

CITATION REPORT

List of articles citing

GROMACS 3.0: a package for molecular simulation and trajectory analysis

DOI: 10.1007/s008940100045

Journal of Molecular Modeling, 2001, 7, 306-317.

Source: <https://exaly.com/paper-pdf/32895100/citation-report.pdf>

Version: 2024-04-24

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

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

#	Paper	IF	Citations
2293	Direct and Fast Assessment of Antimicrobial Surface Activity Using Molecular Dynamics Simulation and Time-Lapse Imaging.		
2292	Restructuring a Deep Eutectic Solvent by Water: The Nanostructure of Hydrated Choline Chloride/Urea.		
2291	On Obtaining Boltzmann-Distributed Configurational Ensembles from Expanded Ensemble Simulations with Fast State Mixing.		
2290	How the Ribosomal ASite Finger Can Lead to tRNA Species-Dependent Dynamics.		
2289	Concerted Two-Electron Reduction of Ubiquinone in Respiratory Complex I.		
2288	Free Energies of Redox Half-Reactions from First-Principles Calculations.		
2287	Structural and Mechanical Properties of Amyloid Beta Fibrils: A Combined Experimental and Theoretical Approach.		
2286	Effect of the Synaptic Plasma Membrane on the Stability of the Amyloid Precursor Protein Homodimer.		
2285	Mesoscale Organization and Dynamics in Binary Ionic Liquid Mixtures.		
2284	Microenvironment of MOF Channel Coordination with Pt NPs for Selective Hydrogenation of Unsaturated Aldehydes.		
2283	Molecular Mechanism behind Solvent Concentration-Dependent Optimal Activity of Thermomyces lanuginosus Lipase in a Biocompatible Ionic Liquid: Interfacial Activation through Arginine Switch.		
2282	Insight into Speciation and Electrochemistry of Uranyl Ions in Deep Eutectic Solvents.		
2281	Combining Molecular and Spin Dynamics Simulations with Solid-State NMR: A Case Study of Amphiphilic LysineLeucine Repeat Peptide Aggregates.		
2280	Probing the Adsorption of Polycyclic Aromatic Compounds onto Water Droplets Using Molecular Dynamics Simulations.		
2279	Markov-State Transition Path Analysis of Electrostatic Channeling.		
2278	Oriental Switch of the Lipase A Enzyme at the OilWater Interface: An Order of Magnitude Increase in Turnover Rate with a Single Surfactant Tag Explained.		
2277	Identifying WaterAnion Correlated Motion in Aqueous Solutions through Van Hove Functions.		

2276 Cascade Kinetics of an Artificial Metabolon by Molecular Dynamics and Kinetic Monte Carlo.

2275 Membrane Fluidity Sensing on the Single Virus Particle Level with Plasmonic Nanoparticle Transducers.

2274 .

2273 Cytoprotective Self-assembled RGD Peptide Nanofilms for Surface Modification of Viable Mesenchymal Stem Cells.

2272 Revisiting Hydrogen Bond Thermodynamics in Molecular Simulations.

2271 Polarizable QM/MM Approach with Fluctuating Charges and Fluctuating Dipoles: The QM/FQF Model.

2270 .

2269 Bioinformatics. Reality simulation--observe while it happens. **2001**, 294, 2304-5

15

2268 Ab initio x-ray scattering of liquid water. **2002**, 117, 9409-9412

35

2267 Theoretical equations of state for temperature and electromagnetic field dependence of fluid systems, based on the quasi-Gaussian entropy theory. **2002**, 116, 4437-4449

16

2266 Vanadate inhibits the ATPase activity and DNA binding capability of bacterial MutS. A structural model for the vanadate-MutS interaction at the Walker A motif. **2002**, 30, 4700-8

52

2265 Structure-activity relationships of linear and cyclic peptides containing the NGR tumor-homing motif. **2002**, 277, 47891-7

144

2264 Structure and flexibility of Streptococcus agalactiae hyaluronate lyase complex with its substrate. Insights into the mechanism of processive degradation of hyaluronan. **2002**, 277, 36678-88

