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2180 Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study.

2180	Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study.		
2179	Suppression of Tumor Growth and Metastases by Targeted Intervention in Urokinase Activity with Cyclic Peptides.		
2178	Molecular modeling of nucleic acid structure: energy and sampling. 2001 , Chapter 7, Unit 7.8		2
2177	GROMACS: fast, flexible, and free. <i>Journal of Computational Chemistry</i> , 2005 , 26, 1701-18	5	10273
2176	Solution structure of the N-terminal zinc fingers of the Xenopus laevis double-stranded RNA-binding protein ZFa. 2005 , 351, 718-30		16
2175	Scalable Algorithms for Molecular Dynamics Simulations on Commodity Clusters. 2006,		469
2174	Drug-Target Binding Investigated by Quantum Mechanical/Molecular Mechanical (QM/MM) Methods. 2006 , 449-479		7
2173	Molecular dynamicsScalable algorithms for molecular dynamics simulations on commodity clusters. 2006 ,		578
2172	Conformation of Glycopeptides and Glycoproteins. 2006 , 187-251		25
2171	Role of Solvent Dynamics in Stabilizing the Transition State of RNA Hydrolysis by Hairpin Ribozyme. 2006 , 2, 858-62		21
2170	Cathepsin D deficiency is associated with a human neurodegenerative disorder. 2006 , 78, 988-98		221
2169	Molecular dynamics: survey of methods for simulating the activity of proteins. 2006 , 106, 1589-615		818
2168	Low-Resolution Molecular Dynamics Simulations of the 30S Ribosomal Subunit. 2006 , 5, 1248-1263		14
2167	Allosteric signaling of ATP hydrolysis in GroEL-GroES complexes. 2006 , 13, 147-52		131
2166	Estimation of Absolute Free Energies of Hydration Using Continuum Methods: Accuracy of Partial Charge Models and Optimization of Nonpolar Contributions. 2006 , 2, 128-39		143
2165	Structural monitoring of oligosaccharides through 13C enrichment and NMR observation of acetyl groups. 2006 , 91, 1952-9		18

(2006-2006)

2164	Phenol red interacts with the protofibril-like oligomers of an amyloidogenic hexapeptide NFGAIL through both hydrophobic and aromatic contacts. 2006 , 91, 3664-72	55
2163	A computational study of nucleosomal DNA flexibility. 2006 , 91, 4121-32	65
2162	Structure and interactions of the ubiquitin-conjugating enzyme variant human Uev1a: implications for enzymatic synthesis of polyubiquitin chains. 2006 , 45, 9866-77	13
2161	Investigation of the influence of spacer arm on the structural evolution of affinity ligands supported on agarose. 2006 , 110, 23564-77	29
2160	HIV-1 protease flaps spontaneously open and reclose in molecular dynamics simulations. 2006 , 103, 915-20	298
2159	Electrostatic, steric, and hydration interactions favor Na(+) condensation around DNA compared with K(+). 2006 , 128, 14506-18	123
2158	Redesign of Schistosoma mansoni NAD+ catabolizing enzyme: active site H103W mutation restores ADP-ribosyl cyclase activity. 2006 , 45, 11867-78	13
2157	Physical and structural basis for the strong interactions of the -ImPy- central pairing motif in the polyamide f-ImPyIm. 2006 , 45, 13551-65	68
2156	Linking ligand-induced alterations in androgen receptor structure to differential gene expression: a first step in the rational design of selective androgen receptor modulators. 2006 , 20, 1201-17	59
2155	Improved Efficiency of Replica Exchange Simulations through Use of a Hybrid Explicit/Implicit Solvation Model. 2006 , 2, 420-33	118
2154	Structural analysis of ligand binding and catalysis in chorismate lyase. 2006 , 445, 72-80	16
2153	Tertiary structure prediction of SARS coronavirus helicase. 2006 , 343, 1101-4	25
2152	Computational studies of H5N1 hemagglutinin binding with SA-alpha-2, 3-Gal and SA-alpha-2, 6-Gal. 2006 , 347, 662-8	38
2151	Quantification of DNA BI/BII backbone states in solution. Implications for DNA overall structure and recognition. 2006 , 128, 9170-7	85
2150	Structural basis for cooperative transcription factor binding to the CBP coactivator. 2006 , 355, 1005-13	144
2149	Structure of the Escherichia coli quorum sensing protein SdiA: activation of the folding switch by acyl homoserine lactones. 2006 , 355, 262-73	143
2148	Induced fit and "lock and key" recognition of 5S RNA by zinc fingers of transcription factor IIIA. 2006 , 357, 275-91	60
2147	Nudged elastic band calculation of minimal energy paths for the conformational change of a GG non-canonical pair. 2006 , 357, 1683-93	37

2146	The unfolded state of the villin headpiece helical subdomain: computational studies of the role of locally stabilized structure. 2006 , 360, 1094-107	46
2145	One protein, two enzymes revisited: a structural entropy switch interconverts the two isoforms of acireductone dioxygenase. 2006 , 363, 823-34	55
2144	Electronic structure theory of DNA: from semi-empirical theory of the Estack to ab initio calculations of the optical conductivity. 2006 , 393-406	
2143	High-Resolution Protein Structure Determination by NMR. 2006 , 59, 235-273	4
2142	Comparison of multiple Amber force fields and development of improved protein backbone parameters. 2006 , 65, 712-25	5087
2141	Histone H3 recognition and presentation by the WDR5 module of the MLL1 complex. 2006 , 13, 704-12	191
2140	Study of charges transferability for use in force fields. 2006 , 420, 497-502	4
2139	Biological and synthetic membranes: What can be learned from a coarse-grained description?. 2006 , 434, 113-176	257
2138	Computational prediction of homodimerization of the A3 adenosine receptor. 2006 , 25, 549-61	25
2137	A study of the interaction of cinnamate analogues with macrophage migration inhibitory factor (MIF) and P1G mutant from molecular dynamics simulations. 2006 , 763, 97-101	1
2136	Molecular quantum mechanics to biodynamics: Essential connections. 2006 , 764, 1-8	6
2135	A suite of Mathematica notebooks for the analysis of protein main chain 15N NMR relaxation data. 2006 , 36, 215-24	52
2134	Graphical exploratory data analysis of RNA secondary structure dynamics predicted by the massively parallel genetic algorithm. 2006 , 25, 514-31	26
2133	Lengsin is a survivor of an ancient family of class I glutamine synthetases re-engineered by evolution for a role in the vertebrate lens. 2006 , 14, 1823-34	26
2132	Modelling study of dimerization in mammalian defensins. 2006 , 7 Suppl 5, S17	24
2131	Synthesis and biological evaluation of bicyclic nucleosides as inhibitors of M. tuberculosis thymidylate kinase. 2006 , 1, 1081-90	28
2130	Correlation of biological activity with active site binding modes of geminal disulfone HIV-1 integrase inhibitors. 2006 , 1, 959-64	7
2129	PREDITOR: a web server for predicting protein torsion angle restraints. 2006 , 34, W63-9	158

2120	Atomic structures of peptide self-assembly mimics. 2006 , 103, 17753-8	55
2127	Conformational transition pathway in the allosteric process of human glucokinase. 2006 , 103, 13368-73	59
2126	Determination of binding site residues responsible for the subunit selectivity of novel marine-derived compounds on kainate receptors. 2006 , 69, 1849-60	28
2125	Understanding the bacterial polysaccharide antigenicity of Streptococcus agalactiae versus Streptococcus pneumoniae. 2006 , 103, 8149-54	39
2124	X-ray diffraction "fingerprinting" of DNA structure in solution for quantitative evaluation of molecular dynamics simulation. 2006 , 103, 3534-9	84
2123	NMR structure of the three quasi RNA recognition motifs (qRRMs) of human hnRNP F and interaction studies with Bcl-x G-tract RNA: a novel mode of RNA recognition. 2006 , 34, 3634-45	77
2122	Generalization of the Gaussian electrostatic model: extension to arbitrary angular momentum, distributed multipoles, and speedup with reciprocal space methods. 2006 , 125, 184101	91
2121	Dynamics of polymer translocation through nanopores: theory meets experiment. 2006 , 96, 118103	113
2120	Analytical electrostatics for biomolecules: beyond the generalized Born approximation. 2006 , 124, 124902	90
2119	An accurate and simple quantum model for liquid water. 2006 , 125, 184507	165
2118	Structure of acyl carrier protein bound to FabI, the FASII enoyl reductase from Escherichia coli. 2006 , 281, 39285-39293	87
		8 ₇
	2006 , 281, 39285-39293	,
2117	2006 , 281, 39285-39293 The characterization and role of zinc binding in yeast Cox4. 2007 , 282, 8926-34	31
2117	2006, 281, 39285-39293 The characterization and role of zinc binding in yeast Cox4. 2007, 282, 8926-34 Databases and Informatics for Glycobiology and Glycomics. 2007, 329-346 Structure of Aquifex aeolicus argonaute highlights conformational flexibility of the PAZ domain as	31
2117 2116 2115	2006, 281, 39285-39293 The characterization and role of zinc binding in yeast Cox4. 2007, 282, 8926-34 Databases and Informatics for Glycobiology and Glycomics. 2007, 329-346 Structure of Aquifex aeolicus argonaute highlights conformational flexibility of the PAZ domain as a potential regulator of RNA-induced silencing complex function. 2007, 282, 13824-32	31 9 41
2117 2116 2115 2114	The characterization and role of zinc binding in yeast Cox4. 2007, 282, 8926-34 Databases and Informatics for Glycobiology and Glycomics. 2007, 329-346 Structure of Aquifex aeolicus argonaute highlights conformational flexibility of the PAZ domain as a potential regulator of RNA-induced silencing complex function. 2007, 282, 13824-32 Crystallographic and NMR analyses of UvsW and UvsW.1 from bacteriophage T4. 2007, 282, 34392-400 Folding free-energy landscape of villin headpiece subdomain from molecular dynamics simulations.	31 9 41 19
2117 2116 2115 2114 2113	The characterization and role of zinc binding in yeast Cox4. 2007, 282, 8926-34 Databases and Informatics for Glycobiology and Glycomics. 2007, 329-346 Structure of Aquifex aeolicus argonaute highlights conformational flexibility of the PAZ domain as a potential regulator of RNA-induced silencing complex function. 2007, 282, 13824-32 Crystallographic and NMR analyses of UvsW and UvsW.1 from bacteriophage T4. 2007, 282, 34392-400 Folding free-energy landscape of villin headpiece subdomain from molecular dynamics simulations. 2007, 104, 4925-30 A proposed signaling motif for nuclear import in mRNA processing via the formation of arginine	31 9 41 19

2110	Particle-particle, particle-scaling function algorithm for electrostatic problems in free boundary conditions. 2007 , 127, 024109	10
2109	Study of the quasicanonical localized orbital method based on protein structures. 2007 , 127, 184106	7
2108	Als3 is a Candida albicans invasin that binds to cadherins and induces endocytosis by host cells. 2007 , 5, e64	398
2107	Substrate specificity of cyclins determined by electrostatics. 2007 , 6, 2219-26	3
2106	The electrostatic characteristics of G.U wobble base pairs. 2007 , 35, 3836-47	32
2105	Free energy of liquid water from a computer simulation via cell theory. 2007 , 126, 064504	62
2104	Sampling of slow diffusive conformational transitions with accelerated molecular dynamics. 2007 , 127, 155102	188
2103	Molecular Modeling of the Biologically Active Alkaloids. 2007, 75-97	1
2102	Molecular dynamics simulations of a single stranded (ss) DNA. 2007, 33, 573-576	5
2101	Sensitivity Analysis of Biomolecular Simulations using Symbolic Models. 2007,	
2100	Photoselected electron transfer pathways in DNA photolyase. 2007 , 104, 802-7	68
2099	Topoisomerase Ilbeta mediated DNA double-strand breaks: implications in doxorubicin cardiotoxicity and prevention by dexrazoxane. 2007 , 67, 8839-46	426
2098	In search of CS2(H2O)(n=1-4) clusters. 2007 , 126, 154320	20
2097	SOFTWARE PACKAGES FOR STUDYING DIFFUSION PATHWAYS OF GASES IN PROTEINS. 2007 , 02, 273-286	1
2096	Computational Enzymology: Insights into Enzyme Mechanism and Catalysis from Modelling. 2007 , 275-304	
2095	On the oligomeric state of DJ-1 protein and its mutants associated with Parkinson Disease. A combined computational and in vitro study. 2007 , 282, 24905-14	26
2094	Structural basis of substrate-binding specificity of human arylamine N-acetyltransferases. 2007 , 282, 30189-97	94
2093	eF-seek: prediction of the functional sites of proteins by searching for similar electrostatic potential and molecular surface shape. 2007 , 35, W398-402	49

(2007-2007)

2092	that targets the viral RNA-dependent RNA polymerase at a hot spot for inhibition of viral replication. 2007 , 81, 11046-53	39
2091	Statistical properties and kinetics of end-end contact formation of unfolded polypeptides: a systematic molecular dynamics study. 2007 , 126, 045108	5
2090	Conformational Analysis of Drugs by Nuclear Magnetic Resonance Spectroscopy. 2007 , 207-254	7
2089	[Receptor-ligand docking simulation for membrane proteins]. 2007, 127, 123-31	7
2088	Agaritine and its derivatives are potential inhibitors against HIV proteases. 2007, 3, 221-6	42
2087	RNA localization signals: deciphering the message with bioinformatics. 2007 , 18, 178-85	18
2086	Molecular dynamics simulations and their application to four-stranded DNA. 2007, 43, 278-90	91
2085	Small molecule inhibitors of histone arginine methyltransferases: homology modeling, molecular docking, binding mode analysis, and biological evaluations. 2007 , 50, 1241-53	88
2084	Coarse-grained protein molecular dynamics simulations. 2007 , 126, 025101	84
2083	Tuning of the FMN binding and oxido-reduction properties by neighboring side chains in Anabaena flavodoxin. 2007 , 467, 206-17	22
2082	Prediction of HIV-1 entry inhibitors neomycin-arginine conjugates interaction with the CD4-gp120 binding site by molecular modeling and multistep docking procedure. 2007 , 1768, 2107-19	14
2081	Discovery of small-molecule HIV-1 fusion and integrase inhibitors oleuropein and hydroxytyrosol: part II. integrase inhibition. 2007 , 354, 879-84	44
2080	Discovery of small-molecule HIV-1 fusion and integrase inhibitors oleuropein and hydroxytyrosol: Part I. fusion [corrected] inhibition. 2007 , 354, 872-8	81
2079	The folding mechanics of a knotted protein. 2007 , 368, 884-93	122
2078	Two-stage folding of HP-35 from ab initio simulations. 2007 , 370, 196-206	80
2077	Embryonic neural inducing factor churchill is not a DNA-binding zinc finger protein: solution structure reveals a solvent-exposed beta-sheet and zinc binuclear cluster. 2007 , 371, 1274-89	20
2076	Biophysical properties of gammaC-crystallin in human and mouse eye lens: the role of molecular dipoles. 2007 , 372, 205-22	27
2075	Structure of the Wilms tumor suppressor protein zinc finger domain bound to DNA. 2007 , 372, 1227-45	82

2074	Structure of the antiviral assembly inhibitor CAP-1 complex with the HIV-1 CA protein. 2007, 373, 355-66	124
2073	Molecular analysis of the HIV-1 resistance development: enzymatic activities, crystal structures, and thermodynamics of nelfinavir-resistant HIV protease mutants. 2007 , 374, 1005-16	65
2072	Predicting the binding properties of cibacron blue F3GA in affinity separation systems. 2007, 41, 430-8	17
2071	QM/MM Methods for Biological Systems. 2006 , 173-290	325
2070	Spontaneous Formation of KCl Aggregates in Biomolecular Simulations: A Force Field Issue?. 2007 , 3, 1851-9	153
2069	Dual binding modes of Congo red to amyloid protofibril surface observed in molecular dynamics simulations. 2007 , 129, 1225-32	141
2068	Efficient estimators for quantum instanton evaluation of the kinetic isotope effects: application to the intramolecular hydrogen transfer in pentadiene. 2007 , 127, 114309	56
2067	Computational design and experimental discovery of an antiestrogenic peptide derived from alpha-fetoprotein. 2007 , 129, 6263-8	23
2066	Azole-bridged diplatinum anticancer compounds. Modulating DNA flexibility to escape repair mechanism and avoid cross resistance. 2007 , 111, 11873-6	28
2065	Refinement of COSMOâBAC and the Applications. 2007 , 46, 7275-7288	148
2064	On the Use of Elevated Temperature in Simulations To Study Protein Unfolding Mechanisms. 2007 , 3, 1476-83	21
2063	General NMR Spectroscopy of Carbohydrates and Conformational Analysis in Solution. 2007 , 101-132	10
2062	Numerical fitting of molecular properties to Hermite Gaussians. 2007 , 111, 12049-56	28
2061	A common, avoidable source of error in molecular dynamics integrators. 2007 , 126, 046101	82
2060	PDB2PQR: expanding and upgrading automated preparation of biomolecular structures for molecular simulations. 2007 , 35, W522-5	1317
2059	Validation of Molecular Dynamics Simulations of Biomolecules Using NMR Spin Relaxation as Benchmarks: Application to the AMBER99SB Force Field. 2007 , 3, 961-75	186
2058	Prediction and rationalization of the pH dependence of the activity and stability of family 11 xylanases. 2007 , 46, 13581-92	22
2057	Interaction simulation of hERG K+ channel with its specific BeKm-1 peptide: insights into the selectivity of molecular recognition. 2007 , 6, 611-20	49

(2007-2007)

2056	Substitution of methionine 435 with leucine, isoleucine, and serine in tumor necrosis factor alpha converting enzyme inactivates ectodomain shedding activity. 2007 , 85, 141-9	15
2055	Open Standards-Based Interoperability of Job Submission and Management Interfaces across the Grid Middleware Platforms gLite and UNICORE. 2007 ,	7
2054	Structure and Raman spectrum of clavulanic acid in aqueous solution. 2007 , 111, 2621-30	10
2053	Coupling of replica exchange simulations to a non-Boltzmann structure reservoir. 2007 , 111, 2415-8	71
2052	Toward quantitative interpretation of methyl side-chain dynamics from NMR by molecular dynamics simulations. 2007 , 129, 14146-7	64
2051	Insights into a mutation-assisted lateral drug escape mechanism from the HIV-1 protease active site. 2007 , 46, 14865-77	23
2050	Computational design of an RNA hexagonal nanoring and an RNA nanotube. 2007, 7, 2328-34	106
2049	Computational modeling of poly(alkylthiophene) conductive polymer insertion into phospholipid bilayers. 2007 , 23, 10672-81	16
2048	DrugScoreRNAknowledge-based scoring function to predict RNA-ligand interactions. 2007, 47, 1868-76	78
2047	A critical assessment of the performance of protein-ligand scoring functions based on NMR chemical shift perturbations. 2007 , 50, 5128-34	32
2046	Ab initio folding of albumin binding domain from all-atom molecular dynamics simulation. 2007 , 111, 5458-63	35
2045	Dispersion terms and analysis of size- and charge dependence in an enhanced Poisson-Boltzmann approach. 2007 , 111, 8910-8	19
2044	Implementation of the SCC-DFTB method for hybrid QM/MM simulations within the amber molecular dynamics package. 2007 , 111, 5655-64	183
2043	Structure of the 1,N2-etheno-2'-deoxyguanosine adduct in duplex DNA at pH 8.6. 2007 , 20, 1601-11	15
2042	Mutagenesis of morphinone reductase induces multiple reactive configurations and identifies potential ambiguity in kinetic analysis of enzyme tunneling mechanisms. 2007 , 129, 13949-56	45
2041	Peptide conformation and supramolecular organization in amylin fibrils: constraints from solid-state NMR. 2007 , 46, 13505-22	487
2040	Chromophore channeling in the G-protein coupled receptor rhodopsin. 2007, 129, 6970-1	61
2039	Consensus adaptation of fields for molecular comparison (AFMoC) models incorporate ligand and receptor conformational variability into tailor-made scoring functions. 2007 , 47, 2383-400	15

2038	Sequence occurrence and structural uniqueness of a G-quadruplex in the human c-kit promoter. 2007 , 35, 5799-808	125
2037	Dopamine D1 receptor agonist and D2 receptor antagonist effects of the natural product (-)-stepholidine: molecular modeling and dynamics simulations. 2007 , 93, 1431-41	33
2036		89
2035	Molecular dynamics and free energy studies on the wild-type and double mutant HIV-1 protease complexed with amprenavir and two amprenavir-related inhibitors: mechanism for binding and drug resistance. 2007 , 50, 1177-88	216
2034	Petaflop Essay Contest. 2007 , 9, 55-59	2
2033	Anisotropic, Polarizable Molecular Mechanics Studies of Inter- and Intramolecular Interactions and Ligand-Macromolecule Complexes. A Bottom-Up Strategy. 2007 , 3, 1960-1986	281
2032	Reconciling the solution and X-ray structures of the villin headpiece helical subdomain: molecular dynamics simulations and double mutant cycles reveal a stabilizing cation-pi interaction. 2007 , 46, 3624-34	23
2031	Secondary structure bias in generalized Born solvent models: comparison of conformational ensembles and free energy of solvent polarization from explicit and implicit solvation. 2007 , 111, 1846-57	105
2030	AMBER Force Field Parameters for the Naturally Occurring Modified Nucleosides in RNA. 2007, 3, 1464-75	128
2029	Molecular Modeling in Glycoscience. 2007 , 347-388	6
	Molecular Modeling in Glycoscience. 2007, 347-388 . 2007,	6
2028	. 2007,	
2028	. 2007, Deployment of Grid Life Sciences Applications. 199-223	6
2028 2027 2026	. 2007, Deployment of Grid Life Sciences Applications. 199-223 . 2007, Tetrabromocinnamic acid (TBCA) and related compounds represent a new class of specific protein kinase CK2 inhibitors. 2007, 8, 129-39	7
2028 2027 2026 2025	. 2007, Deployment of Grid Life Sciences Applications. 199-223 . 2007, Tetrabromocinnamic acid (TBCA) and related compounds represent a new class of specific protein kinase CK2 inhibitors. 2007, 8, 129-39	7
2028 2027 2026 2025	. 2007, Deployment of Grid Life Sciences Applications. 199-223 . 2007, Tetrabromocinnamic acid (TBCA) and related compounds represent a new class of specific protein kinase CK2 inhibitors. 2007, 8, 129-39 Peptide design and structural characterization of a GPCR loop mimetic. 2007, 86, 298-310 Automated docking to explore subsite binding by glycoside hydrolase family 6 cellobiohydrolases	6 7 104

	DNA-Binding Protein JBP1. 2007 , 119, 2897-2901	4
2019	Binding of 5-phospho-D-arabinonohydroxamate and 5-phospho-D-arabinonate inhibitors to zinc phosphomannose isomerase from Candida albicans studied by polarizable molecular mechanics and quantum mechanics. <i>Journal of Computational Chemistry</i> , 2007 , 28, 938-57	40
2018	Can a physics-based, all-atom potential find a protein's native structure among misfolded structures? I. Large scale AMBER benchmarking. <i>Journal of Computational Chemistry</i> , 2007 , 28, 2059-66 ^{3.5}	59
2017	Comparison of thermodynamic properties of coarse-grained and atomic-level simulation models. 2007 , 8, 452-61	92
2016	Long-range interactions and parallel scalability in molecular simulations. 2007, 176, 14-22	34
2015	A fine grained parallel smooth particle mesh Ewald algorithm for biophysical simulation studies: Application to the 6-D torus QCDOC supercomputer. 2007 , 177, 362-377	7
2014	Validation of an automated procedure for the prediction of relative free energies of binding on a set of aldose reductase inhibitors. 2007 , 15, 7865-77	87
2013	Fluorinated NSC as a Cdc25 inhibitor. 2007 , 17, 2351-4	31
2012	Structure-based design of benzylamino-acridine compounds as G-quadruplex DNA telomere targeting agents. 2007 , 17, 2293-8	58
2011	Free energy calculations of counterion partitioning between DNA and chloride solutions. 2007 , 17, 97-99	5
2010	Free energy calculations of counterion partitioning between DNA and chloride solutions. 2007 , 17, 97-99 Conformational behaviour of acetamide derivatives studied by NMR spectroscopic and computational methods. 2007 , 834-836, 349-354	5
2010	Conformational behaviour of acetamide derivatives studied by NMR spectroscopic and	
2010	Conformational behaviour of acetamide derivatives studied by NMR spectroscopic and computational methods. 2007, 834-836, 349-354 Virtual screening on large scale grids. 2007, 33, 289-301	4
2010	Conformational behaviour of acetamide derivatives studied by NMR spectroscopic and computational methods. 2007 , 834-836, 349-354 Virtual screening on large scale grids. 2007 , 33, 289-301 Stepwise dissection and visualization of the catalytic mechanism of haloalkane dehalogenase LinB	4
2010	Conformational behaviour of acetamide derivatives studied by NMR spectroscopic and computational methods. 2007, 834-836, 349-354 Virtual screening on large scale grids. 2007, 33, 289-301 Stepwise dissection and visualization of the catalytic mechanism of haloalkane dehalogenase LinB using molecular dynamics simulations and computer graphics. 2007, 26, 643-51 Molecular dynamics simulation of human LOX-1 provides an explanation for the lack of OxLDL	4 16 31
2010 2009 2008 2007 2006	Conformational behaviour of acetamide derivatives studied by NMR spectroscopic and computational methods. 2007, 834-836, 349-354 Virtual screening on large scale grids. 2007, 33, 289-301 Stepwise dissection and visualization of the catalytic mechanism of haloalkane dehalogenase LinB using molecular dynamics simulations and computer graphics. 2007, 26, 643-51 Molecular dynamics simulation of human LOX-1 provides an explanation for the lack of OxLDL binding to the Trp150Ala mutant. 2007, 7, 73 Binding of antifusion peptides with HIVgp41 from molecular dynamics simulations: quantitative	4 16 31 24
2010 2009 2008 2007 2006	Conformational behaviour of acetamide derivatives studied by NMR spectroscopic and computational methods. 2007, 834-836, 349-354 Virtual screening on large scale grids. 2007, 33, 289-301 Stepwise dissection and visualization of the catalytic mechanism of haloalkane dehalogenase LinB using molecular dynamics simulations and computer graphics. 2007, 26, 643-51 Molecular dynamics simulation of human LOX-1 provides an explanation for the lack of OxLDL binding to the Trp150Ala mutant. 2007, 7, 73 Binding of antifusion peptides with HIVgp41 from molecular dynamics simulations: quantitative correlation with experiment. 2007, 67, 630-42 FLIPDock: docking flexible ligands into flexible receptors. 2007, 68, 726-37	4 16 31 24 39

2002	A potential molecular switch in an alpha-helical coiled coil. 2008 , 70, 25-30	10
2001	Molecular dynamics simulation study for LRH-1: interaction with fragments of SHP and function of phospholipid ligand. 2008 , 70, 1527-39	4
2000	The point mutation A34F causes dimerization of GB1. 2008, 71, 1420-31	31
1999	Conformational dynamics of human alpha-fetoprotein-derived heptapeptide LDSYQCT analogs. 2007 , 72, 529-39	6
1998	Molecular dynamics of human alpha-fetoprotein fragment LDSYQCT and its analogs at different dielectric constants. 2007 , 52, 365-374	
1997	Sequence-specific dynamics modulate recognition specificity in WW domains. 2007, 14, 325-31	52
1996	Enteropathogenic Escherichia coli Tir is an SH2/3 ligand that recruits and activates tyrosine kinases required for pedestal formation. 2007 , 63, 1748-68	53
1995	Molecular dynamics of the DNA-binding domain of the papillomavirus E2 transcriptional regulator uncover differential properties for DNA target accommodation. 2007 , 274, 2385-95	10
1994	Binding pathways of ligands to HIV-1 protease: coarse-grained and atomistic simulations. 2007 , 69, 5-13	59
1993	Nucleic acid solvation: from outside to insight. 2007 , 17, 325-33	114
1993 1992	Nucleic acid solvation: from outside to insight. 2007, 17, 325-33 Hydrophobic sliding: a possible mechanism for drug resistance in human immunodeficiency virus type 1 protease. 2007, 15, 225-33	114 69
	Hydrophobic sliding: a possible mechanism for drug resistance in human immunodeficiency virus	
1992	Hydrophobic sliding: a possible mechanism for drug resistance in human immunodeficiency virus type 1 protease. 2007 , 15, 225-33 Hydrophobic potential of mean force as a solvation function for protein structure prediction. 2007 ,	69
1992 1991	Hydrophobic sliding: a possible mechanism for drug resistance in human immunodeficiency virus type 1 protease. 2007 , 15, 225-33 Hydrophobic potential of mean force as a solvation function for protein structure prediction. 2007 , 15, 727-40 Characterization and localization of Plasmodium falciparum homolog of prokaryotic ClpQ/HslV	69
1992 1991 1990	Hydrophobic sliding: a possible mechanism for drug resistance in human immunodeficiency virus type 1 protease. 2007, 15, 225-33 Hydrophobic potential of mean force as a solvation function for protein structure prediction. 2007, 15, 727-40 Characterization and localization of Plasmodium falciparum homolog of prokaryotic ClpQ/HslV protease. 2007, 152, 139-48 Coumarin-based inhibitors of human NAD(P)H:quinone oxidoreductase-1. Identification,	69 41 40
1992 1991 1990	Hydrophobic sliding: a possible mechanism for drug resistance in human immunodeficiency virus type 1 protease. 2007, 15, 225-33 Hydrophobic potential of mean force as a solvation function for protein structure prediction. 2007, 15, 727-40 Characterization and localization of Plasmodium falciparum homolog of prokaryotic ClpQ/HslV protease. 2007, 152, 139-48 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	69 41 40 56
1992 1991 1990 1989	Hydrophobic sliding: a possible mechanism for drug resistance in human immunodeficiency virus type 1 protease. 2007, 15, 225-33 Hydrophobic potential of mean force as a solvation function for protein structure prediction. 2007, 15, 727-40 Characterization and localization of Plasmodium falciparum homolog of prokaryotic ClpQ/HslV protease. 2007, 152, 139-48 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 Structural models for the KCNQ1 voltage-gated potassium channel. 2007, 46, 14141-52 Clustering Molecular Dynamics Trajectories: 1. Characterizing the Performance of Different	69 41 40 56 82

1984	Vibrational averaging of chemical shift anisotropies in model peptides. 2007 , 38, 255-66	27
1983	Density functional theory and molecular dynamics investigations on substituted banana-shaped compounds. 2007 , 13, 907-17	16
1982	Homology modeling and examination of the effect of the D92E mutation on the H5N1 nonstructural protein NS1 effector domain. 2007 , 13, 1237-44	39
1981	Comparative (1)H NMR and molecular modeling study of hydroxy protons of beta-D-Galp-(1>4)-beta-D-GlcpNAc-(1>2)-alpha-D-Manp-(1>0)(CH(2))(7)CH(3) analogues in aqueous solution. 2007 , 342, 597-609	6
1980	Molecular modeling of modified peptides, potent inhibitors of the xWNT8 and hWNT8 proteins. 2008 , 26, 1179-87	
1979	Structures, fragmentation, and protonation of trideoxynucleotide CCC mono- and dianions. 2008 , 19, 987-96	4
1978	Secondary structure prediction of beta-hairpin peptide tryptophan zipper-I. 2008, 387, 3537-3545	
1977	A tool for the prediction of structures of complex sugars. 2008 , 42, 241-56	21
1976	A dual-purpose protein ligand for effective therapy and sensitive diagnosis of anthrax. 2008 , 27, 292-302	12
1975	The 3D structure of the defense-related rice protein Pir7b predicted by homology modeling and ligand binding studies. 2008 , 14, 559-69	4
1974	Modeling structure and flexibility of Candida antarctica lipase B in organic solvents. 2008, 8, 9	125
1973	Viral cystatin evolution and three-dimensional structure modelling: a case of directional selection acting on a viral protein involved in a host-parasitoid interaction. 2008 , 6, 38	28
1972	Structural adaptation of endonuclease I from the cold-adapted and halophilic bacterium Vibrio salmonicida. 2008 , 64, 368-76	22
1971	QSAR Study of Cyclic Urea Type HIV-1 PR Inhibitors Using Ab Initio MO Calculation of Their Complex Structures with HIV-1 PR. 2008 , 27, 694-703	27
1970	Simple Formulas for Improved Point-Charge Electrostatics in Classical Force Fields and Hybrid Quantum Mechanical/Molecular Mechanical Embedding. 2008 , 108, 1905-1912	51
1969	Carbohydrate-binding modules from family 11: Understanding the binding mode of polysaccharides. 2008 , 108, 2030-2040	20
1968	Functionalization and molecular dynamics study of carboxy-terminated poly(1-vinylpyrrolidin-2-one): A potential soluble carrier of biomolecules. 2008 , 46, 1683-1698	6
1967	Second step of hydrolytic dehalogenation in haloalkane dehalogenase investigated by QM/MM methods. 2008 , 70, 707-17	24

1966	An efficient conformational sampling method for homology modeling. 2008 , 71, 175-88	20
1965	Structural characterization of the zinc binding domain in cytosolic PSD-95 interactor (cypin): Role of zinc binding in guanine deamination and dendrite branching. 2008 , 70, 873-81	15
1964	Molecular basis of inhibitory peptide maurotoxin recognizing Kv1.2 channel explored by ZDOCK and molecular dynamic simulations. 2008 , 70, 844-54	49
1963	Probing ligand binding modes of human cytochrome P450 2J2 by homology modeling, molecular dynamics simulation, and flexible molecular docking. 2008 , 71, 938-49	41
1962	Evaluating the potency of HIV-1 protease drugs to combat resistance. 2008 , 71, 1163-74	103
1961	An insight into the general relationship between the three dimensional structures of enzymes and their electronic wave functions: Implication for the prediction of functional sites of enzymes. 2008 , 71, 1940-54	15
1960	Protein-protein docking by simulating the process of association subject to biochemical constraints. 2008 , 71, 1955-69	24
1959	Comparative molecular dynamics simulations of histone deacetylase-like protein: binding modes and free energy analysis to hydroxamic acid inhibitors. 2008 , 73, 134-49	40
1958	Computational evidence for the catalytic mechanism of glutaminyl cyclase. A DFT investigation. 2008 , 73, 527-38	19
1957	Structure of HP0564 from Helicobacter pylori identifies it as a new transcriptional regulator. 2008 , 73, 265-8	4
1957 1956	73, 265-8	159
	73, 265-8	
1956	73, 265-8 Principles of flexible protein-protein docking. 2008, 73, 271-89 Electrostatic stabilization and general base catalysis in the active site of the human protein	159
1956 1955	73, 265-8 Principles of flexible protein-protein docking. 2008, 73, 271-89 Electrostatic stabilization and general base catalysis in the active site of the human protein disulfide isomerase a domain monitored by hydrogen exchange. 2008, 9, 768-78 Linear analogues of human beta-defensin 3: concepts for design of antimicrobial peptides with	159 20
1956 1955 1954	Principles of flexible protein-protein docking. 2008, 73, 271-89 Electrostatic stabilization and general base catalysis in the active site of the human protein disulfide isomerase a domain monitored by hydrogen exchange. 2008, 9, 768-78 Linear analogues of human beta-defensin 3: concepts for design of antimicrobial peptides with reduced cytotoxicity to mammalian cells. 2008, 9, 964-73	159 20 65
1956 1955 1954 1953	Principles of flexible protein-protein docking. 2008, 73, 271-89 Electrostatic stabilization and general base catalysis in the active site of the human protein disulfide isomerase a domain monitored by hydrogen exchange. 2008, 9, 768-78 Linear analogues of human beta-defensin 3: concepts for design of antimicrobial peptides with reduced cytotoxicity to mammalian cells. 2008, 9, 964-73 Web resources for the glycoscientist. 2008, 9, 2155-60	159 20 65 22
1956 1955 1954 1953 1952	Principles of flexible protein-protein docking. 2008, 73, 271-89 Electrostatic stabilization and general base catalysis in the active site of the human protein disulfide isomerase a domain monitored by hydrogen exchange. 2008, 9, 768-78 Linear analogues of human beta-defensin 3: concepts for design of antimicrobial peptides with reduced cytotoxicity to mammalian cells. 2008, 9, 964-73 Web resources for the glycoscientist. 2008, 9, 2155-60 Determinants of the unexpected stability of RNA fluorobenzene self pairs. 2008, 9, 2619-22 Hydrogen-bond detection, configuration assignment and rotamer correction of side-chain amides	159 20 65 22 36

1948	Exploring acyclic nucleoside analogues as inhibitors of Mycobacterium tuberculosis thymidylate kinase. 2008 , 3, 1083-93		24	
1947	Structure-based discovery and experimental verification of novel AI-2 quorum sensing inhibitors against Vibrio harveyi. 2008 , 3, 1242-9		53	
1946	Thiobarbiturates as sirtuin inhibitors: virtual screening, free-energy calculations, and biological testing. 2008 , 3, 1965-76		56	•
1945	Identification of the first germline mutation in the extracellular domain of the follitropin receptor responsible for spontaneous ovarian hyperstimulation syndrome. 2008 , 29, 91-8		50	
1944	Molecular mechanics parameters for the FapydG DNA lesion. <i>Journal of Computational Chemistry</i> , 2008 , 29, 17-23	3.5	10	
1943	Parameterization of azole-bridged dinuclear platinum anticancer drugs via a QM/MM force matching procedure. <i>Journal of Computational Chemistry</i> , 2008 , 29, 38-49	3.5	30	
1942	Accurate prediction of protonation state as a prerequisite for reliable MM-PB(GB)SA binding free energy calculations of HIV-1 protease inhibitors. <i>Journal of Computational Chemistry</i> , 2008 , 29, 673-85	3.5	59	
1941	Charge parameterization of the metal centers in cytochrome c oxidase. <i>Journal of Computational Chemistry</i> , 2008 , 29, 753-67	3.5	45	
1940	Asynchronous replica exchange for molecular simulations. <i>Journal of Computational Chemistry</i> , 2008 , 29, 788-94	3.5	34	
1939	A versatile AMBER-Gaussian QM/MM interface through PUPIL. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1564-73	3.5	36	
1938	CHARMM-GUI: a web-based graphical user interface for CHARMM. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1859-65	3.5	2877	
1937	Induction correction model for rotation of two or three dihedral angles. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1905-11	3.5	4	
1936	Structure and dynamics of phosphate ion in aqueous solution: an ab initio QMCF MD study. <i>Journal of Computational Chemistry</i> , 2008 , 29, 2330-4	3.5	60	
1935	Multiscale modeling of nucleic acids: insights into DNA flexibility. 2008 , 89, 722-31		29	
1934	Structural insights for designed alanine-rich helices: comparing NMR helicity measures and conformational ensembles from molecular dynamics simulation. 2008 , 89, 747-60		23	
1933	Structure-Based Insight into the Asymmetric Bioreduction of the C=C Double Bond of alpha,beta-Unsaturated Nitroalkenes by Pentaerythritol Tetranitrate Reductase. 2008 , 350, 2789-2803		78	
1932	Binding modes of CCR5-targetting HIV entry inhibitors: partial and full antagonists. 2008 , 26, 1287-95		21	
1931	Nanosecond molecular dynamics simulations of Cdc25B and its complex with a 1,4-naphthoquinone inhibitor: implications for rational inhibitor design. 2008 , 27, 13-9		5	

