual screening and molecular dynamics simulations for detecting novel candidates for allosteric inhibition of EGFRT790M. 1-27	0
15	Fragment-based investigation of thiourea derivatives as VEGFR-2 inhibitors: a cross-validated approach of ligand-based and structure-based molecular modeling studies. 1-17	0
14	Structure-guided engineering of a receptor-agonist pair for inducible activation of the ABA adaptive response to drought. **2023**, 9,	0
13	The Impact of Supervised Learning Methods in Ultralarge High-Throughput Docking.	0
12	Hybridization into a Bitopic Ligand Increased Muscarinic Receptor Activation for Isopilocarpine but Not for Pilocarpine Derivatives.	0
11	In silico drug repurposing by combining machine learning classification model and molecular dynamics to identify a potential OGT inhibitor. 1-12	0
10	AI-Driven Discovery of SARS-CoV-2 Main Protease Fragment-like Inhibitors with Antiviral Activity In Vitro.	0
9	An in silico approach to unveil peptides from Acheta domesticus with potential bioactivity against hypertension, diabetes, cardiac and pulmonary fibrosis. **2023**, 112847	0
8	Vutiglabridin Modulates Paraoxonase 1 and Ameliorates Diet-Induced Obesity in Hyperlipidemic Mice. **2023**, 13, 687	0
7	In-Silico Approaches for the Screening and Discovery of Broad-Spectrum Marine Natural Product Antiviral Agents Against Coronaviruses. Volume 16, 2321-2338	0
6	Reinventing Therapeutic Proteins: Mining a Treasure of New Therapies. **2023**, 3, 72-94	0
5	Developments in molecular docking technologies for application of polysaccharide-based materials: A review. 1-13	0
4	Synergistic Combination of Citrus Flavanones as Strong Antioxidant and COX-Inhibitor Agent. **2023**, 12, 972	0
3	Identification of fungus-growing termite-associated halogenated-PKS maduralactomycin a as a potential inhibitor of MurF protein of multidrug-resistant Acinetobacter baumannii. 10,	0
2	Synthesis, in vitro □glucosidase and □amylase activities, and an in silico molecular docking study of triazinoindole-thiazolidinone hybrid derivatives. **2023**, 45, 101035	0
1	Development of heterodimeric estrogen receptor alpha antagonists to target simultaneously the ligand and coactivator binding site.	0