63

2263 FAD is a preferred substrate and an inhibitor of Escherichia coli general NAD(P)H:flavin oxidoreductase. **2002**, 277, 39450-5

23

2262 Mechanism of hyaluronan degradation by Streptococcus pneumoniae hyaluronate lyase. Structures of complexes with the substrate. **2002**, 277, 28287-97

92

2261 Probing the hirudin-thrombin interaction by incorporation of noncoded amino acids and molecular dynamics simulation. **2002**, 41, 13556-69

23

2260 Determining Limonene Diffusion in Molten Polyethylene from within 0.1 Å Molecular Dynamics Trajectories. **2002**, 35, 7453-7459

10

2259 Convergence of sampling in protein simulations. **2002**, 65, 031910

283

2258	Pentapeptide amides interfere with the aggregation of beta-amyloid peptide of Alzheimer's disease. 2002 , 292, 931-6	58
2257	Determining the shear viscosity of model liquids from molecular dynamics simulations. 2002 , 116, 209	509
2256	Flexible constraints: An adiabatic treatment of quantum degrees of freedom, with application to the flexible and polarizable mobile charge densities in harmonic oscillators model for water. 2002 , 116, 9602-9610	27
2255	Structures of neat and hydrated 1-octanol from computer simulations. 2002 , 124, 15085-93	101
2254	Orientation and interactions of dipolar molecules during transport through OmpF porin. 2002 , 528, 53-7	49
2253	Cholesterol-induced modifications in lipid bilayers: a simulation study. 2002 , 83, 1842-53	210
2252	Molecular dynamics simulation of spontaneous membrane fusion during a cubic-hexagonal phase transition. 2002 , 83, 2386-92	72
2251	Homology modeling and molecular dynamics study of NAD-dependent glycerol-3-phosphate dehydrogenase from <i>Trypanosoma brucei rhodesiense</i> , a potential target enzyme for anti-sleeping sickness drug development. 2002 , 82, 2906-15	5
2250	Water permeation through gramicidin A: desformylation and the double helix: a molecular dynamics study. 2002 , 82, 2934-42	80
2249	Molecular basis of voltage gating of OmpF porin. 2002 , 80, 517-23	37
2248	Calculation of the free energy of solvation for neutral analogs of amino acid side chains. 2002 , 23, 548-53	157
2247	Mapping of possible binding sequences of two beta-sheet breaker peptides on beta amyloid peptide of Alzheimer's disease. 2002 , 10, 1587-93	38
2246	Molecular dynamics simulations of a mixed DOPC/DOPG bilayer. 2003 , 12 Suppl 1, S135-40	21
2245	Dynamic molecules: molecular dynamics for everyone. An internet-based access to molecular dynamic simulations: basic concepts. <i>Journal of Molecular Modeling</i> , 2003 , 9, 308-15	2 19
2244	Analysis of the effect of electrostatic energy truncation in molecular dynamics simulations of immunoglobulin G light chain dimer. <i>Journal of Molecular Modeling</i> , 2003 , 9, 316-24	2 6
2243	Pound-wise but penny-foolish: How well do micromolecules fare in macromolecular refinement?. 2003 , 11, 1051-9	85
2242	Comparison of various implicit solvent models in molecular dynamics simulations of immunoglobulin G light chain dimer. 2003 , 24, 531-46	19
2241	Calculation of the water-cyclohexane transfer free energies of neutral amino acid side-chain analogs using the OPLS all-atom force field. 2003 , 24, 1930-5	98