1930	Molecular dynamics simulation study on the structural stabilities of polyglutamine peptides. 2008 , 32, 102-10	29
1929	A biophysical perspective on the cellulosome: new opportunities for biomass conversion. 2008 , 19, 218-27	79
1928	Geometry and Excitation Energy Fluctuations of NMA in Aqueous Solution with CHARMM, AMBER, OPLS, and GROMOS Force Fields: Implications for Protein Ultraviolet Spectra Simulation. 2008 , 452, 78-83	15
1927	Potential of mean force for human lysozymeâ@amelid vhh hl6 antibody interaction studies. 2008 , 455, 284-288	7
1926	Molecular simulation evidence for processive motion of Trichoderma reesei Cel7A during cellulose depolymerization. 2008 , 460, 284-288	27
1925	Effects of vibrational motion on core-level spectra of prototype organic molecules. 2008, 467, 195-199	47
1924	Modifying the N-terminus of polyamides: PylmPylm has improved sequence specificity over f-lmPylm. 2008 , 16, 5266-76	13
1923	Specific binding capacity of beta-cyclodextrin with cis and trans enalapril: physicochemical characterization and structural studies by molecular modeling. 2008 , 16, 8403-12	15
1922	Screening of herbal constituents for aromatase inhibitory activity. 2008 , 16, 8466-70	43
1921	Pyrogallol and its analogs can antagonize bacterial quorum sensing in Vibrio harveyi. 2008 , 18, 1567-72	82
1920	In silico multi-filter screening approaches for developing novel beta-secretase inhibitors. 2008 , 18, 2771-5	7
1919	Identification of novel inhibitors of extracellular signal-regulated kinase 2 based on the structure-based virtual screening. 2008 , 18, 5372-6	7
1918	Determining the solution conformational entropy of O-linked oligosaccharides at quasi-physiological conditions: size-exclusion chromatography and molecular dynamics. 2008 , 343, 132-8	15
1917	Solvent structure and hammerhead ribozyme catalysis. 2008 , 15, 332-42	92
1916	Vulnerability in Popular Molecular Dynamics Packages Concerning Langevin and Andersen Dynamics. 2008 , 4, 1669-1680	68
1915	Computational chemistry approaches to drug discovery in signal transduction. 2008 , 3, 452-70	19
1914	Towards a molecular dynamics consensus view of B-DNA flexibility. 2008 , 36, 2379-94	128
1913	Comparison of protein force fields for molecular dynamics simulations. 2008 , 443, 63-88	132

1912	Hit identification and binding mode predictions by rigorous free energy simulations. 2008 , 51, 6654-64	56
1911	Molecular model of the Wnt protein binding site on the surface of dimeric CRD domain of the hFzd8 receptor. 2008 , 419, 75-8	4
1910	Structure of the putative 32 kDa myrosinase-binding protein from Arabidopsis (At3g16450.1) determined by SAIL-NMR. 2008 , 275, 5873-84	25
1909	Molecular dynamic investigation of the interaction of supported affinity ligands with monoclonal antibodies. 2008 , 24, 527-39	29
1908	Visual Abstractions of Solvent Pathlines near Protein Cavities. 2008, 27, 935-942	20
1907	The MuLV 4070A G541R Env mutation decreases the stability and alters the conformation of the TM ectodomain. 2008 , 371, 165-74	1
1906	Stability of the core domain of p53: insights from computer simulations. 2008 , 9 Suppl 1, S17	14
1905	Imidazo[4,5-c]pyridines inhibit the in vitro replication of the classical swine fever virus and target the viral polymerase. 2008 , 77, 114-9	25
1904	Molecular modeling and experimental evidence for hypericin as a substrate for mitochondrial complex III; mitochondrial photodamage as demonstrated using specific inhibitors. 2008 , 45, 1581-90	14
1903	Catalytic mechanism of human DNA polymerase lambda with Mg2+ and Mn2+ from ab initio quantum mechanical/molecular mechanical studies. 2008 , 7, 1824-34	50
1902	Molecular dynamics simulations of nucleic acid-protein complexes. 2008 , 18, 194-9	135
		135
	Molecular dynamics simulations of nucleic acid-protein complexes. 2008 , 18, 194-9	
1901	Molecular dynamics simulations of nucleic acid-protein complexes. 2008 , 18, 194-9 Iterative assembly of helical proteins by optimal hydrophobic packing. 2008 , 16, 1257-66 Computational methods in nanostructure design: replica exchange simulations of self-assembling	10
1901 1900	Molecular dynamics simulations of nucleic acid-protein complexes. 2008 , 18, 194-9 Iterative assembly of helical proteins by optimal hydrophobic packing. 2008 , 16, 1257-66 Computational methods in nanostructure design: replica exchange simulations of self-assembling peptides. 2008 , 474, 133-51 Efficient and direct generation of multidimensional free energy surfaces via adiabatic dynamics	10
1901 1900 1899	Molecular dynamics simulations of nucleic acid-protein complexes. 2008, 18, 194-9 Iterative assembly of helical proteins by optimal hydrophobic packing. 2008, 16, 1257-66 Computational methods in nanostructure design: replica exchange simulations of self-assembling peptides. 2008, 474, 133-51 Efficient and direct generation of multidimensional free energy surfaces via adiabatic dynamics without coordinate transformations. 2008, 112, 15742-57 Extension of the GLYCAM06 Biomolecular Force Field to Lipids, Lipid Bilayers and Glycolipids. 2008,	10 3 134
1901 1900 1899 1898	Molecular dynamics simulations of nucleic acid-protein complexes. 2008, 18, 194-9 Iterative assembly of helical proteins by optimal hydrophobic packing. 2008, 16, 1257-66 Computational methods in nanostructure design: replica exchange simulations of self-assembling peptides. 2008, 474, 133-51 Efficient and direct generation of multidimensional free energy surfaces via adiabatic dynamics without coordinate transformations. 2008, 112, 15742-57 Extension of the GLYCAM06 Biomolecular Force Field to Lipids, Lipid Bilayers and Glycolipids. 2008, 34, 349-363 Prediction of Molecular Interactions from 3D-Structures: From Small Ligands to Large Protein	10 3 134 80

1894	Osmotic pressure and packaging structure of caged DNA. 2008 , 94, 737-46	33
1893	Analyzing the flexibility of RNA structures by constraint counting. 2008 , 94, 4202-19	40
1892	Development of a physics-based force field for the scoring and refinement of protein models. 2008 , 94, 3227-40	37
1891	Hydration effects on the HET-s prion and amyloid-beta fibrillous aggregates, studied with three-dimensional molecular theory of solvation. 2008 , 95, 4540-8	42
1890	Insights into subunit interactions in the heterotetrameric structure of potato ADP-glucose pyrophosphorylase. 2008 , 95, 3628-39	22
1889	Interactions between neuronal fusion proteins explored by molecular dynamics. 2008, 94, 3436-46	22
1888	Observation of noncooperative folding thermodynamics in simulations of 1BBL. 2008 , 94, 4837-46	29
1887	Molecular dynamics simulations of GABA binding to the GABAC receptor: the role of Arg104. 2008 , 95, 4115-23	27
1886	Conformation and free energy analyses of the complex of calcium-bound calmodulin and the Fas death domain. 2008 , 95, 5913-21	23
1885	MD simulations of papillomavirus DNA-E2 protein complexes hints at a protein structural code for DNA deformation. 2008 , 95, 1108-17	11
1884	Starting structure dependence of NMR order parameters derived from MD simulations: implications for judging force-field quality. 2008 , 95, L04-6	33
1883	Pressure effects on the ensemble dynamics of ubiquitin inspected with molecular dynamics simulations and isotropic reorientational eigenmode dynamics. 2008 , 95, 3943-55	10
1882	Flexible fitting of high-resolution x-ray structures into cryoelectron microscopy maps using biased molecular dynamics simulations. 2008 , 95, 5692-705	83
1881	Evaluation of Salt Bridge Structure and Energetics in Peptides Using Explicit, Implicit, and Hybrid Solvation Models. 2008 , 4, 488-98	31
1880	An analytical approach to computing biomolecular electrostatic potential. I. Derivation and analysis. 2008 , 129, 075101	23
1879	Enzyme kinetic and molecular modelling studies of sulphur-containing substrates of phenylalanine 4-monooxygenase. 2008 , 23, 958-63	11
1878	What governs the charge transfer in DNA? The role of DNA conformation and environment. 2008 , 112, 8788-98	109
1877	Implicit Solvent Models in Molecular Dynamics Simulations: A Brief Overview. 2008 , 4, 125-137	63

1876	Molecular dynamics simulations. 2008 , 443, 3-23	40
1875	Revised charge equilibration potential for liquid alkanes. 2008 , 112, 8298-310	34
1874	Evaluating rotational diffusion from protein MD simulations. 2008 , 112, 6013-24	114
1873	DeltaF508 mutation increases conformational flexibility of CFTR protein. 2008 , 7, 295-300	35
1872	Recent progress in linear-scaling density functional calculations with plane waves and pseudopotentials: the ONETEP code. 2008 , 20, 064209	17
1871	Specific ion binding to nonpolar surface patches of proteins. 2008 , 130, 11582-3	114
1870	Persistence of camptothecin analog-topoisomerase I-DNA ternary complexes: a molecular dynamics study. 2008 , 130, 17928-37	20
1869	Computational techniques at the organic-inorganic interface in biomineralization. 2008 , 108, 4823-54	103
1868	Development of an ion mobility quadrupole time of flight mass spectrometer. 2008 , 80, 6336-44	69
1867	In silico mutagenesis and docking studies of Pseudomonas aeruginosa PA-IIL lectin predicting binding modes and energies. 2008 , 48, 2234-42	15
1866	Is Alanine Dipeptide a Good Model for Representing the Torsional Preferences of Protein Backbones?. 2008 , 4, 1555-64	65
1865	Different residues in channel turret determining the selectivity of ADWX-1 inhibitor peptide between Kv1.1 and Kv1.3 channels. 2008 , 7, 4890-7	43
1864	Modeling and biochemical analysis of the activity of antibiofilm agent Dispersin B. 2008, 59, 439-51	15
1863	Molecular Modeling of Proteins. 2008,	27
1862	Structure and Conformation of Carbohydrates. 2008 , 3-55	8
1861	Computational and experimental determination of the alpha-helix unfolding reaction coordinate. 2008 , 47, 2046-50	8
1860	Composites with Micro- and Nano-Structure. 2008,	4
1859	Characterization of domain-peptide interaction interface: a case study on the amphiphysin-1 SH3 domain. 2008 , 376, 1201-14	179

1858	Molecular dynamics simulation of the Escherichia coli NikR protein: equilibrium conformational fluctuations reveal interdomain allosteric communication pathways. 2008 , 378, 1155-73	59
1857	A unique mode of microtubule stabilization induced by peloruside A. 2008 , 378, 1016-30	107
1856	Unusual role of a cysteine residue in substrate binding and activity of human AP-endonuclease 1. 2008 , 379, 28-37	31
1855	Molecular dynamics-solvated interaction energy studies of protein-protein interactions: the MP1-p14 scaffolding complex. 2008 , 379, 787-802	115
1854	Structural basis of PxxDY motif recognition in SH3 binding. 2008 , 382, 167-78	33
1853	Importance of accurate DNA structures in solution: the Jun-Fos model. 2008 , 382, 956-70	37
1852	Stability and ATP binding of the nucleotide-binding domain of the Wilson disease protein: effect of the common H1069Q mutation. 2008 , 383, 1097-111	27
1851	Amyloid beta-protein monomer folding: free-energy surfaces reveal alloform-specific differences. 2008 , 384, 450-64	197
1850	Differential tapasin dependence of MHC class I molecules correlates with conformational changes upon peptide dissociation: a molecular dynamics simulation study. 2008 , 45, 3714-22	46
1849	Mutations in growth factor independent-1 associated with human neutropenia block murine granulopoiesis through colony stimulating factor-1. 2008 , 28, 370-80	68
1848	Geometrical and electronic structure variability of the sugar-phosphate backbone in nucleic acids. 2008 , 112, 8188-97	50
1847	The NMR structure and dynamics of the two-domain tick carboxypeptidase inhibitor reveal flexibility in its free form and stiffness upon binding to human carboxypeptidase B. 2008 , 47, 7066-78	15
1846	Biomolecular simulation and modelling: status, progress and prospects. 2008 , 5 Suppl 3, S173-90	62
1845	Chapter 2 Electrostatics in Biomolecular Simulations: Where Are We Now and Where Are We Heading?. 2008 , 60, 49-89	55
1844	Discovery of the first SecA inhibitors using structure-based virtual screening. 2008 , 368, 839-45	42
1843	Catalytic mechanism of inulinase from Arthrobacter sp. S37. 2008 , 371, 600-5	18
1842	Target flexibility: an emerging consideration in drug discovery and design. 2008, 51, 6237-55	244
1841	Automated molecular simulation based binding affinity calculator for ligand-bound HIV-1 proteases. 2008 , 48, 1909-19	43

1840	Chapter 4 Molecular Dynamics Simulation of Lipidâ P rotein Interactions. 2008 , 111-130	12
1839	Determination of alkali and halide monovalent ion parameters for use in explicitly solvated biomolecular simulations. 2008 , 112, 9020-41	1985
1838	Molecular dynamics simulations of nanoparticles. 2008 , 104, 142	39
1837	Treating entropy and conformational changes in implicit solvent simulations of small molecules. 2008 , 112, 938-46	97
1836	Molecular dynamics and principal components analysis of human telomeric quadruplex multimers. 2008 , 95, 296-311	169
1835	Patchy proteins, anions and the Hofmeister series. 2008 , 20, 494218	40
1834	A test on peptide stability of AMBER force fields with implicit solvation. 2008, 112, 6878-86	117
1833	Structure-activity studies on splitomicin derivatives as sirtuin inhibitors and computational prediction of binding mode. 2008 , 51, 1203-13	147
1832	Aqueous solutions of ionic liquids: study of the solution/vapor interface using molecular dynamics simulations. 2008 , 10, 5765-75	55
1831	Accelerating Molecular Dynamics Simulations with Reconfigurable Computers. 2008, 19, 764-778	21
1830	Hunting for predictive computational drug-discovery models. 2008 , 6, 291-3	
1829	The post-SCF quantum chemistry characteristics of the guanine-guanine stacking B-DNA. 2008, 10, 2665-72	24
1828	Energetics and kinetics of primary charge separation in bacterial photosynthesis. 2008, 112, 10322-42	48
1827	Targeting telomerase and telomeres: a click chemistry approach towards highly selective G-quadruplex ligands. 2008 , 4, 629-42	35
1826	The catalytic activity of proline racemase: a quantum mechanical/molecular mechanical study. 2008 , 112, 1057-9	13
1825	Flavodoxin-mediated electron transfer from photosystem I to ferredoxin-NADP+ reductase in Anabaena: role of flavodoxin hydrophobic residues in protein-protein interactions. 2008 , 47, 1207-17	25
1824	The structural basis of the difference in sensitivity for PNGase F in the de-N-glycosylation of the native bovine pancreatic ribonucleases B and BS. 2008 , 47, 3435-46	14
1823	Simulations of a protein crystal: explicit treatment of crystallization conditions links theory and experiment in the streptavidin-biotin complex. 2008 , 47, 12065-77	32

1822	Structural properties of polyglutamine aggregates investigated via molecular dynamics simulations. 2008 , 112, 16843-50	18
1821	CHARMMing: a new, flexible web portal for CHARMM. 2008 , 48, 1920-9	105
1820	2D NMR study of the DNA duplex d(CTCTC*A*ACTTCC).d(GGAAGTTGAGAG) cross-linked by the antitumor-active dirhodium(II,II) unit at the cytosine-adenine step. 2008 , 47, 2265-76	27
1819	Studies of the mechanism of selectivity of protein tyrosine phosphatase 1B (PTP1B) bidentate inhibitors using molecular dynamics simulations and free energy calculations. 2008 , 48, 2030-41	22
1818	Polyionic charge density plays a key role in differential recognition of mobile ions by biopolymers. 2008 , 112, 9135-45	20
1817	Aqueous Partial Molar Volumes from Simulation and Individual Group Contributions. 2008, 47, 5169-5174	19
1816	Induced disorder in protein-ligand complexes as a drug-design strategy. 2008 , 5, 430-7	19
1815	Molecular dynamics simulations of functional group effects on solvation thermodynamics of model solutes in decane and tricaprylin. 2008 , 5, 1023-36	19
1814	3'-Intercalation of a N2-dG 1R-trans-anti-benzo[c]phenanthrene DNA adduct in an iterated (CG)3 repeat. 2008 , 21, 1348-58	9
1813	Glassy protein dynamics and gigantic solvent reorganization energy of plastocyanin. 2008, 112, 5218-27	39
1812	Developing improved MD codes for understanding processive cellulases. 2008 , 125, 012049	2
1811	Ground- and Excited-State Pinched Cone Equilibria in Calix[4]arenes Bearing Two Perylene Bisimide Dyes. 2008 , 112, 14626-14638	7 2
1810	Potential intra- and intermolecular interactions involving the unique-5' region of the HIV-1 5'-UTR. 2008 , 47, 13064-73	39
1809	Structure and dynamics of the Abeta(21-30) peptide from the interplay of NMR experiments and molecular simulations. 2008 , 130, 6145-58	142
1808	Dimerization affects collective dynamics of triosephosphate isomerase. 2008 , 47, 1358-68	32
1807	Approach for the Simulation and Modeling of Flexible Rings: Application to the Đ-Arabinofuranoside Ring, a Key Constituent of Polysaccharides from. 2008 , 4, 184-191	22
1806	Identification of phosphorylation sites of TOPORS and a role for serine 98 in the regulation of ubiquitin but not SUMO E3 ligase activity. 2008 , 47, 13887-96	8
1805	Open science grid study of the coupling between conformation and water content in the interior of a protein. 2008 , 48, 2021-9	18

(2008-2008)

1804	simulation study. 2008 , 112, 4583-93	26
1803	Structure of aqueous sodium perchlorate solutions. 2008 , 112, 15417-25	18
1802	The solution structure of the amino-terminal domain of human DNA polymerase epsilon subunit B is homologous to C-domains of AAA+ proteins. 2008 , 36, 5102-10	21
1801	Folding processes of the B domain of protein A to the native state observed in all-atom ab initio folding simulations. 2008 , 128, 235105	31
1800	Ciliary neurotrophic factor, cardiotrophin-like cytokine, and neuropoietin share a conserved binding site on the ciliary neurotrophic factor receptor alpha chain. 2008 , 283, 30341-50	16
1799	Structural glycobiology: a game of snakes and ladders. 2008 , 18, 426-40	124
1798	Calculation of protein-ligand binding free energy by using a polarizable potential. 2008, 105, 6290-5	197
1797	His-311 and Arg-559 are key residues involved in fatty acid oxygenation in pathogen-inducible oxygenase. 2008 , 283, 24962-71	21
1796	Digging a hole: Scaled-particle theory and cavity solvation in organic solvents. 2008 , 129, 174505	15
1795	Synthesis and investigation of the 5-formylcytidine modified, anticodon stem and loop of the human mitochondrial tRNAMet. 2008 , 36, 6548-57	41
1794	Left handed beta helix models for mammalian prion fibrils. 2008 , 2, 81-90	24
1793	Molecular basis for agonist selectivity and activation of the orphan bombesin receptor subtype 3 receptor. 2008 , 324, 463-74	18
1792	The NMR structures of the major intermediates of the two-domain tick carboxypeptidase inhibitor reveal symmetry in its folding and unfolding pathways. 2008 , 283, 27110-20	9
1791	New insights into the mechanism of RNA degradation by ribonuclease II: identification of the residue responsible for setting the RNase II end product. 2008 , 283, 13070-6	38
1790	Structural domains within the 3' untranslated region of Turnip crinkle virus. 2008, 82, 8706-20	59
1789	Differential roles of phosphatidylserine, PtdIns(4,5)P2, and PtdIns(3,4,5)P3 in plasma membrane targeting of C2 domains. Molecular dynamics simulation, membrane binding, and cell translocation studies of the PKCalpha C2 domain. 2008 , 283, 26047-58	73
1788	Measuring the dynamic surface accessibility of RNA with the small paramagnetic molecule TEMPOL. 2008 , 36, e20	22
1787	Rett syndrome-causing mutations in human MeCP2 result in diverse structural changes that impact folding and DNA interactions. 2008 , 283, 20523-34	48

1786	Dynamics of RASSF1A/MOAP-1 association with death receptors. 2008, 28, 4520-35	66
1785	Mismatched dNTP incorporation by DNA polymerase beta does not proceed via globally different conformational pathways. 2008 , 36, 2948-57	19
1784	PBEQ-Solver for online visualization of electrostatic potential of biomolecules. 2008 , 36, W270-5	163
1783	Adaptively biased molecular dynamics for free energy calculations. 2008 , 128, 134101	138
1782	Redox entropy of plastocyanin: developing a microscopic view of mesoscopic polar solvation. 2008 , 128, 155106	19
1781	The fast-folding HP35 double mutant has a substantially reduced primary folding free energy barrier. 2008 , 129, 155104	21
1780	Nitrile and thiocyanate IR probes: molecular dynamics simulation studies. 2008 , 128, 154504	113
1779	RNAJunction: a database of RNA junctions and kissing loops for three-dimensional structural analysis and nanodesign. 2008 , 36, D392-7	126
1778	Intramolecular cohesion of coils mediated by phenylalanineglycine motifs in the natively unfolded domain of a nucleoporin. 2008 , 4, e1000145	43
1777	Comparing ion distributions around RNA and DNA helical and loop-loop motifs. 2008 , 1130, 50501	
1776	Three consecutive arginines are important for the mycobacterial peptide deformylase enzyme activity. 2008 , 283, 23754-64	5
1775	Cofilin is a pH sensor for actin free barbed end formation: role of phosphoinositide binding. 2008 , 183, 865-79	147
1774	Structural insight into the mechanisms of Wnt signaling antagonism by Dkk. 2008 , 283, 23364-70	53
1773	A minimalist network model for coarse-grained normal mode analysis and its application to biomolecular x-ray crystallography. 2008 , 105, 15358-63	40
1772	Atomic-resolution conformational analysis of the GM3 ganglioside in a lipid bilayer and its implications for ganglioside-protein recognition at membrane surfaces. 2009 , 19, 344-55	52
1771	A molecular dynamics simulation study on trapping ions in a nanoscale Paul trap. 2008 , 19, 195702	16
1771	A molecular dynamics simulation study on trapping ions in a nanoscale Paul trap. 2008 , 19, 195702 Milestones in Molecular Dynamics Simulations of RNA Systems. 2008 , 363-399	16

(2009-2008)

1768	CReF. 2008 ,	9
1767	Analyzing dynamical simulations of intrinsically disordered proteins using spectral clustering. 2008,	6
1766	Nanostructure design: methods and protocols. Preface. 2008 , 474, v-vii	6
1765	Assessment of Protein Structure Predictions. 2008 , 89-109	3
1764	Bioinformatics based Ligand-Docking and in-silico screening. 2008 , 56, 742-4	18
1763	Insights into the substrate specificity of plant peptide deformylase, an essential enzyme with potential for the development of novel biotechnology applications in agriculture. 2008 , 413, 417-27	12
1762	. 2008,	6
1761	HIV-1 capsid assembly inhibitor (CAI) peptide: structural preferences and delivery into human embryonic lung cells and lymphocytes. 2008 , 5, 230-9	5
1760	Dinfinica molecular: teoria e aplicales em planejamento de ffimacos. 2008 , 33, 13-24	20
1759	Methods for Studying Nucleic Acid Structure. 2008 , 1-19	5
1758	Net positive charge of HIV-1 CRF01_AE V3 sequence regulates viral sensitivity to humoral immunity. 2008 , 3, e3206	33
1757	The internal sequence of the peptide-substrate determines its N-terminus trimming by ERAP1. 2008 , 3, e3658	67
1756	Chemical Structure Indices in In Silico Molecular Design. 2008 , 76, 101-132	6
1755	. 2009,	2
1754	. 2009,	9
1753	Functional analysis and molecular dynamics simulation of LOX-1 K167N polymorphism reveal alteration of receptor activity. 2009 , 4, e4648	47
1752	Lys169 of human glucokinase is a determinant for glucose phosphorylation: implication for the atomic mechanism of glucokinase catalysis. 2009 , 4, e6304	25
1751	Toward the discovery of vaccine adjuvants: coupling in silico screening and in vitro analysis of antagonist binding to human and mouse CCR4 receptors. 2009 , 4, e8084	46

1750 Molecular Dynamics Computations for Proteins: A Case Study in Membrane Ion Permeation. 2009,

1749	Article Commentary: Graphical User Interfaces for Molecular DynamicsâQuo Vadis?. 2009 , 3, BBI.S3332	5
1748	Residue network in protein native structure belongs to the universality class of a three-dimensional critical percolation cluster. 2009 , 79, 020901	18
1747	A cooperative combinatorial Particle Swarm Optimization algorithm for side-chain packing. 2009,	4
1746	In silico relationship between configurational entropy and soft degrees of freedom in proteins and peptides. 2009 , 102, 118108	39
1745	Influence of structural disorder and large-scale geometric fluctuations on the coherent transport of metallic junctions and molecular wires. 2009 , 80,	11
1744	Coarse-grained ions without charges: reproducing the solvation structure of NaCl in water using short-ranged potentials. 2009 , 131, 034107	61
1743	LOOS: an extensible platform for the structural analysis of simulations. 2009 , 2009, 2332-5	52
1742	Human mitochondrial thymidine kinase is selectively inhibited by 3'-thiourea derivatives of beta-thymidine: identification of residues crucial for both inhibition and catalytic activity. 2009 , 75, 1127-36	10
1741	A mechanism for S-adenosyl methionine assisted formation of a riboswitch conformation: a small molecule with a strong arm. 2009 , 37, 6528-39	43
1740	Atomistic Simulation of Ionic Liquids. 2009 , 421-493	5
1739	Solution NMR structure of the C-terminal EF-hand domain of human cardiac sodium channel NaV1.5. 2009 , 284, 6436-45	57
1738	Design of peptide-based inhibitors for human immunodeficiency virus type 1 strains resistant to T-20. 2009 , 284, 4914-20	37
1737	Solution structure of an ABC collagen heterotrimer reveals a single-register helix stabilized by electrostatic interactions. 2009 , 284, 26851-9	69
1736	Structural and functional analysis of Campylobacter jejuni PseG: a udp-sugar hydrolase from the pseudaminic acid biosynthetic pathway. 2009 , 284, 20989-1000	15
1735	Recent advances in computer-aided drug design. 2009 , 10, 579-91	164
1734	Hole-transfer Mechanism in Hydrated DNA Duplexes: Direct Ab Initio Molecular Dynamics Simulation. 2009 , 16, 53-64	
1733	Dimerization of the core domain of the p53 family: a computational study. 2009 , 8, 137-48	12

(2009-2009)

1732	Dual folding pathways of an alpha/beta protein from all-atom ab initio folding simulations. 2009 , 131, 165105	20
1731	The Kir channel immunoglobulin domain is essential for Kir1.1 (ROMK) thermodynamic stability, trafficking and gating. 2009 , 3, 57-68	22
1730	Conformational sampling and energetics of drug-like molecules. 2009 , 16, 3381-413	56
1729	COARSE GRAINED MODELING OF BIOPOLYMERS AND PROTEINS: METHODS AND APPLICATIONS. 2009 , 01, 113-136	11
1728	Integrating statistical predictions and experimental verifications for enhancing protein-chemical interaction predictions in virtual screening. 2009 , 5, e1000397	47
1727	Solvent dependent structural perturbations of chemical reaction intermediates visualized by time-resolved x-ray diffraction. 2009 , 130, 154502	33
1726	Coarse-grained molecular dynamics of ligands binding into protein: The case of HIV-1 protease inhibitors. 2009 , 130, 215102	24
1725	Chapter 2 Elements of High-Performance Reconfigurable Computing. 2009 , 113-157	1
1724	Free energy calculations of glycosaminoglycan-protein interactions. 2009 , 19, 1103-15	51
1723	Rapid sampling of molecular motions with prior information constraints. 2009 , 5, e1000295	46
1722	Structural basis for subversion of cellular control mechanisms by the adenoviral E1A oncoprotein. 2009 , 106, 13260-5	102
1721	Determination of key residues for catalysis and RNA cleavage specificity: one mutation turns RNase II into a "SUPER-ENZYME". 2009 , 284, 20486-98	33
1720	Mechanism of CB1954 reduction by Escherichia coli nitroreductase. 2009 , 37, 413-8	23
	The children of the section by Eschericina commercial cases and the section of th	
1719	Investigation of the interaction between the large and small subunits of potato ADP-glucose pyrophosphorylase. 2009 , 5, e1000546	20
1719 1718	Investigation of the interaction between the large and small subunits of potato ADP-glucose	
	Investigation of the interaction between the large and small subunits of potato ADP-glucose pyrophosphorylase. 2009 , 5, e1000546 Characterization of domain-peptide interaction interface: a generic structure-based model to	20
1718	Investigation of the interaction between the large and small subunits of potato ADP-glucose pyrophosphorylase. 2009, 5, e1000546 Characterization of domain-peptide interaction interface: a generic structure-based model to decipher the binding specificity of SH3 domains. 2009, 8, 639-49 Molecular dynamics simulations and coupled nucleotide substitution experiments indicate the nature of A{middle dot}A base pairing and a putative structure of the coralyne-induced homo-adenine duplex. 2009, 37, 7715-27	20

1714	DOCK 6: combining techniques to model RNA-small molecule complexes. 2009 , 15, 1219-30		510
1713	Molecular-genetic PET imaging using an HSV1-tk mutant reporter gene with enhanced specificity to acycloguanosine nucleoside analogs. 2009 , 50, 409-16		27
1712	Flavodoxin: a compromise between efficiency and versatility in the electron transfer from Photosystem I to Ferredoxin-NADP(+) reductase. 2009 , 1787, 144-54		34
1711	Identification of aspartic acid-203 in human thymidine phosphorylase as an important residue for both catalysis and non-competitive inhibition by the small molecule "crystallization chaperone" 5'-O-tritylinosine (KIN59). 2009 , 78, 231-40		10
1710	Theoretical mimicry of biomembranes. 2009 , 583, 1909-15		18
1709	Asymmetric Reduction of Activated Alkenes by Pentaerythritol Tetranitrate Reductase: Specificity and Control of Stereochemical Outcome by Reaction Optimisation. 2009 , 351, 2976-2990		100
1708	Asymmetric Reduction of Activated Alkenes by Pentaerythritol Tetranitrate Reductase: Specificity and Control of Stereochemical Outcome by Reaction Optimisation. 2009 , 351, 2976-2990		49
1707	Barrier Compression Enhances an Enzymatic Hydrogen-Transfer Reaction. 2009 , 121, 1480-1482		5
1706	Polymerase-catalysed incorporation of glucose nucleotides into a DNA duplex. 2009 , 15, 5463-70		18
1705	Parallel pathways and free-energy landscapes for enzymatic hydride transfer probed by hydrostatic pressure. 2009 , 10, 1379-84		22
1704	Structurally minimized mu-conotoxin analogues as sodium channel blockers: implications for designing conopeptide-based therapeutics. 2009 , 4, 406-14		45
1703	Design and discovery of plasmepsin II inhibitors using an automated workflow on large-scale grids. 2009 , 4, 1164-73		38
1702	Modeling the separation of macromolecules: a review of current computer simulation methods. 2009 , 30, 792-818		116
1701	Accelerating molecular dynamic simulation on the cell processor and Playstation 3. <i>Journal of Computational Chemistry</i> , 2009 , 30, 268-74	3.5	21
1700	GridMAT-MD: a grid-based membrane analysis tool for use with molecular dynamics. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1952-8	3.5	214
1699	RedMDreduced molecular dynamics package. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2364-73	3.5	18
1698	Force-field parameters of the Psi and Phi around glycosidic bonds to oxygen and sulfur atoms. Journal of Computational Chemistry, 2009 , 30, 2656-65	3.5	
1697	Refinement of the primary hydration shell model for molecular dynamics simulations of large proteins. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2635-44	3.5	4

1696	Current performance gains from utilizing the GPU or the ASIC MDGRAPE-3 within an enhanced Poisson Boltzmann approach. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2351-7	3.5	15
1695	Roles of K151 and D180 in L-2-haloacid dehalogenase from Pseudomonas sp. YL: analysis by molecular dynamics and ab initio fragment molecular orbital calculations. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2625-34	3.5	24
1694	CHARMM: the biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-61	4 3.5	5515
1693	An N log N approximation based on the natural organization of biomolecules for speeding up the computation of long range interactions. <i>Journal of Computational Chemistry</i> , 2010 , 31, 691-706	3.5	11
1692	CHARMM general force field: A force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields. <i>Journal of Computational Chemistry</i> , 2010 , 31, 671-90	3.5	2953
1691	Fast and accurate predictions of binding free energies using MM-PBSA and MM-GBSA. <i>Journal of Computational Chemistry</i> , 2010 , 31, 797-810	3.5	377
1690	Conformational populations of ligand-sized molecules by replica exchange molecular dynamics and temperature reweighting. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1357-67	3.5	14
1689	Basic ingredients of free energy calculations: a review. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1569-82	3.5	225
1688	Including receptor flexibility and induced fit effects into the design of MMP-2 inhibitors. 2010 , 23, 173-8	32	22
1687	Sulindac Inhibits Canonical Wnt Signaling by Blocking the PDZ Domain of the Protein Dishevelled. 2009 , 121, 6570-6574		4
1686	Barrier compression enhances an enzymatic hydrogen-transfer reaction. 2009 , 48, 1452-4		51
1685	Sulindac inhibits canonical Wnt signaling by blocking the PDZ domain of the protein Dishevelled. 2009 , 48, 6448-52		74
1684	Flexibility of the MHC class II peptide binding cleft in the bound, partially filled, and empty states: a molecular dynamics simulation study. 2009 , 91, 14-27		50
1683	Mechanistic studies of displacer-protein binding in chemically selective displacement systems using NMR and MD simulations. 2009 , 102, 1428-37		10
1682	Optimized conditions for 2-aminobenzamide labeling and high-performance liquid chromatography analysis of N-acylated monosaccharides. 2010 , 24, 343-6		5
1681	Computer-based design of novel HIV-1 entry inhibitors: neomycin conjugated to arginine peptides at two specific sites. 2009 , 15, 281-94		8
1680	Molecular dynamic simulations of the metallo-beta-lactamase from Bacteroides fragilis in the presence and absence of a tight-binding inhibitor. 2009 , 15, 133-45		21
1679	Structural and energetic heterogeneities of canonical and oxidized central guanine triad of B-DNA telomeric fragments. 2009 , 15, 607-13		5

1678	Homology modeling of a novel epoxide hydrolase (EH) from Aspergillus niger SQ-6: structure-activity relationship in expoxides inhibiting EH activity. 2009 , 15, 1125-32	2
1677	Molecular dynamics simulations and MM-PBSA calculations of the lectin from snowdrop (Galanthus nivalis). 2009 , 15, 1501-7	8
1676	Convergence of calculated nuclear magnetic resonance chemical shifts in a protein with respect to quantum mechanical model size. 2009 , 898, 56-61	16
1675	Molecular modeling of ligand-receptor interactions in GABA C receptor. 2009 , 27, 813-21	19
1674	Computer simulation and SERR detection of cytochrome c dynamics at SAM-coated electrodes. 2009 , 54, 4963-4970	30
1673	T cell receptor cross-reactivity directed by antigen-dependent tuning of peptide-MHC molecular flexibility. 2009 , 31, 885-96	140
1672	Structural models in the assessment of protein druggability based on HTS data. 2009 , 23, 583-92	17
1671	Studies of chirality effect of 4-(phenylamino)-pyrrolo[2,1-f][1,2,4]triazine on p38alpha by molecular dynamics simulations and free energy calculations. 2009 , 23, 737-45	5
1670	Structural dynamics of protein backbone phi angles: extended molecular dynamics simulations versus experimental (3) J scalar couplings. 2009 , 45, 17-21	29
1669	Mechanical signaling on the single protein level studied using steered molecular dynamics. 2009 , 55, 141-52	26
1668	Docking and molecular dynamics studies on the stereoselectivity in the enzymatic synthesis of carbohydrates. 2009 , 122, 283-296	15
1667	Characterizing ion mobility-mass spectrometry conformation space for the analysis of complex biological samples. 2009 , 394, 235-44	165
1666	Crystal structures of g-type lysozyme from Atlantic cod shed new light on substrate binding and the catalytic mechanism. 2009 , 66, 2585-98	42
1665	Integrity of H1 helix in prion protein revealed by molecular dynamic simulations to be especially vulnerable to changes in the relative orientation of H1 and its S1 flank. 2009 , 38, 601-11	7
1664	Molecular dynamics guided study of salt bridge length dependence in both fluorinated and non-fluorinated parallel dimeric coiled-coils. 2009 , 74, 612-29	22
1663	Predicting drug resistance of the HIV-1 protease using molecular interaction energy components. 2009 , 74, 837-46	72
1662	Clarifying allosteric control of flap conformations in the 1TW7 crystal structure of HIV-1 protease. 2009 , 74, 872-80	8
1661	Molecular dynamics study of chemically engineered green fluorescent protein mutants: comparison of intramolecular fluorescence resonance energy transfer rate. 2009 , 75, 28-39	12

(2009-2009)

1000	Trapping open and closed forms of FitE: a group III periplasmic binding protein. 2009 , 75, 598-609	26
1659	G protein inactive and active forms investigated by simulation methods. 2009 , 75, 919-30	24
1658	Conformational dynamics of the EGFR kinase domain reveals structural features involved in activation. 2009 , 76, 375-86	23
1657	Solution structure of Apo-YjaB from Escherichia coli. 2009 , 76, 261-5	1
1656	The role of conserved water molecules in the catalytic domain of protein kinases. 2009 , 76, 527-35	37
1655	Identification of specificity and promiscuity of PDZ domain interactions through their dynamic behavior. 2009 , 77, 796-811	49
1654	Adaptively biased molecular dynamics: An umbrella sampling method with a time-dependent potential. 2009 , 109, 3666-3678	27
1653	C-terminal domain of SARS-CoV main protease can form a 3D domain-swapped dimer. 2009 , 18, 839-44	19
1652	ALDH1A2 (RALDH2) genetic variation in human congenital heart disease. 2009 , 10, 113	30
1651	Modeling of solvent-dependent conformational transitions in Burkholderia cepacia lipase. 2009 , 9, 38	53
1650	Comparison of molecular dynamics and superfamily spaces of protein domain deformation. 2009 , 9, 6	29
	Comparison of molecular dynamics and superfamily spaces of protein domain deformation. 2009 , 9, 6 Shape: automatic conformation prediction of carbohydrates using a genetic algorithm. 2009 , 1, 16	29
1649	Shape: automatic conformation prediction of carbohydrates using a genetic algorithm. 2009, 1, 16 A small molecule blocking oncogenic protein EWS-FLI1 interaction with RNA helicase A inhibits	20
1649 1648	Shape: automatic conformation prediction of carbohydrates using a genetic algorithm. 2009, 1, 16 A small molecule blocking oncogenic protein EWS-FLI1 interaction with RNA helicase A inhibits growth of Ewing's sarcoma. 2009, 15, 750-6	20
1649 1648 1647	Shape: automatic conformation prediction of carbohydrates using a genetic algorithm. 2009 , 1, 16 A small molecule blocking oncogenic protein EWS-FLI1 interaction with RNA helicase A inhibits growth of Ewing's sarcoma. 2009 , 15, 750-6 Dynamic proteomics in modeling of the living cell. Protein-protein interactions. 2009 , 74, 1586-607 Binding estimation after refinement, a new automated procedure for the refinement and rescoring	20 320 21
1649 1648 1647 1646	Shape: automatic conformation prediction of carbohydrates using a genetic algorithm. 2009, 1, 16 A small molecule blocking oncogenic protein EWS-FLI1 interaction with RNA helicase A inhibits growth of Ewing's sarcoma. 2009, 15, 750-6 Dynamic proteomics in modeling of the living cell. Protein-protein interactions. 2009, 74, 1586-607 Binding estimation after refinement, a new automated procedure for the refinement and rescoring of docked ligands in virtual screening. 2009, 73, 283-6 Activity prediction and structural insights of extracellular signal-regulated kinase 2 inhibitors with	20 320 21 87

1642	Novel C-seco-taxoids possessing high potency against paclitaxel-resistant cancer cell lines overexpressing class III beta-tubulin. 2009 , 19, 3300-4	34
1641	Modelling beta-1,3-exoglucanase-saccharide interactions: structure of the enzyme-substrate complex and enzyme binding to the cell wall. 2009 , 27, 908-20	8
1640	Computational screening and design of S100B ligand to block S100B-p53 interaction. 2009 , 27, 969-77	10
1639	Ab initio molecular orbital calculations on specific interactions between urokinase-type plasminogen activator and its receptor. 2009 , 28, 46-53	6
1638	Characterization of an inhibitory dynamic pharmacophore for the ERCC1-XPA interaction using a combined molecular dynamics and virtual screening approach. 2009 , 28, 113-30	28
1637	Molecular modeling of human cytochrome P450 2W1 and its interactions with substrates. 2009 , 28, 170-6	16
1636	The role of polarization interactions in the wrapping/unwrapping of nucleosomal DNA around the histone octamer: implications to gene regulation. 2009 , 258, 229-39	3
1635	Structure and function of the glycopeptide N-methyltransferase MtfA, a tool for the biosynthesis of modified glycopeptide antibiotics. 2009 , 16, 401-10	33
1634	Context-specific target definition in influenza a virus hemagglutinin-glycan receptor interactions. 2009 , 16, 803-14	22
1633	Molecular modeling of protein A affinity chromatography. 2009 , 1216, 8678-86	36
1632	Understanding ligand-protein interactions in affinity membrane chromatography for antibody purification. 2009 , 1216, 8687-96	31
1631	Calcium uptake by casein embedded in polyelectrolyte multilayer. 2009 , 343, 118-126	15
1630	A program for performing exact quantum dynamics calculations using cylindrical polar coordinates: A nanotube application. 2009 , 180, 459-465	4
1629	TiReX: Replica-exchange molecular dynamics using Tinker. 2009 , 180, 2013-2019	12
1628	Single-molecule DNA conductance in water solutions: Role of DNA low-frequency dynamics. 2009 , 467, 369-374	12
1627	The 1.4 A crystal structure of the large and cold-active Vibrio sp. alkaline phosphatase. 2009 , 1794, 297-308	42
1626	Introducing temperature dependence in an enhanced PoissonâBoltzmann approach. 2009, 480, 313-317	7
1625	Identification of new Hsp90 inhibitors by structure-based virtual screening. 2009 , 19, 4839-42	13

(2009-2009)

1624	Metadynamics modelling of the solvent effect on primary hydroxyl rotamer equilibria in hexopyranosides. 2009 , 344, 1575-81	24
1623	Expression and molecular dynamics studies on effect of amino acid substitutions at Arg344 in human cathepsin A on the protein local conformation. 2009 , 1794, 1693-9	2
1622	Identification and characterization of an intermediate taxol binding site within microtubule nanopores and a mechanism for tubulin isotype binding selectivity. 2009 , 49, 424-36	49
1621	Protein NMR chemical shift calculations based on the automated fragmentation QM/MM approach. 2009 , 113, 10380-8	79
1620	Molecular dynamics simulations of the dynamic and energetic properties of alkali and halide ions using water-model-specific ion parameters. 2009 , 113, 13279-90	354
1619	Sensitivity of 2D IR spectra to peptide helicity: a concerted experimental and simulation study of an octapeptide. 2009 , 113, 12037-49	39
1618	Reduced Catalytic Activity of P450 2A6 Mutants with Coumarin: A Computational Investigation. 2009 , 5, 1411-20	22
1617	Deuterium spin probes of backbone order in proteins: 2H NMR relaxation study of deuterated carbon alpha sites. 2009 , 131, 15853-65	34
1616	Thermostat artifacts in replica exchange molecular dynamics simulations. 2009 , 5, 1393-1399	72
1615	Apo and nickel-bound forms of the Pyrococcus horikoshii species of the metalloregulatory protein: NikR characterized by molecular dynamics simulations. 2009 , 48, 12024-33	13
1614	Dihydroorotase from the hyperthermophile Aquifex aeolicus is activated by stoichiometric association with aspartate transcarbamoylase and forms a one-pot reactor for pyrimidine biosynthesis. 2009 , 48, 766-78	33
1613	Homology modelling and molecular dynamics study of human fatty acid amide hydrolase. 2009 , 35, 1201-1208	36
1612	Reaction mechanism of the epsilon subunit of E. coli DNA polymerase III: insights into active site metal coordination and catalytically significant residues. 2009 , 131, 1550-6	52
1611	Prediction of and experimental support for the three-dimensional structure of replication protein A. 2009 , 48, 7892-905	4
1610	Free energy and kinetics of conformational transitions from Voronoi tessellated milestoning with restraining potentials. 2009 , 5, 2589-2594	46
1609	Steering protein-ligand docking with quantitative NMR chemical shift perturbations. 2009 , 49, 2260-71	32
1608	Structure-activity relations of nanolipoblockers with the atherogenic domain of human macrophage scavenger receptor A. 2009 , 10, 1381-91	22
1607	Bad Seeds Sprout Perilous Dynamics: Stochastic Thermostat Induced Trajectory Synchronization in Biomolecules. 2009 , 5, 1624-31	123

1606	Electrostatic control of the photoisomerization efficiency and optical properties in visual pigments: on the role of counterion quenching. 2009 , 131, 5172-86	116
1605	The cis-(5R,6S)-thymine glycol lesion occupies the wobble position when mismatched with deoxyguanosine in DNA. 2009 , 48, 9722-33	19
1604	Mechanistic insight into the role of transition-state stabilization in cyclophilin A. 2009, 131, 147-52	49
1603	Solvent fluctuations drive the hole transfer in DNA: a mixed quantum-classical study. 2009 , 113, 13107-17	68
1602	Structure-based CoMFA as a predictive model - CYP2C9 inhibitors as a test case. 2009 , 49, 853-64	24
1601	A dictionary for protein side-chain entropies from NMR order parameters. 2009, 131, 7226-7	60
1600	Water-induced polaron formation at the pentacene surface: Quantum mechanical molecular mechanics simulations. 2009 , 79,	42
1599	Trans-cis switching mechanisms in proline analogues and their relevance for the gating of the 5-HT3 receptor. 2009 , 113, 12148-53	40
1598	Nucleic acid folding determined by mesoscale modeling and NMR spectroscopy: solution structure of d(GCGAAAGC). 2009 , 113, 6881-93	7
1597	Structural basis of pathway-dependent force profiles in stretched DNA. 2009 , 113, 15364-71	11
1596	Short-range coherence of internal protein dynamics revealed by high-precision in silico study. 2009 , 131, 14610-1	56
1595	Deciphering intrinsic deactivation/isomerization routes in a phytochrome chromophore model. 2009 , 113, 15067-73	27
1594	Dynamics of the streptavidin-biotin complex in solution and in its crystal lattice: distinct behavior revealed by molecular simulations. 2009 , 113, 6971-85	30
1593	Conformational Studies of Methyl 떤-Arabinofuranoside Using the AMBER/GLYCAM Approach. 2009 , 5, 430-8	16
1592	A combined crystallographic and molecular dynamics study of cathepsin L retrobinding inhibitors. 2009 , 52, 6335-46	10
1591	Polarization effects in molecular mechanical force fields. 2009 , 21, 333102	192
1590	Critical role of the solvent environment in galectin-1 binding to the disaccharide lactose. 2009 , 48, 786-91	20
1589	Essential role of hydration in aggregation of misfolded prion proteins: quantification by molecular theory of solvation. 2009 , 72, 1060-8	

(2009-2009)

1588	Synergistic regulation and ligand-induced conformational changes of tryptophan synthase. 2009 , 48, 9921-31	21
1587	Functional roles of a structural element involving Na+-pi interactions in the catalytic site of T1 lipase revealed by molecular dynamics simulations. 2009 , 131, 16697-705	20
1586	Carbohydrate-binding proteins: Dissecting ligand structures through solvent environment occupancy. 2009 , 113, 8717-24	30
1585	Ab Initio Raman Spectra of Lactamase Inhibitor Intermediates Bound to E166A SHV Lactamase. 2009 , 5, 2158-72	12
1584	Correlated dynamics between protein HN and HC bonds observed by NMR cross relaxation. 2009 , 131, 3668-78	36
1583	Deciphering the structural properties that confer stability to a DNA nanocage. 2009 , 3, 1813-22	22
1582	Catalytic Mechanism of Diaminopimelate Epimerase: A QM/MM Investigation. 2009 , 5, 1915-30	11
1581	Improved Hydrogen Bonding at the NDDO-Type Semiempirical Quantum Mechanical/Molecular Mechanical Interface. 2009 , 5, 2206-11	18
1580	Ion specific effects of sodium and potassium on the catalytic activity of HIV-1 protease. 2009 , 11, 7599-604	35
1579	Tuning of copper-loop flexibility in Bacillus subtilis CopZ copper chaperone: role of conserved residues. 2009 , 113, 1919-32	12
1578	Differential roles of Met10, Thr11, and Lys60 in structural dynamics of human copper chaperone Atox1. 2009 , 48, 960-72	17
1577	Structural perturbations induced by the alpha-anomer of the aflatoxin B(1) formamidopyrimidine adduct in duplex and single-strand DNA. 2009 , 131, 16096-107	20
1576	Free energy calculation of modified base-pair formation in explicit solvent: A predictive model. 2009 , 15, 2278-87	36
1575	The cluster of hydrophobic residues controls the entrance to the active site of choline oxidase. 2009 , 48, 9599-605	24
1574	Charges for Large Scale Binding Free Energy Calculations with the Linear Interaction Energy Method. 2009 , 5, 380-95	12
1573	New pyrrole-based histone deacetylase inhibitors: binding mode, enzyme- and cell-based investigations. 2009 , 41, 235-47	20
1572	A novel sequence variation in the transactivation regulating domain of the human androgen receptor. 2009 , 92, 390.e9-390.e11	7
1571	Non-genetic global optimization methods in molecular science: An overview. 2009 , 45, 8-15	16

1570	Study of bradykinin conformation in the presence of model membrane by Nuclear Magnetic Resonance and molecular modelling. 2009 , 1788, 708-16	24
1569	Insight into the molecular switch mechanism of human Rab5a from molecular dynamics simulations. 2009 , 390, 608-12	79
1568	Solution structure of Hyp10Pro variant of conomarphin, a cysteine-free and D-amino-acid containing conopeptide. 2009 , 54, 153-60	13
1567	A short guide for molecular dynamics simulations of RNA systems. 2009 , 47, 187-97	60
1566	Ectodomain orientation, conformational plasticity and oligomerization of ErbB1 receptors investigated by molecular dynamics. 2009 , 167, 117-28	39
1565	A mechanistic model of the cysteine synthase complex. 2009 , 386, 37-59	66
1564	Statics of the ribosomal exit tunnel: implications for cotranslational peptide folding, elongation regulation, and antibiotics binding. 2009 , 387, 502-17	60
1563	Distinct glycan topology for avian and human sialopentasaccharide receptor analogues upon binding different hemagglutinins: a molecular dynamics perspective. 2009 , 387, 465-91	67
1562	Structural and dynamic implications of an effector-induced backbone amide cis-trans isomerization in cytochrome P450cam. 2009 , 388, 801-14	25
1561	Configurational entropy in protein-peptide binding: computational study of Tsg101 ubiquitin E2 variant domain with an HIV-derived PTAP nonapeptide. 2009 , 389, 315-35	70
1560	Structural and functional model for ionic (K(+)/Na(+)) and pH dependence of GTPase activity and polymerization of FtsZ, the prokaryotic ortholog of tubulin. 2009 , 390, 17-25	34
1559	Crystal structure of the HEAT domain from the Pre-mRNA processing factor Symplekin. 2009 , 392, 115-28	15
1558	Minimum-energy path for a u6 RNA conformational change involving protonation, base-pair rearrangement and base flipping. 2009 , 391, 894-905	31
1557	Ligand entry and exit pathways in the beta2-adrenergic receptor. 2009 , 392, 1102-15	80
1556	Predicting Raman spectra using density functional theory. 2009 , 63, 733-41	23
1555	Association of cytochrome c with membrane-bound cytochrome c oxidase proceeds parallel to the membrane rather than in bulk solution. 2009 , 96, 1721-32	17
1554	Affinity and specificity of levamlodipine-human serum albumin interactions: insights into its carrier function. 2009 , 96, 3917-25	28
1553	All-atom contact model for understanding protein dynamics from crystallographic B-factors. 2009 , 96, 3074-81	30

(2009-2009)

1552	Molecular renormalization group coarse-graining of polymer chains: application to double-stranded DNA. 2009 , 96, 4044-52	70
1551	Evaluating the performance of the ff99SB force field based on NMR scalar coupling data. 2009 , 97, 853-6	182
1550	Roles of boundary conditions in DNA simulations: analysis of ion distributions with the finite-difference Poisson-Boltzmann method. 2009 , 97, 554-62	25
1549	Focused functional dynamics of supramolecules by use of a mixed-resolution elastic network model. 2009 , 97, 1178-87	42
1548	Analysis of sub-tauc and supra-tauc motions in protein Gbeta1 using molecular dynamics simulations. 2009 , 97, 2513-20	11
1547	Solution and crystal molecular dynamics simulation study of m4-cyanovirin-N mutants complexed with di-mannose. 2009 , 97, 2532-40	32
1546	Binding of the bacteriophage P22 N-peptide to the boxB RNA motif studied by molecular dynamics simulations. 2009 , 97, 3139-49	25
1545	Overview of computational methods employed in early-stage drug discovery. 2009 , 1, 49-63	8
1544	Boxed molecular dynamics: a simple and general technique for accelerating rare event kinetics and mapping free energy in large molecular systems. 2009 , 113, 16603-11	65
1543	Ras conformational switching: simulating nucleotide-dependent conformational transitions with accelerated molecular dynamics. 2009 , 5, e1000325	136
1542	SINGLE-MOLECULE DNA CONDUCTANCE IN WATER SOLUTIONS: ROLE OF EXPLICIT WATERâ©OUNTERION SHEATH AND CHEMICAL MODIFICATION OF NUCLEOBASES. 2009 , 04, 231-243	3
1541	Solution conformation of C-linked antifreeze glycoprotein analogues and modulation of ice recrystallization. 2009 , 131, 15745-53	53
1540	Docking Ligands on Protein Surfaces: The Case Study of Prion Protein. 2009 , 5, 2565-73	30
1539	The AGBNP2 Implicit Solvation Model. 2009 , 5, 2544-2564	101
1538	Human islet amyloid polypeptide monomers form ordered beta-hairpins: a possible direct amyloidogenic precursor. 2009 , 131, 18283-92	180
1537	Quantum dynamical effects in liquid water: A semiclassical study on the diffusion and the infrared absorption spectrum. 2009 , 131, 164509	69
1536	A docking study using atomistic conformers generated via elastic network model for cyclosporin A/cyclophilin A complex. 2009 , 27, 13-26	40
1535	Structure and Dynamics of Lipid Monolayers: Theory and Applications. 2009 , 75-99	7

1534	The electronegativity equalization method and the split charge equilibration applied to organic systems: parametrization, validation, and comparison. 2009 , 131, 044127	77
1533	Matrix metalloproteinase 2 inhibition: combined quantum mechanics and molecular mechanics studies of the inhibition mechanism of (4-phenoxyphenylsulfonyl)methylthiirane and its oxirane analogue. 2009 , 48, 9839-47	53
1532	CPDB: a database of circular permutation in proteins. 2009 , 37, D328-32	47
1531	Pattern Recognition in Bioinformatics. 2009,	
1530	Importance of dispersion and electron correlation in ab initio protein folding. 2009 , 113, 5290-300	61
1529	Predictions of binding for dopamine D2 receptor antagonists by the SIE method. 2009 , 49, 2369-75	22
1528	Computational study of the conformational structures of saccharides in solution based on J couplings and the "fast sugar structure prediction software". 2009 , 10, 3081-8	7
1527	Validating CHARMM parameters and exploring charge distribution rules in structure-based drug design. 2009 , 5, 1680-1691	10
1526	WISDOM-II: screening against multiple targets implicated in malaria using computational grid infrastructures. 2009 , 8, 88	22
1525	Computational Approaches in Peptide and Protein Design: An Overview. 2009 , 5-48	2
1524	Characterizing loop dynamics and ligand recognition in human- and avian-type influenza neuraminidases via generalized born molecular dynamics and end-point free energy calculations. 2009 , 131, 4702-9	117
1523	Assessment of QM/MM scoring functions for molecular docking to HIV-1 protease. 2009 , 49, 913-24	41
1522	A Multiscale Treatment of Angeli's Salt Decomposition. 2009 , 5, 37-46	11
1521	Molecular insights on the two fluorescence lifetimes displayed by warfarin from fluorescence anisotropy and molecular dynamics studies. 2009 , 113, 7945-9	16
152 0	Differential harmaterials interesting induced by this other interest of DNA areas links in the	
1520	Differential base stacking interactions induced by trimethylene interstrand DNA cross-links in the 5'-CpG-3' and 5'-GpC-3' sequence contexts. 2009 , 22, 1810-6	9
1519		9
	5'-CpG-3' and 5'-GpC-3' sequence contexts. 2009 , 22, 1810-6 Structure and dynamics of monomer-template complexation: an explanation for molecularly	

1516	Unique tautomeric and recognition properties of thioketothymines?. 2009 , 131, 12845-53	4
1515	Computations of Absolute Solvation Free Energies of Small Molecules Using Explicit and Implicit Solvent Model. 2009 , 5, 919-30	125
1514	In silico selection of RNA aptamers. 2009 , 37, e87	102
1513	Conantokin-Br from Conus brettinghami and selectivity determinants for the NR2D subunit of the NMDA receptor. 2009 , 48, 4063-73	25
1512	Performance Analysis of ClearSpeed's CSX600 Interconnects. 2009 ,	
1511	Motions of ions in a nanoscale Paul trap from molecular dynamics. 2009 , 35, 812-821	1
1510	Tracing conformational changes in proteins. 2009,	1
1509	Determination of phosphorylation sites for NADP-specific isocitrate dehydrogenase from mycobacterium tuberculosis. 2009 , 26, 741-54	15
1508	Microhydration of guaninecytosine base pairs, a theoretical Study on the role of water in stability, structure and tautomeric equilibrium. 2009 , 11, 3430-5	13
1507	Structural basis for recruitment of CBP/p300 coactivators by STAT1 and STAT2 transactivation domains. 2009 , 28, 948-58	108
1506	Hepcidin revisited, disulfide connectivity, dynamics, and structure. 2009 , 284, 24155-67	159
1505	Diazo transfer-click reaction route to new, lipophilic teicoplanin and ristocetin aglycon derivatives with high antibacterial and anti-influenza virus activity: an aggregation and receptor binding study. 2009 , 52, 6053-61	34
1504	jSimMacs for GROMACS: a Java application for advanced molecular dynamics simulations with remote access capability. 2009 , 49, 2412-7	10
1503	Conformational flexibility of soluble cellulose oligomers: chain length and temperature dependence. 2009 , 131, 14786-94	94
1502	The impact of monovalent ion force field model in nucleic acids simulations. 2009 , 11, 10596-607	59
1501	Molecular Simulation of Cross-Linked Epoxy and Epoxyâ P OSS Nanocomposite. 2009 , 42, 4319-4327	147
1500	An Improved Reaction Coordinate for Nucleic Acid Base Flipping Studies. 2009 , 5, 3105-13	49
1499	Computational approaches for the design of peptides with anti-breast cancer properties. 2009 , 1, 201-12	6

1498	Novel Quantitative Structure-Activity Studies of HIV-1 Protease Inhibitors of the Cyclic Urea Type Using Descriptors Derived from Molecular Dynamics and Molecular Orbital Calculations. 2009 , 5, 38-55	29
1497	Support Vector Machine Prediction of N- and O-glycosylation Sites Using Whole Sequence Information and Subcellular Localization. 2009 , 2, 25-35	15
1496	Analysis of the secondary structure of a protein's N-terminal. 2009 , 182, 012008	
1495	The copper-responsive repressor CopR of Lactococcus lactis is a 'winged helix' protein. 2009 , 417, 493-9	18
1494	Structural insight on the control of urea synthesis: identification of the binding site for N-acetyl-L-glutamate, the essential allosteric activator of mitochondrial carbamoyl phosphate synthetase. 2009 , 424, 211-20	22
1493	FAMSD: A powerful protein modeling platform that combines alignment methods, homology modeling, 3D structure quality estimation and molecular dynamics. 2009 , 57, 1335-42	5
1492	Predicting Carbohydrate 3D Structures Using Theoretical Methods. 359-388	2
1491	Potential of Nurr1 interactions to disclose new Parkinsonâl therapeutics. 2009, 4, 161-165	
1490	Chaperone therapy for neuronopathic lysosomal diseases: competitive inhibitors as chemical chaperones for enhancement of mutant enzyme activities. 2009 , 3, 7-19	44
1489	Steroid hormone binding receptors: application of homology modeling, induced fit docking, and molecular dynamics to study structure-function relationships. 2009 , 9, 844-53	14
1488	Serum albumin complexation of acetylsalicylic acid metabolites. 2009 , 10, 448-58	5
1487	Protein Structure Calculation using Ambiguous Restraints. 2010 ,	3
1486	Dimer-tetramer transition controls RUNX1/ETO leukemogenic activity. 2010 , 116, 603-13	35
1485	Mining the protein data bank with CReF to predict approximate 3-D structures of polypeptides. 2010 , 4, 281-99	8
1484	On using many-particle interatomic potentials to compute elastic properties of graphene and diamond. 2010 , 45, 815-834	17
1483	Molecular basis of the interaction for an essential subunit PA-PB1 in influenza virus RNA polymerase: insights from molecular dynamics simulation and free energy calculation. 2010 , 7, 75-85	68
1482	PSMB8 encoding the \$\mathbf{F}\$ i proteasome subunit is mutated in joint contractures, muscle atrophy, microcytic anemia, and panniculitis-induced lipodystrophy syndrome. 2010 , 87, 866-72	252
1481	Simulations of the Structure of Cellulose. 2010 , 17-53	19

1480 Modeling the Cellulosome Using Multiscale Methods. **2010**, 75-98

1479 Water in the polar and nonpolar cavities of the protein interleukin-1 #2010 , 114, 16290-7	37
1478 Practical considerations for building GROMOS-compatible small-molecule topologies. 2010 , 50, 2	2221-35 154
1477 Bioinformatics and molecular modeling in glycobiology. 2010 , 67, 2749-72	73
Rationalizing perhydrolase activity of aryl-esterase and subtilisin Carlsberg mutants by molecular dynamics simulations of the second tetrahedral intermediate state. 2010 , 125, 375-386	r 9
Asymmetric synthesis of (S)-3-chloro-1-phenyl-1-propanol using Saccharomyces cerevisiae reductase with high enantioselectivity. 2010 , 87, 185-93	25
1474 Fis-protein induces rod-like DNA bending. 2010 , 500, 318-322	
1473 Developing Force Fields from the Microscopic Structure of Solutions. 2010 , 290, 43	48
The first low microM SecA inhibitors. 2010 , 18, 1617-25	47
Identification of small molecule compounds with higher binding affinity to guanine deaminase (cypin) than guanine. 2010 , 18, 6748-55	16
1470 A RNA-based nanodevice recording temperature over time. 2010 , 369, 91-95	3
1469 NMR in structural proteomics and beyond. 2010 , 56, 247-66	29
Pyridine-containing chiral macrocycles for the enantioselective recognition of amino acid derivatives and their molecular dynamics simulations. 2010 , 21, 990-996	9
Relative stability of complexes of six-carbon-rings with variable numbers of double bonds: DFT a ab initio results. 2010 , 941, 78-84	nd 2
Specific interactions between aryl hydrocarbon receptor and dioxin congeners: ab initio fragmen molecular orbital calculations. 2010 , 29, 197-205	nt 10
Structural and energetic consequences of oxidation of d(ApGpGpGpTpT) telomere repeat unit in complex with TRF1 protein. 2010 , 16, 1797-807	2
Dynamics of \oplus ocopherol Acetate: Proton Relaxation Studies Supported by Molecular Dynamics Simulations. 2010 , 39, 273-283	1
Insight into herbicide resistance of W574L mutant Arabidopsis thaliana acetohydroxyacid syntha molecular dynamics simulations and binding free energy calculations. 2010 , 53, 91-102	se: 8

1462	Computational Study of Macroscopic Properties of Macromolecules with Industrial Interest. 2010 , 87, 271-279	1
1461	Major groove width variations in RNA structures determined by NMR and impact of 13C residual chemical shift anisotropy and 1H-13C residual dipolar coupling on refinement. 2010 , 47, 205-19	60
1460	A computational workflow for the design of irreversible inhibitors of protein kinases. 2010 , 24, 183-94	9
1459	Rapid prediction of solvation free energy. 3. Application to the SAMPL2 challenge. 2010 , 24, 373-83	15
1458	Dependency of ligand free energy landscapes on charge parameters and solvent models. 2010 , 24, 699-712	6
1457	Phosphorylation and ATP-binding induced conformational changes in the PrkC, Ser/Thr kinase from B. subtilis. 2010 , 24, 733-47	5
1456	T-Analyst: a program for efficient analysis of protein conformational changes by torsion angles. 2010 , 24, 819-27	24
1455	Influence of metal cofactors and water on the catalytic mechanism of creatininase-creatinine in aqueous solution from molecular dynamics simulation and quantum study. 2010 , 24, 879-86	4
1454	Conformational Analysis of a Synthetic Antimicrobial Peptide in Water and Membrane-Mimicking Solvents: A Molecular Dynamics Simulation Study. 2010 , 16, 223-231	7
1453	Standards-Based Job Management in Grid Systems. 2010 , 8, 19-45	5
1452	Parameter Sweep Workflows for Modelling Carbohydrate Recognition. 2010 , 8, 587-601	15
1451	Oxidation of human cytochrome P450 1A2 substrates by Bacillus megaterium cytochrome P450 BM3. 2010 , 63, 179-187	20
1450	A toxin-antitoxin module as a target for antimicrobial development. 2010 , 63, 31-9	61
1449	Computational glycoscience: characterizing the spatial and temporal properties of glycans and glycan-protein complexes. 2010 , 20, 575-83	68
1448	Structural insight into the zinc finger CW domain as a histone modification reader. 2010 , 18, 1127-39	93
1447	Creating PWMs of transcription factors using 3D structure-based computation of protein-DNA free binding energies. 2010 , 11, 225	18
1446	Optimizing structural modeling for a specific protein scaffold: knottins or inhibitor cystine knots. 2010 , 11, 535	7
1445	Differences in the transactivation domains of p53 family members: a computational study. 2010 , 11 Suppl 1, S5	22

1444	Mining flexible-receptor docking experiments to select promising protein receptor snapshots. 2010 , 11 Suppl 5, S6		15	
1443	A ligand predication tool based on modeling and reasoning with imprecise probabilistic knowledge. 2010 , 98, 45-54			
1442	Molecular simulations of carbohydrates and protein-carbohydrate interactions: motivation, issues and prospects. 2010 , 15, 596-609		141	
1441	Dual role of FMN in flavodoxin function: electron transfer cofactor and modulation of the protein-protein interaction surface. 2010 , 1797, 262-71		16	
1440	Design and evaluation of antiretroviral peptides corresponding to the C-terminal heptad repeat region (C-HR) of human immunodeficiency virus type 1 envelope glycoprotein gp41. 2010 , 405, 157-64		2	
1439	Discovery of potent vascular endothelial growth factor receptor-2 inhibitors. 2010 , 5, 118-29		8	
1438	Pyrrolidine derivatives as plasmepsin inhibitors: binding mode analysis assisted by molecular dynamics simulations of a highly flexible protein. 2010 , 5, 443-54		14	
1437	Structure-based virtual screening and electrophysiological evaluation of new chemotypes of K(v)1.5 channel blockers. 2010 , 5, 1353-8		7	
1436	The role of fluorine atoms in a fluorinated prostaglandin agonist. 2010 , 5, 1254-7		16	
1435	Understanding the key factors that control the inhibition of type II dehydroquinase by (2R)-2-benzyl-3-dehydroquinic acids. 2010 , 5, 1726-33		20	
1434	Computational analysis of missense mutations causing Snyder-Robinson syndrome. 2010 , 31, 1043-9		66	
1433	The polarity of the amino acid residue 118 of calcineurin B is closely linked to calcineurin enzyme activity. 2010 , 62, 561-7		5	
1432	Symmetrization of the AMBER and CHARMM force fields. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1402-9	3.5	26	
1431	A toolkit to assist ONIOM calculations. <i>Journal of Computational Chemistry</i> , 2010 , 31, 2363-9	3.5	42	
1430	vmdICE: a plug-in for rapid evaluation of molecular dynamics simulations using VMD. <i>Journal of Computational Chemistry</i> , 2010 , 31, 2868-73	3.5	34	
1429	Less is more when simulating unsulfated glycosaminoglycan 3D-structure: comparison of GLYCAM06/TIP3P, PM3-CARB1/TIP3P, and SCC-DFTB-D/TIP3P predictions with experiment. <i>Journal of Computational Chemistry</i> , 2010 , 31, 2932-47	3.5	24	
1428	Selective Recognition of Mannosides by Synthetic Tripodal Receptors: A 3D View of the Recognition Mode by NMR. 2010 , 2010, 64-71		21	
1427	Computational Methods for the Development of Polymeric Biomaterials. 2010 , 12, B3-B17		15	

1426	Multimeric lactoside "click clusters" as tools to investigate the effect of linker length in specific interactions with peanut lectin, galectin-1, and -3. 2010 , 11, 1430-42	38
1425	Mimicking chitin: chemical synthesis, conformational analysis, and molecular recognition of the beta(1>3) N-acetylchitopentaose analogue. 2010 , 16, 4239-49	7
1424	Synthesis and molecular modelling of double-functionalised nucleosides with aromatic moieties in the 5'-(S)-position and minor groove interactions in DNA zipper structures. 2010 , 16, 12904-19	19
1423	Synthesis and molecular modeling of a nitrogen mustard DNA interstrand crosslink. 2010 , 16, 12100-3	29
1422	NMR-Based Protein Potentials. 2010 , 122, 6930-6932	25
1421	NMR-based protein potentials. 2010 , 49, 6778-80	154
1420	Characterization of a clinical polymer-drug conjugate using multiscale modeling. 2010, 93, 936-51	19
1419	Complexation of sulfonamides with beta-cyclodextrin studied by experimental and theoretical methods. 2010 , 99, 3166-76	28
1418	Comparison of the complexation between methylprednisolone and different cyclodextrins in solution by 1H-NMR and molecular modeling studies. 2010 , 99, 3863-73	20
1417	Asymmetric synthesis of (S)-ethyl-4-chloro-3-hydroxy butanoate using a Saccharomyces cerevisiae reductase: enantioselectivity and enzyme-substrate docking studies. 2010 , 1804, 1841-9	12
1416	Molecular dynamics simulations of Krytox-SilicaâNafion composite for high temperature fuel cell electrolyte membranes. 2010 , 51, 4632-4638	19
1415	Ensemble-based virtual screening reveals dual-inhibitors for the p53-MDM2/MDMX interactions. 2010 , 28, 555-68	50
1414	Force field design and molecular dynamics simulations of factor-inhibiting HIF-1 and its complex with known inhibitors: implications for rational inhibitor design. 2010 , 29, 221-8	2
1413	Insights into the folding pathway of the Engrailed Homeodomain protein using replica exchange molecular dynamics simulations. 2010 , 29, 481-91	10
1412	Study of the inclusion of the (R)- and (S)-camphor enantiomers in alpha-cyclodextrin by X-ray crystallography and molecular dynamics. 2010 , 345, 1034-40	15
1411	A synthetic and in silico study on the highly regioselective DielsâAlder reaction of the polyenic antifungal antibiotics natamycin and flavofungin. 2010 , 51, 4968-4971	2
1410	Fragment molecular orbital (FMO) study on stabilization mechanism of neuro-oncological ventral antigen (NOVA)âRNA complex system. 2010 , 962, 45-55	16
1409	Biochemical and structural consequences of a glycine deletion in the alpha-8 helix of protoporphyrinogen oxidase. 2010 , 1804, 1548-56	44

1408	Small-molecule ligands of GD2 ganglioside, designed from NMR studies, exhibit induced-fit binding and bioactivity. 2010 , 17, 183-94	11
1407	3D structure-based protein retention prediction for ion-exchange chromatography. 2010 , 1217, 1343-53	59
1406	Pyrazolone-fused combretastatins and their precursors: synthesis, cytotoxicity, antitubulin activity and molecular modeling studies. 2010 , 18, 2375-87	34
1405	Discovery of highly selective inhibitors of human fatty acid binding protein 4 (FABP4) by virtual screening. 2010 , 20, 3675-9	22
1404	Homology modeling, docking, and molecular dynamics reveal HR1039 as a potent inhibitor of 2009 A(H1N1) influenza neuraminidase. 2010 , 147, 74-80	22
1403	A 3D-structural model of unsulfated chondroitin from high-field NMR: 4-sulfation has little effect on backbone conformation. 2010 , 345, 291-302	41
1402	Solvation of Biomolecules by the Soft Sticky Dipole-Quadrupole-Octupole Water Model. 2010 , 486, 70-73	8
1401	AtomSim: web-deployed atomistic dynamics simulator. 2010 , 43, 1553-1559	1
1400	Elucidation of the conformational free energy landscape in H.pylori LuxS and its implications to catalysis. 2010 , 10, 27	17
1399	Tracing conformational changes in proteins. 2010 , 10 Suppl 1, S1	48
1398	Computational model of hepatitis B virus DNA polymerase: molecular dynamics and docking to understand resistant mutations. 2010 , 19, 796-807	34
1397	Solvent-induced lid opening in lipases: a molecular dynamics study. 2010 , 19, 2122-30	101
1396	Site-specific inhibition of integrin alpha v beta 3-vitronectin association by a ser-asp-val sequence through an Arg-Gly-Asp-binding site of the integrin. 2010 , 10, 72-80	25
1395	Focus on composition and interaction potential of single-pass transmembrane domains. 2010 , 10, 4196-208	42
1394	Protein-protein interactions at an enzyme-substrate interface: characterization of transient reaction intermediates throughout a full catalytic cycle of Escherichia coli thioredoxin reductase. 2010 , 78, 36-51	14
1393	Comparative binding energy analysis for binding affinity and target selectivity prediction. 2010 , 78, 135-53	18
1392	A novel approach to segregate and identify functional loop regions in protein structures using their	
	Ramachandran maps. 2010 , 78, 900-16	6
1391		5

1390	Structural facets of disease-linked human prion protein mutants: a molecular dynamic study. 2010 , 78, 3270-80	41
1389	Computational study of the molecular mechanisms of caffeine action: Caffeine complexes with adenosine receptors. 2010 , 110, 681-688	19
1388	PM01183, a new DNA minor groove covalent binder with potent in vitro and in vivo anti-tumour activity. 2010 , 161, 1099-110	8o
1387	Degradation of tropoelastin by matrix metalloproteinasescleavage site specificities and release of matrikines. 2010 , 277, 1939-56	67
1386	Keratin mutations in patients with epidermolysis bullosa simplex: correlations between phenotype severity and disturbance of intermediate filament molecular structure. 2010 , 162, 1004-13	18
1385	Structural basis of G-tract recognition and encaging by hnRNP F quasi-RRMs. 2010 , 17, 853-61	112
1384	Conical intersection dynamics of the primary photoisomerization event in vision. 2010 , 467, 440-3	651
1383	Rapid desensitization of the rat 日 nAChR is facilitated by the presence of a proline residue in the outer 動heet. 2010 , 588, 4415-29	21
1382	GUI-BioPASED: A program for molecular dynamics simulations of biopolymers with a graphical user interface. 2010 , 44, 648-654	21
1381	In silico drug discovery approaches on grid computing infrastructures. 2010 , 5, 37-46	9
1380	Small molecules showing significant protection of mice against botulinum neurotoxin serotype A. 2010 , 5, e10129	33
1379	Binding of the human nucleotide excision repair proteins XPA and XPC/HR23B to the 5R-thymine glycol lesion and structure of the cis-(5R,6S) thymine glycol epimer in the 5'-GTgG-3' sequence: destabilization of two base pairs at the lesion site. 2010 , 38, 428-40	60
1378	BioDrugScreen: a computational drug design resource for ranking molecules docked to the human proteome. 2010 , 38, D765-73	28
1377	DNA structures from phosphate chemical shifts. 2010 , 38, e18	22
1377 1376	DNA structures from phosphate chemical shifts. 2010 , 38, e18 Antidiabetic sulfonylureas modulate farnesoid X receptor activation and target gene transcription. 2010 , 2, 575-86	22
	Antidiabetic sulfonylureas modulate farnesoid X receptor activation and target gene transcription.	
1376	Antidiabetic sulfonylureas modulate farnesoid X receptor activation and target gene transcription. 2010, 2, 575-86 Solution NMR structure of the C-terminal DNA binding domain of Mcm10 reveals a conserved MCM	4