2240	Monitoring folding transitions of synthetic, branched-chain polypeptides by capillary zone electrophoresis. 2003 , 24, 794-800	11
2239	Molecular dynamics studies of alanine racemase: a structural model for drug design. 2003 , 70, 186-200	18
2238	Lead conformer prediction based on a library of flexible molecules. 2003 , 666-667, 645-649	5
2237	Investigations on the predictability of the formation of glassy solid solutions of drugs in sugar alcohols. 2003 , 252, 167-79	38
2236	Use of essential and molecular dynamics to study gammaB-crystallin unfolding after non-enzymic post-translational modifications. 2003 , 27, 507-10	9
2235	Nonequilibrium, multiple-timescale simulations of ligand-receptor interactions in structured protein systems. 2003 , 52, 339-48	12
2234	Relative stability of protein structures determined by X-ray crystallography or NMR spectroscopy: a molecular dynamics simulation study. 2003 , 53, 111-20	44
2233	Novel use of a genetic algorithm for protein structure prediction: searching template and sequence alignment space. 2003 , 53 Suppl 6, 424-9	27
2232	Orientation restraints in molecular dynamics simulations using time and ensemble averaging. 2003 , 164, 19-27	50
2231	Extending the structure of an ABC transporter to atomic resolution: modeling and simulation studies of MsbA. 2003 , 42, 3666-73	53
2230	Monolayer ice. 2003 , 91, 025502	195
2229	Characteristic domain motion in the ribosome recycling factor revealed by 15N NMR relaxation experiments and molecular dynamics simulations. 2003 , 42, 4101-7	23
2228	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution. guanine: surprising stabilization of rare tautomers in aqueous solution. 2003 , 125, 7678-88	192
2227	Water structure as a function of temperature from X-ray scattering experiments and ab initio molecular dynamics. 2003 , 5, 1981	173
2226	On the evaluation and optimization of protein X-ray structures for pKa calculations. 2003 , 12, 313-26	97
2225	Surface tension from molecular dynamics simulation: Adsorption at the gas-liquid interface. 2003 , 43, 393-397	5
2224	Spontaneous Insertion of DNA Oligonucleotides into Carbon Nanotubes. 2003 , 3, 471-473	397
2223	Electrolytic Transport in Modified Carbon Nanotubes. 2003 , 3, 1399-1403	164

2222	Mixing Distributions within the Quasi-Gaussian Entropy Theory: Multistate Thermal Equations of State Valid for Large Temperature Ranges. 2003 , 107, 1410-1422	5
2221	Force Field Influence on the Observation of β -Helical Protein Structures in Molecular Dynamics Simulations. 2003 , 107, 2831-2836	186
2220	Conformational studies of a bombolitin III-derived peptide mimicking the four-helix bundle structural motif of proteins. 2003 , 125, 15314-23	5
2219	The Flexing/Twirling Helix: Exploring the Flexibility about Molecular Hinges Formed by Proline and Glycine Motifs in Transmembrane Helices. 2003 , 107, 627-636	50
2218	Brute-Force Molecular Dynamics Simulations of Villin Headpiece: Comparison with NMR Parameters. 2003 , 107, 11178-11187	58
2217	Anomalously Immobilized Water: A New Water Phase Induced by Confinement in Nanotubes. 2003 , 3, 589-592	377
2216	Understanding binding affinity: a combined isothermal titration calorimetry/molecular dynamics study of the binding of a series of hydrophobically modified benzamidine chloride inhibitors to trypsin. 2003 , 125, 10570-9	90
2215	The structure of the aquaporin-1 water channel: a comparison between cryo-electron microscopy and X-ray crystallography. 2003 , 325, 485-93	45
2214	Molecular dynamics studies of a molecular switch in the glucocorticoid receptor. 2003 , 328, 325-34	17
2213	Membrane protein dynamics versus environment: simulations of OmpA in a micelle and in a bilayer. 2003 , 329, 1035-53	125
2212	NMR studies of protein hydration and TEMPOL accessibility. 2003 , 332, 437-47	35
2211	Molecular dynamics simulations of a K ⁺ channel blocker: Tc1 toxin from <i>Tityus cambridgei</i> . 2003 , 535, 29-33	17
2210	Interdomain dynamics and ligand binding: molecular dynamics simulations of glutamine binding protein. 2003 , 550, 168-74	59
2209	Structural basis of the lisinopril-binding specificity in N- and C-domains of human somatic ACE. 2003 , 308, 219-26	25
2208	The mechanism of proton exclusion in the aquaporin-1 water channel. 2003 , 333, 279-93	233
2207	Structural requirements of the fructan-lipid interaction. 2003 , 84, 3147-54	67
2206	The implementation of slab geometry for membrane-channel molecular dynamics simulations. 2003 , 85, 97-107	64
2205	Molecular dynamics simulations of the bacterial outer membrane protein FhuA: a comparative study of the ferrichrome-free and bound states. 2003 , 85, 1406-20	85

2204	Conformational dynamics of the F1-ATPase beta-subunit: a molecular dynamics study. 2003 , 85, 1482-91	38
2203	A tree-based algorithm for determining the effects of solvation on the structure of salivary gland tripeptide NH ₃ ⁺ -D-PHE-D-GLU-GLY-COO ⁻ . 2003 , 85, 1503-11	2
2202	Investigating lipid composition effects on the mechanosensitive channel of large conductance (MscL) using molecular dynamics simulations. 2003 , 85, 1512-24	86
2201	Effect of sodium chloride on a lipid bilayer. 2003 , 85, 1647-55	452
2200	Potassium channel, ions, and water: simulation studies based on the high resolution X-ray structure of KcsA. 2003 , 85, 2787-800	99
2199	Mixed bilayer containing dipalmitoylphosphatidylcholine and dipalmitoylphosphatidylserine: lipid complexation, ion binding, and electrostatics. 2003 , 85, 3120-31	140
2198	Structure of sphingomyelin bilayers: a simulation study. 2003 , 85, 3624-35	127
2197	Gramicidin A channel as a test ground for molecular dynamics force fields. 2003 , 84, 2159-68	102
2196	Molecular dynamics simulations of phospholipid bilayers with cholesterol. 2003 , 84, 2192-206	411
2195	Molecular dynamics studies of caspase-3. 2003 , 84, 2207-15	29
2194	Molecular dynamics simulations of lipid bilayers: major artifacts due to truncating electrostatic interactions. 2003 , 84, 3636-45	363
2193	Molecular dynamics simulation of a dipalmitoylphosphatidylcholine bilayer with NaCl. 2003 , 84, 3743-50	205
2192	Atypical Dependence of Electroosmotic Transport on Surface Charge in a Single-wall Carbon Nanotube. 2003 , 3, 1013-1017	78
2191	Simulation of pore formation in lipid bilayers by mechanical stress and electric fields. 2003 , 125, 6382-3	363
2190	Molecular dynamics simulations of pentapeptides at interfaces: salt bridge and cation-pi interactions. 2003 , 42, 8976-87	97
2189	Molecular dynamics simulation of the formation, structure, and dynamics of small phospholipid vesicles. 2003 , 125, 15233-42	263
2188	Nonequilibrium molecular-dynamics study of the vibrational energy relaxation of peptides in water. 2003 , 119, 11350-11358	78
2187	Dynamic properties of water/alcohol mixtures studied by computer simulation. 2003 , 119, 7308-7317	238