1372	Identification of novel peptide inhibitors for human trypsins. 2010 , 391, 283-293	15
1371	Glycosylation of {beta}2 subunits regulates GABAA receptor biogenesis and channel gating. 2010 , 285, 31348-61	34
1370	Structural characterization of the TCR complex by electron microscopy. 2010 , 22, 897-903	16
1369	Predicting loop-helix tertiary structural contacts in RNA pseudoknots. 2010 , 16, 538-52	32
1368	A Framework for End-to-End Simulation of High-performance Computing Systems. 2010 , 86, 331-350	13
1367	Design and characterization of a mutation outside the active site of human thymidylate synthase that affects ligand binding. 2010 , 23, 81-9	5
1366	An isoform-specific PDZ-binding motif targets type I PIP5 kinase beta to the uropod and controls polarization of neutrophil-like HL60 cells. 2010 , 24, 3381-92	13
1365	Combining molecular simulation techniques to predict the binding modes of oseltamivir, zanamivir and natural herb products with the neuramindase of the H1N1 influenza A virus. 2010 ,	
1364	RNA stability under different combinations of amber force fields and solvation models. 2010 , 28, 431-41	43
1363	Ab initio fragment molecular orbital calculations on the specific interactions between human, mouse and rat PPAR and GW409544. 2010 , 36, 644-656	1
1362	Assessing the thermodynamic signatures of hydrophobic hydration for several common water models. 2010 , 132, 124504	64
1361	Modulation of electronic structures of bases through DNA recognition of protein. 2010 , 22, 152101	1
1360	FAST MOLECULAR SOLVATION ENERGETICS AND FORCE COMPUTATION. 2010 , 31, 4524-4552	13
1359	The therapeutically anti-prion active antibody-fragment scFv-W226: paramagnetic relaxation-enhanced NMR spectroscopy aided structure elucidation of the paratope-epitope interface. 2010 , 28, 13-22	12
1358	Inhibitor-induced structural change in the HCV IRES domain IIa RNA. 2010 , 107, 7263-8	47
1357	Chemical validation of phosphodiesterase C as a chemotherapeutic target in Trypanosoma cruzi, the etiological agent of Chagas' disease. 2010 , 54, 3738-45	29
1356	Insights into the Role of Conformational Transitions and Metal Ion Binding in RNA Catalysis from Molecular Simulations. 2010 , 6, 168-200	1
1355	Particle Swarm Optimization for multimodal combinatorial problems and its application to protein design. 2010 ,	1

1354	Molecular dynamics studies on troponin (TnI-TnT-TnC) complexes: insight into the regulation of muscle contraction. 2010 , 28, 159-74	37
1353	A novel p53 phosphorylation site within the MDM2 ubiquitination signal: II. a model in which phosphorylation at SER269 induces a mutant conformation to p53. 2010 , 285, 37773-86	18
1352	Molecular interfaces of the galactose-binding protein Tectonin domains in host-pathogen interaction. 2010 , 285, 9898-9907	18
1351	Catalytic mechanism of heparinase II investigated by site-directed mutagenesis and the crystal structure with its substrate. 2010 , 285, 20051-61	39
1350	An antibody as surrogate receptor reveals determinants of activity of an innate immune peptide antibiotic. 2010 , 285, 35750-8	6
1349	Insights into function, catalytic mechanism, and fold evolution of selenoprotein methionine sulfoxide reductase B1 through structural analysis. 2010 , 285, 33315-33323	20
1348	Structure and mechanism of sanguinarine reductase, an enzyme of alkaloid detoxification. 2010 , 285, 18397-406	32
1347	Identification of dynamical hinge points of the L1 ligase molecular switch. 2010 , 16, 769-80	6
1346	On the origins of the weak folding cooperativity of a designed 脚ltrafast protein FSD-1. 2010 , 6, e1000998	13
1345	A computational simulation study of benzamidine derivatives binding to arginine-specific gingipain (HRgpA) from periodontopathogen Porphyromonas gingivalis. 2010 , 11, 3252-65	
1344	Molecular structures of quiescently grown and brain-derived polymorphic fibrils of the Alzheimer amyloid abeta9-40 peptide: a comparison to agitated fibrils. 2010 , 6, e1000693	49
1343	A mechanistic view of the role of E3 in sumoylation. 2010 , 6, e1000913	16
1342	The role of oligomerization and cooperative regulation in protein function: the case of tryptophan synthase. 2010 , 6, e1000994	31
1341	How cations can assist DNase I in DNA binding and hydrolysis. 2010 , 6, e1001000	42
1340	Interpolation schemes for peptide rearrangements. 2010 , 132, 054101	13
1339	A wave-function based approach for polarizable charge model: Systematic comparison of polarization effects on protic, aprotic, and ionic liquids. 2010 , 132, 044106	30
1338	Communication: Molecular dynamics simulations of the interfacial structure of alkali metal fluoride solutions. 2010 , 133, 061103	14
1337	Activation of integrins by urea in perfused rat liver. 2010 , 285, 29348-56	13

1336	Unique gating properties of C. elegans ClC anion channel splice variants are determined by altered CBS domain conformation and the R-helix linker. 2010 , 4, 289-301	8
1335	Deciphering the role of glucosamine-6-phosphate in the riboswitch action of glmS ribozyme. 2010 , 16, 2455-63	42
1334	DockFlow: Achieving interoperability of protein docking tools across heterogeneous Grid middleware. 2010 , 6, 235	3
1333	Aromatic N versus aromatic F: bioisosterism discovered in RNA base pairing interactions leads to a novel class of universal base analogs. 2010 , 38, 3133-46	35
1332	Atomistic basis for the on-off signaling mechanism in SAM-II riboswitch. 2010 , 38, 1392-400	23
1331	Identifying software usage at HPC centers with the automatic library tracking database. 2010,	4
1330	Coarse-grained models to study dynamics of nanoscale biomolecules and their applications to the ribosome. 2010 , 22, 453101	30
1329	Towards accurate free energy calculations in ligand protein-binding studies. 2010 , 17, 767-85	116
1328	Engineering bacterial cytochrome P450 (P450) BM3 into a prototype with human P450 enzyme activity using indigo formation. 2010 , 38, 732-9	48
1327	Molecular dynamics of membrane peptides and proteins: principles and comparison to experimental data. 2010 , 654, 403-21	4
1326	Dissociation of NaCl in water from ab initio molecular dynamics simulations. 2010 , 132, 114510	95
1325	Theoretical and Computational Approaches to Biomolecular Structure. 2010 , 237-264	
1324	Investigation of the catalytic mechanism of Sir2 enzyme with QM/MM approach: SN1 vs SN2?. 2010 , 114, 11927-33	19
1323	Structural basis of multivalent binding to wheat germ agglutinin. 2010 , 132, 8704-19	152
1322	Combining 3-D quantitative structure-activity relationship with ligand based and structure based alignment procedures for in silico screening of new hepatitis C virus NS5B polymerase inhibitors. 2010 , 50, 662-76	52
1321	In silico identification of the potential drug resistance sites over 2009 influenza A (H1N1) virus neuraminidase. 2010 , 7, 894-904	55
1320	Docking validation resources: protein family and ligand flexibility experiments. 2010 , 50, 1986-2000	120
1319	Structure of the p53 transactivation domain in complex with the nuclear receptor coactivator binding domain of CREB binding protein. 2010 , 49, 9964-71	129

1318	Clay minerals mediate folding and regioselective interactions of RNA: a large-scale atomistic simulation study. 2010 , 132, 13750-64	56
1317	Structure, dynamics, and energetics of siRNA-cationic vector complexation: a molecular dynamics study. 2010 , 114, 9220-30	44
1316	Association thermodynamics and conformational stability of beta-sheet amyloid beta(17-42) oligomers: effects of E22Q (Dutch) mutation and charge neutralization. 2010 , 98, 282-96	46
1315	Folding simulations of a de novo designed protein with a betaalphabeta fold. 2010 , 98, 321-9	13
1314	Statistics and physical origins of pK and ionization state changes upon protein-ligand binding. 2010 , 98, 872-80	38
1313	Molecular dynamics free energy calculations to assess the possibility of water existence in protein nonpolar cavities. 2010 , 98, 2974-83	8
1312	Structure-function perturbation and dissociation of tetrameric urate oxidase by high hydrostatic pressure. 2010 , 98, 2365-73	48
1311	MD simulations of the dsRBP DGCR8 reveal correlated motions that may aid pri-miRNA binding. 2010 , 99, 248-56	12
1310	pK(a) values for the unfolded state under native conditions explain the pH-dependent stability of PGB1. 2010 , 99, 3365-73	12
1309	Folding network of villin headpiece subdomain. 2010 , 99, 3374-84	14
1308	Structural insight into the role of thrombospondin-1 binding to calreticulin in calreticulin-induced focal adhesion disassembly. 2010 , 49, 3685-94	35
1307	Multi-Level Ewald: A hybrid multigrid / Fast Fourier Transform approach to the electrostatic particle-mesh problem. 2010 , 6, 443-58	24
1306	Cholic acid micellescontrolling the size of the aqueous cavity by PEGylation. 2010 , 12, 1589-94	12
1305	Accurate ensemble molecular dynamics binding free energy ranking of multidrug-resistant HIV-1 proteases. 2010 , 50, 890-905	70
1304	Influence of side chain conformations on local conformational features of amino acids and implication for force field development. 2010 , 114, 5840-50	36
1303	Development of molecular simulation methods to accurately represent protein-surface interactions: The effect of pressure and its determination for a system with constrained atoms. 2010 , 5, 85-95	22
1302	NSC114792, a novel small molecule identified through structure-based computational database screening, selectively inhibits JAK3. 2010 , 9, 36	13
1301	Three-dimensional molecular theory of solvation coupled with molecular dynamics in Amber. 2010 , 6, 607-624	197

1300	Crucial roles of the subnanosecond local dynamics of the flap tips in the global conformational changes of HIV-1 protease. 2010 , 114, 3060-9	26
1299	The tail wagging the dog: insights into catalysis in R67 dihydrofolate reductase. 2010 , 49, 9078-88	20
1298	Structure-based design of peptides against G3BP with cytotoxicity on tumor cells. 2010 , 50, 380-7	22
1297	Development of a rotamer library for use in beta-peptide foldamer computational design. 2010 , 132, 7312-20	30
1296	Metadynamics as a tool for mapping the conformational and free-energy space of peptidesthe alanine dipeptide case study. 2010 , 114, 5632-42	50
1295	Systematic docking study of the carbohydrate binding module protein of Cel7A with the cellulose Ialpha crystal model. 2010 , 114, 49-58	30
1294	Atmospheric implications for formation of clusters of ammonium and 1-10 water molecules. 2010 , 114, 4266-71	33
1293	Entropy localization in proteins. 2010 , 114, 16036-44	47
1292	Inhibition of pancreatic elastase by polyphenolic compounds. 2010 , 58, 10668-76	39
1291	Reducing the Secondary Structure Bias in the Generalized Born Model via R6 Effective Radii. 2010 , 6, 3613-3630	44
1290	Determination of energies and sites of binding of PFOA and PFOS to human serum albumin. 2010 , 114, 14860-74	80
1289	Interdomain interactions modulate collective dynamics of the metal-binding domains in the Wilson disease protein. 2010 , 114, 1836-48	18
1288	Merging Implicit with Explicit Solvent Simulations: Polyethylene Glycol. 2010 , 6, 1871-83	8
1287	Using molecular dynamics to probe the structural basis for enhanced stability in thermal stable cytochromes P450. 2010 , 49, 6680-6	23
1286	Dynamic origins of differential RNA binding function in two dsRBDs from the miRNA "microprocessor" complex. 2010 , 49, 10728-36	19
1285	Atomistic modeling of collagen proteins in their fibrillar environment. 2010 , 114, 13263-70	25
1284	Experimental and theoretical investigation of effect of spacer arm and support matrix of synthetic affinity chromatographic materials for the purification of monoclonal antibodies. 2010 , 114, 9367-80	28
1283	Presentation of membrane-anchored glycosphingolipids determined from molecular dynamics simulations and NMR paramagnetic relaxation rate enhancement. 2010 , 132, 1334-8	54

1282	Can peptide folding simulations provide predictive information for aggregation propensity?. 2010 , 114, 11899-908	11
1281	A revised density function for molecular surface definition in continuum solvent models. 2010 , 6, 1157-1169	25
1280	Explicit Water Models Affect the Specific Solvation and Dynamics of Unfolded Peptides While the Conformational Behavior and Flexibility of Folded Peptides Remain Intact. 2010 , 6, 3569-79	75
1279	Structure of the 1,N(2)-etheno-2'-deoxyguanosine lesion in the 3'-G(epsilon dG)T-5' sequence opposite a one-base deletion. 2010 , 49, 2615-26	8
1278	Multilevel Fragment-Based Approach (MFBA): A Novel Hybrid Computational Method for the Study of Large Molecules. 2010 , 6, 91-9	55
1277	Simulations of a protein crystal with a high resolution X-ray structure: evaluation of force fields and water models. 2010 , 114, 12811-24	61
1276	PACE Force Field for Protein Simulations. 2. Folding Simulations of Peptides. 2010 , 6, 3390-402	39
1275	Heparin mimicking polymer promotes myogenic differentiation of muscle progenitor cells. 2010 , 11, 3294-300	49
1274	Quantum mechanical pairwise decomposition analysis of protein kinase B inhibitors: validating a new tool for guiding drug design. 2010 , 50, 651-61	15
1273	HIV-1 TAR RNA spontaneously undergoes relevant apo-to-holo conformational transitions in molecular dynamics and constrained geometrical simulations. 2010 , 50, 1489-501	28
1272	Magnetic resonance studies of a redox probe in a reverse sodium bis(2-ethylhexyl)sulfosuccinate/octane/water microemulsion. 2010 , 114, 12558-64	11
1271	Monopeptide versus monopeptoid: insights on structure and hydration of aqueous alanine and sarcosine via X-ray absorption spectroscopy. 2010 , 114, 4702-9	13
127 0	What is adenine doing in photolyase?. 2010 , 114, 4101-6	37
1269	Structural basis of ubiquitin recognition by translesion synthesis DNA polymerase [2010, 49, 10198-207	25
1268	Vinylcatechin dimers are much better copigments for anthocyanins than catechin dimer procyanidin b3. 2010 , 58, 3159-66	18
1267	Molecular basis of coupled protein and electron transfer dynamics of cytochrome c in biomimetic complexes. 2010 , 132, 5769-78	61
1266	Inverse correlation of thermal lability and conversion efficiency for five prion protein polymorphic variants. 2010 , 49, 1448-59	23
1265	Exchange Often and Properly in Replica Exchange Molecular Dynamics. 2010 , 6, 2804-8	89

1264	Variation in quadrupole couplings or alpha deuterons in ubiquitin suggests the presence of C(alpha)-H(alpha)O=C hydrogen bonds. 2010 , 132, 7709-19	23
1263	Constant pH replica exchange molecular dynamics in biomolecules using a discrete protonation model. 2010 , 6, 1401-1412	79
1262	Rescue of K12G triosephosphate isomerase by ammonium cations: the reaction of an enzyme in pieces. 2010 , 132, 13525-32	34
1261	Calculations of the free energy of interaction of the c-Fos-c-Jun coiled coil: effects of the solvation model and the inclusion of polarization effects. 2010 , 50, 2201-12	14
1260	Coarse-grained model for simulation of RNA three-dimensional structures. 2010 , 114, 13497-506	73
1259	Current status of the AMOEBA polarizable force field. 2010 , 114, 2549-64	914
1258	Structure of nanoscale truncated octahedral DNA cages: variation of single-stranded linker regions and influence on assembly yields. 2010 , 4, 1367-76	42
1257	From laws of inference to protein folding dynamics. 2010 , 82, 021914	2
1256	Conformational Analysis of Arabinofuranosides: Prediction of (3)JH,H Using MD Simulations with DFT-Derived Spin-Spin Coupling Profiles. 2010 , 6, 212-22	21
1255	Origins of resistance to the HIVgp41 viral entry inhibitor T20. 2010 , 49, 3575-92	29
1254	A computational approach to the study of the binding mode of dual ACE/NEP inhibitors. 2010 , 50, 388-96	16
1253	Understanding the binding of procyanidins to pancreatic elastase by experimental and computational methods. 2010 , 49, 5097-108	33
1252	Structure-function analysis of RAMP1-RAMP3 chimeras. 2010 , 49, 522-31	7
1251	The molecular recognition mechanism for superoxide dismutase presequence binding to the mitochondrial protein import receptor Tom20 from Oryza sativa involves an LRTLA motif. 2010 , 114, 13839-46	14
1250	Balancing simulation accuracy and efficiency with the Amber united atom force field. 2010 , 114, 2886-93	8
1249	Copper-transfer mechanism from the human chaperone Atox1 to a metal-binding domain of Wilson disease protein. 2010 , 114, 3698-706	42
1248	A Mixed QM/MM Scoring Function to Predict Protein-Ligand Binding Affinity. 2010 , 6, 3079-3091	63
1247	Structural and functional characterization of the monomeric U-box domain from E4B. 2010 , 49, 347-55	27

1246	A systematic molecular dynamics study of nearest-neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA. 2010 , 38, 299-313	299
1245	Correlation analyses on binding affinity of substituted benzenesulfonamides with carbonic anhydrase using ab initio MO calculations on their complex structures. 2010 , 50, 850-60	33
1244	Molecular order in a chromonic liquid crystal: a molecular simulation study of the anionic azo dye sunset yellow. 2010 , 132, 7794-802	108
1243	The R.E.D. tools: advances in RESP and ESP charge derivation and force field library building. 2010 , 12, 7821-39	631
1242	Pairwise decomposition of residue interaction energies of single chain Fv with HIV-1 p17 epitope variants. 2010 , 47, 982-90	21
1241	Crystal structure and molecular modeling study of N-carbamoylsarcosine amidase Ta0454 from Thermoplasma acidophilum. 2010 , 169, 304-11	13
1240	Sequence-dependent DNA flexibility mediates DNase I cleavage. 2010 , 395, 123-33	34
1239	Glycine-rich loop of mitochondrial processing peptidase alpha-subunit is responsible for substrate recognition by a mechanism analogous to mitochondrial receptor Tom20. 2010 , 396, 1197-210	21
1238	Structural basis for the recognition and cleavage of polysialic acid by the bacteriophage K1F tailspike protein EndoNF. 2010 , 397, 341-51	35
1237	Solution structure of histone chaperone ANP32B: interaction with core histones H3-H4 through its acidic concave domain. 2010 , 401, 97-114	23
1236	The occluding loop of cathepsin B prevents its effective inhibition by human kininogens. 2010 , 400, 1022-35	12
1235	The unique binding mode of cellulosomal CBM4 from Clostridium thermocellum cellobiohydrolase A. 2010 , 402, 374-87	25
1234	Molecular mechanisms modulating glutamate kinase activity. Identification of the proline feedback inhibitor binding site. 2010 , 404, 890-901	20
1233	Selective and potent furin inhibitors protect cells from anthrax without significant toxicity. 2010 , 42, 987-95	33
1232	Molecular dynamics simulations of protein dynamics and their relevance to drug discovery. 2010 , 10, 738-44	109
1231	Conformational coupling, bridge helix dynamics and active site dehydration in catalysis by RNA polymerase. 2010 , 1799, 575-87	26
1230	Functional characterization of two human receptor activity-modifying protein 3 variants. 2010 , 31, 579-84	9
1229	Molecular dynamics simulations of A旷ibril interactions with 歌heet breaker peptides. 2010 , 31, 2100-8	19

1228	Carbohydrate Moieties as Vaccine Candidates: meeting summary. 2010 , 28, 1121-31	14
1227	Electronic energy changes associated with Guanine quadruplex formation: an investigation at the atomic level. 2010 , 114, 9833-9	18
1226	Statistical thermodynamics of biomembranes. 2010 , 60, 80-90	9
1225	Rapid Prediction of Solvation Free Energy. 2. The First-Shell Hydration (FiSH) Continuum Model. 2010 , 6, 1622-37	27
1224	Rapid Prediction of Solvation Free Energy. 1. An Extensive Test of Linear Interaction Energy (LIE). 2010 , 6, 1608-21	12
1223	Efficient, Regularized, and Scalable Algorithms for Multiscale Coarse-Graining. 2010 , 6, 954-65	95
1222	New insights into the structures of ligand-quadruplex complexes from molecular dynamics simulations. 2010 , 114, 15301-10	35
1221	Molecular characterization of the interaction between siRNA and PAMAM G7 dendrimers by SAXS, ITC, and molecular dynamics simulations. 2010 , 11, 3571-7	70
1220	Structure and dynamics of multiple cationic vectors-siRNA complexation by all-atomic molecular dynamics simulations. 2010 , 114, 9231-7	41
1219	Accurate predictions of water cluster formation, (HâD)(n=2-10). 2010 , 114, 11725-37	183
1219	Accurate predictions of water cluster formation, (HâD)(n=2-10). 2010 , 114, 11725-37 Computational identification of uncharacterized cruzain binding sites. 2010 , 4, e676	183
1218	Computational identification of uncharacterized cruzain binding sites. 2010 , 4, e676 Correlation analyses on binding affinity of sialic acid analogues with influenza virus	34
1218	Computational identification of uncharacterized cruzain binding sites. 2010 , 4, e676 Correlation analyses on binding affinity of sialic acid analogues with influenza virus neuraminidase-1 using ab initio MO calculations on their complex structures. 2010 , 50, 1796-805 Influence of the acetylcholinesterase active site protonation on omega loop and active site	34
1218 1217 1216	Computational identification of uncharacterized cruzain binding sites. 2010 , 4, e676 Correlation analyses on binding affinity of sialic acid analogues with influenza virus neuraminidase-1 using ab initio MO calculations on their complex structures. 2010 , 50, 1796-805 Influence of the acetylcholinesterase active site protonation on omega loop and active site dynamics. 2010 , 28, 393-403	34 35 39
1218 1217 1216 1215	Computational identification of uncharacterized cruzain binding sites. 2010, 4, e676 Correlation analyses on binding affinity of sialic acid analogues with influenza virus neuraminidase-1 using ab initio MO calculations on their complex structures. 2010, 50, 1796-805 Influence of the acetylcholinesterase active site protonation on omega loop and active site dynamics. 2010, 28, 393-403 The Sequence of HIV-1 TAR RNA Helix Controls Cationic Distributionâ 2010, 114, 5506-5512 Intramolecular cation-pi interactions as the driving force to restrict the conformation of certain	34 35 39
1218 1217 1216 1215	Computational identification of uncharacterized cruzain binding sites. 2010, 4, e676 Correlation analyses on binding affinity of sialic acid analogues with influenza virus neuraminidase-1 using ab initio MO calculations on their complex structures. 2010, 50, 1796-805 Influence of the acetylcholinesterase active site protonation on omega loop and active site dynamics. 2010, 28, 393-403 The Sequence of HIV-1 TAR RNA Helix Controls Cationic Distributionâ 2010, 114, 5506-5512 Intramolecular cation-pi interactions as the driving force to restrict the conformation of certain nucleosides. 2010, 75, 1974-81 Computer-aided identification of Trypanosoma brucei uridine diphosphate galactose 4'-epimerase	34 35 39 12 5

1210	Membrane Protein Structure Determination. 2010,	4
1209	Linking the structure and thermal stability of beta-galactoside-binding protein galectin-1 to ligand binding and dimerization equilibria. 2010 , 49, 7652-8	15
1208	Editing mechanism of aminoacyl-tRNA synthetases operates by a hybrid ribozyme/protein catalyst. 2010 , 132, 2751-8	34
1207	Advancements in Molecular Dynamics Simulations of Biomolecules on Graphical Processing Units. 2010 , 2-19	17
1206	Effect of oligonucleotide length on the assembly of DNA materials: molecular dynamics simulations of layer-by-layer DNA films. 2010 , 26, 17339-47	28
1205	Investigations of enzyme-catalysed reactions with combined quantum mechanics/molecular mechanics (QM/MM) methods. 2010 , 29, 65-133	89
1204	Comparison of intrinsic stacking energies of ten unique dinucleotide steps in A-RNA and B-DNA duplexes. Can we determine correct order of stability by quantum-chemical calculations?. 2010 , 114, 1191-203	87
1203	G-Quadruplex DNA. 2010 ,	8
1202	Explicitly solvated ligand contribution to continuum solvation models for binding free energies: selectivity of theophylline binding to an RNA aptamer. 2010 , 114, 2227-37	15
1201	Structure-activity relationships of monomeric C2-aryl pyrrolo[2,1-c][1,4]benzodiazepine (PBD) antitumor agents. 2010 , 53, 2927-41	36
1200	Towards a universal method for calculating hydration free energies: a 3D reference interaction site model with partial molar volume correction. 2010 , 22, 492101	89
1199	Determination of Three-Dimensional Structures of Nucleic Acids by NMR. 2010 , 247-278	
1198	Quantifying interactions between G-quadruplex DNA and transition-metal complexes. 2010 , 608, 223-55	6
1197	Knowledge-Guided Docking of Flexible Ligands to SH2 Domain Proteins. 2010 ,	1
1196	Comparison between molecular dynamic based and knowledge based potentials for protein side chains. 2010 , 17, 943-52	4
1195	Guanine-aspartic acid interactions probed with IR-UV resonance spectroscopy. 2010 , 12, 3597-605	14
1194	A replica-exchange approach to computing peptide conformational free energies. 2010 , 36, 505-515	3
1193	Importance of loop dynamics in the neocarzinostatin chromophore binding and release mechanisms. 2010 , 12, 3443-9	4

1192	Adenine deactivation in DNA resolved at the CASPT2//CASSCF/ AMBER level. 2010 , 12, 5016-23	71
1191	Certification of Molecular Dynamics Trajectories with NMR Chemical Shifts. 2010 , 1, 246-248	70
1190	Assignment of the vibrational spectra of enzyme-bound tryptophan tryptophyl quinones using a combined QM/MM approach. 2010 , 114, 1212-7	7
1189	Recent advances in jointed quantum mechanics and molecular mechanics calculations of biological macromolecules: schemes and applications coupled to ab initio calculations. 2010 , 22, 413101	4
1188	Charge migration through DNA molecules in the presence of mismatches. 2010 , 82,	15
1187	Evaluation of the interaction of cyclin-dependent kinase 5 with activator p25 and with p25-derived inhibitor CIP. 2010 , 17, 707-21	2
1186	Abstractions for Loosely-Coupled and Ensemble-Based Simulations on Azure. 2010,	9
1185	Crystal structure versus solution for two new lutetium thiocyanato complexes. 2011 , 35, 2755	9
1184	A molecular dynamics study of the interprotein interactions in collagen fibrils. 2011 , 7, 3373-3382	34
1183	Elastomechanical properties of resilin. 2011 , 7, 11006	12
1182	Dynamics of lysine side-chain amino groups in a protein studied by heteronuclear 1Hâd5N NMR spectroscopy. 2011 , 133, 909-19	63
1182 1181		10
	spectroscopy. 2011 , 133, 909-19 A single nucleotide polymorphism in transcobalamin II (I5V) induces structural changes in the	
1181	A single nucleotide polymorphism in transcobalamin II (I5V) induces structural changes in the protein as revealed by molecular modeling studies. 2011 , 50, 1396-402	10
1181	A single nucleotide polymorphism in transcobalamin II (I5V) induces structural changes in the protein as revealed by molecular modeling studies. 2011, 50, 1396-402 Modeling of intracellular transport and compartmentation. 2012, 127, 221-49 Insights on the permeability of wide protein channels: measurement and interpretation of ion	10 7
1181 1180 1179	A single nucleotide polymorphism in transcobalamin II (I5V) induces structural changes in the protein as revealed by molecular modeling studies. 2011, 50, 1396-402 Modeling of intracellular transport and compartmentation. 2012, 127, 221-49 Insights on the permeability of wide protein channels: measurement and interpretation of ion selectivity. 2011, 3, 159-72 Expanding the accessible chemical space by solid phase synthesis of bicyclic homodetic peptides.	10 7 44
1181 1180 1179 1178	A single nucleotide polymorphism in transcobalamin II (I5V) induces structural changes in the protein as revealed by molecular modeling studies. 2011, 50, 1396-402 Modeling of intracellular transport and compartmentation. 2012, 127, 221-49 Insights on the permeability of wide protein channels: measurement and interpretation of ion selectivity. 2011, 3, 159-72 Expanding the accessible chemical space by solid phase synthesis of bicyclic homodetic peptides. 2011, 47, 12634-6 Accounting for non-optimal interactions in molecular recognition: a study of ion-Etomplexes using	10 7 44 16

1174	Unraveling the similarity of the photoabsorption of deprotonated p-coumaric acid in the gas phase and within the photoactive yellow protein. 2011 , 13, 1585-9	37
1173	R.E.D. Server: a web service for deriving RESP and ESP charges and building force field libraries for new molecules and molecular fragments. 2011 , 39, W511-7	508
1172	3-Phosphono-L-alanine as pyrophosphate mimic for DNA synthesis using HIV-1 reverse transcriptase. 2011 , 9, 111-9	20
1171	Power shifting in Thrifty Interconnection Network. 2011 ,	14
1170	3D-RISM-KH approach for biomolecular modelling at nanoscale: thermodynamics of fibril formation and beyond. 2011 , 37, 718-728	15
1169	Comparing experimental and computational alanine scanning techniques for probing a prototypical protein-protein interaction. 2011 , 24, 197-207	62
1168	Molecular modeling of the interaction between heparan sulfate and cellular growth factors: bringing pieces together. 2011 , 21, 1181-93	39
1167	The protein folding network indicates that the ultrafast folding mutant of villin headpiece subdomain has a deeper folding funnel. 2011 , 134, 205104	12
1166	The Arabidopsis cell cycle F-box protein SKP2A binds to auxin. 2010 , 22, 3891-904	106
1165	Peptide synthesis and self-assembly. 2012 , 310, 27-69	32
	Peptide synthesis and self-assembly. 2012 , 310, 27-69 Examining docking interactions on ERK2 with modular peptide substrates. 2011 , 50, 9500-10	32 30
1164	Examining docking interactions on ERK2 with modular peptide substrates. 2011 , 50, 9500-10 A New Efficient Method for Generating Conformations of Unfolded Proteins with Diverse	30
1164	Examining docking interactions on ERK2 with modular peptide substrates. 2011 , 50, 9500-10 A New Efficient Method for Generating Conformations of Unfolded Proteins with Diverse Main-Chain Dihedral-Angle Distributions. 2011 , 7, 2126-36	30
1164 1163 1162	Examining docking interactions on ERK2 with modular peptide substrates. 2011 , 50, 9500-10 A New Efficient Method for Generating Conformations of Unfolded Proteins with Diverse Main-Chain Dihedral-Angle Distributions. 2011 , 7, 2126-36 Redox-promoting protein motions in rubredoxin. 2011 , 115, 8925-36 Molecular Mechanics Investigation of an Adenine-Adenine Non-Canonical Pair Conformational	30 4 12
1164 1163 1162 1161	Examining docking interactions on ERK2 with modular peptide substrates. 2011, 50, 9500-10 A New Efficient Method for Generating Conformations of Unfolded Proteins with Diverse Main-Chain Dihedral-Angle Distributions. 2011, 7, 2126-36 Redox-promoting protein motions in rubredoxin. 2011, 115, 8925-36 Molecular Mechanics Investigation of an Adenine-Adenine Non-Canonical Pair Conformational Change. 2011, 7, 3779-3792 EHydroxy-1,N2-propano-2'-deoxyguanosine DNA adduct conjugates the N-terminal amine of the	30 4 12
1164 1163 1162 1161 1160	Examining docking interactions on ERK2 with modular peptide substrates. 2011, 50, 9500-10 A New Efficient Method for Generating Conformations of Unfolded Proteins with Diverse Main-Chain Dihedral-Angle Distributions. 2011, 7, 2126-36 Redox-promoting protein motions in rubredoxin. 2011, 115, 8925-36 Molecular Mechanics Investigation of an Adenine-Adenine Non-Canonical Pair Conformational Change. 2011, 7, 3779-3792 EHydroxy-1,N2-propano-2'-deoxyguanosine DNA adduct conjugates the N-terminal amine of the KWKK peptide via a carbinolamine linkage. 2011, 24, 1123-33 A computational and experimental approach to investigate bepridil binding with cardiac troponin.	30 4 12 12

1156	Refinement of the Cornell et al. Nucleic Acids Force Field Based on Reference Quantum Chemical Calculations of Glycosidic Torsion Profiles. 2011 , 7, 2886-2902	569
1155	Male-specific sesquiterpenes from Phyllotreta flea beetles. 2011 , 74, 585-95	8
1154	Mechanistic studies on transcriptional coactivator protein arginine methyltransferase 1. 2011 , 50, 3332-45	38
1153	LeuRS synthetase: a first-principles investigation of the water-mediated editing reaction. 2011 , 115, 12276-86	19
1152	Molecular dynamics simulations of CXCL-8 and its interactions with a receptor peptide, heparin fragments, and sulfated linked cyclitols. 2011 , 51, 335-58	29
1151	Significant enhancement of docking sensitivity using implicit ligand sampling. 2011 , 51, 693-706	23
1150	Atomistic simulations reveal structural disorder in the RAP74-FCP1 complex. 2011 , 115, 13731-9	17
1149	On the mechanism of dimethylarginine dimethylaminohydrolase inactivation by 4-halopyridines. 2011 , 133, 10951-9	16
1148	Molecular and structural insight into the role of key residues of thrombospondin-1 and calreticulin in thrombospondin-1-calreticulin binding. 2011 , 50, 566-73	14
1147	Molecular Dynamics Simulations of the Self-Assembly of Tetraphenylporphyrin-Based Monolayers and Bilayers at a Silver Interface. 2011 , 115, 18434-18444	17
1146	Insights on the mechanism of amine oxidation catalyzed by D-arginine dehydrogenase through pH and kinetic isotope effects. 2011 , 133, 18957-65	15
1145	Importance of polar solvation for cross-reactivity of antibody and its variants with steroids. 2011 , 115, 7661-9	32
1144	Quantifying the stabilizing energy of the intraprotein hydrogen bond due to local mutation. 2011 , 115, 12230-3	20
1143	Hydration thermodynamics using the reference interaction site model: speed or accuracy?. 2011 , 115, 6011-22	53
1142	Simulative Analysis of a Truncated Octahedral DNA Nanocage Family Indicates the Single-Stranded Thymidine Linkers as the Major Player for the Conformational Variability. 2011 , 115, 16819-16827	14
1141	Theoretical study of the mechanism of proton transfer in the esterase EstB from Burkholderia gladioli. 2011 , 115, 13019-25	8
1140	Induced fit or conformational selection? The role of the semi-closed state in the maltose binding protein. 2011 , 50, 10530-9	76
1139	NMR spectroscopy and molecular dynamics simulation of r(CCGCUGCGG)âlreveal a dynamic UU internal loop found in myotonic dystrophy type 1. 2011 , 50, 599-601	23

1138	Contribution of active site residues to substrate hydrolysis by USP2: insights into catalysis by ubiquitin specific proteases. 2011 , 50, 4775-85	19
1137	Modeling DNA-bending in the nucleosome: role of AA periodicity. 2011 , 115, 8638-44	10
1136	Effect of counterions on the protonation state in a poly(G)-poly(C) radical cation. 2011 , 115, 14885-90	4
1135	Structure of the HIV-1 frameshift site RNA bound to a small molecule inhibitor of viral replication. 2011 , 6, 857-64	48
1134	Identification of RNA pseudoknot-binding ligand that inhibits the -1 ribosomal frameshifting of SARS-coronavirus by structure-based virtual screening. 2011 , 133, 10094-100	90
1133	High-temperature behavior of cellulose I. 2011 , 115, 2155-66	110
1132	Solvent interaction energy calculations on molecular dynamics trajectories: increasing the efficiency using systematic frame selection. 2011 , 51, 2680-9	20
1131	An n log n Generalized Born Approximation. 2011 , 7, 544-59	12
1130	Helix stabilization of poly(ethylene glycol)-peptide conjugates. 2011 , 12, 2729-34	49
1129	Using J-coupling constants for force field validation: application to hepta-alanine. 2011 , 115, 15221-7	20
1128	Structural Instability of the Active Site of T1 Lipase Induced by Replacement of Na(+) with Water Complexed with the Phenylalanine Aromatic Ring. 2011 , 7, 2593-9	3
1127	Formation of a N2-dG:N2-dG carbinolamine DNA cross-link by the trans-4-hydroxynonenal-derived (6S,8R,11S) 1,N2-dG adduct. 2011 , 133, 16101-10	10
1126	Halide affinity for the water-air interface in aqueous solutions of mixtures of sodium salts. 2011 , 115, 5895-9	25
1125	Predicting the Solubility of the Sparingly Soluble Solids 1,2,4,5-Tetramethylbenzene, Phenanthrene, and Fluorene in Various Organic Solvents by Molecular Simulation. 2011 , 56, 1587-1595	15
1124	An integrated computational analysis of the structure, dynamics, and ligand binding interactions of the human galectin network. 2011 , 51, 1918-30	21
1123	Alzheimer's disease drug candidates stabilize A-睁rotein native structure by interacting with the hydrophobic core. 2011 , 100, 1076-82	27
1122	Systematic examination of polymorphism in amyloid fibrils by molecular-dynamics simulation. 2011 , 100, 2234-42	46
1121	Reengineering rate-limiting, millisecond enzyme motions by introduction of an unnatural amino acid. 2011 , 101, 411-20	13