2186	Bilayer ice and alternate liquid phases of confined water. 2003 , 119, 1694-1700	114
2185	Structure-oriented rational design of chymotrypsin inhibitor models. 2003 , 16, 673-81	7
2184	The weighted-volume derivative of a space-filling diagram. 2003 , 100, 2203-8	40
2183	Identification of the C-signal, a contact-dependent morphogen coordinating multiple developmental responses in <i>Myxococcus xanthus</i> . 2003 , 17, 2151-61	105
2182	EF loop conformational change triggers ligand binding in beta-lactoglobulins. 2003 , 278, 38840-6	62
2181	A fast multipole method combined with a reaction field for long-range electrostatics in molecular dynamics simulations: The effects of truncation on the properties of water. 2003 , 118, 10847-10860	77
2180	An algorithm to describe molecular scale rugged surfaces and its application to the study of a water/lipid bilayer interface. 2003 , 119, 2199-2205	85
2179	Ion concentrations and velocity profiles in nanochannel electroosmotic flows. 2003 , 118, 4692-4701	263
2178	Quasiequilibrium unfolding thermodynamics of a small protein studied by molecular dynamics simulation with an explicit water model. 2003 , 67, 061903	5
2177	Trapping site structures of HARF and HKrF in solid rare gases. 2003 , 119, 7356-7364	24
2176	Liquid-vapor oscillations of water in hydrophobic nanopores. 2003 , 100, 7063-8	377
2175	Large scale simulation of protein mechanics and function. 2003 , 66, 195-247	30
2174	Expression of Na ⁺ ,K ⁺ -ATPase in <i>Pichia pastoris</i> : analysis of wild type and D369N mutant proteins by Fe ²⁺ -catalyzed oxidative cleavage and molecular modeling. 2003 , 278, 46064-73	34
2173	Intermolecular interactions between peptidic and nonpeptidic agonists and the third extracellular loop of the cholecystokinin 1 receptor. 2003 , 46, 3476-82	16
2172	Modelling Carbon Nanotube Based Bio-Nano Systems: A Molecular Dynamics Study. 2003 , 773, 851	6
2171	Foldamer simulations: novel computational methods and applications to poly-phenylacetylene oligomers. 2004 , 121, 12760-71	26
2170	Heat capacity effects associated with the hydrophobic hydration and interaction of simple solutes: a detailed structural and energetical analysis based on molecular dynamics simulations. 2004 , 120, 10605-17	69
2169	A computer simulation study of water drying at the interface of protein chains. 2004 , 121, 1969-77	9

2168	Network equilibration and first-principles liquid water. 2004 , 121, 11136-44	148
2167	Structure and dielectric properties of polar fluids with extended dipoles: results from numerical simulations. 2004 , 102, 599-609	42
2166	Spontaneous three-dimensional nanostructure formation of perfluoroalkyl terminated liquid crystal: a molecular dynamics simulation study. 2004 , 121, 7520-5	5
2165	Correlations among hydrogen bonds in liquid water. 2004 , 93, 087801	58
2164	Temperature dependence of the hydrophobic hydration and interaction of simple solutes: an examination of five popular water models. 2004 , 120, 6674-90	241
2163	Model for the dynamics of a water cluster in an x-ray free electron laser beam. 2004 , 70, 051904	65
2162	Combined Monte Carlo and molecular dynamics simulation of hydrated 18:0 sphingomyelin-cholesterol lipid bilayers. 2004 , 120, 9841-7	68
2161	Electrofreezing of confined water. 2004 , 120, 7123-30	99
2160	Heme-ligand tunneling in group I truncated hemoglobins. 2004 , 279, 21520-5	107
2159	Toc12, a novel subunit of the intermembrane space preprotein translocon of chloroplasts. 2004 , 15, 5130-44	91
2158	Solution structure of the Kaposi's sarcoma-associated herpesvirus K3 N-terminal domain reveals a Novel E2-binding C4HC3-type RING domain. 2004 , 279, 53840-7	77
2157	Conformational transitions induced by the binding of MgATP to the vitamin B12 ATP-binding cassette (ABC) transporter BtuCD. 2004 , 279, 45013-9	76
2156	Molecular modeling correctly predicts the functional importance of Phe594 in transmembrane helix 11 of the multidrug resistance protein, MRP1 (ABCC1). 2004 , 279, 463-8	53
2155	Linkage of interactions in sickle hemoglobin fiber assembly: inhibitory effect emanating from mutations in the AB region of the alpha-chain is annulled by a mutation at its EF corner. 2004 , 279, 20018-27	3
2154	Conservation of the biochemical properties of InCA from Chlamydia trachomatis and Chlamydia caviae: oligomerization of InCA mediates interaction between facing membranes. 2004 , 279, 46896-906	73
2153	Jararhagin-derived RKKH peptides induce structural changes in alpha1I domain of human integrin alpha1beta1. 2004 , 279, 7962-70	33
2152	Differential peptide dynamics is linked to major histocompatibility complex polymorphism. 2004 , 279, 28197-201	74
2151	Deformation of helix C in the low temperature L-intermediate of bacteriorhodopsin. 2004 , 279, 2147-58	66