1120	Three force fields' views of the 3(10) helix. 2011 , 101, 1766-71	42
1119	Smoothing protein energy landscapes by integrating folding models with structure prediction. 2011 , 101, 2251-9	7
1118	Molecular simulation uncovers the conformational space of the ICro dimer in solution. 2011 , 101, 2516-24	11
1117	Modulation of microtubule interprotofilament interactions by modified taxanes. 2011 , 101, 2970-80	26
1116	Toward a universal model to calculate the solvation thermodynamics of druglike molecules: the importance of new experimental databases. 2011 , 8, 1423-9	36
1115	Discovering conformational sub-states relevant to protein function. 2011 , 6, e15827	53
1114	Thermodynamics of liquids: standard molar entropies and heat capacities of common solvents from 2PT molecular dynamics. 2011 , 13, 169-81	113
1113	Using molecular dynamics to study liquid phase behavior: simulations of the ternary sodium laurate/sodium oleate/water system. 2011 , 27, 11381-93	28
1112	Modeling and Simulation of Nanoscale Materials. 2011 , 175-198	
1111	Small-molecule inhibitor leads of ribosome-inactivating proteins developed using the doorstop approach. 2011 , 6, e17883	30
1110	Assessing the performance of the MM/PBSA and MM/GBSA methods. 1. The accuracy of binding free energy calculations based on molecular dynamics simulations. 2011 , 51, 69-82	1511
1109	Advances in automated NMR protein structure determination. 2011 , 44, 257-309	65
1108	Simulation studies of protein folding/unfolding equilibrium under polar and nonpolar confinement. 2011 , 133, 15157-64	48
1107	Block Covariance Overlap Method and Convergence in Molecular Dynamics Simulation. 2011 , 7, 2464-72	47
1106	Virtual screening identification of nonfolate compounds, including a CNS drug, as antiparasitic agents inhibiting pteridine reductase. 2011 , 54, 211-21	52
1105	Molecular dynamics and docking studies on cardiac troponin C. 2011 , 29, 123-35	17
1104	Coarse-graining entropy, forces, and structures. 2011 , 135, 214101	103
1103	Investigating protein variants using structural calculation techniques. 2012 , 857, 313-30	

1102	Araiosamines A-D: tris-bromoindole cyclic guanidine alkaloids from the marine sponge Clathria (Thalysias) araiosa. 2011 , 76, 5515-23	30
1101	Dynamics, flexibility and ligand-induced conformational changes in biological macromolecules: a computational approach. 2011 , 3, 2079-100	27
1100	Molecular dynamics simulation, free energy calculation and structure-based 3D-QSAR studies of B-RAF kinase inhibitors. 2011 , 51, 680-92	64
1099	Understanding the specificity of a docking interaction between JNK1 and the scaffolding protein JIP1. 2011 , 115, 1491-502	29
1098	Software and resources for computational medicinal chemistry. 2011 , 3, 1057-85	120
1097	Theoretical Investigations on the Conformation of the 粗-Arabinofuranoside Ring. 2011 , 7, 420-32	17
1096	Computational ligand-based rational design: Role of conformational sampling and force fields in model development. 2011 , 2, 356-370	58
1095	Probing the early events associated with liquid ammonia pretreatment of native crystalline cellulose. 2011 , 115, 9782-8	29
1094	Effect of solvation on the vertical ionization energy of thymine: from microhydration to bulk. 2011 , 115, 6028-38	84
1093	Drug discovery using chemical systems biology: weak inhibition of multiple kinases may contribute to the anti-cancer effect of nelfinavir. 2011 , 7, e1002037	126
1092	Catalytic chameleon dendrimers. 2011 , 133, 14359-67	49
1091	Peptide and Protein Analysis Using Ion MobilityâMass Spectrometry. 2011 , 139-174	3
1090	Combination of spectroscopic and computational methods to get an understanding of supramolecular chemistry of drugs: from simple host systems to biomolecules. 2011 , 13, 20893-905	25
1089	A normal mode-based geometric simulation approach for exploring biologically relevant conformational transitions in proteins. 2011 , 51, 1604-22	53
1088	Insight into G-DNA structural polymorphism and folding from sequence and loop connectivity through free energy analysis. 2011 , 133, 14270-9	53
1087	Computational screening and design of DNA-linked molecular nanowires. 2011 , 11, 604-8	4
1086	A Grid-enabled web portal for NMR structure refinement with AMBER. 2011 , 27, 2384-90	51
1085	Post-synthetic modification of epitaxially grown, highly oriented functionalized MOF thin films. 2011 , 47, 11210-2	52

1084	Structure of (5'S)-8,5'-cyclo-2'-deoxyguanosine in DNA. 2011 , 133, 20357-68	38
1083	Understanding the molecular mechanism of enzyme dynamics of ribonuclease A through protonation/deprotonation of HIS48. 2011 , 133, 17727-37	18
1082	Initial stage of cheese production: a molecular modeling study of bovine and camel chymosin complexed with peptides from the chymosin-sensitive region of Lasein. 2011 , 59, 5636-47	22
1081	Nonequilibrium water transport in a nonionic microemulsion system. 2011 , 115, 6503-8	1
1080	Correlation between electron localization and metal ion mutagenicity in DNA synthesis from QM/MM calculations. 2011 , 13, 11239-47	18
1079	Handling Protein Flexibility in Docking and High-Throughput Docking: From Algorithms to Applications. 2011 , 245-262	4
1078	Product formation in rhodopsin by fast hydrogen motions. 2011 , 13, 3645-8	66
1077	Secondary structures of native and pathogenic huntingtin N-terminal fragments. 2011 , 115, 11597-608	30
1076	Functional and Structural Proteomics of Glycoproteins. 2011,	7
1075	Network Biology. 2011 ,	3
1075	Network Biology. 2011, Preparation and refinement of model protein-ligand complexes. 2012, 857, 351-73	3
, ,		
1074	Preparation and refinement of model protein-ligand complexes. 2012 , 857, 351-73 Conformational flexibility and binding energy profile of c-Abl tyrosine kinase complexed with	
1074	Preparation and refinement of model protein-ligand complexes. 2012, 857, 351-73 Conformational flexibility and binding energy profile of c-Abl tyrosine kinase complexed with Imatinib: an insight from MD study. 2011, 37, 1151-1163 A negative cooperativity mechanism of human CYP2E1 inferred from molecular dynamics	11
1074 1073 1072	Preparation and refinement of model protein-ligand complexes. 2012, 857, 351-73 Conformational flexibility and binding energy profile of c-Abl tyrosine kinase complexed with Imatinib: an insight from MD study. 2011, 37, 1151-1163 A negative cooperativity mechanism of human CYP2E1 inferred from molecular dynamics simulations and free energy calculations. 2011, 51, 3217-25 Construction and test of ligand decoy sets using MDock: community structure-activity resource	11 1 31
1074 1073 1072	Preparation and refinement of model protein-ligand complexes. 2012, 857, 351-73 Conformational flexibility and binding energy profile of c-Abl tyrosine kinase complexed with Imatinib: an insight from MD study. 2011, 37, 1151-1163 A negative cooperativity mechanism of human CYP2E1 inferred from molecular dynamics simulations and free energy calculations. 2011, 51, 3217-25 Construction and test of ligand decoy sets using MDock: community structure-activity resource benchmarks for binding mode prediction. 2011, 51, 2107-14 Data-driven high-throughput prediction of the 3-D structure of small molecules: review and	11 1 31 17
1074 1073 1072 1071	Preparation and refinement of model protein-ligand complexes. 2012, 857, 351-73 Conformational flexibility and binding energy profile of c-Abl tyrosine kinase complexed with Imatinib: an insight from MD study. 2011, 37, 1151-1163 A negative cooperativity mechanism of human CYP2E1 inferred from molecular dynamics simulations and free energy calculations. 2011, 51, 3217-25 Construction and test of ligand decoy sets using MDock: community structure-activity resource benchmarks for binding mode prediction. 2011, 51, 2107-14 Data-driven high-throughput prediction of the 3-D structure of small molecules: review and progress. 2011, 51, 760-76	11 31 17

1066	Structural basis of specific binding between Aurora A and TPX2 by molecular dynamics simulations. 2011 , 51, 2626-35	6
1065	A Multibox Splitting Scheme: Robust Approximation For ab Initio Molecular Dynamics. 2011 , 7, 3872-83	2
1064	Conformational Analysis of Oligoarabinofuranosides: Overcoming Torsional Barriers with Umbrella Sampling. 2011 , 7, 2989-3000	18
1063	GROMOS++ Software for the Analysis of Biomolecular Simulation Trajectories. 2011 , 7, 3379-90	160
1062	On-the-fly Numerical Surface Integration for Finite-Difference Poisson-Boltzmann Methods. 2011 , 7, 3608-3619	21
1061	Hydrogen exchange study on the hydroxyl groups of serine and threonine residues in proteins and structure refinement using NOE restraints with polar side-chain groups. 2011 , 133, 17420-7	20
1060	Heat conductivity of DNA double helix. 2011 , 83,	37
1059	Structure of long human telomeric RNA (TERRA): G-quadruplexes formed by four and eight UUAGGG repeats are stable building blocks. 2011 , 50, 6455-61	62
1058	Least constraint approach to the extraction of internal motions from molecular dynamics trajectories of flexible macromolecules. 2011 , 135, 084110	14
1057	Normal mode analysis with molecular geometry restraints: bridging molecular mechanics and elastic models. 2011 , 508, 64-71	10
1056	Membrane binding of an acyl-lactoferricin B antimicrobial peptide from solid-state NMR experiments and molecular dynamics simulations. 2011 , 1808, 2019-30	26
1055	Role of pH on dimeric interactions for DENV envelope protein: an insight from molecular dynamics study. 2011 , 1814, 1796-801	16
1054	Structure of human telomeric DNA in crowded solution. 2011 , 133, 9824-33	264
1053	Indolylarylsulfones as HIV-1 non-nucleoside reverse transcriptase inhibitors: new cyclic substituents at indole-2-carboxamide. 2011 , 54, 1587-98	112
1052	Solvated interaction energy (SIE) for scoring protein-ligand binding affinities. 2. Benchmark in the CSAR-2010 scoring exercise. 2011 , 51, 2066-81	37
1051	Molecular dynamics study and electronic structure evolution of a DNA duplex d(CCCGATCGGG)2. 2011 , 115, 1760-6	3
1050	Assaying the Energies of Biological Halogen Bonds. 2011 , 11, 5087-5095	43
1049	Comparison of molecular dynamics simulation methods for amyloid ∰1-42) monomers containing D-aspartic acid residues for predicting retention times in chromatography. 2011 , 879, 3337-43	18

1048	Juvenile hormone synthesis: "esterify then epoxidize" or "epoxidize then esterify"? Insights from the structural characterization of juvenile hormone acid methyltransferase. 2011 , 41, 228-35	35
1047	Stabilizing the eIF4G1 Helix increases its binding affinity with eIF4E: implications for peptidomimetic design strategies. 2011 , 405, 736-53	19
1046	Solution NMR structure of Apo-calmodulin in complex with the IQ motif of human cardiac sodium channel NaV1.5. 2011 , 406, 106-19	92
1045	The recognition specificity of the CHD1 chromodomain with modified histone H3 peptides. 2011 , 406, 527-41	9
1044	Alternative allosteric mechanisms can regulate the substrate and E2 in SUMO conjugation. 2011 , 406, 620-30	8
1043	Dynamics of preferential substrate recognition in HIV-1 protease: redefining the substrate envelope. 2011 , 410, 726-44	56
1042	Molecular dynamics simulations of viral RNA polymerases link conserved and correlated motions of functional elements to fidelity. 2011 , 410, 159-81	73
1041	A concerted mechanism for opening the GDP binding pocket and release of the nucleotide in hetero-trimeric G-proteins. 2011 , 411, 298-312	26
1040	Arg149 is involved in switching the low affinity, open state of the binding protein AfProX into its high affinity, closed state. 2011 , 411, 36-52	22
1039	Allosteric drugs: the interaction of antitumor compound MKT-077 with human Hsp70 chaperones. 2011 , 411, 614-32	137
1038	Common structural traits across pathogenic mutants of the human prion protein and their implications for familial prion diseases. 2011 , 411, 700-12	54
1037	Comparison of SARS and NL63 papain-like protease binding sites and binding site dynamics: inhibitor design implications. 2011 , 414, 272-88	17
1036	Disparate degrees of hypervariable loop flexibility control T-cell receptor cross-reactivity, specificity, and binding mechanism. 2011 , 414, 385-400	56
1035	Development of CHARMM polarizable force field for nucleic acid bases based on the classical Drude oscillator model. 2011 , 115, 580-96	105
1034	New in vitro tools to study human constitutive androstane receptor (CAR) biology: discovery and comparison of human CAR inverse agonists. 2011 , 8, 2424-33	32
1033	Gyration- and inertia-tensor-based collective coordinates for metadynamics. Application on the conformational behavior of polyalanine peptides and Trp-cage folding. 2011 , 115, 11455-65	41
1032	Entropy Calculations of Single Molecules by Combining the Rigid-Rotor and Harmonic-Oscillator Approximations with Conformational Entropy Estimations from Molecular Dynamics Simulations. 2011 , 7, 2638-53	46
1031	Algorithm improvements for molecular dynamics simulations. 2011 , 1, 93-108	26

1030	Solution structure of a DNA duplex containing the potent anti-poxvirus agent cidofovir. 2011 , 133, 2264-74	23
1029	Correlation analyses on binding affinity of sialic acid analogues and anti-influenza drugs with human neuraminidase using ab initio MO calculations on their complex structuresLERE-QSAR analysis (IV). 2011 , 51, 2706-16	33
1028	Aromatic-aromatic interactions in proteins: beyond the dimer. 2011 , 51, 1623-33	93
1027	Simulating water with rigid non-polarizable models: a general perspective. 2011 , 13, 19663-88	640
1026	Free energies and folding mechanics between human prion fragment	1
1025	. 2011,	26
1024	Simulations. 2011 , 1431-1469	
1023	Virtual Screening for DNA Repair Inhibitors. 2011 ,	3
1022	Protein Modeling. 2011,	
1021	A QM/MM-based computational investigation on the catalytic mechanism of saccharopine reductase. 2011 , 16, 8569-89	6
1020	Amelogenin supramolecular assembly in nanospheres defined by a complex helix-coil-PPII helix 3D-structure. 2011 , 6, e24952	39
1019	Catalytic mechanism investigation of lysine-specific demethylase 1 (LSD1): a computational study. 2011 , 6, e25444	36
1018	Evolutionarily conserved linkage between enzyme fold, flexibility, and catalysis. 2011 , 9, e1001193	77
1017	Electrostatically biased binding of kinesin to microtubules. 2011 , 9, e1001207	45
1016	Stoichiometry of HLA class II-invariant chain oligomers. 2011 , 6, e17257	18
1015	In silico and in vitro investigations of the mutability of disease-causing missense mutation sites in spermine synthase. 2011 , 6, e20373	45
1014	Biochemical, structural and molecular dynamics analyses of the potential virulence factor RipA from Yersinia pestis. 2011 , 6, e25084	13
1013	The Energy-Based Fragmentation Approach for Ab Initio Calculations of Large Systems. 2011 , 225-258	3

1012	Drug design by generalized-ensemble simulations. 2011 , 17, 1758-72	2
1011	Modeling of HIV-1 TAR RNA-ligand complexes. 2011 , 7, 301-8	2
1010	Support vector machine based prediction of P. falciparum proteasome inhibitors and development of focused library by molecular docking. 2011 , 14, 898-907	5
1009	Molecular recognition in the case of flexible targets. 2011 , 17, 1663-71	39
1008	Probing the S1 specificity pocket of the aminopeptidases that generate antigenic peptides. 2011 , 435, 411-20	74
1007	Molecular Dynamics Study on Evaporation Coefficient of Long-Chain Molecules. 2011 , 77, 1826-1833	2
1006	Computational analysis on the binding of epitope peptide to human leukocyte antigen class I molecule A*2402 subtype. 2011 , 59, 1254-62	4
1005	Nanoinformatics: an emerging area of information technology at the intersection of bioinformatics, computational chemistry and nanobiotechnology. 2011 , 44, 43-51	23
1004	Quantum diffusive dynamics of macromolecular transitions. 2011 , 135, 034103	6
1003	Structural modelling of red cell surface proteins. 2011 , 100, 129-39	7
1003	Structural modelling of red cell surface proteins. 2011 , 100, 129-39 Intrinsic local disorder and a network of charge-charge interactions are key to actinoporin membrane disruption and cytotoxicity. 2011 , 278, 2080-9	7
	Intrinsic local disorder and a network of charge-charge interactions are key to actinoporin	
1002	Intrinsic local disorder and a network of charge-charge interactions are key to actinoporin membrane disruption and cytotoxicity. 2011 , 278, 2080-9 Assessing protein kinase selectivity with molecular dynamics and mm-pbsa binding free energy	20
1002	Intrinsic local disorder and a network of charge-charge interactions are key to actinoporin membrane disruption and cytotoxicity. 2011 , 278, 2080-9 Assessing protein kinase selectivity with molecular dynamics and mm-pbsa binding free energy calculations. 2011 , 78, 252-9 Pyrone-based inhibitors of metalloproteinase types 2 and 3 may work as conformation-selective	20
1002	Intrinsic local disorder and a network of charge-charge interactions are key to actinoporin membrane disruption and cytotoxicity. 2011 , 278, 2080-9 Assessing protein kinase selectivity with molecular dynamics and mm-pbsa binding free energy calculations. 2011 , 78, 252-9 Pyrone-based inhibitors of metalloproteinase types 2 and 3 may work as conformation-selective inhibitors. 2011 , 78, 191-8 Non-bisphosphonate inhibitors of isoprenoid biosynthesis identified via computer-aided drug	20 26 12
1002 1001 1000	Intrinsic local disorder and a network of charge-charge interactions are key to actinoporin membrane disruption and cytotoxicity. 2011 , 278, 2080-9 Assessing protein kinase selectivity with molecular dynamics and mm-pbsa binding free energy calculations. 2011 , 78, 252-9 Pyrone-based inhibitors of metalloproteinase types 2 and 3 may work as conformation-selective inhibitors. 2011 , 78, 191-8 Non-bisphosphonate inhibitors of isoprenoid biosynthesis identified via computer-aided drug design. 2011 , 78, 323-32 Influence of intramolecular interactions on conformational and dynamic properties of analogs of	20 26 12 34
1002 1001 1000 999 998	Intrinsic local disorder and a network of charge-charge interactions are key to actinoporin membrane disruption and cytotoxicity. 2011, 278, 2080-9 Assessing protein kinase selectivity with molecular dynamics and mm-pbsa binding free energy calculations. 2011, 78, 252-9 Pyrone-based inhibitors of metalloproteinase types 2 and 3 may work as conformation-selective inhibitors. 2011, 78, 191-8 Non-bisphosphonate inhibitors of isoprenoid biosynthesis identified via computer-aided drug design. 2011, 78, 323-32 Influence of intramolecular interactions on conformational and dynamic properties of analogs of heptapeptide AFP(14-20). 2011, 76, 1321-36 Molecular dynamics method for proteins with ionization-conformation coupling and equilibrium	20 26 12 34

994	Structural model and trans-interaction of the entire ectodomain of the olfactory cell adhesion molecule. 2011 , 19, 203-11	22
993	Optimal mutation sites for PRE data collection and membrane protein structure prediction. 2011 , 19, 484-95	22
992	Tracing protein evolution through ancestral structures of fish galectin. 2011 , 19, 711-21	13
991	Status of GPCR modeling and docking as reflected by community-wide GPCR Dock 2010 assessment. 2011 , 19, 1108-26	243
990	Multiscale methods for nanochemistry and biophysics in solution. 2011 , 164, 101-112	18
989	Spectral accuracy in fast Ewald-based methods for particle simulations. 2011 , 230, 8744-8761	39
988	Molecular modeling and molecular dynamics simulation studies on pyrrolopyrimidine-based ⊞elix mimetic as dual inhibitors of MDM2 and MDMX. 2011 , 30, 167-78	16
987	HBonanza: a computer algorithm for molecular-dynamics-trajectory hydrogen-bond analysis. 2011 , 31, 5-9	59
986	Identification of amino acid residues of a designed ankyrin repeat protein potentially involved in intermolecular interactions with CD4: analysis by molecular dynamics simulations. 2011 , 31, 65-75	4
985	Use of run time predictions for automatic co-allocation of multi-cluster resources for iterative parallel applications. 2011 , 71, 1388-1399	9
984	Theoretical analyses of photoinduced electron transfer in medium chain acyl-CoA dehydrogenase: Electron transfer in the normal region. 2011 , 224, 80-90	7
983	Lignans as food constituents with estrogen and antiestrogen activity. 2011 , 72, 2396-405	41
982	Discovering and validating unknown phospho-sites from p38 and HuR protein kinases in vitro by Phosphoproteomic and Bioinformatic tools. 2011 , 1, 16	9
981	Elucidating the molecular mechanism of PAMAM-siRNA dendriplex self-assembly: effect of dendrimer charge density. 2011 , 416, 410-8	71
980	Dielectric Boundary Forces in Numerical Poisson-Boltzmann Methods: Theory and Numerical Strategies. 2011 , 514, 368-373	27
979	Potentially increasing the metabolic stability of drug candidates via computational site of metabolism prediction by CYP2C9: The utility of incorporating protein flexibility via an ensemble of structures. 2011 , 46, 3953-63	22
978	P-glycoprotein limits the absorption of the anti-HIV drug zidovudine through rat intestinal segments. 2011 , 43, 151-9	20
977	Structural properties of so-called NSAID-phospholipid-complexes. 2011 , 44, 103-16	33

976	Exploring the molecular basis of dsRNA recognition by NS1 protein of influenza A virus using molecular dynamics simulation and free energy calculation. 2011 , 92, 424-33	10
975	Use of comprehensive screening methods to detect selective human CAR activators. 2011 , 82, 1994-2007	34
974	A computational analysis of the insertion of carbon nanotubes into cellular membranes. 2011 , 32, 7079-85	48
973	Synthesis, structural, and biological evaluation of bis-heteroarylmaleimides and bis-heterofused imides. 2011 , 19, 5291-9	23
972	Bioassay-guided identification of an anti-inflammatory prenylated acylphloroglucinol from Melicope ptelefolia and molecular insights into its interaction with 5-lipoxygenase. 2011 , 19, 6340-7	25
971	Disulfide and amide-bridged cyclic peptide analogues of the VEGFâBBâBIFragment: synthesis, conformational analysis and biological evaluation. 2011 , 19, 7526-33	21
970	Molecular dynamics simulations and MM/GBSA methods to investigate binding mechanisms of aminomethylpyrimidine inhibitors with DPP-IV. 2011 , 21, 6630-5	12
969	Nucleosomal DNA: Kinked, Not Kinked, or Self-Healing Material?. 2011 , 69-92	3
968	Semiempirical quantum mechanical method PM6-DH2X describes the geometry and energetics of CK2-inhibitor complexes involving halogen bonds well, while the empirical potential fails. 2011 , 115, 8581-9	75
967	Development of an optimized intermolecular potential for sulfur dioxide. 2011 , 115, 4949-54	52
966	Quaternary ∰-oxoazepane ⊞mino acids: synthesis from ornithine-derived ¶actams and incorporation into model dipeptides. 2011 , 76, 6592-603	30
965	Excited-State Electronic Structure with Configuration Interaction Singles and Tamm-Dancoff Time-Dependent Density Functional Theory on Graphical Processing Units. 2011 , 7, 1814-1823	154
964	A critical assessment of combined ligand- and structure-based approaches to HERG channel blocker modeling. 2011 , 51, 2948-60	47
963	Identification of a negative allosteric site on human 智和 and 日暮 neuronal nicotinic acetylcholine receptors. 2011 , 6, e24949	16
962	Molecular dynamics simulation and free energy calculation studies of the binding mechanism of allosteric inhibitors with p38HMAP kinase. 2011 , 51, 3235-46	63
961	Evaluation of DNA Force Fields in Implicit Solvation. 2011 , 7, 3181-3198	34
960	Conformational selection in the recognition of phosphorylated substrates by the catalytic domain of human Pin1. 2011 , 50, 9605-15	22
959	Force fields for homology modeling. 2012 , 857, 83-106	9

958	MSCALE: A General Utility for Multiscale Modeling. 2011 , 7, 1208-1219	38
957	Probing the stability-limiting regions of an antibody single-chain variable fragment: a molecular dynamics simulation study. 2011 , 24, 649-57	22
956	A molecular dynamics investigation of structure and dynamics of SDS and SDBS micelles. 2011 , 7, 9148	83
955	Accelerating molecular docking calculations using graphics processing units. 2011 , 51, 865-76	26
954	Loading of Two Related Metal-Organic Frameworks (MOFs), [Cu2(bdc)2(dabco)] and [Cu2(ndc)2(dabco)], with Ferrocene. 2011 , 3, 1565-1574	22
953	Preferential binding of peptides to graphene edges and planes. 2011 , 133, 14480-3	151
952	Why boys will be boys: two pathways of fetal testicular androgen biosynthesis are needed for male sexual differentiation. 2011 , 89, 201-18	174
951	Computer-aided drug design platform using PyMOL. 2011 , 25, 13-9	278
950	Molecular and structural determinants of adamantyl susceptibility to HLA-DRs allelic variants: an in silico approach to understand the mechanism of MLEs. 2011 , 25, 81-101	20
949	The molecular mechanism studies of chirality effect of PHA-739358 on Aurora kinase A by molecular dynamics simulation and free energy calculations. 2011 , 25, 171-80	19
948	Structural-dynamical investigation of the ZnuA histidine-rich loop: involvement in zinc management and transport. 2011 , 25, 181-94	14
947	Structure-activity relationships of diphenyl-ether as protoporphyrinogen oxidase inhibitors: insights from computational simulations. 2011 , 25, 213-22	16
946	Transferable scoring function based on semiempirical quantum mechanical PM6-DH2 method: CDK2 with 15 structurally diverse inhibitors. 2011 , 25, 223-35	46
945	Towards a rational spacer design for bivalent inhibition of estrogen receptor. 2011 , 25, 253-62	13
944	Molecular dynamics and docking simulations as a proof of high flexibility in E. coli FabH and its relevance for accurate inhibitor modeling. 2011 , 25, 371-93	15
943	VSDMIP 1.5: an automated structure- and ligand-based virtual screening platform with a PyMOL graphical user interface. 2011 , 25, 813-24	18
942	Binding of novel fullerene inhibitors to HIV-1 protease: insight through molecular dynamics and molecular mechanics Poisson-Boltzmann surface area calculations. 2011 , 25, 959-76	41
941	NMR order parameters calculated in an expanding reference frame: identifying sites of short- and long-range motion. 2011 , 50, 59-70	2

940	Binding free energy calculation with QM/MM hybrid methods for Abl-Kinase inhibitor. 2011, 37, 69-78	29
939	Neutron crystallographic and molecular dynamics studies of the structure of ammonia-cellulose I: rearrangement of hydrogen bonding during the treatment of cellulose with ammonia. 2011 , 18, 191-206	33
938	Molecular dynamics directed CoMFA studies on carbocyclic neuraminidase inhibitors. 2011 , 15, 979-87	8
937	Computational characterization of how the VX nerve agent binds human serum paraoxonase 1. 2011 , 17, 97-109	24
936	Studying the mechanism that enables paullones to selectively inhibit glycogen synthase kinase 3 rather than cyclin-dependent kinase 5 by molecular dynamics simulations and free-energy calculations. 2011 , 17, 795-803	15
935	ATP and its Nâtsubstituted analogues: parameterization, molecular dynamics simulation and conformational analysis. 2011 , 17, 1081-90	O
934	Identification of ligand binding site on RXR using molecular docking and dynamics methods. 2011 , 17, 1259-65	2
933	Multiple templates-based homology modeling enhances structure quality of AT1 receptor: validation by molecular dynamics and antagonist docking. 2011 , 17, 1565-77	32
932	Prediction of zanamivir efficiency over the possible 2009 influenza A (H1N1) mutants by multiple molecular dynamics simulations and free energy calculations. 2011 , 17, 2465-73	21
931	RNA and protein 3D structure modeling: similarities and differences. 2011 , 17, 2325-36	67
930	A comparative study of HIV-1 and HTLV-I protease structure and dynamics reveals a conserved residue interaction network. 2011 , 17, 2693-705	7
929	Exploration of the binding mode of m ype small acid soluble proteins (SASPs) with DNA. 2011 , 17, 3183-93	2
928	Molecular dynamics simulations of the growth of poly(chloro-para-xylylene) films. 2011, 17, 2725-33	4
927	Predicting binding energies of CDK6 inhibitors in the hit-to-lead process. 2011 , 128, 807-823	6
926	An MD simulation of the decoy action of EpsteinâBarr virus LMP1 protein mimicking the CD40 interaction with TRAF3. 2011 , 130, 401-410	2
925	Antigenâlntibody interactions of influenza virus hemagglutinin revealed by the fragment molecular orbital calculation. 2011 , 130, 1197-1202	16
924	Systematic mutational analysis of an ubiquitin ligase (MDM2)-binding peptide: computational studies. 2011 , 130, 1145-1154	4
923	Towards a synthetic avidin mimic. 2011 , 400, 1397-404	8

922	Molecular dynamics of ribosomal elongation factors G and Tu. 2011 , 40, 289-303	6
921	Improving the description of salt bridge strength and geometry in a Generalized Born model. 2011 , 29, 676-84	15
920	Relaxed complex scheme suggests novel inhibitors for the lyase activity of DNA polymerase beta. 2011 , 29, 702-16	31
919	Comparative CYP1A1 and CYP1B1 substrate and inhibitor profile of dietary flavonoids. 2011 , 19, 2842-9	73
918	Intramolecular hydrogen bonding in articaine can be related to superior bone tissue penetration: a molecular dynamics study. 2011 , 154, 18-25	29
917	Molecular mechanism of action for reversible P2Y12 antagonists. 2011 , 155, 74-81	10
916	The effect of pH on PAMAM dendrimer-siRNA complexation: endosomal considerations as determined by molecular dynamics simulation. 2011 , 158, 126-33	70
915	Molecular dynamics simulations and drug discovery. 2011 , 9, 71	615
914	Validating clustering of molecular dynamics simulations using polymer models. 2011 , 12, 445	23
913	FReDoWS: a method to automate molecular docking simulations with explicit receptor flexibility and snapshots selection. 2011 , 12 Suppl 4, S6	11
912	Effect of the explicit flexibility of the InhA enzyme from Mycobacterium tuberculosis in molecular docking simulations. 2011 , 12 Suppl 4, S7	13
911	Validating and improving elastic network models with molecular dynamics simulations. 2011 , 79, 23-34	41
910	A computational investigation on the role of glycosylation in the binding of alpha1 nicotinic acetylcholine receptor with two alpha-neurotoxins. 2011 , 79, 142-52	5
909	Exploring coumarin egress channels in human cytochrome P450 2A6 by random acceleration and steered molecular dynamics simulations. 2011 , 79, 271-81	70
908	Structure of the Mycobacterium tuberculosis OmpATb protein: a model of an oligomeric channel in the mycobacterial cell wall. 2011 , 79, 645-61	21
907	Dynamic communication between androgen and coactivator: mutually induced conformational perturbations in androgen receptor ligand-binding domain. 2011 , 79, 1154-71	19
906	Molecular dynamics of EF-G during translocation. 2011 , 79, 1478-86	33
905	Virtual screening using molecular simulations. 2011 , 79, 1940-51	128

(2011-2011)

904	A missense mutation in CLIC2 associated with intellectual disability is predicted by in silico modeling to affect protein stability and dynamics. 2011 , 79, 2444-54	50
903	Trifluoperazine regulation of calmodulin binding to Fas: a computational study. 2011 , 79, 2543-56	12
902	Molecular dynamics study of small molecule inhibitors of the Bcl-2 family. 2011 , 79, 2624-36	24
901	Statistical mechanics-based method to extract atomic distance-dependent potentials from protein structures. 2011 , 79, 2648-61	43
900	The active-inactive transition of human thymidylate synthase: targeted molecular dynamics simulations. 2011 , 79, 2886-99	13
899	Structural and biochemical analysis of mammalian methionine sulfoxide reductase B2. 2011 , 79, 3123-31	11
898	An optimized MM/PBSA virtual screening approach applied to an HIV-1 gp41 fusion peptide inhibitor. 2011 , 79, 3221-35	31
897	pH replica-exchange method based on discrete protonation states. 2011 , 79, 3420-36	89
896	Theoretical study on the mechanism of the DNA repair protein Fpg. 2011, 111, 2454-2463	4
895	Design of novel ligands of CDP-methylerythritol kinase by mimicking direct protein-protein and solvent-mediated interactions. 2011 , 24, 71-80	4
894	Retinal release from opsin in molecular dynamics simulations. 2011 , 24, 350-8	31
893	Human dipeptidyl peptidase III: insights into ligand binding from a combined experimental and computational approach. 2011 , 24, 804-14	18
892	Identification of selective ligands for human fibrin recognition using high-throughput docking. 2011 , 24, 824-32	
891	Docking and Molecular Dynamics Calculations of Pyrrolidinone Analog MMK16 Bound to COX and LOX Enzymes. 2011 , 30, 473-86	8
890	Addressing the Conformational Flexibility of Serine Racemase by Combining Targeted Molecular Dynamics, Conformational Sampling and Docking Studies. 2011 , 30, 317-28	6
889	Molecular Dynamics Simulations Using Graphics Processing Units. 2011 , 30, 498-504	21
888	Conformational Properties and Energetic Analysis of Aliskiren in Solution and Receptor Site. 2011 , 30, 973-85	11
887	Blind Dockings of Benzothiazoles to Multiple Receptor Conformations of Triosephosphate Isomerase from Trypanosoma cruzi and Human. 2011 , 30, 986-95	7

886	Asymmetric Synthesis of New		6
885	The role of the N-terminal domain in the regulation of the "constitutively active" conformation of protein kinase CK2&insight from a molecular dynamics investigation. 2011 , 6, 1207-16		5
884	Effect of ligand binding on the intraminimum dynamics of proteins. <i>Journal of Computational Chemistry</i> , 2011 , 32, 483-96	3.5	8
883	The first branching point in porphyrin biosynthesis: a systematic docking, molecular dynamics and quantum mechanical/molecular mechanical study of substrate binding and mechanism of uroporphyrinogen-III decarboxylase. <i>Journal of Computational Chemistry</i> , 2011 , 32, 822-34	3.5	15
882	Assessing the performance of the molecular mechanics/Poisson Boltzmann surface area and molecular mechanics/generalized Born surface area methods. II. The accuracy of ranking poses generated from docking. <i>Journal of Computational Chemistry</i> , 2011 , 32, 866-77	3.5	484
881	Multipole electrostatics in hydration free energy calculations. <i>Journal of Computational Chemistry</i> , 2011 , 32, 967-77	3.5	60
880	Crystal molecular dynamics simulations to speed up MM/PB(GB)SA evaluation of binding free energies of di-mannose deoxy analogs with P51G-m4-Cyanovirin-N. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1043-53	3.5	35
879	Non-Boltzmann sampling and Bennett's acceptance ratio method: how to profit from bending the rules. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1082-90	3.5	60
878	Wordom: a user-friendly program for the analysis of molecular structures, trajectories, and free energy surfaces. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1183-94	3.5	187
877	Specific interactions between lactose repressor protein and DNA affected by ligand binding: ab initio molecular orbital calculations. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1661-70	3.5	4
876	MDAnalysis: a toolkit for the analysis of molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2319-27	3.5	1205
875	Calculation of free energy landscapes: a histogram reweighted metadynamics approach. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2084-96	3.5	25
874	Avoiding the van der Waals endpoint problem using serial atomic insertion. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2449-58	3.5	14
873	Theoretical modulation of the color of light emitted by firefly oxyluciferin. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2654-63	3.5	28
872	Ab initio prediction of protein-ligand binding structures by replica-exchange umbrella sampling simulations. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2810-21	3.5	48
871	Molecular dynamics simulation reveals structural and thermodynamic features of kinase activation by cancer mutations within the epidermal growth factor receptor. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2843-52	3.5	21
870	Surveying implicit solvent models for estimating small molecule absolute hydration free energies. Journal of Computational Chemistry, 2011 , 32, 2909-23	3.5	58
869	Glycan Reader: automated sugar identification and simulation preparation for carbohydrates and glycoproteins. <i>Journal of Computational Chemistry</i> , 2011 , 32, 3135-41	3.5	118

(2011-2011)

868	Peptoid conformational free energy landscapes from implicit-solvent molecular simulations in AMBER. 2011 , 96, 639-50	43
867	Brownian dynamics study of the association between the 70S ribosome and elongation factor G. 2011 , 95, 616-27	18
866	Furan-oxidation-triggered inducible DNA cross-linking: acyclic versus cyclic furan-containing building blockson the benefit of restoring the cyclic sugar backbone. 2011 , 17, 6940-53	24
865	Conformational analysis of bivalent estrogen receptor ligands: from intramolecular to intermolecular binding. 2011 , 12, 2587-98	27
864	Enhanced reactivity of Lys182 explains the limited efficacy of biogenic amines in preventing the inactivation of glucose-6-phosphate dehydrogenase by methylglyoxal. 2011 , 19, 1613-22	6
863	Synthesis and biological testing of novel pyridoisothiazolones as histone acetyltransferase inhibitors. 2011 , 19, 3678-89	38
862	Correlation analyses on binding affinity of substituted benzenesulfonamides with carbonic anhydrase using ab initio MO calculations on their complex structures (II). 2011 , 21, 141-4	18
861	Structural basis for ligand recognition in a mushroom lectin: solvent structure as specificity predictor. 2011 , 346, 939-48	19
860	Assessment of dynamic properties of water around a monovalent ion: A classical molecular dynamics simulation study. 2011 , 966, 26-30	11
859	Applications of computational science for understanding enzymatic deconstruction of cellulose. 2011 , 22, 231-8	111
858	Flexibility of human cytochrome P450 enzymes: molecular dynamics and spectroscopy reveal important function-related variations. 2011 , 1814, 58-68	45
857	Effect of polarization on the stability of a helix dimer. 2011 , 501, 508-512	2
856	The DF-LCCSD(T0) correction of the Aforce field dihedral parameters significantly influences the free energy profile of the alanine dipeptide. 2011 , 503, 301-304	8
855	Molecular modelling studies on Arylthioindoles as potent inhibitors of tubulin polymerization. 2011 , 46, 3519-25	13
854	Molecular dynamics simulations of metalâdyanide complexes: Fundamental considerations in gold hydrometallurgy. 2011 , 106, 64-70	24
853	Free energy perturbation approach for the rational engineering of the antibody for human hepatitis B virus. 2011 , 29, 643-9	7
852	Exploring the conformational changes of the ATP binding site of gyrase B from Escherichia coli complexed with different established inhibitors by using molecular dynamics simulation: protein-ligand interactions in the light of the alanine scanning and free energy decomposition	33
851	methods. 2011 , 29, 726-39 The effects of amino-acid mutations on specific interactions between urokinase-type plasminogen activator and its receptor: Ab initio molecular orbital calculations. 2011 , 29, 975-84	10

850	Multiscale molecular dynamics using the matched interface and boundary method. 2011 , 230, 435-457	51
849	Interpreting protein chemical shift data. 2011 , 58, 62-87	171
848	Structure determination and dynamics of protein-RNA complexes by NMR spectroscopy. 2011 , 58, 1-61	74
847	Prediction of peptides binding to the PKA RIIalpha subunit using a hierarchical strategy. 2011 , 27, 1814-21	54
846	Novel neuraminidase inhibitors: identification, biological evaluation and investigations of the binding mode. 2011 , 3, 437-50	30
845	ClickMD: an intuitive web-oriented molecular dynamics platform. 2011 , 3, 923-31	4
844	Enabling and scaling biomolecular simulations of 100 million atoms on petascale machines with a multicore-optimized message-driven runtime. 2011 ,	16
843	Treecode-based generalized Born method. 2011 , 134, 064107	8
842	Therapeutic targeting of HCV internal ribosomal entry site RNA. 2011 , 21, 117-28	31
841	Mixed time slicing in path integral simulations. 2011 , 134, 074112	14
840	Review of computer-aided models for predicting collagen stability. 2011 , 7, 287-303	2
839	Optimization methods for virtual screening on novel computational architectures. 2011 , 7, 44-52	20
838	Explaining the varied glycosidic conformational, G-tract length and sequence preferences for anti-parallel G-quadruplexes. 2011 , 39, 4499-512	105
837	Is an intuitive convergence definition of molecular dynamics simulations solely based on the root mean square deviation possible?. 2011 , 18, 997-1005	46
836	Non-Markovian Theory of Vibrational Energy Relaxation and its Applications to Biomolecular Systems. 2011 , 1-33	6
835	Structure and stability of RNA/RNA kissing complex: with application to HIV dimerization initiation signal. 2011 , 17, 2130-43	30
834	Rapid and accurate ranking of binding affinities of epidermal growth factor receptor sequences with selected lung cancer drugs. 2011 , 8, 1114-27	29
833	Reaction of vascular adhesion protein-1 (VAP-1) with primary amines: mechanistic insights from isotope effects and quantitative structure-activity relationships. 2011 , 286, 29584-93	10

832	Crystal structures of bacterial peptidoglycan amidase AmpD and an unprecedented activation mechanism. 2011 , 286, 31714-22	41
831	Structural basis for the dual RNA-recognition modes of human Tra2-RRM. 2011 , 39, 1538-53	54
830	Integrating diffusion maps with umbrella sampling: application to alanine dipeptide. 2011 , 134, 135103	55
829	Transient binding of an activator BH3 domain to the Bak BH3-binding groove initiates Bak oligomerization. 2011 , 194, 39-48	116
828	MDpocket: open-source cavity detection and characterization on molecular dynamics trajectories. 2011 , 27, 3276-85	190
827	Calculated vibrational properties of pigments in protein binding sites. 2011 , 108, 10526-31	14
826	Mechanistic insight into human ether-^-go-go-related gene (hERG) K+ channel deactivation gating from the solution structure of the EAG domain. 2011 , 286, 6184-91	78
825	Structure and binding analysis of Polyporus squamosus lectin in complex with the Neu5Ac{alpha}2-6Gal{beta}1-4GlcNAc human-type influenza receptor. 2011 , 21, 973-84	51
824	BEAR, a novel virtual screening methodology for drug discovery. 2011 , 16, 129-33	28
823	Is N-acetyl-D-glucosamine a rigid 4C1 chair?. 2011 , 21, 1651-62	44
822	Structural and mechanistic insight into covalent substrate binding by Escherichia coli dihydroxyacetone kinase. 2011 , 108, 1302-7	32
821	Solution structure of the Zbeta domain of human DNA-dependent activator of IFN-regulatory factors and its binding modes to B- and Z-DNAs. 2011 , 108, 6921-6	30
820	Identification of a novel functional domain of ricin responsible for its potent toxicity. 2011 , 286, 12166-71	28
819	Cytokine-induced paracrystals prolong the activity of signal transducers and activators of transcription (STAT) and provide a model for the regulation of protein solubility by small ubiquitin-like modifier (SUMO). 2011 , 286, 18731-46	40
818	Communication: The electrostatic polarization is essential to differentiate the helical propensity in polyalanine mutants. 2011 , 134, 171101	20
817	Dynamic aspects of antibody:oligosaccharide complexes characterized by molecular dynamics simulations and saturation transfer difference nuclear magnetic resonance. 2011 , 21, 1570-9	16
816	Comparative modeling: the state of the art and protein drug target structure prediction. 2011, 14, 532-47	33
815	Receptors, signaling networks, and disease. 2011 , 4, mr3	3

814	Effects of backbone substitutions on the conformational behavior of Shigella flexneri O-antigens: implications for vaccine strategy. 2011 , 21, 109-21	29
813	Human 1-acylglycerol-3-phosphate O-acyltransferase isoforms 1 and 2: biochemical characterization and inability to rescue hepatic steatosis in Agpat2(-/-) gene lipodystrophic mice. 2011 , 286, 37676-91	56
812	Dietary isothiocyanate-induced apoptosis via thiol modification of DNA topoisomerase IIE 2011 , 286, 33591-600	37
811	The molecular basis of distinct aggregation pathways of islet amyloid polypeptide. 2011 , 286, 6291-300	94
810	Structure of surface layer homology (SLH) domains from Bacillus anthracis surface array protein. 2011 , 286, 26042-9	63
809	Loss of T cell antigen recognition arising from changes in peptide and major histocompatibility complex protein flexibility: implications for vaccine design. 2011 , 286, 40163-73	42
808	Probing carbohydrate product expulsion from a processive cellulase with multiple absolute binding free energy methods. 2011 , 286, 18161-9	64
807	Autocatalytic cleavage of human gamma-glutamyl transpeptidase is highly dependent on N-glycosylation at asparagine 95. 2011 , 286, 28876-28888	29
806	Protein-protein interface-binding peptides inhibit the cancer therapy target human thymidylate synthase. 2011 , 108, E542-9	66
805	Heat shock protein 70 kDa chaperone/DnaJ cochaperone complex employs an unusual dynamic interface. 2011 , 108, 18966-71	101
805 804		101
	interface. 2011 , 108, 18966-71	
804	interface. 2011, 108, 18966-71 Grids, Clouds and Virtualization. 2011, CScore: a simple yet effective scoring function for protein-ligand binding affinity prediction using	12
804	interface. 2011, 108, 18966-71 Grids, Clouds and Virtualization. 2011, CScore: a simple yet effective scoring function for protein-ligand binding affinity prediction using modified CMAC learning architecture. 2011, 9 Suppl 1, 1-14 Dual chaperone role of the C-terminal propeptide in folding and oligomerization of the	12 30
804 803 802	Grids, Clouds and Virtualization. 2011, CScore: a simple yet effective scoring function for protein-ligand binding affinity prediction using modified CMAC learning architecture. 2011, 9 Suppl 1, 1-14 Dual chaperone role of the C-terminal propeptide in folding and oligomerization of the pore-forming toxin aerolysin. 2011, 7, e1002135 Studies of new fused benzazepine as selective dopamine D3 receptor antagonists using 3D-QSAR,	12 30 45
804 803 802	Grids, Clouds and Virtualization. 2011, CScore: a simple yet effective scoring function for protein-ligand binding affinity prediction using modified CMAC learning architecture. 2011, 9 Suppl 1, 1-14 Dual chaperone role of the C-terminal propeptide in folding and oligomerization of the pore-forming toxin aerolysin. 2011, 7, e1002135 Studies of new fused benzazepine as selective dopamine D3 receptor antagonists using 3D-QSAR, molecular docking and molecular dynamics. 2011, 12, 1196-221	1230459
804 803 802 801	Grids, Clouds and Virtualization. 2011, CScore: a simple yet effective scoring function for protein-ligand binding affinity prediction using modified CMAC learning architecture. 2011, 9 Suppl 1, 1-14 Dual chaperone role of the C-terminal propeptide in folding and oligomerization of the pore-forming toxin aerolysin. 2011, 7, e1002135 Studies of new fused benzazepine as selective dopamine D3 receptor antagonists using 3D-QSAR, molecular docking and molecular dynamics. 2011, 12, 1196-221 Application-Level Interoperability Across Grids and Clouds. 2011, 199-229	12 30 45 9

796	In silico elucidation of the recognition dynamics of ubiquitin. 2011 , 7, e1002035	40
795	Mutation D816V alters the internal structure and dynamics of c-KIT receptor cytoplasmic region: implications for dimerization and activation mechanisms. 2011 , 7, e1002068	59
794	A dynamic data structure for flexible molecular maintenance and informatics. 2011 , 27, 55-62	8
793	Towards high-throughput, high-performance computational estimation of binding affinities for patient specific HIV-1 protease sequences. 2011 ,	
792	Two-dimensional replica exchange approach for peptide-peptide interactions. 2011 , 134, 064112	15
791	pH-dependent x-ray absorption spectra of aqueous boron oxides. 2011 , 134, 154503	35
790	Multiple time scale molecular dynamics for fluids with orientational degrees of freedom. I. Microcanonical ensemble. 2011 , 135, 114110	9
7 ⁸ 9	Mathematical analysis of the boundary-integral based electrostatics estimation approximation for molecular solvation: exact results for spherical inclusions. 2011 , 135, 124107	9
788	Energy-aware metrics for benchmarking heterogeneous systems. 2011 , 38, 88-94	4
787	Nucleotide binding switches the information flow in ras GTPases. 2011 , 7, e1001098	27
786	Computational methods for studying serpin conformational change and structural plasticity. 2011 , 501, 295-323	5
7 ⁸ 5	Convergent transmission of RNAi guide-target mismatch information across Argonaute internal allosteric network. 2012 , 8, e1002693	9
784	A syn-anti conformational difference allows SRSF2 to recognize guanines and cytosines equally well. 2012 , 31, 162-74	93
783	Serine phosphorylation and proline isomerization in RNAP II CTD control recruitment of Nrd1. 2012 , 26, 1891-6	76
782	A structural systems biology approach for quantifying the systemic consequences of missense mutations in proteins. 2012 , 8, e1002738	17
781	Biological applications of hybrid quantum mechanics/molecular mechanics calculation. 2012 , 2012, 236157	7
7 ⁸ 0	Recognition of asymmetrically dimethylated arginine by TDRD3. 2012 , 40, 11748-55	33
779	Coupling between catalytic loop motions and enzyme global dynamics. 2012 , 8, e1002705	35

778	Combining molecular docking and molecular dynamics to predict the binding modes of flavonoid derivatives with the neuraminidase of the 2009 H1N1 influenza A virus. 2012 , 13, 4496-507	24
777	Conformational control of the binding of the transactivation domain of the MLL protein and c-Myb to the KIX domain of CREB. 2012 , 8, e1002420	31
776	A scoring function based on solvation thermodynamics for protein structure prediction. 2012 , 8, 127-38	1
775	Target molecular simulations of RecA family protein filaments. 2012 , 13, 7138-48	2
774	Computational design of a PDZ domain peptide inhibitor that rescues CFTR activity. 2012 , 8, e1002477	89
773	Energetic selection of topology in ferredoxins. 2012 , 8, e1002463	26
77²	A Molecular Dynamics (MD) and Quantum Mechanics/Molecular Mechanics (QM/MM) study on Ornithine Cyclodeaminase (OCD): a tale of two iminiums. 2012 , 13, 12994-3011	9
771	Disease-associated mutations disrupt functionally important regions of intrinsic protein disorder. 2012 , 8, e1002709	95
770	A computational investigation on the connection between dynamics properties of ribosomal proteins and ribosome assembly. 2012 , 8, e1002530	16
769	Modeling holo-ACP:DH and holo-ACP:KR complexes of modular polyketide synthases: a docking and molecular dynamics study. 2012 , 12, 10	14
768	Ca2+ improves organization of single-stranded DNA bases in human Rad51 filament, explaining stimulatory effect on gene recombination. 2012 , 40, 4904-13	15
767	Multiple cholesterol recognition/interaction amino acid consensus (CRAC) motifs in cytosolic C tail of Slo1 subunit determine cholesterol sensitivity of Ca2+- and voltage-gated K+ (BK) channels. 2012 , 287, 20509-21	74
766	Structure of Musashi1 in a complex with target RNA: the role of aromatic stacking interactions. 2012 , 40, 3218-31	57
765	Drug hypersensitivity caused by alteration of the MHC-presented self-peptide repertoire. 2012 , 109, 9959-64	29 0
764	Solution structure of IseA, an inhibitor protein of DL-endopeptidases from Bacillus subtilis, reveals a novel fold with a characteristic inhibitory loop. 2012 , 287, 44736-48	10
763	Ca2+/calmodulin-dependent protein kinase II-based regulation of voltage-gated Na+ channel in cardiac disease. 2012 , 126, 2084-94	92
762	Structure-based analysis of the molecular recognitions between HIV-1 TAR-RNA and transcription factor nuclear factor-kappaB (NFkB). 2012 , 12, 814-27	9
761	Semiclassical evaluation of kinetic isotope effects in 13-atomic system. 2012 , 137, 134107	23

(2012-2012)

760	Plasticity of the trefoil protein fold in the recognition and control of invertebrate predators and parasites by a fungal defence system. 2012 , 8, e1002706	54
759	Modeling and simulation studies of human B adrenergic receptor and its interactions with agonists. 2012 , 8, 283-95	4
758	Permeation pathway of homomeric connexin 26 and connexin 30 channels investigated by molecular dynamics. 2012 , 29, 985-98	44
757	Combining computational chemistry and crystallography for a better understanding of the structure of cellulose. 2012 , 67, 19-93	25
756	MOLECULAR DYNAMICS SIMULATIONS OF HELIX BUNDLE PROTEINS USING UNRES FORCE FIELD AND ALL-ATOM FORCE FIELD. 2012 , 11, 1201-1215	4
755	PHF20 is an effector protein of p53 double lysine methylation that stabilizes and activates p53. 2012 , 19, 916-24	63
754	Molecular dynamics simulations for microscopic behavior of water molecules in the vicinity of zwitterionic self-assembled monolayers. 2012 , 44, 1149-1153	19
753	Structural insights into charge pair interactions in triple helical collagen-like proteins. 2012 , 287, 8039-47	61
75 ²	Cyanobacterial metallochaperone inhibits deleterious side reactions of copper. 2012 , 109, 95-100	81
751	Resolving the negative potential side (n-side) water-accessible proton pathway of F-type ATP synthase by molecular dynamics simulations. 2012 , 287, 36536-43	13
750	Product binding varies dramatically between processive and nonprocessive cellulase enzymes. 2012 , 287, 24807-13	49
749	A unique sugar-binding site mediates the distinct anti-influenza activity of pig surfactant protein D. 2012 , 287, 26666-77	19
748	Human IgA-binding peptides selected from random peptide libraries: affinity maturation and application in IgA purification. 2012 , 287, 43126-36	25
747	Identification of a small molecule that modulates platelet glycoprotein Ib-von Willebrand factor interaction. 2012 , 287, 9461-72	12
746	H++ 3.0: automating pK prediction and the preparation of biomolecular structures for atomistic molecular modeling and simulations. 2012 , 40, W537-41	876
745	Proteome-wide detection of Abl1 SH3-binding peptides by integrating computational prediction and peptide microarray. 2012 , 11, O111.010389	20
744	DR_bind: a web server for predicting DNA-binding residues from the protein structure based on electrostatics, evolution and geometry. 2012 , 40, W249-56	34
743	The role of electrostatic interactions on klentaq1 insight for domain separation. 2012 , 6, 225-34	2

742	Role of Flexibility in Protein-DNA-Drug Recognition: The Case of Asp677Gly-Val703Ile Topoisomerase Mutant Hypersensitive to Camptothecin. 2012 , 2012, 206083	12
741	Applications of Potential Energy Surfaces in the Study of Enzymatic Reactions. 2012 , 2012, 1-15	11
740	Computational analyses of the catalytic and heparin-binding sites and their interactions with glycosaminoglycans in glycoside hydrolase family 79 endo-即-glucuronidase (heparanase). 2012 , 22, 35-55	40
739	Nucleotide-dependent mechanism of Get3 as elucidated from free energy calculations. 2012 , 109, 7759-64	47
738	Fibril structure of human islet amyloid polypeptide. 2012 , 287, 5235-41	122
737	A sugar isomerization reaction established on various (胎印arrel scaffolds is based on substrate-assisted catalysis. 2012 , 25, 751-60	6
736	Biomimetic Insights: Structure-Toughness Relations in Spider Silk Nanocrystals. 2012 , 622-623, 1799-1802	2
735	NMSim web server: integrated approach for normal mode-based geometric simulations of biologically relevant conformational transitions in proteins. 2012 , 40, W310-6	64
734	Proteome-wide inference of human endophilin 1-binding peptides. 2012 , 19, 1094-102	7
733	Homology Modeling and Antagonist Binding Site Study of the Human Histamine H2 Receptor. 2012 , 8, 1084-1092	2
732	New Cathepsin D Inhibitor Library Utilizing Hydroxyethyl Isosteres with Cyclic Tertiary Amines. 2012 , 8, 1146-1154	1
731	Recent Progress in Molecular Dynamics Simulations of Dihydrofolate Reductase. 2012 , 8, 140-149	4
730	Coarse Grained Approach to First Principles Modeling of Radiation Cascade in Large Fe Supercells. 2012 , 402, 012011	1
729	Synthetic tripodal receptors for carbohydrates. Pyrrole, a hydrogen bonding partner for saccharidic hydroxyls. 2012 , 77, 7548-54	26
728	Synthesis and biological evaluation of 2-substituted-4-(3',4',5'-trimethoxyphenyl)-5-aryl thiazoles as anticancer agents. 2012 , 20, 7083-94	49
727	Rational design of peptide ligands against a glycolipid by NMR studies. 2012 , 928, 39-52	1
726	Utilizing experimental data for reducing ensemble size in flexible-protein docking. 2012 , 52, 187-98	34
725	A common single nucleotide polymorphism in endoplasmic reticulum aminopeptidase 2 induces a specificity switch that leads to altered antigen processing. 2012 , 189, 2383-92	76

(2019-2012)

724	A structural model of the E. coli PhoB dimer in the transcription initiation complex. 2012, 12, 3	3
723	Comparative binding effects of aspirin and anti-inflammatory Cu complex in the active site of LOX-1. 2012 , 52, 3293-301	8
722	Using metadynamics and path collective variables to study ligand binding and induced conformational transitions. 2012 , 819, 501-13	19
721	A toolkit and benchmark study for FRET-restrained high-precision structural modeling. 2012 , 9, 1218-25	296
720	Idealized models of protofilaments of human islet amyloid polypeptide. 2012 , 52, 2983-91	7
719	Biomolecular electrostatics and solvation: a computational perspective. 2012 , 45, 427-91	132
718	Fast estimation of solvation free energies for diverse chemical species. 2012 , 116, 3772-9	16
717	Dynamic cholesterol redistribution favors membrane fusion pore constriction.	Ο
716	Novel methods to characterise spatial distribution and enantiomeric composition of usnic acids in four Icelandic lichens 2022 , 113210	1
715	Data_Sheet_1.pdf. 2020 ,	
714	Data_Sheet_1.PDF. 2020 ,	
713	Data_Sheet_1.PDF. 2018 ,	
712	Data_Sheet_1.PDF. 2020 ,	
711	Data_Sheet_1.pdf. 2019 ,	
710	Data_Sheet_1.docx. 2019 ,	
709	Image_1.TIF. 2019 ,	
708	Image_2.TIF. 2019 ,	
707	Image_3.TIF. 2019 ,	

```
Image_4.TIF. 2019,
706
      Table_1.xlsx. 2019,
705
      Table_2.docx. 2019,
704
      Data_Sheet_1.docx. 2019,
703
      Presentation_1.pdf. 2019,
702
      Data_Sheet_1.PDF. 2020,
701
700
      Data_Sheet_1.docx. 2020,
      Data_Sheet_1.pdf. 2020,
699
698
      Data_Sheet_1.PDF. 2020,
697
      Image_1.TIF. 2018,
      Image_2.TIF. 2018,
696
      Image_3.TIF. 2018,
695
694
      Image_4.TIF. 2018,
      Image_5.TIF. 2018,
693
      Image_6.TIF. 2018,
692
691
      Image_7.TIF. 2018,
690
      Image_8.TIF. 2018,
689
      Image_9.TIF. 2018,
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688	Presentation_1.PDF. 2018 ,		
687	Table_1.DOCX. 2018 ,		
686	Data_Sheet_1.ZIP. 2019 ,		
685	Data_Sheet_2.docx. 2019 ,		
684	Data_Sheet_1.PDF. 2018 ,		
683	Table_1.XLS. 2018 ,		
682	Table_2.XLS. 2018 ,		
681	Table_3.XLS. 2018 ,		
680	Table_4.XLS. 2018 ,		
679	Table_5.XLS. 2018 ,		
678	Table_6.XLSX. 2018 ,		
677	DataSheet_1.pdf. 2019 ,		
676	prepareforleap: An automated tool for fast PDB-to-parameter generation <i>Journal of Computational Chemistry</i> , 2022 ,	3.5	
675	Promiscuous Catalytic Activity of a Binuclear: Peptide and Phosphoester Hydrolyses 2022,		1
674	Identification of potential bioactive natural compounds from Indonesian medicinal plants against 3-chymotrypsin-like protease (3CL) of SARS-CoV-2: molecular docking, ADME/T, molecular dynamic simulations, and DFT analysis 2022 , 1-18		1
673	Surface Ig variable domain glycosylation affects autoantigen binding and acts as threshold for human autoreactive B cell activation 2022 , 8, eabm1759		4
672	Genetic diversity of the melanocortin-1 receptor in an admixed population of Rio de Janeiro: Structural and functional impacts of Cys35Tyr variant 2022 , 17, e0267286		
671	Theoretical Study of the Hydrogen-Bond Interactions of CO2 in the Organic Absorbent 1,3-Diphenylguanidine.		

670	OUP accepted manuscript.	1
669	Principles of cholesterol regulation of ion channels. 2022 , 169-204	
668	OUP accepted manuscript.	О
667	Spontaneous Reactivation of OPC-Inhibited BChE Mutants: Modeling of Mechanisms. 2022 , 16, 103-108	O
666	Redox Profiling of Selected Apulian Red Wines in a Single Minute. 2022 , 11, 859	О
665	Computational Insight into Biotransformation Profiles of Organophosphorus Flame Retardants to Their Diester Metabolites by Cytochrome P450 2022 , 27,	
664	Alchemical free energy simulations without speed limits. A generic framework to calculate free energy differences independent of the underlying molecular dynamics program <i>Journal of 2.5 Computational Chemistry</i> , 2022 ,	О
663	Design and Development of Novel Nutraceuticals: Current Trends and Methodologies. 2022 , 2, 71-90	1
662	Design of D-Amino Acids SARS-CoV-2 Main Protease Inhibitors Using the Cationic Peptide from Rattlesnake Venom as a Scaffold. 2022 , 15, 540	О
661	Development of Neuropeptide Y and Cell-Penetrating Peptide MAP Adsorbed onto Lipid Nanoparticle Surface 2022 , 27,	O
660	Discovery of METTL3 Small Molecule Inhibitors by Virtual Screening of Natural Products 2022 , 13, 878135	2
659	Advancement of Computer-Aided Design Software and Simulation Tools for Nucleic Acid Nanostructures and DNA Origami. 2022 , 75-99	
658	Quantum Mechanics/Molecular Mechanics Studies on the Catalytic Mechanism of a Novel Esterase (FmtA) of 2022 ,	4
657	Drug repurposing for SARS-CoV-2: a high-throughput molecular docking, molecular dynamics, machine learning, and DFT study 2022 , 1-23	O
656	Moving Average-Based Multitasking In Silico Classification Modeling: Where Do We Stand and What Is Next?. 2022 , 23,	2
655	Endogenous pannexin1 channels form functional intercellular cell-cell channels with characteristic voltage-dependent properties 2022 , 119, e2202104119	O
654	Heteroplasmic and homoplasmic m.616T>C in mitochondria tRNAPhe promote isolated chronic kidney disease and hyperuricemia 2022 ,	1
653	Mechanism of integrin activation by talin and its cooperation with kindlin 2022 , 13, 2362	2

652	Reversible Monoacylglycerol Lipase Inhibitors: Discovery of a New Class of Benzylpiperidine Derivatives 2022 ,	O
651	Molecular modeling of lactoferrin for food and nutraceutical applications: insights from techniques 2022 , 1-24	1
650	Structure-based discovery of Licoflavone B and Ginkgetin targeting c-Myc G-quadruplex to suppress c-Myc transcription and myeloma growth 2022 ,	O
649	Force Field Dependent DNA Breathing Dynamics: A Case Study of Hoogsteen Base Pairing in A6-DNA.	
648	Nearest-Neighbor dsDNA Stability Analysis Using Alchemical Free-Energy Simulations 2022,	
647	Structural snapshots of nitrosoglutathione binding and reactivity underlying S-nitrosylation of photosynthetic GAPDH.	
646	Ensemble Simulations and Experimental Free Energy Distributions: Evaluation and Characterization of Isoxazole Amides as SMYD3 Inhibitors 2022 ,	0
645	Plant-derived active compounds as a potential nucleocapsid protein inhibitor of SARS-CoV-2: an study 2022 , 1-16	
644	Molecular basis for coordinating secondary metabolite production by bacterial and plant signaling molecules 2022 , 102027	
643	Enhanced Removal of Extracellular Microcystin-LR using Chitosan Coagulation-Ultrafiltration: Performance and Mechanisms. 2022 , 107902	O
642	Discovery and characterization of a first-in-field transcription factor BRN2 inhibitor for the treatment of neuroendocrine prostate cancer.	O
641	Stretching of Long Double-Stranded DNA and RNA Described by the Same Approach 2022,	O
640	Vaccinomics to Design a Multi-Epitopes Vaccine for 2022 , 19,	4
639	Critical Extracellular Ca Dependence of the Binding between PTH1R and a G-Protein Peptide Revealed by MD Simulations 2022 ,	O
638	Understanding the P-Loop Conformation in the Determination of Inhibitor Selectivity Toward the Hepatocellular Carcinoma-Associated Dark Kinase STK17B. 2022 , 9,	1
637	Identification of VEGFR2 as the Histatin-1 receptor in endothelial cells 2022, 115079	O
636	Conformational adjustment overcomes multiple drug-resistance mutants of tropomyosin receptor kinase 2022 , 237, 114406	O
635	Investigation of the binding and dynamic features of A.30 variant revealed higher binding of RBD for hACE2 and escapes the neutralizing antibody: A molecular simulation approach 2022 , 146, 105574	1

634	New Evidence on a Distinction between A#0 and A#2 Amyloids: Thioflavin T Binding Modes, Clustering Tendency, Degradation Resistance, and Cross-Seeding. 2022 , 23, 5513	0
633	Long-ranged heterogeneous structure in aqueous solutions of the deep eutectic solvent choline and geranate at the liquid-vapor interface.	1
632	Polymer-coated carbon nanotube hybrids with functional peptides for gene delivery into plant mitochondria 2022 , 13, 2417	1
631	Active site geometry stabilization of a presenilin homolog by the lipid bilayer promotes intramembrane proteolysis 2022 , 11,	
630	Modulation of beta-amyloid aggregation using ascorbic acid 2022,	1
629	Statistic Copolymers Working as Growth Factor-Binding Mimics of Fibronectin 2022 , e2200775	2
628	Conformational dynamics of the hepatitis B virus pre-genomic RNA on multiple time scales: implications for viral replication. 2022 , 167633	1
627	Water-Regulated Mechanisms for Degradation of Pesticides Paraoxon and Parathion by Phosphotriesterase: Insight from QM/MM and MD Simulations 2022 ,	O
626	Benchmarking Adaptive Steered Molecular Dynamics (ASMD) on CHARMM Force Fields 2022,	O
625	Talazoparib Dual-targeting on Poly (ADP-ribose) Polymerase-1 and -16 Enzymes Offers a Promising Therapeutic Strategy in Small Cell Lung Cancer Therapy: Insight from Biophysical Computations 2022 ,	O
624	Origins of glycan selectivity in streptococcal Siglec-like adhesins suggest mechanisms of receptor adaptation 2022 , 13, 2753	
623	Cholesterol binds the amphipathic helix of IFITM3 and regulates antiviral activity.	
622	Rational Design Yields Molecular Insights on Leaf-Binding of Anchor Peptides.	О
621	Cryo-EM structure of the agonist-bound Hsp90-XAP2-AHR complex.	O
620	A Proteomics-MM/PBSA Dual Approach for the Analysis of SARS-CoV-2 Main Protease Substrate Peptide Specificity. 2022 , 170814	
619	Difluorobenzene-Based Locally Concentrated Ionic Liquid Electrolyte Enabling Stable Cycling of Lithium Metal Batteries with Nickel-Rich Cathode. 2200862	7
618	LAWS: Local Alignment for Water Sites âltracking ordered water in simulations.	
617	Assessment of mutations on RBD in the Spike protein of SARS-CoV-2 Alpha, Delta and Omicron variants. 2022 , 12,	2

616	Comparative QM/MM study on the inhibition mechanism of	O
615	Multiscale Computational Modelling of MesoBioNano Systems. 2022 , 95-136	
614	Structure and Ɗynamics of Ɓio- and Macromolecules. 2022 , 137-199	
613	Multiscale Modeling of 1rradiation-Driven Chemistry Processes. 2022 , 347-388	
612	Atomistic Molecular Dynamics Simulations of DNA in Complex 3D Arrangements for Comparison with Lower Resolution Structural Experiments. 2022 , 95-109	
611	Proteome-Wide and Protein-Specific Multi-Epitope Vaccine Constructs Against the Rift Valley Fever Virus Outbreak Using Integrated Omics Approaches. 2022 , 13,	
610	Structure-based discovery of selective histone deacetylase (HDAC) 3 and 4 inhibitors.	
609	DNA Sequence Specificity Reveals a Role of the HLTF HIRAN Domain in the Recognition of Trinucleotide Repeats.	О
608	Specific Pupylation as IDEntity Reporter (SPIDER) for the identification of Protein-Biomolecule interactions.	
607	Can Membrane Composition Traffic Toxins? Mycolactone and Preferential Membrane Interactions.	
606	Markov State Modeling Analysis Captures Changes in the Temperature-Sensitive N-Terminal and 町urn Regions of the p53 DNA-Binding Domain.	
605	A conserved subunit vaccine designed against SARS-CoV-2 variants showed evidence in neutralizing the virus.	1
604	Modeling the molecular dynamics of cytochrome C in aqueous and waterâthethanol environment. 2022 , 32, 336-337	
603	Never Cared for What They Do: High Structural Stability of Guanine-Quadruplexes in the Presence of Strand-Break Damage. 2022 , 27, 3256	O
602	ADAMTS4-specific MR probe to assess aortic aneurysms in vivo using synthetic peptide libraries. 2022 , 13,	1
601	Crystal Structure of an Intramolecular Mesaconyl-Coenzyme A Transferase From the 3-Hydroxypropionic Acid Cycle of Roseiflexus castenholzii. 2022 , 13,	1
600	The structure of yeast Npl3 bound to RNA reveals a cooperative sequence-specific recognition and an RNA chaperone role in splicing.	
599	Mapping the Structural Drivers of Insulin Recognition and Specificity Using Molecular Dynamics and Free Energy Calculations.	

598	Immunoinformatics Approach Toward the Introduction of a Novel Multi-Epitope Vaccine Against Clostridium difficile. 2022 , 13,	1
597	Accelerating Ab Initio Quantum Mechanical and Molecular Mechanical (QM/MM) Molecular Dynamics Simulations with Multiple Time Step Integration and a Recalibrated Semiempirical QM/MM Hamiltonian.	
596	Classical Force-Field Parameters for CsPbBr3 Perovskite Nanocrystals.	1
595	Lysosomal dysfunction in Down Syndrome and Alzheimer mouse models is caused by selective v-ATPase inhibition by Tyr682 phosphorylated APP ETF.	1
594	Identification and validation of potent inhibitor of Escherichia coli DHFR from MMV pathogen box. 1-10	
593	Prolyl Isomerization-Mediated Conformational Changes Define ATR Subcellular Compartment-Specific Functions. 10,	O
592	Neglected N-Truncated Amyloid-₽eptide and Its Mixed Cuâ⊠n Complexes.	O
591	Staufen-2 functions as a cofactor for enhanced Rev-mediated nucleocytoplasmic trafficking of HIV-1 genomic RNA via the CRM1 pathway.	O
590	Synthesis and In Silico Evaluation of Potential Insecticide Activity of Benzamides.	
589	Multistructural Microiteration Combined with QM/MM-ONIOM Electrostatic Embedding.	
588	Uncovering the Molecular Basis for the Better Gefitinib Sensitivity of EGFR with Complex Mutations over Single Rare Mutation: Insights from Molecular Simulations. 2022 , 27, 3844	O
587	Recent advances in RNA structurome.	1
586	Identifying a Feasible Transition Pathway between Two Conformational States for a Protein.	
585	Protein structural bioinformatics: An overview. 2022 , 105695	O
584	Concentrated electrolytes enabling stable aqueous ammonium-ion batteries. 2201877	1
583	Structural basis for the unique multifaceted interaction of DPPA3 with the UHRF1 PHD finger.	
582	Identification of PRMT5 inhibitors with novel scaffold structures through virtual screening and biological evaluations. 2022 , 28,	O
581	Ionization of D571 Is Coupled with SARS-CoV-2 Spike Up/Down Equilibrium Revealing the pH-Dependent Allosteric Mechanism of Receptor-Binding Domains.	1

580	Insights into the Interaction between Polyphenols and 且actoglobulin through Molecular Docking, MD Simulation, and QM/MM Approaches.	2
579	1H, 13C, and 15N resonance assignments and solution structures of the KH domain of human ribosome binding factor A, mtRbfA, involved in mitochondrial ribosome biogenesis.	O
578	A metal ion-dependent conformational switch modulates activity of the Plasmodium M17 aminopeptidase 2022 , 102119	
577	Activation mechanism of the human Smoothened receptor.	
576	G-quadruplex structure of the C. elegans telomeric repeat: a two tetrads basket type conformation stabilized by a non-canonical Câll base-pair.	Ο
575	Automatic Learning of Hydrogen-Bond Fixes in the AMBER RNA Force Field.	3
574	Binding and unbinding pathways of peptide substrate on SARS-CoV-2 3CL protease.	O
573	Accelerators for Classical Molecular Dynamics Simulations of Biomolecules.	1
572	Toward High-level Machine Learning Potential for Water Based on Quantum Fragmentation and Neural Networks. 2022 , 126, 3926-3936	О
571	Superimmunity by pan-sarbecovirus nanobodies. 2022 , 111004	O
570	Sizing up DNA nanostructure assembly with native mass spectrometry and ion mobility. 2022, 13,	1
569	In Vitro and in Silico Analyses of the Adiponectin Receptor Agonistic Action of Soybean Tripeptides.	1
568	Molecular Rectifiers with a Very High Rectification Ratio Enabled by Oxidative Damage in Double-Stranded DNA.	
567	Solution structure of NPSL2, a regulatory element in the oncomiR-1 RNA. 2022, 167688	O
566	De Novo design of potential inhibitors against SARS-CoV-2 Mpro. 2022 , 147, 105728	1
565	Allosteric regulation of the inactive to active state conformational transition in CDPK1 protein of Plasmodium falciparum. 2022 , 215, 489-500	1
565 564		1

562	Theoretical and experimental perspectives of interaction mechanism between zein and lysozyme. 2022 , 132, 107876	1
561	Targeting Pseudomonas aeruginosa MvfR in the battle against biofilm formation: a multi-level computational approach.	
560	Behaviors of Water Molecules in Polyvinyl Alcohol Gel Amid Stretch and Temperature Changes: A Molecular Dynamics Study.	
559	Deciphering the functional mechanism of zinc ions of PARP1 binding with single strand breaks and double strand breaks. 2022 , 12, 19029-19039	
558	An intermolecular salt bridge linking substrate binding and P1 substrate specificity switch of arterivirus 3C-like proteases. 2022 , 20, 3409-3421	
557	Modularity of the hydrophobic core and evolution of functional diversity in fold A glycosyltransferases. 2022 , 102212	1
556	Small Molecules Promote Selective Denaturation and Degradation of Tubulin Heterodimers through a Low-Barrier Hydrogen Bond. 2022 , 65, 9159-9173	
555	Insights into the Allosteric Effect of SENP1 Q597A Mutation on the Hydrolytic Reaction of SUMO1 via an Integrated Computational Study. 2022 , 27, 4149	
554	Critical Evaluation of Reactive Force Fields for Vibrational Spectra: Case Study of Crystalline Cellulose I⊞	0
553	Simulation and Machine Learning Methods for Ion-Channel Structure Determination, Mechanistic Studies and Drug Design. 13,	1
552	Leveraging structural and 2D-QSAR to investigate the role of functional group substitutions, conserved surface residues and desolvation in triggering the small molecule-induced dimerization of hPD-L1. 2022 , 16,	
551	Repurposing antiviral phytochemicals from the leaf extracts of Spondias mombin (Linn) towards the identification of potential SARSCOV-2 inhibitors. 2022 , 12,	
550	Molecular Modeling Approaches Can Reveal the Molecular Interactions Established between a Biofilm and the Bioactive Compounds of the Essential Oil of Piper divaricatum. 2022 , 27, 4199	0
549	Riboflavin, a Potent Neuroprotective Vitamin: Focus on Flavivirus and Alphavirus Proteases. 2022 , 10, 1331	
548	A Physics-Guided Neural Network for Predicting Proteinâlligand Binding Free Energy: From Hostâlluest Systems to the PDBbind Database. 2022 , 12, 919	0
547	Zinc finger structure determination by NMR: why zinc fingers can be a handful. 2022,	0
546	Hinge disulfides in human IgG2 CD40 antibodies modulate receptor signaling by regulation of conformation and flexibility. 2022 , 7,	1
545	Implications of conformational flexibility, lipid binding, and regulatory domains in cell traversal-protein CelTOS for apicomplexan migration. 2022 , 102241	O

544	Insights into the structural stability of major groove RNA triplexes by WAXS-guided MD simulations. 2022 , 100971	1
543	Machine Learning and Artificial Intelligence: A paradigm shift in Big Data-Driven Drug Design and Discovery 2022 , 22,	1
542	Restoring and Enhancing the Potency of Existing Antibiotics against Drug-Resistant Gram-Negative Bacteria through the Development of Potent Small-Molecule Adjuvants.	O
541	Multifaceted Computational Modeling in Glycoscience.	7
540	An entropic safety catch controls Hepatitis C virus entry and antibody resistance. 11,	О
539	Dynamics of Human Serum Transferrin in Varying Physicochemical Conditions Explored by Using Molecular Dynamics Simulations.	
538	Cryo neutron crystallography demonstrates influence of RNA 2?-OH orientation on conformation, sugar pucker and water structure.	
537	The Effects of RNA.DNA-DNA Triple Helices on Nucleosome Structures and Dynamics.	
536	Topological bio-scaling analysis as a universal measure of protein folding. 2022, 9,	
535	Benchmarking AlphaFold for protein complex modeling reveals accuracy determinants. 2022, 31,	5
534	Structural and functional characterization of DdrC, a novel DNA damage-induced nucleoid associated protein involved in DNA compaction.	0
533	Computational analysis uncovers the deleterious SNPs along with the mutational spectrum of p53 gene and its differential expression pattern in pan-cancer. 2022 , 46,	
	gene and its annerentiate expression pattern in pair cancer, 1011 , 10,	
532	pH Effect on Ligand Binding to an Enzyme Active Site.	
532 531		
	pH Effect on Ligand Binding to an Enzyme Active Site. Structural and thermodynamics properties of pure phase alkanes, monoamides and	4
531	pH Effect on Ligand Binding to an Enzyme Active Site. Structural and thermodynamics properties of pure phase alkanes, monoamides and alkane/monoamide mixtures with an ab initio based force-field model. 2022, 119797	4
531	pH Effect on Ligand Binding to an Enzyme Active Site. Structural and thermodynamics properties of pure phase alkanes, monoamides and alkane/monoamide mixtures with an ab initio based force-field model. 2022, 119797 Zinc-Ion Hybrid Supercapacitors Employing Acetate-Based Water-in-Salt Electrolytes. 2201563	4

526	A plausible contributor to multiple sclerosis; presentation of antigenic myelin protein epitopes by major histocompatibility complexes. 2022 , 148, 105856	O
525	A review on computational approaches that support the researches on traditional Chinese medicines (TCM) against COVID-19. 2022 , 104, 154324	O
524	Discovery of novel human lactate dehydrogenase inhibitors: Structure-based virtual screening studies and biological assessment. 2022 , 240, 114605	O
523	Molecular insight into the systematic affinity and selectivity of partner recognition sites between the WW1 and WW2 domains of human KIBRA neuroprotein. 2022 , 116, 108258	
522	Eugenol Ester Derivatives: Synthesis, Insecticidal Activity and Computational Studies.	
521	Engineering of enzymes using non-natural amino acids.	
520	Synthesis, Characterization, Molecular Docking and Molecular Dynamics Simulations of Benzamide Derivatives as Potential Anti-Ovarian Cancer Agents. 2022 , 133785	10
519	Cholesterol binds the amphipathic helix of IFITM3 and regulates antiviral activity. 2022 , 167759	O
518	Mechanistic Insights into the Mechanism of Inhibitor Selectivity toward the Dark Kinase STK17B against Its High Homology STK17A. 2022 , 27, 4655	O
517	Computational Characterization of Homologous Ligands Binding to a Deep Hydrophobic Pocket in Shigella flexneri pilot protein MxiM.	
516	Performance Evaluation and Molecular Dynamics Simulation in the Liquid-Liquid Extraction Process of Low Transition Temperature Mixture +n-Hexane+1,2-Dichloroethane. 2022 , 119913	О
515	Use of Solvent Mapping for Characterizing the Binding Site and for Predicting the Inhibition of the Human Ether-EGo-Go-Related K+ Channel.	O
514	A strategy to optimize the peptide-based inhibitors against different mutants of the spike protein of SARS-CoV-2. 1-12	O
513	Computational design of a sensitive, selective phase-changing sensor protein for the VX nerve agent. 2022 , 8,	
512	Identification and structural analysis of a selective tropomyosin receptor kinase C (TRKC) inhibitor. 2022 , 241, 114601	
511	Binding mechanism of oseltamivir and influenza neuraminidase suggests perspectives for the design of new anti-influenza drugs. 2022 , 18, e1010343	
510	Estimating near-wall diffusion coefficients of arbitrarily shaped rigid macromolecules. 2022, 106,	О
509	Discovery of BRAF/HDAC Dual Inhibitors Suppressing Proliferation of Human Colorectal Cancer Cells. 10,	1

508 $\,$ Modeling of the Interaction of Cytochrome c with the Lipid Bilayer. **2022,** 67, 590-593

507	A Closed-Form, Analytical Approximation for Apparent Surface Charge and Electric Field of Molecules. 2022 , 7, 26123-26136	1
506	Structural Insights into the Role of B nAChR Subunit in the Activation of Nicotinic Receptors. 2022 , 27, 4642	0
505	Solvent Sites Improve Docking Performance of Proteinâ B rotein Complexes and Proteinâ B rotein Interface-Targeted Drugs. 2022 , 62, 3577-3588	
504	Discovery of a lectin domain that regulates enzyme activity in mouse N-acetylglucosaminyltransferase-IVa (MGAT4A). 2022 , 5,	О
503	The neuropeptide cycloprolylglycine can form a complex with AMPA receptors. 2022 , 32, 436-438	
502	Nanoscale Technologies in the Fight against COVID-19: From Innovative Nanomaterials to Computer-Aided Discovery of Potential Antiviral Plant-Derived Drugs. 2022 , 12, 1060	О
501	Computational chemistry of cluster: Understanding the mechanism of atmospheric new particle formation at the molecular level. 2022 , 136109	
500	Computational Modeling of Molecular Mechanics for the Experimentally Inclined.	
499	Natural inhibitors for severe acute respiratory syndrome coronavirus 2 main protease from Moringa oleifera, Aloe vera, and Nyctanthes arbor-tristis: molecular docking and ab initio fragment molecular orbital calculations.	О
498	Insights into the stability of engineered mini-proteins from their dynamic electronic properties.	0
497	Structural and Functional Characterization of Orcokinin B-like Neuropeptides in the Cuttlefish (Sepia officinalis). 2022 , 20, 505	
496	Binding Models of A#2 Peptide with Membranes Explored by Molecular Simulations.	2
495	CHARMM-GUI high-throughput simulator for efficient evaluation of proteinâlgand interactions with different force fields. 2022 , 31,	2
494	A Universal Framework for Featurization of Atomistic Systems. 7911-7919	О
493	TD-DFT modeling of electronic spectra of biliverdins in different environments.	
492	Preserving the Integrity of Empirical Force Fields. 2022 , 62, 3825-3831	1
491	A Fe2+-dependent self-inhibited state influences the druggability of human collagen lysyl hydroxylase (LH/PLOD) enzymes. 9,	O

490	Unraveling the Tomaralimab Epitope on the Toll-like Receptor 2 via Molecular Dynamics and Deep Learning. 2022 , 7, 28226-28237	1
489	Screening and Remodeling of Enone Oxidoreductase for High Production of 2(or 5)-Ethyl-5(or 2)-methyl-4-hydroxy-3(2H)-Furanone in Saccharomyces Cerevisiae. 2022 , 70, 9888-9897	
488	Understanding the Separation of Timescales in Rhodococcus erythropolis Proteasome Core Particle Assembly. 2022 ,	O
487	Molecularly Imprinted Nanoparticles towards MMP9 for Controlling Cardiac ECM after Myocardial Infarction: A Predictive Experimental-Computational Chemistry Investigation. 2022 , 10, 2070	2
486	Understanding gilteritinib resistance to FLT3-F691L mutation through an integrated computational strategy. 2022 , 28,	O
485	Molecular mechanisms of spontaneous curvature and softening in complex lipid bilayer mixtures. 2022 ,	O
484	Virtual Screening Identifies Novel and Potent Inhibitors of Mycobacterium tuberculosis PknB with Antibacterial Activity.	1
483	Characterizing (un)binding mechanism of USP7 inhibitors to unravel the cause of enhanced binding potencies at allosteric checkpoint. 2022 , 31,	2
482	CRISPR/Cas9-mediated F1534S substitution in the voltage-gated sodium channel reveals its necessity and sufficiency for deltamethrin resistance in Aedes albopictus.	
481	A Homozygous Missense Variant in K25 Underlying Overlapping Phenotype with Woolly Hair and Dental Anomalies. 2022 ,	O
480	Stability and Existence of Noncanonical I-motif DNA Structures in Computer Simulations Based on Atomistic and Coarse-Grained Force Fields. 2022 , 27, 4915	
479	Molecular Basis of Inhibitory Mechanism of Naltrexone and Its Metabolites through Structural and Energetic Analyses. 2022 , 27, 4919	
478	Predicting the mutation effects of proteinaligand interactions via end-point binding free energy calculations: strategies and analyses. 2022 , 14,	2
477	Total Synthesis of the Antimycobacterial Natural Product Chlorflavonin and Analogs via a Late-Stage Ruthenium(II)-Catalyzed ortho-C(sp2)-H-Hydroxylation. 2022 , 15, 984	
476	Mutagenic Activation of Glutathione Peroxidase-4: Approaches toward Rational Design of Allosteric Drugs.	O
475	Protein Design: From the Aspect of Water Solubility and Stability.	7
474	Pharmacophore-based virtual screening from phytocannabinoids as antagonist r-CB1. 2022, 28,	
473	Virulence and biofilm inhibition of 3-methoxycinnamic acid against Agrobacterium tumefaciens.	

472	Carbon Nanodots from an In Silico Perspective. 2022, 122, 13709-13799	2
471	Engineering human JMJD2A tudor domains for an improved understanding of histone peptide recognition.	
470	Evaluation of the active constituents of Nilavembu Kudineer for viral replication inhibition against SARS - CoV -2: An approach to targeting RNA -dependent RNA polymerase (RdRp).	О
469	Interdisciplinary in silico studies to understand in-depth molecular level mechanism of drug resistance involving NS3-4A protease of HCV. 1-20	
468	Phylogeny analysis of Pakistani SARS-CoV2 strains and screening of a list of natural compounds as the antiviral targets for viral M pro protein.	
467	131I-C19 Iodide Radioisotope and Synthetic I-C19 Compounds as K-Ras4BâPDE6Inhibitors: A Novel Approach against Colorectal CancerâBiological Characterization, Biokinetics and Dosimetry. 2022 , 27, 5446	1
466	Fundamental Redesign of the TIGER2hs Kernel to Address Severe Parameter Sensitivity.	2
465	A Versatile Class of 1,4,4-Trisubstituted Piperidines Block Coronavirus Replication In Vitro. 2022, 15, 1021	
464	Rational Design and Identification of Novel Piperine Derivatives as Multichitinase Inhibitors. 2022 , 70, 10326-10336	1
463	Modeling intermediates of BamA folding an outer membrane protein. 2022,	O
462	Structural Significance of Conformational Preferences and Ribose-Ring-Puckering of Hyper Modified Nucleotide 5âEMonophosphate 2-Methylthio Cyclic N6-Threonylcarbamoyladenosine (p-ms2ct6A) Present at 37th Position in Anticodon Loop of tRNALys.	
461	Potential Mechanisms of Biejiajian Pill in the Treatment of Diabetic Atherosclerosis Based on Network Pharmacology, Molecular Docking, and Molecular Dynamics Simulation. 2022 , 2022, 1-14	1
460	Prediction of Peptide-Induced Silica Formation under a Wide pH Range by Molecular Descriptors. 2022 , 130030	
459	Plant-derived compounds effectively inhibit the main protease of SARS-CoV-2: An in silico approach. 2022 , 17, e0273341	1
458	Halogenation of tyrosine perturbs large-scale protein self-organization. 2022, 13,	1
457	Discovery of natural products to block SARS-CoV-2 S-protein interaction with Neuropilin-1 receptor: A molecular dynamics simulation approach. 2022 , 170, 105701	
456	Screening of immune epitope in the proteome of the Dabie bandavirus, SFTS, to design a protein-specific and proteome-wide vaccine for immune response instigation using an immunoinformatics approaches. 2022 , 148, 105893	O
455	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	

454	A computational study to reveal selpercatinib resistance to RET kinase double mutant V804M/Y806C.	0
453	Pan-Genome-Assisted Computational Design of a Multi-Epitopes-Based Vaccine Candidate against Helicobacter cinaedi. 2022 , 19, 11579	O
452	Self-assembling branched amphiphilic peptides for targeted delivery of small molecule anticancer drugs. 2022 , 179, 137-146	O
451	Met/Val129 polymorphism of the full-length human prion protein dictates distinct pathways of amyloid formation. 2022 , 298, 102430	O
450	Structure of MotA, a flagellar stator protein, from hyperthermophile. 2022, 631, 78-85	O
449	Protein tyrosine phosphatase 1B inhibitory activity of compounds from Justicia spicigera (Acanthaceae). 2022 , 203, 113410	2
448	Combining structure-based pharmacophore modeling and machine learning for the identification of novel BTK inhibitors. 2022 , 222, 239-250	2
447	Silybin A enhances circadian clock by targeting CRY1 and disrupting its interaction with CLOCK. 2022 , 5, 100159	O
446	Computational tools for aptamer identification and optimization. 2022, 157, 116767	0
445	Residue interaction network and molecular dynamics simulation study on the binding of S239D/I332E Fc variant with enhanced affinity to FcRIIIa receptor. 2023 , 118, 108327	1
444	Recognition between CD147 and cyclophilin A deciphered by accelerated molecular dynamics simulations. 2022 , 24, 18905-18914	1
443	In-cell DNP NMR reveals multiple targeting effect of antimicrobial peptide. 2022, 6, 100074	O
442	On modeling and utilizing chemical compound information with deep learning technologies: A task-oriented approach. 2022 , 20, 4288-4304	0
441	Bioinformatics Resources, Tools, and Strategies in Designing Therapeutic Proteins. 2022 , 91-123	O
440	A molecular simulation study of hepatitis B virus core protein and the nuclear protein allosteric modulators of phthalazinone derivatives. 2022 , 24, 23209-23225	O
439	Computational Methods for Peptide Macrocycle Drug Design. 2022 , 79-161	O
438	Molecular dynamics simulation of several typical molecular ferroelectrics based on PCC charge model.	O
437	Conformational fluctuations in the molten globule state of <code>Hactalbumin</code> . 2022 , 24, 21348-21357	O

436	Proof-of-concept Study of the Secondary Structure of Influenza A, B M2, and MERS-, SARS-CoV E Transmembrane Peptides Using Folding Molecular Dynamics Simulations in Membrane Mimetic Solvent.	O
435	Effect of temperature variation on the structure of gene-translated thermostable lipase by molecular dynamic simulation. 2022 ,	O
434	In silico Molecular Docking, ADMET Property, Molecular Dynamic Simulation Evaluation of N,N?-bis(2-Hydroxybenzylidene)-1,2-diaminobenzene and its Metal Complexes against SARS-CoV-2. 2022 , 34, 2573-2582	0
433	Conformational Exchange Divergence Along the Evolutionary Pathway of Eosinophil-Associated Ribonucleases.	O
432	Probing the Energy Landscapes of Biomolecular Folding and Function. 2022 , 61-82	Ο
431	End-to-end differentiable construction of molecular mechanics force fields.	1
430	Zymography assisted quick purification, characterization and inhibition analysis of K. pneumoniae alkaline phosphatase by mercury and thiohydroxyal compounds. 2023 , 201, 106185	O
429	In-depth analysis of the interactions of various aryl hydrocarbon receptor ligands from a computational perspective. 2023 , 118, 108339	O
428	Computational investigation of peptidomimetics as potential inhibitors of SARS-CoV-2 spike protein. 1-14	O
427	Molecular explorations of the Leishmania donovani 6-phosphogluconolactonase enzyme, a key player in the pentose phosphate pathway. 2022 ,	O
426	Determination of Molecule Category of Ligands Targeting the Ligand-Binding Pocket of Nuclear Receptors with Structural Elucidation and Machine Learning. 2022 , 62, 3993-4007	1
425	Transient Crosslinking Mass Spectrometry: Taking Conformational Snapshots of Proteins.	O
424	Deciphering Conformational Changes of the GDP-Bound NRAS Induced by Mutations G13D, Q61R, and C118S through Gaussian Accelerated Molecular Dynamic Simulations. 2022 , 27, 5596	7
423	Novel Hits for N-Myristoyltransferase Inhibition Discovered by Docking-Based Screening. 2022 , 27, 5478	O
422	Applications of Molecular Dynamics Simulation in Protein Study. 2022 , 12, 844	1
421	The cancer-associated RBM39 bridges the pre-mRNA, U1 and U2 snRNPs to regulate alternative splicing.	O
420	A Molecular Mechanics Energy Partitioning Software for Biomolecular Systems. 2022 , 27, 5524	O
419	Bitosterol could serve as a dual inhibitor of Trypanosoma congolense sialidase and phospholipase A2: in vitro kinetic analyses and molecular dynamic simulations.	O

418	Assessment of Reversibility for Covalent Cysteine Protease Inhibitors Using Quantum Mechanics/Molecular Mechanics Free Energy Surfaces. 2022 , 62, 4083-4094	0
417	Structural basis for the interaction between the first SURP domain of the SF3A1 subunit in U2 snRNP and the human splicing factor SF1. 2022 , 31,	Ο
416	In Silico Study towards Repositioning of FDA-Approved Drug Candidates for Anticoronaviral Therapy: Molecular Docking, Molecular Dynamics and Binding Free Energy Calculations. 2022 , 27, 5988	2
415	Computational benchmarking of putative KIFC1 inhibitors.	Ο
414	Anticancer 5-arylidene-2-(4-hydroxyphenyl)aminothiazol-4(5 H)-ones as tubulin inhibitors.	1
413	Comprehensive evaluation of end-point free energy techniques in carboxylated-pillar[6]arene hostâguest binding: I. Standard procedure.	1
412	Structural changes and adaptative evolutionary constraints in FLOWERING LOCUS T and TERMINAL FLOWER1-like genes of flowering plants. 13,	0
411	Linker-Dependent Folding Rationalizes PROTAC Cell Permeability.	2
410	Pronounced sequence specificity of the TET enzyme catalytic domain guides its cellular function. 2022 , 8,	0
409	Contribution of Molecular Dynamics in pNMR for the Structural Determination of AnV and AnVI Complexes in Solution.	O
408	Bottom-up Coarse-Graining: Principles and Perspectives.	6
407	Microsecond MD Simulations to Explore the Structural and Energetic Differences between the Human RXR⊕PARѾs. RXR⊕PARѾNA. 2022 , 27, 5778	Ο
406	Structural insights into the elevator-type transport mechanism of a bacterial ZIP metal transporter.	0
405	Computational modelling of diatom silicic acid transporters predicts a conserved fold with implications for their function and evolution. 2022 , 184056	O
404	Probing the effect of NEK7 and cofactor interactions on dynamics of NLRP3 monomer using molecular simulation. 2022 , 31,	0
403	Modeling peptide-protein complexes: docking, simulations, and machine learning. 1-54	O
402	3dDNA: A Computational Method of Building DNA 3D Structures. 2022 , 27, 5936	1
401	Homology modeling of Forkhead box protein C2: identification of potential inhibitors using ligand and structure-based virtual screening.	Ο

400	PLAS-5k: Dataset of Protein-Ligand Affinities from Molecular Dynamics for Machine Learning Applications. 2022 , 9,	0
399	Computational Insights into the Sequence-Activity Relationships of the NGF(1â114) Peptide by Molecular Dynamics Simulations. 2022 , 11, 2808	O
398	Structural basis of adhesion GPCR GPR110 activation by stalk peptide and G-proteins coupling. 2022 , 13,	О
397	Semi-rational engineering membrane binding domain of L-amino acid deaminase from Proteus vulgaris for enhanced ⊞etoisocaproate. 13,	O
396	Combination of ligand and structure based virtual screening approaches for the discovery of potential PARP1 inhibitors. 2022 , 17, e0272065	0
395	Mechanism of enhanced sensitivity of mutated <code>adrenergic-like</code> octopamine receptor to amitraz in honeybee Apis mellifera: An insight from MD simulations.	O
394	Discovery of novel IDH1-R132C inhibitors through structure-based virtual screening. 13,	О
393	High-Resolution Conformational Analysis of RGDechi-Derived Peptides Based on a Combination of NMR Spectroscopy and MD Simulations. 2022 , 23, 11039	Ο
392	Peptidomimetics designed to bind to RAS effector domain are promising cancer therapeutic compounds. 2022 , 12,	О
391	A Novel FadL Homolog, AltL, Mediates Transport of Long-Chain Alkanes and Fatty Acids in Acinetobacter venetianus RAG-1.	O
390	Studies on the Phytochemical Profile of Ocimum basilicum var. minimum (L.) Alef. Essential Oil, Its Larvicidal Activity and In Silico Interaction with Acetylcholinesterase against Aedes aegypti (Diptera: Culicidae). 2022 , 23, 11172	О
389	RNA recognition by Npl3p reveals U2 snRNA-binding compatible with a chaperone role during splicing.	Ο
388	Machine Learning-Based Virtual Screening for the Identification of Cdk5 Inhibitors. 2022 , 23, 10653	2
387	CHARMM-GUI Implicit Solvent Modeler for Various Generalized Born Models in Different Simulation Programs. 2022 , 126, 7354-7364	Ο
386	Computational Dissection of the Role of Trp305 in the Regulation of the Death-Associated Protein Kinaseâtalmodulin Interaction. 2022 , 12, 1395	Ο
385	OCT4 interprets and enhances nucleosome flexibility.	1
384	Assessing the effect of forcefield parameter sets on the accuracy of relative binding free energy calculations. 9,	О
383	In silico high throughput screening of ZINC database of natural compounds to identify novel histone deacetylase inhibitors.	O

382	Accurate Prediction for Proteinâ B eptide Binding Based on High-Temperature Molecular Dynamics Simulations.	0
381	Computational insights into the differentiated binding affinities of Myc, Max, and Omomyc dimers to the E-boxes of DNA. 2022 , 28,	Ο
380	LAWS: Local alignment for water sitesâllracking ordered water in simulations. 2022,	О
379	CHARMM-GUI Enhanced Sampler for Various Collective Variables and Enhanced Sampling Methods.	Ο
378	Force-Field-Dependent DNA Breathing Dynamics: A Case Study of Hoogsteen Base Pairing in A6-DNA.	1
377	Structure and Diffusive Properties of Water in Polymer Hydrogels.	1
376	Pre-Training of Equivariant Graph Matching Networks with Conformation Flexibility for Drug Binding. 2203796	0
375	Comparison of the conformational dynamics of an N-glycan in implicit and explicit solvents. 2022 , 108700	Ο
374	Probabilistic Interpretation of NMR J-Couplings Determines Blâ B II State Equilibria in DNA.	0
373	A New Formulation for the Concerted Alchemical Calculation of van der Waals and Coulomb Components of Solvation Free Energies.	O
372	Regulating substrate preference of phosphatase by reshaping the âdap domainâlfor multi-enzymatic biosynthesis of high-purity monosaccharides.	0
371	Differential Boric Acid and Water Transport in Type I and Type II Pores of Arabidopsis Nodulin 26-Intrinsic Protein.	O
370	Comparison of the United- and All-Atom Representations of (Halo)alkanes Based on Two Condensed-Phase Force Fields Optimized against the Same Experimental Data Set.	2
369	Hydrogen-bonds mediate liquid-liquid phase separation of mussel derived adhesive peptides. 2022 , 13,	1
368	Computationally guided conversion of the specificity of E-selectin to mimic that of Siglec-8. 2022 , 119,	O
367	Mixed computational-experimental study to reveal the anti-metastasis and anti-angiogenesis effects of Astragalin in human breast cancer. 2022 , 150, 106131	O
366	Agathisflavone, a natural biflavonoid that inhibits SARS-CoV-2 replication by targeting its proteases. 2022 , 222, 1015-1026	2
365	Interatomic potentials: achievements and challenges. 2023, 8,	O

364	Evaluation of Novel HIV-1 Protease Inhibitors with DRV-resistance by Utilizing 3D-QSAR Molecular Docking and Molecular Dynamics Simulation.	O
363	Predicting the configuration and energy of DNA in a nucleosome by coarse-grain modelling. 2022 , 24, 26124-26133	O
362	Disrupting Cu trafficking as a potential therapy for cancer. 9,	O
361	Does Generic Cyclic Kinase Insert Domain of Receptor Tyrosine Kinase KIT Clone Its Native Homologue?. 2022 , 23, 12898	O
360	Can membrane composition traffic toxins? Mycolactone and preferential membrane interactions. 2022 ,	0
359	Bisindolylmaleimides New Ligands of CaM Protein. 2022 , 27, 7161	O
358	Improving the Synthesis Efficiency of Amino Acids Such as L-Lysine by Assembling Artificial Cellulosome Elements Dockerin Protein In Vivo. 2022 , 8, 578	0
357	Profiling of the 瞪lucosidases identified in the genome ofPenicillium funiculosum: Insights from genomics, transcriptomics, proteomics and homology modelling studies.	O
356	Multitargeted Molecular Docking and Dynamic Simulation Studies of Bioactive Compounds from Rosmarinus officinalis against Alzheimerâ Disease. 2022 , 27, 7241	O
355	On the fluorescence enhancement of arch neuronal optogenetic reporters. 2022, 13,	O
354	Establishing the catalytic and regulatory mechanism of RNA -based machineries.	O
353	Structure-Based Virtual Screening and De Novo Design to Identify Submicromolar Inhibitors of G2019S Mutant of Leucine-Rich Repeat Kinase 2. 2022 , 23, 12825	1
352	Functional variant rs12614 in CFB confers a low risk of IgA nephropathy by attenuating complement alternative pathway activation in Han Chinese. 13,	О
351	Understanding the effectiveness of enzyme pre-reaction state by a quantum-based machine learning model. 2022 , 101128	1
350	Virtual Drug Repositioning as a Tool to Identify Natural Small Molecules That Synergize with Lumacaftor in F508del-CFTR Binding and Rescuing. 2022 , 23, 12274	O
349	From plant scent defense to biopesticide discovery: Evaluation of toxicity and acetylcholinesterase docking properties for Lamiaceae monoterpenes. 2022 , 106126	1
348	mRNA-Based Vaccine Designing against Epstein-Barr Virus to Induce an Immune Response Using Immunoinformatic and Molecular Modelling Approaches. 2022 , 19, 13054	О
347	Accurate Quantum-Mechanically Derived Force-Fields through a Fragment-Based Approach: Balancing Specificity and Transferability in the Prediction of Self-Assembly in Soft Matter.	O

346	Extraction desulfurization with mixed solvents of organic solvent + organic solvent or deep eutectic solvent as extractants: Liquid-liquid equilibrium experiments and molecular dynamics simulations. 2022 , 113655	O
345	Arylcoumarin perturbs SARS-CoV-2 pathogenesis by targeting the S-protein/ACE2 interaction. 2022 , 12,	O
344	The gut microbe Bacteroides fragilis ameliorates renal fibrosis in mice. 2022, 13,	1
343	Optimization of Resveratrol Used as a Scaffold to Design Histone Deacetylase (HDAC-1 and HDAC-2) Inhibitors. 2022 , 15, 1260	О
342	Liposomal Formulations Loaded with a Eugenol Derivative for Application as Insecticides: Encapsulation Studies and In Silico Identification of Protein Targets. 2022 , 12, 3583	О
341	The emergence of protein dynamics simulations: how computational statistical mechanics met biochemistry. 2022 , 47,	O
340	Programmed Aptamer Screening, Characterization, and Rapid Detection for £Conotoxin Ml. 2022 , 14, 706	О
339	Structural insights into adhesion GPCR ADGRL3 activation and Gq, Gs, Gi, and G12 coupling. 2022 ,	O
338	HDOCK update for modeling protein- RNA / DNA complex structures. 2022, 31,	О
337	Improving Condensed-Phase Water Dynamics with Explicit Nuclear Quantum Effects: The Polarizable Q-AMOEBA Force Field. 2022 , 126, 8813-8826	1
336	Application of Molecular Dynamics to Expand Docking Programâ® Exploratory Capabilities and to Evaluate Its Predictions. 2023 , 75-101	О
335	Potential effects of metal ion induced two-state allostery on the regulatory mechanism of add adenine riboswitch. 2022 , 5,	O
334	Angiotensin converting enzyme inhibitors from medicinal plants: a molecular docking and dynamic simulation approach. 2022 , 10,	О
333	Exploring the Binding Process of Cognate Ligand to Add Adenine Riboswitch Aptamer by Using Explicit Solvent Molecular Dynamics (MD) Simulation. 2023 , 103-122	O
332	Mechanism studies of the activation of DNA methyltransferase DNMT1 triggered by histone H3 ubiquitination, revealed by multi-scale molecular dynamics simulations.	О
331	Variable Regions of p53 Isoforms Allosterically Hard Code DNA Interaction. 2022 , 126, 8495-8507	O
330	Qualitative Estimation of Proteinâlligand Complex Stability through Thermal Titration Molecular Dynamics Simulations.	4
329	Behaviors of water molecules in polyvinyl alcohol gel amid stretch and temperature changes: a molecular dynamics study. 2022 , 104834	O

328	Molecular dynamics simulation of the interaction of food proteins with small molecules. 2022, 134824	1
327	Sequence-Specific Structural Features and Solvation Properties of Transcription Factor Binding DNA Motifs: Insights from Molecular Dynamics Simulation.	О
326	Characterization of the Gateway Decarboxylase for Psilocybin Biosynthesis.	O
325	In silico study of local anesthetics analogues on sodium channel Nav 1.7 a pharmacological target on inflamed dental pulp. 2022 , 101117	O
324	An understanding of coronavirus and exploring the molecular dynamics simulations to find promising candidates against the Mpro of nCoV to combat the COVID-19: A systematic review. 2022 , 15, 1326-1349	О
323	Improving the preclinical and clinical success rates of LMW drugs depends on radical revisions to the status quo scientific foundations of medicinal chemistry: a case study on COVID Mpro inhibition.	O
322	Persistent cross-species SARS-CoV-2 variant infectivity predicted via comparative molecular dynamics simulation. 2022 , 9,	О
321	Unravelling viral dynamics through molecular dynamics simulations - A brief overview. 2022 , 291, 106908	1
320	Peptide inhibitors of angiotensin-I converting enzyme based on angiotensin (1â11) with selectivity for the C-terminal domain. 2022 , 129, 106204	О
319	Discovery and optimization of 4-anilinoquinazoline derivatives spanning ATP binding site and allosteric site as effective EGFR-C797S inhibitors. 2022 , 244, 114856	O
318	Thyroid hormone activities of neutral and anionic hydroxylated polybrominated diphenyl ethers to thyroid receptor #A molecular dynamics study. 2023 , 311, 136920	0
317	Structural and energetic basis of interaction between human estrogen-related receptor land environmental endocrine disruptors from multiple molecular dynamics simulations and free energy predictions. 2023, 443, 130174	3
316	Interaction mechanism between zein and <code>#actoglobulin</code> : Insights from multi-spectroscopy and molecular dynamics simulation methods. 2023 , 135, 108226	1
315	Biochemical characterization and molecular insights into substrate recognition of pectin methylesterase from Phytophthora infestans. 2022 , 20, 6023-6032	O
314	The impact of simulation time in predicting binding free energies using end-point approaches. 2022 , 20,	1
313	Molecular Dynamics with Conformationally Dependent, Distributed Charges.	O
312	Molecular Dynamics Methods for Antibody Design. 2023 , 109-124	О
311	Molecular Dynamics Simulations of the Cardiac Ryanodine Receptor Type 2 (RyR2) Gating Mechanism.	O

310	Quantifying the Effects of Lossy Compression on Energies Calculated from Molecular Dynamics Trajectories.	О
309	pH Regulates Ligand Binding to an Enzyme Active Site by Modulating Intermediate Populations.	Ο
308	Cryo-EM structure of the agonist-bound Hsp90-XAP2-AHR cytosolic complex. 2022, 13,	1
307	Complexes++: Efficient and versatile coarse-grained simulations of protein complexes and their dense solutions.	O
306	A Rapid and Sensitive Aptamer-Based Biosensor for Amnesic Shellfish Toxin Domoic Acid. 2022 , 9, 684	0
305	Identification of Small Molecular Chaperones Binding P23H Mutant Opsin through an In Silico Structure-Based Approach.	1
304	Characterization of binding properties of ephedrine derivatives to human alpha-1-acid glycoprotein. 2022 , 106333	Ο
303	Efficient Interrogation of the Kinetic Barriers Demarcating Catalytic States of a Tyrosine Kinase with Optimal Physical Descriptors and Mixture Models.	Ο
302	Selectivity and ranking of tight-binding JAK-STAT inhibitors using Markovian milestoning with Voronoi tessellations.	0
301	Understanding VPAC receptor family peptide binding and selectivity. 2022, 13,	Ο
300	Insight into the Inhibitory Mechanism of Aryl Formyl Piperidine Derivatives on Monoacylglycerol Lipase through Molecular Dynamics Simulations. 2022 , 27, 7512	0
299	Binding selectivity-dependent molecular mechanism of inhibitors towards CDK2 and CDK6 investigated by multiple short molecular dynamics and free energy landscapes. 2023 , 38, 84-99	3
298	Dynamic and thermodynamic impact of L94A, W100A, and W100L mutations on the D2 dopamine receptor bound to risperidone.	0
297	Comprehensive evaluation of end-point free energy techniques in carboxylated-pillar[6]arene hostâguest binding: II. regression and dielectric constant.	2
296	Could artificial intelligence revolutionize the development of nanovectors for gene therapy and mRNA vaccines?. 2022 , 47, 101665	O
295	A redox switch regulates the assembly and anti-CRISPR activity of AcrIIC1. 2022, 13,	O
294	p38EKinase Auto-Activation through Its Conformational Transition Induced by Tyr323 Phosphorylation.	1
293	Structure-Guided Design of Halofuginone Derivatives as ATP-Aided Inhibitors Against Bacterial Prolyl-tRNA Synthetase.	O

292	Inter-Site Cooperativity of Calmodulin N-Terminal Domain and Phosphorylation Synergistically Improve the Affinity and Selectivity for Uranyl. 2022 , 12, 1703	O
291	Enhancing Biomolecular Simulations with Hybrid Potentials Incorporating NMR Data.	O
29 0	Correlated Coevolving Mutations at Proteinâ B rotein Interfaces. 2022 , 39-52	O
289	How binding to surfaces affects disorder?. 2023 , 455-489	O
288	Molecular basis of ssDNA recognition by RBM45 protein of neurodegenerative disease from multiple molecular dynamics simulations and energy predictions. 2022 , 108377	0
287	Dynamic and thermodynamic impact of L94A, W100A, and W100L mutations on the D2 dopamine receptor bound to risperidone. 2022 , 12, 34359-34368	O
286	Bispecific antibodiesâlffects of point mutations on CH3-CH3 interface stability. 2022, 35,	0
285	Discovery of allosteric SHP2 inhibitors through ensemble-based consensus molecular docking, endpoint and absolute binding free energy calculations. 2023 , 152, 106442	O
284	A novel binding site in the nicotinic acetylcholine receptor for MB327 can explain its allosteric modulation relevant for organophosphorus-poisoning treatment. 2023 , 373, 160-171	0
283	Role of supramolecular steric compression during photoinduced intramolecular hydrogen abstraction reactions of ketones and thioketones. 2023 , 437, 114442	O
282	New insights into the effect of mutations on affibody-Fc interaction, a molecular dynamics simulation approach. 2023 , 215, 107925	O
281	Structural basis of Nrf2 activation by flavonolignans from silymarin. 2023 , 119, 108393	O
280	Identification and Characterization of a Novel Dual Inhibitor of Indoleamine 2,3-dioxygenase 1 and Tryptophan 2,3-dioxygenase. 2022 , 15, 117864692211384	0
279	Structural and conformational dynamics of human milk oligosaccharides, lacto-N-fucopentaose I and II, through molecular dynamics simulation. 2022 , 41, 385-404	O
278	Investigating RNAâprotein recognition mechanisms through supervised molecular dynamics (SuMD) simulations. 2022 , 4,	2
277	Orthogonal glycolytic pathway enables directed evolution of noncanonical cofactor oxidase. 2022 , 13,	O
276	A universal graph deep learning interatomic potential for the periodic table. 2022, 2, 718-728	0
275	Reverse engineering approach: a step towards a new era of vaccinology with special reference to Salmonella. 2022 , 21, 1763-1785	O

274	Deciphering the impact of Mutations in the RBD of the Omicron Variant (BA.2) with Medicinal compound to disrupt the RBD-hACE2 complex using computational approaches.	О
273	QM/MM Investigation to Identify the Hallmarks of Superior PET Biodegradation Activity of PETase over Cutinase. 2022 , 10, 15857-15868	Ο
272	Wound Healing Potential and In Silico Appraisal of Convolvulus arvensis L. Methanolic Extract. 2022 , 2022, 1-16	0
271	Molecular Dynamics Simulation of the Thermal Behavior of Hydroxyapatite. 2022 , 12, 4244	Ο
270	Boosting the Full Potential of PyMOL with Structural Biology Plugins. 2022 , 12, 1764	2
269	Computational screening of natural products to identify potential inhibitors for human neuropilin-1 (NRP1) receptor to abrogate the binding of SARS-CoV-2 and host cell. 1-10	Ο
268	Combinatorial Oligonucleotide FISH (COMBO-FISH): Computer Designed Probe Sets for Microscopy Research of Chromatin in Cell Nuclei.	0
267	PHARMACOKINETIC PREDICTIONS AND MOLECULAR DYNAMIC ANALYSIS OF TERPENOID AND FLAVONOID COMPOUNDS FROM MIANA LEAVES (PLECTRANTHUS SCUTELLARIOIDES (L.) R. BR.) AS AN ANTIMALARIAL CANDIDATES ON PLASMEPSIN II RECEPTOR. 142-150	Ο
266	Computational Study of Helicase from SARS-CoV-2 in RNA-Free and Engaged Form. 2022 , 23, 14721	0
265	Evolution of drug resistance drives progressive destabilizations in functionally conserved molecular dynamics of the flap region of the HIV-1 protease.	Ο
264	Effects of Conformational Constraint on Peptide Solubility Limits. 2022, 126, 10510-10518	0
263	Deciphering the active constituents of Dabushen decoction of ameliorating osteoarthritis via PPARIpreservation by targeting DNMT1. 13,	Ο
262	Molecular dynamics and free energy calculations of clozapine bound to D2 and H1 receptors reveal a cardiometabolic mitigated derivative. 1-13	0
261	Biological Characterization of Natural Peptide BcI-1003 from Boana cordobae (anura): Role in Alzheimerâ Disease and Microbial Infections. 2023 , 29,	O
260	Structural basis for the unique multifaceted interaction of DPPA3 with the UHRF1 PHD finger. 2022 , 50, 12527-12542	O
259	N-Terminally Lipidated Sialorphin Analogsâßynthesis, Molecular Modeling, In Vitro Effect on Enkephalins Degradation by NEP and Treatment of Intestinal Inflammation in Mice. 2022 , 23, 14450	O
258	Molecular basis for anti-insomnia drug design from structure of lemborexant-bound orexin 2 receptor. 2022 , 30, 1582-1589.e4	0
257	LAST: Latent Space-Assisted Adaptive Sampling for Protein Trajectories.	Ο

256	Structural plasticity of omicron BA.5 and BA.2.75 for enhanced ACE-dependent entry into cells. 1-12	O
255	Proteinâlligand Binding Free-Energy Calculations with ARROW-A Purely First-Principles Parameterized Polarizable Force Field. 2022 , 18, 7751-7763	O
254	Biodegradation of 2,5-Dihydroxypyridine by 2,5-Dihydroxypyridine Dioxygenase and Its Mutants: Insights into Oâ® Bond Activation and Flexible Reaction Mechanisms from QM/MM Simulations. 2022 , 61, 20501-20512	О
253	Hexokinase 2 localizes to the nucleus in response to glucose limitation but does not regulate gene expression.	O
252	Annonaceous acetogenins: A computational study into their antitumor activity in multidrug resistant enzymes.	O
251	N-terminal 點trand in YAP is critical for stronger binding to Scalloped relative to TEAD transcription factor.	O
250	Effect of the Thermal Fluctuations of the Photophysics of GC and CG DNA Steps: A Computational Dynamical Study. 2022 , 126, 10608-10621	1
249	Artificial intelligence for template-free protein structure prediction: a comprehensive review.	O
248	Network Analysis of Molecular Dynamics Sectors in the p53 Protein.	0
247	Understanding the Allosteric Modulation of PTH1R by a Negative Allosteric Modulator. 2023 , 12, 41	O
246	Activation-induced cytidine deaminase, an antibody diversification enzyme, interacts with chromatin modifier UBN1 in B-cells.	O
245	Probing Conformational Landscapes and Mechanisms of Allosteric Communication in the Functional States of the ABL Kinase Domain Using Multiscale Simulations and Network-Based Mutational Profiling of Allosteric Residue Potentials.	O
244	Vaccinomics to design a multi-epitope-based vaccine against monkeypox virus using surface-associated proteins. 1-10	2
243	Markov State Models Underlying the N-Terminal Premodel of TOPK/PBK. 2022 , 126, 10662-10671	O
242	Probing conformational landscapes and mechanisms of allosteric communication in the functional states of the ABL kinase domain using multiscale simulations and network-based mutational profiling of allosteric residue potentials. 2022 , 157, 245101	O
241	Structural and binding studies of 2?- and 3-fucosyllactose and its complexes with norovirus capsid protein by molecular dynamics simulations. 1-14	O
240	A deep transfer learning-based protocol accelerates full quantum mechanics calculation of protein.	0
239	Simulation Reveals the Chameleonic Behavior of Macrocycles.	O

238	Thermodynamic characterization of a macrocyclic Zika virus NS2B/NS3 protease inhibitor and its acyclic analogs.	Ο
237	Triazole-Based Estradiol Dimers Prepared via CuAAC from 17Æthinyl Estradiol with Five-Atom Linkers Causing G2/M Arrest and Tubulin Inhibition. 2022 , 106334	Ο
236	Activation Mechanism of RhoA Caused by Constitutively Activating Mutations G14V and Q63L. 2022 , 23, 15458	Ο
235	Carbonyl-Containing Solid Polymer Electrolyte Host Materials: Conduction and Coordination in Polyketone, Polyester, and Polycarbonate Systems. 2022 , 55, 10940-10949	2
234	Chemoenzymatic synthesis of sulfur-linked sugar polymers as heparanase inhibitors. 2022, 13,	Ο
233	Destabilizers of the thymidylate synthase homodimer accelerate its proteasomal degradation and inhibit cancer growth. 11,	O
232	Study of Human Lipoxygenase by the Method of Molecular and Quantum Mechanics. 2022, 16, 1089-1093	Ο
231	DNA Aptamer Selected against Esophageal Squamous Cell Carcinoma for Tissue Imaging and Targeted Therapy with Integrin # as a Molecular Target. 2022 , 94, 17212-17222	O
230	Computational investigation on the effect of the lysine 2-hydroxyisobutyrylation on argininosuccinate synthetase 1 conformational dynamics in Botrytis cinerea. 2023 , 29,	Ο
229	Substitution of PINK1 Gly411 modulates substrate receptivity and turnover. 1-22	1
228	Bispecific Aptamer-Based Recognition-then-Conjugation Strategy for PD1/PDL1 Axis Blockade and Enhanced Immunotherapy.	О
227	Extending the applicability of popular force fields for describing water/metal interfaces: application to water/Pd(111). 2023 , 98, 015009	O
226	Binding and Unbinding Pathways of Peptide Substrates on the SARS-CoV-2 3CL Protease.	0
225	Efficient Antibacterial/Antifungal Activities: Synthesis, Molecular Docking, Molecular Dynamics, Pharmacokinetic, and Binding Free Energy of Galactopyranoside Derivatives. 2023 , 28, 219	4
224	The architecture of the 10-23 DNA zyme and its implications for DNA -mediated catalysis.	Ο
223	A combined ligand and target-based virtual screening strategy to repurpose drugs as putrescine uptake inhibitors with trypanocidal activity.	O
222	Mapping allosteric pathway in NIa-Pro using computational approach. 2023 , 0	Ο
221	Ligands-Induced Open-Close Conformational Change during DapE Catalysis: Insights from Molecular Dynamics Simulations.	Ο

220	Dimeric Lectin Chimeras as Novel Candidates for Gb3-Mediated Transcytotic Drug Delivery through Cellular Barriers. 2023 , 15, 225	О
219	Bioinformatic Approaches for Characterizing Molecular Structure and Function of Food Proteins. 2023 , 14,	О
218	Allosteric Signaling in PDZ Energetic Networks: Embedding Error Analysis.	O
217	A role of salt bridges in mediating drug potency: A lesson from the N-myristoyltransferase inhibitors. 9,	O
216	Single-Molecule Fluorescence Spectroscopy of Intrinsically Disordered Proteins. 2022,	0
215	Specific zinc binding to heliorhodopsin.	1
214	Development of a QM/MM(ABEEM) method combined with a polarizable force field to investigate the excision reaction mechanism of damaged thymine.	О
213	Valproate Coenzyme-A Conjugate Blocks Opening of Receptor Binding Domains in the Spike Trimer of SARS-CoV-2 through an Allosteric Mechanism. 2023 ,	1
212	Study on endogenous inhibitors against PD-L1: cAMP as a potential candidate. 2023 , 123266	О
211	The Inhibitory Properties of a Novel, Selective LMTK3 Kinase Inhibitor. 2023 , 24, 865	О
210	Generating Antiaromaticity: Thermally-selective Skeletal Rearrangements at Interfaces.	О
209	Structure of pre-miR-31 reveals an active role in Dicer processing.	О
208	In Silico Discovery of Aptamers with An Enhanced Library Design Strategy. 2023,	0
207	Conformational exchange divergence along the evolutionary pathway of eosinophil-associated ribonucleases. 2023 ,	О
206	Acetylcholinesterase inhibition of Alzheimerâl disease: identification of potential phytochemicals and designing more effective derivatives to manage disease condition. 1-13	О
205	Atomistic Simulations of Chitosan as Possible Carrier System for miRNA Transport.	О
204	Structural Analysis, Multi-Conformation Virtual Screening and Molecular Simulation to Identify Potential Inhibitors Targeting pS273R Proteases of African Swine Fever Virus. 2023 , 28, 570	О
203	Use of Apatinib as a Bait to Fish Its Unexpected Kinase Targets from the Hepatocellular Carcinoma Druggable Kinome.	О

202	Interaction of Chondroitin and Hyaluronan Glycosaminoglycans with Surfaces of Carboxylated Carbon Nanotubes Studied Using Molecular Dynamics Simulations. 2023 , 28, 826	0
201	Deciphering the Structural Determinants Critical in Attaining the FXR Partial Agonism.	O
200	Mtodos computacionales para estimar la afinidad de un complejo ligando-receptor. 2023 , 5, 27-46	0
199	Exploration on Ononin and Corylin molecule Against Anti-Influenza H1N1 A Virus via Molecular Docking, Molecular dynamics simulation and Binding free energy calculations.	O
198	The Inhibitory Mechanism of 7H-Pyrrolo[2,3-d]pyrimidine Derivatives as Inhibitors of P21-Activated Kinase 4 through Molecular Dynamics Simulation. 2023 , 28, 413	О
197	Transthyretin binds soluble endoglin and increases its uptake by hepatocytes: A possible role for transthyretin in preeclampsia?. 2023 , 562, 111851	O
196	Non-classical digestive lipase BmTGL selected by gene amplification reduces the effects of mulberry inhibitor during silkworm domestication. 2023 , 229, 589-599	О
195	The role of post-transcriptional modification on a new tRNAIle(GAU) identified from Ganoderma lucidum in its fragmentsâltytotoxicity on cancer cells. 2023 , 229, 885-895	O
194	EGCG attenuates Bynuclein protofibril-membrane interactions and disrupts the protofibril. 2023 , 230, 123194	О
193	Role of distal sites in enzyme engineering. 2023 , 63, 108094	O
193	Role of distal sites in enzyme engineering. 2023, 63, 108094 Deacetylation of K481 and K484 on Penaeid Shrimp Hemocyanin Is Critical for Antibacterial Activity. 2022, 209, 476-487	0
	Deacetylation of K481 and K484 on Penaeid Shrimp Hemocyanin Is Critical for Antibacterial	
192	Deacetylation of K481 and K484 on Penaeid Shrimp Hemocyanin Is Critical for Antibacterial Activity. 2022 , 209, 476-487 Free energy and kinetic rate calculation via non-equilibrium molecular simulation: application to	0
192 191	Deacetylation of K481 and K484 on Penaeid Shrimp Hemocyanin Is Critical for Antibacterial Activity. 2022, 209, 476-487 Free energy and kinetic rate calculation via non-equilibrium molecular simulation: application to biomolecules. 2022, 14, 1303-1314 Insights into pralsetinib resistance to the non-gatekeeper RET kinase G810C mutation through	0
192 191 190	Deacetylation of K481 and K484 on Penaeid Shrimp Hemocyanin Is Critical for Antibacterial Activity. 2022, 209, 476-487 Free energy and kinetic rate calculation via non-equilibrium molecular simulation: application to biomolecules. 2022, 14, 1303-1314 Insights into pralsetinib resistance to the non-gatekeeper RET kinase G810C mutation through molecular dynamics simulations. 2023, 29, Solution Nuclear Magnetic Resonance Structures of ATTTT and ATTTC Pentanucleotide Repeats	0 0
192 191 190	Deacetylation of K481 and K484 on Penaeid Shrimp Hemocyanin Is Critical for Antibacterial Activity. 2022, 209, 476-487 Free energy and kinetic rate calculation via non-equilibrium molecular simulation: application to biomolecules. 2022, 14, 1303-1314 Insights into pralsetinib resistance to the non-gatekeeper RET kinase G810C mutation through molecular dynamics simulations. 2023, 29, Solution Nuclear Magnetic Resonance Structures of ATTTT and ATTTC Pentanucleotide Repeats Associated with SCA37 and FAMEs. 2023, 14, 289-299 High-Affinity Antibodies Designing of SARS-CoV-2 Based on Molecular Dynamics Simulations. 2023,	o o o
192 191 190 189	Deacetylation of K481 and K484 on Penaeid Shrimp Hemocyanin Is Critical for Antibacterial Activity. 2022, 209, 476-487 Free energy and kinetic rate calculation via non-equilibrium molecular simulation: application to biomolecules. 2022, 14, 1303-1314 Insights into pralsetinib resistance to the non-gatekeeper RET kinase G810C mutation through molecular dynamics simulations. 2023, 29, Solution Nuclear Magnetic Resonance Structures of ATTTT and ATTTC Pentanucleotide Repeats Associated with SCA37 and FAMEs. 2023, 14, 289-299 High-Affinity Antibodies Designing of SARS-CoV-2 Based on Molecular Dynamics Simulations. 2023, 24, 481 Cooperation of structural motifs controls drug selectivity in cyclin-dependent kinases: an advanced	0 0 0

184	Different pKa Shifts of Internal GLU8 in Human 眭ndorphin Amyloid Revealing a Coupling of Internal Ionization and Stepwise Fibril Disassembly. 2023 , 127, 1089-1096	O
183	A universal deep-learning model for zinc finger design enables transcription factor reprogramming.	O
182	Probing the bioactive compounds of Kigelia africana as novel inhibitors of TNF-Econverting enzyme using HPLC/GCMS analysis, FTIR and molecular modelling. 1-25	O
181	Molecular dynamics simulations depict structural motions of the whole human aryl hydrocarbon receptor influencing its binding of ligands and HSP90. 1-16	O
180	Loading and Co-Solvent-Triggered Release of Okanin, a C4 Plant Key Enzyme Inhibitor, into/from Functional Microgels. 2023 , 141631	O
179	Assessment of Different Parameters on the Accuracy of Computational Alanine Scanning of Proteina Protein Complexes with the Molecular Mechanics/Generalized Born Surface Area Method. 2023 , 127, 944-954	O
178	MD Investigation on the Interaction between Carbamazepine and Two CYP Isoforms, CYP3A4 and CYP3A5. 2023 , 24, 2188	O
177	Attenuation of Lipopolysaccharide-Induced Inflammatory Responses through Inhibition of the NF-B Pathway and the Increased NRF2 Level by a Flavonol-Enriched n-Butanol Fraction from Uvaria alba.	O
176	âDual Anta-Inhibitorsâlof the A2A Adenosine Receptor and Casein Kinase CK1delta: Synthesis, Biological Evaluation, and Molecular Modeling Studies. 2023 , 16, 167	0
175	Influencing Molecular Dynamics Simulations of Ion-Exchange Membranes by Considering Comonomer Propagation.	O
174	Structure-based approach: molecular insight of pyranocumarins against £glucosidase through computational studies. 2023 , 13, 3438-3447	0
173	Exploring the interaction sites in glucose and galactose using phenol as a probe.	Ο
172	Molecular Dynamics and Raman Optical Activity Spectra Reveal Nucleotide Conformation Ratios in Solution.	0
171	Solvation Structure and Dynamics of Aqueous Solutions of Au+ Ions: A Molecular Dynamics Simulation Study.	O
170	Regulation of Intersubunit Interactions in Homotetramer of Glyceraldehyde-3-Phosphate Dehydrogenases upon Its Immobilization in Proteinâkappa-Carrageenan Gels. 2023 , 15, 676	0
169	Why do some fungi want to be sterile? The role of dysfunctional Pro1 in the rice blast fungus.	O
168	Aggregation of Nucleobases and Metabolites: Adenine-Theobromine trimers.	O
167	Is the Association of the Rare rs35667974 IFIH1 Gene Polymorphism With Autoimmune Diseases a Case of RNA Epigenetics?.	O

166	Structural insights into the elevator-type transport mechanism of a bacterial ZIP metal transporter. 2023 , 14,	O
165	SUMO interacting motif (SIM) of S100A1 is critical for S100A1 post-translational protein stability.	O
164	Induction effects on the absorption maxima of photoreceptor proteins. 2023,	O
163	MetaDOCK: A Combinatorial Molecular Docking Approach.	O
162	Wordom update 2: A user-friendly program for the analysis of molecular structures and conformational ensembles. 2023 , 21, 1390-1402	0
161	Aggregation of Asphaltene Subfractions A1 and A2 in Different Solvents from the Perspective of Molecular Dynamics Simulations.	O
160	Synthesis and Biophysical Properties of Phosphorodiamidate Piperidino Oligomers.	О
159	Modeling of the Interaction of Cytochrome c with Cardiolipin. 2022 , 67, 892-896	О
158	State-of-the-art experimental and computational approaches to investigate structure, substrate recognition, and catalytic mechanism of enzymes. 2023 , 75-107	0
157	Binding modes of GDP, GTP and GNP to NRAS deciphered by using Gaussian accelerated molecular dynamics simulations. 2023 , 34, 65-89	3
156	Thermal Titration Molecular Dynamics (TTMD): Not Your Usual Post-Docking Refinement. 2023, 24, 3596	1
155	Identifying Mutational Hotspots using Differences in Atomic Fluctuations combined with Positional Variability.	O
154	Variants inACTC1underlie distal arthrogryposis accompanied by congenital heart defects.	O
153	Probing Altered Receptor Specificities of Antigenically Drifting Human H3N2 Viruses by Chemoenzymatic Synthesis, NMR and Modeling.	O
152	3D-QSAR, molecular docking, and molecular dynamics analysis of dihydrodiazaindolone derivatives as PARP-1 inhibitors. 2023 , 29,	0
151	Electronegative clusters modulate folding status and RNA binding of unstructured RNA -binding proteins.	O
150	Solution NMR structure of cementum protein 1 derived peptide (CEMP1-p1) and its role in the mineralization process.	0
149	Oxidation of Dueling Cysteine Promotes Subunit Exchange in SOD1.	O

148	Proposal of novel ApoE4 inhibitors from the natural spice Cinnamon for the treatment of Alzheimer's disease: Ab initio molecular simulations. 2023 , 296, 106990	O
147	A critical review on molecular dynamics applied to structure fracture and failure analysis. 2023 , 150, 413-422	О
146	Structure-based design of promising natural products to inhibit thymidylate kinase from Monkeypox virus and validation using free energy calculations. 2023 , 158, 106797	0
145	Identification of medicinal plant-based phytochemicals as a potential inhibitor for SARS-CoV-2 main protease (Mpro) using molecular docking and deep learning methods. 2023 , 157, 106785	O
144	How can machine learning and multiscale modeling benefit ocular drug development?. 2023, 196, 114772	О
143	New anticancer potential Pt complex with tertamyl dithiocarbamate ligand: Synthesis, DNA targeting behavior, molecular dynamic, and biological activity. 2023 , 379, 121651	O
142	Molecular dynamics simulation study on interfacial behaviors of betaines and extended surfactants. 2023 , 666, 131323	0
141	Docking Studies of Natural Product Derived Carvacrol Type Aromatic Monoterpenes Against COVID-19 and Comparison with Used Synthetic Drugs: Potential of Carvacryl Acetate Against SARS-CoV-2 (COVID-19). 2023 , 12, 1-14	O
140	Isothermal titration calorimetry and molecular modeling study of the complex formation of daclatasvir by Etyclodextrin and trimethyl-tyclodextrin. 2023 , 313, 120870	О
139	Synthesis, Insecticidal Activity and Computational Studies of Eugenol-Based Insecticides.	О
138	Calculated vibrational properties of pigments in protein binding sites 2: Semiquinones in photosynthetic proteins. 2023 , 295, 122518	0
137	Propitious Indazole Compounds as 歌etoacyl-ACP Synthase Inhibitors and Mechanisms Unfolded for TB Cure: Integrated Rational Design and MD Simulations. 2023 , 8,	О
136	Rational design of a novel halotolerant ATP regeneration system for biocatalytic CTP production. 2023 , 98, 1025-1031	О
135	â⊞itâlto lead optimization and chemoinformatic studies for a new series of Autotaxin inhibitors. 2023 , 249, 115130	O
134	Turning thermostability of Aspergillus terreus (R)-selective transaminase At-ATA by synthetic shuffling. 2023 , 364, 66-74	О
133	Binding Affinity and Mechanisms of Antagonists Targeting Human NMDA Receptors.	O
132	CHARMM-GUI PDB Manipulator: Various PDB Structural Modifications for Biomolecular Modeling and Simulation. 2023 , 167995	O
131	Discovery of Isojacareubin as a covalent inhibitor of SARS-CoV-2 main protease using structural and experimental approaches. 2023 , 95,	О

130	4-Hydroxy Enigmol, a 1-Deoxyphytosphingolipid that Exhibit Good Activity against Prostate and Colon Cancer. 2023 , 8,	О
129	Statistical Mechanical Design Principles for Coarse-Grained Interactions across Different Conformational Free Energy Surfaces. 2023 , 14, 1354-1362	O
128	Analogue and structure based approaches for modelling HIV-1 integrase inhibitors. 1-11	O
127	Structure of Geobacter cytochrome OmcZ identifies mechanism of nanowire assembly and conductivity. 2023 , 8, 284-298	О
126	Computational assessment of the impact of Cu(II) and Al(III) on the myloid42 fibrils: Binding sites, structural stability, and possible physiological implications. 17,	0
125	Antiplasmodial activity of coumarins isolated from Polygala boliviensis: in vitro and in silico studies. 1-21	O
124	The cofactors and domains of a staphylococcal capsule-producing enzyme preserve its structure, stability, shape and dimerization ability.	0
123	Mitochondrial Peroxiredoxin 3 Is Rapidly Oxidized and Hyperoxidized by Fatty Acid Hydroperoxides. 2023 , 12, 408	O
122	Bioinformatics and Cheminformatics Tools in Early Drug Discovery. 2023, 147-181	0
121	Two distinct binding modes provide the RNA-binding protein RbFox with extraordinary sequence specificity. 2023 , 14,	O
120	Molecular Dynamics Refinement of Open State Serotonin 5-HT3A Receptor Structures. 2023 , 63, 1196-1207	0
119	Molecular docking and molecular simulation studies for N-degron selectivity of chloroplastic ClpS from Chlamydomonas reinhardtii. 2023 , 103, 107825	O
118	How Does the Study MD of pH-Dependent Exposure of Nanoparticles Affect Cellular Uptake of Anticancer Drugs?. 2023 , 24, 3479	O
117	MDSuite: comprehensive post-processing tool for particle simulations. 2023 , 15,	O
116	An Efficient Multilayer Approach to Model DNA-Based Nanobiosensors. 2023 , 127, 1513-1525	O
115	Melatonin Activation by Cytochrome P450 Isozymes: How Does CYP1A2 Compare to CYP1A1?. 2023 , 24, 3651	O
114	Flexural behavior and microstructural material properties of sandwich foam core under arctic temperature conditions. 109963622311570	0
113	Exploring the Effects of Mutagenesis on FusionRed by Using Excited-State QM/MM Dynamics and Classical Force Field Simulations.	О

112	Virtual Screening of Hepatitis B Virus Pre-Genomic RNA as a Novel Therapeutic Target. 2023, 28, 1803	О
111	MDBuilder: a PyMOL plugin for the preparation of molecular dynamics simulations. 2023 , 24,	O
110	In Silico Investigation of the Molecular Mechanism of PARP1 Inhibition for the Treatment of BRCA-Deficient Cancers. 2023 , 28, 1829	1
109	Site-Specific Phosphorylation of RTK KIT Kinase Insert Domain: Interactome Landscape Perspectives. 2023 , 1, 39-71	О
108	Molecular Design of Interfaces of Model Food Nanoemulsions: A Combined Experimental and Theoretical Approach. 2023 , 12, 484	O
107	The 5?UTR of HCoV-OC43 adopts a topologically constrained structure to intrinsically repress translation. 2023 , 299, 103028	O
106	Artificial Intelligence uncovers Evolutionarily Conserved Intracellular Allosteric Modulators of GPCR-Ginterface.	O
105	The effects of RNA.DNA-DNA triple helices on nucleosome structures and dynamics. 2023 , 122, 1229-1239	O
104	Computational aided design of a halotolerant CMP kinase for enzymatic synthesis of cytidine triphosphate. 2023 , 46, 499-505	0
103	Phosphorylation Modification Force Field FB18CMAP Improving Conformation Sampling of Phosphoproteins. 2023 , 63, 1602-1614	O
102	Molecular dynamic simulations identifying the mechanism of holoenzyme formation by O-GlcNAc transferase and active p38 ∃2023 , 25, 8090-8102	0
101	Direct Proton-Coupled Electron Transfer between Interfacial Tyrosines in Ribonucleotide Reductase. 2023 , 145, 4784-4790	O
100	Structural basis of the activation of PPARIby the plasticizer metabolites MEHP and MINCH. 2023 , 173, 107822	O
99	Phosphorylation-Competent Metastable State of Escherichia coli Toxin HipA. 2023 , 62, 989-999	O
98	Study of novel androgen receptor V770 variant in androgen insensitivity syndrome patients reveals the transitional state of the androgen receptor ligand binding domain homodimer. 2023 , 32,	O
97	Evaluation of polyanionic cyclodextrins as high affinity binding scaffolds for fentanyl. 2023, 13,	O
96	Understanding Drug Resistance of Wild-Type and L38HL Insertion Mutant of HIV-1 C Protease to Saquinavir. 2023 , 14, 533	O
95	Comparative mutational analysis of the Zika virus genome from different geographical locations and its effect on the efficacy of Zika virus-specific neutralizing antibodies. 14,	O

94	Concentration-Dependent Inhibition of Mesophilic PETases on Poly(ethylene terephthalate) Can Be Eliminated by Enzyme Engineering. 2023 , 16,	O
93	A Competition between Relative Stability and Binding Energy in Caffeine Phenyl-Glucose Aggregates: Implications in Biological Mechanisms. 2023 , 24, 4390	O
92	Simple and Effective Conformational Sampling Strategy for Intrinsically Disordered Proteins Using the UNRES Web Server. 2023 , 127, 2177-2186	0
91	Enzyme adaptation to habitat thermal legacy shapes the thermal plasticity of marine microbiomes. 2023 , 14,	O
90	Structure-Based Virtual Screening of Furan-1,3,4-Oxadiazole Tethered N-phenylacetamide Derivatives as Novel Class of hTYR and hTYRP1 Inhibitors. 2023 , 16, 344	O
89	Multiscale simulations of nanofluidics: Recent progress and perspective.	O
88	Million-atom molecular dynamics simulations reveal the interfacial interactions and assembly of plant PSII-LHCII supercomplex. 2023 , 13, 6699-6712	O
87	A mutant R70V/E166A of short manganese peroxidase showing Mn2+-independent dye decolorization. 2023 , 107, 2303-2319	O
86	Computational Insights into the Allosteric Modulation of a Phthalate-Degrading Hydrolase by Distal Mutations. 2023 , 13, 443	O
85	A generic binding pocket for small moleculeIKsactivators at the extracellular inter-subunit interface of KCNQ1 and KCNE1 channel complexes.	O
84	Routine Molecular Dynamics Simulations Including Nuclear Quantum Effects: From Force Fields to Machine Learning Potentials. 2023 , 19, 1432-1445	O
83	The Importance of Epigallocatechin as a Scaffold for Drug Development against Flaviviruses. 2023 , 15, 803	O
82	Towards a Rational Design of Antibody-Recruiting Molecules through a Computational Microscopy View of their Interactions with the Target Antibody.	O
81	Insights at the atomistic resolution of lantibiotics using multiscale simulations. 2023, 241-253	O
80	In silico approaches for xenobiotic polymers and their degradation mechanism. 2023, 479-501	O
79	Identification of Dietary Bioflavonoids as Potential Inhibitors against KRAS G12D Mutantâ l lovel Insights from Computer-Aided Drug Discovery. 2023 , 45, 2136-2156	O
78	Celastrol attenuates hepatitis C virus translation and inflammatory response in mice by suppressing heat shock protein 90#	O
77	Activation mechanism of the human Smoothened receptor. 2023 , 122, 1400-1413	O

76	Computational Methods for Molecular Understanding of the Antibiotic-Aminoacyl tRNA Synthetase Interaction. 2023 , 3,	0
75	Hepatic COX1 loss leads to impaired autophagic flux and exacerbates nonalcoholic steatohepatitis. 2023 ,	О
74	Decrypting the programming of methylation in virginiamycin M biosynthesis. 2023, 14,	О
73	Lawsonia inermis flower aqueous extract expressed better anti-alpha-glucosidase and anti-acetylcholinesterase activity and their molecular dynamics. 1-14	О
72	Structural insight into TIPE1 functioning as a lipid transfer protein. 1-14	0
71	Synergism for lowering interfacial tensions between betaines and extended surfactants: The role of self-regulating molecular size. 2023 , 378, 121605	О
70	In silico modelling of the function of disease-related CAZymes. 2023 , 67, 355-372	1
69	Deciphering Selectivity Mechanism of BRD9 and TAF1(2) toward Inhibitors Based on Multiple Short Molecular Dynamics Simulations and MM-GBSA Calculations. 2023 , 28, 2583	O
68	A [4Fe-4S] cluster resides at the active center of phosphomevalonate dehydratase, a key enzyme in the archaeal modified mevalonate pathway. 14,	0
67	SARS-CoV-2 envelope protein attain Kac mediated dynamical interaction network to adopt âlistone mimicâlat BRD4 interface. 1-15	O
66	Modulation of the catalytic activity and thermostability of a highly thermostable GH7 endoglucanase by engineering the key loop B3.	O
65	Virtual Screening of Novel 24-Dehydroxysterol Reductase (DHCR24) Inhibitors and the Biological Evaluation of Irbesartan in Cholesterol-Lowering Effect. 2023 , 28, 2643	О
64	In silico investigation of a novel anti EGFR Scfv âll. 24 fusion protein induces apoptosis in malignant cells.	O
63	Comprehensive Evaluation of End-Point Free Energy Techniques in Carboxylated-Pillar[6]arene Hostâtuest Binding: III. Force-Field Comparison, Three-Trajectory Realization and Further Dielectric Augmentation. 2023 , 28, 2767	0
62	Pharmacological Chaperones and Protein Conformational Diseases: Approaches of Computational Structural Biology. 2023 , 24, 5819	О
61	Deciphering the mechanistic basis for perfluoroalkyl-protein interactions.	O
60	Structural and dynamic properties of the YTH domain in complex with N\$lt;sup\$gt;6\$lt;/sup\$gt;-methyladenosine RNA studied by accelerated molecular dynamics simulations. 2023 , 11, 72	О
59	A Single Active-Site Mutagenesis Confers Enhanced Activity and/or Changed Product Distribution to a Pentalenene Synthase from Streptomyces sp. PSKA01. 2023 , 10, 392	O

58	Exploiting the co-crystal ligands shape, features and structure-based approaches for identification of SARS-CoV-2 Mpro inhibitors. 1-14	O
57	Intermolecular And Dynamic Investigation of The Mechanism of Action of Reldesemtiv on Fast Skeletal Muscle Troponin Complex Toward the Treatment of Impaired Muscle Function.	O
56	Enhanced Solid-State Fluorescence of Flavin Derivatives by Incorporation in the Metal-Organic Frameworks MIL-53(Al) and MOF-5. 2023 , 28, 2877	О
55	Structural basis of tRNAPro acceptor stem recognition by a bacterialtrans-editing domain.	O
54	New experimental evidence for pervasive dynamics in proteins. 2023 , 32,	О
53	High Accuracy Prediction of PROTAC Complex Structures. 2023, 145, 7123-7135	O
52	Pharmacotherapeutic Potential of Natural Products to Target the SARS-CoV-2 PLpro Using Molecular Screening and Simulation Approaches.	О
51	Impacts of Mutations in the P-Loop on Conformational Alterations of KRAS Investigated with Gaussian Accelerated Molecular Dynamics Simulations. 2023 , 28, 2886	Ο
50	Unraveling an Alternative Mechanism in Polymer Self-Assemblies: An OrderâDrder Transition with Unusual Molecular Interactions between Hydrophilic and Hydrophobic Polymer Blocks. 2023 , 17, 6932-6942	О
49	Identification of Potential Lead Compounds Targeting Novel Druggable Cavity of SARS-CoV-2 Spike Trimer by Molecular Dynamics Simulations. 2023 , 24, 6281	Ο
48	Active Site Aromatic Residues Play a Dual Role in the Substrate Interaction and Protein Structure in Functional Dimers of CYP121A1 of Mycobacterium tuberculosis. 2023 , 9, 827-839	О
47	Structures and Dynamics of DNA Mini-Dumbbells Are Force Field Dependent.	O
46	Next Generation of Ovarian Cancer Detection Using Aptamers. 2023 , 24, 6315	О
45	Comprehensive Approach to Simulating Large Scale Conformational Changes in Biological Systems Utilizing a Path Collective Variable and New Barrier Restraint.	O
44	Repurposing FIASMAs against Acid Sphingomyelinase for COVID-19: A Computational Molecular Docking and Dynamic Simulation Approach. 2023 , 28, 2989	О
43	Sensitivity of the RNA Structure to Ion Conditions as Probed by Molecular Dynamics Simulations of Common Canonical RNA Duplexes. 2023 , 63, 2133-2146	О
42	A lysine-based 2:1-[Paza]-pseudopeptide series used as additives in polymeric membranes for CO2 capture: synthesis, structural studies, and application. 2023 , 13, 10051-10067	0
41	Inhibition of Human Cholinesterases and in vitro Amyloid Aggregation by Rationally Designed Peptides.	O

40	Spectroscopy, docking and molecular dynamics studies on the interaction between cis and trans palladium-alanine complexes with calf-thymus DNA and antitumor activities. 1-24	О
39	Evaluation of autophagy inhibition to combat cancer: (vanadium complex)âprotein interactions, parameterization, and validation of a new force field. 2023 , 29,	O
38	Targeting Olokizumab-Interleukin 6 interaction interface to discover novel IL-6 inhibitors. 1-13	О
37	A General Picture of Cucurbit[8]uril Hostâ©uest Binding: Recalibrating Bonded Interactions. 2023 , 28, 3124	0
36	Large-scale Annotation of Biochemically Relevant Pockets and Tunnels in Cognate Enzyme-Ligand Complexes.	0
35	All -atom simulations of the trimeric spike protein of SARS-CoV -2 in aqueous medium: Nature of interactions, conformational stability and free energy diagrams for conformational transition of the protein.	0
34	Oncogene-mediated nuclear accumulation of lactate promotes epigenetic alterations to induce cancer cell proliferation. 2023 , 124, 495-519	0
33	The diversity of splicing modifiers acting on A-1bulged 5âEsplice sites reveals rules to guide rational design.	Ο
32	Computational Investigations into Two-Photon Fibril Imaging Using the DANIR-2c Probe. 2023 , 127, 311	9-31250
31	A Computational Biology Study on the Structure and Dynamics Determinants of Thermal Stability of the Chitosanase from Aspergillus fumigatus. 2023 , 24, 6671	Ο
30	Identifying novel selective PPO inhibitors through structure-based virtual screening and bio-evaluation. 2023 , 13, 10873-10883	0
29	Discovery of a novel drug using lipid-based formulation targeting G12D-mutated KRAS4B through non-covalent bonds.	O
28	Selectivity and Ranking of Tight-Binding JAK-STAT Inhibitors Using Markovian Milestoning with Voronoi Tessellations.	0
27	Multilevel interrogation of H3.3 reveals a primordial role in transcription regulation. 2023, 16,	O
26	Modeling the role of charged residues in thermophilic proteins by rotamer and dynamic cross correlation analysis. 2023 , 29,	0
25	Computational and structural insights into the pre- and post-hydrolysis states of bovine multidrug resistance-associated protein 1.	O
24	Enhanced Thermostability and Catalytic Activity of Streptomyces mobaraenesis Transglutaminase by Rationally Engineering Its Flexible Regions.	0
23	Tool and Techniques on Computer-Aided Drug Design for Targeted Cancer Therapy. 2023 , 781-829	Ο

22	In Silico Analysis of a GH3 ��Glucosidase from Microcystis aeruginosa CACIAM 03. 2023 , 11, 998	0
21	Targeting the I7L Protease: A Rational Design for Anti-Monkeypox Drugs?. 2023 , 24, 7119	O
20	Modular development of deep potential for complex solid solutions. 2023, 107,	0
19	Vitamin D analog calcitriol for breast cancer therapy; an integrated drug discovery approach. 1-27	O
18	The CDR3 region as the major driver of TREM-1 interaction with its ligands, an in silico characterization. 2023 , 21, 2579-2590	O
17	Probing mutation-induced conformational transformation of the GTP/M-RAS complex through Gaussian accelerated molecular dynamics simulations. 2023 , 38,	O
16	Synthesis, antiviral activity, and computational study of 瞪-xylofuranosyl nucleoside phosphonates. 2023 , 115379	O
15	Identification of Potential p38Inhibitors via In Silico Screening, In Vitro Bioassay and Molecular Dynamics Simulation Studies. 2023 , 24, 7360	O
14	Interactions between carbon nanotubes and external structures of SARS-CoV-2 using molecular docking and molecular dynamics. 2023 , 1286, 135604	O
13	A Retrospective on the Development of Methods for the Analysis of Protein Conformational Ensembles.	O
12	Bioisosteric Design Identifies Inhibitors of Mycobacterium tuberculosis DNA Gyrase ATPase Activity.	O
11	The structural basis of tRNA recognition by arginyl-tRNA-protein transferase. 2023, 14,	O
10	Decoding CRISPRâlīas PAM recognition with UniDesign.	O
9	Effect of double chain anionic surfactant on the dynamic interfacial tensions of betaine solutions. 2023 , 121866	O
8	Allosteric modulation of GluN1/GluN3 NMDA receptors by GluN1-selective competitive antagonists. 2023 , 155,	0
7	Discovery of Selective P2Y6R Antagonists with High Affinity and In Vivo Efficacy for Inflammatory Disease Therapy.	O
6	Gmx_qk: An Automated Protein/Proteinâlligand Complex Simulation Workflow Bridged to MM/PBSA, Based on Gromacs and Zenity-Dependent GUI for Beginners in MD Simulation Study.	О
5	Controlled sulfur-based engineering confers mouldability to phosphorothioate antisense oligonucleotides.	O

CITATION REPORT

4	Molecular Dynamics Simulations of Ionic Liquid Crystals. 2023 ,	О
3	Molecular dynamics simulations to investigate the effects of organic amines on biogas clathrate hydrate formation. 2023 , 382, 122015	O
2	Design and Identification of Inhibitors for the Spike-ACE2 Target of SARS-CoV-2. 2023 , 24, 8814	O
1	Catalytic Reaction Mechanism of Glyoxalase II: A Quantum Mechanics/Molecular Mechanics Study.	O