2150	Molecular dynamics simulations of beta-turn forming tetra- and hexapeptides. 2004 , 21, 761-70	7
2149	Simulations of the role of water in the protein-folding mechanism. 2004 , 101, 6456-61	170
2148	ISIM: A Program for Grand Canonical Monte Carlo Simulations of the Ionic Environment of Biomolecules. 2004 , 30, 45-61	19
2147	NMR and molecular dynamics studies of an autoimmune myelin basic protein peptide and its antagonist: structural implications for the MHC II (I-Au)-peptide complex from docking calculations. 2004 , 271, 3399-413	18
2146	Structural model of the UbcH5B/CNOT4 complex revealed by combining NMR, mutagenesis, and docking approaches. 2004 , 12, 633-44	103
2145	The N-terminus moiety of the cystatin SmCys from <i>Schistosoma mansoni</i> regulates its inhibitory activity in vitro and in vivo. 2004 , 134, 65-73	20
2144	Molecular dynamics simulations of bovine lactoferricin: turning a helix into a sheet. 2004 , 17, 217-23	22
2143	Molecular-dynamics simulation of amphiphilic bilayer membranes and wormlike micelles: a multi-scale modelling approach to the design of viscoelastic surfactant solutions. 2004 , 362, 1625-38	25
2142	Development of a 3D model for the human cannabinoid CB1 receptor. 2004 , 47, 3048-57	77
2141	Charge inversion and flow reversal in a nanochannel electro-osmotic flow. 2004 , 92, 198301	182
2140	Molecular dynamics simulations of glycosyltransferase LgtC. 2004 , 339, 995-1006	10
2139	Binding and insertion of alpha-helical anti-microbial peptides in POPC bilayers studied by molecular dynamics simulations. 2004 , 132, 113-32	58
2138	Potential impact of an X-ray free electron laser on structural biology. 2004 , 71, 905-916	53
2137	BODIL: a molecular modeling environment for structure-function analysis and drug design. 2004 , 18, 401-19	185
2136	Interactive essential dynamics. 2004 , 18, 433-6	77
2135	Atomic insight into the CD4 binding-induced conformational changes in HIV-1 gp120. 2004 , 55, 582-93	36
2134	A simple topological representation of protein structure: implications for new, fast, and robust structural classification. 2004 , 56, 487-501	22
2133	Molecular modeling of the core of Abeta amyloid fibrils. 2004 , 57, 357-64	55

2132	Conformational sampling and dynamics of membrane proteins from 10-nanosecond computer simulations. 2004 , 57, 783-91	86
2131	A molecular dynamics study of the structural stability of HIV-1 protease under physiological conditions: the role of Na ⁺ ions in stabilizing the active site. 2005 , 58, 450-8	19
2130	Energy landscape of a small peptide revealed by dihedral angle principal component analysis. 2005 , 58, 45-52	302
2129	Theoretical investigations of prostatic acid phosphatase. 2005 , 58, 295-308	14
2128	Water dynamics simulation as a tool for probing proton transfer pathways in a heptahelical membrane protein. 2005 , 58, 528-37	28
2127	Dynamics and energetics of water permeation through the aquaporin channel. 2004 , 55, 924-31	41
2126	Reorganization in apo- and holo-beta-lactoglobulin upon protonation of Glu89: molecular dynamics and pKa calculations. 2004 , 54, 744-58	49
2125	Computer simulations of voltage-gated potassium channel KvAP. 2004 , 100, 1071-1078	14
2124	Dynamite: a simple way to gain insight into protein motions. 2004 , 60, 2280-7	80
2123	The molecular basis of electroporation. 2004 , 5, 10	309
2122	Mutation of exposed hydrophobic amino acids to arginine to increase protein stability. 2004 , 5, 9	82
2121	Synthesis, conformation, and immunoreactivity of new carrier molecules based on repeated tuftsin-like sequence. 2004 , 73, 645-56	27
2120	Quantifying the complexity of chaos in multibasin multidimensional dynamics of molecular systems. 2004 , 10, 40-46	5
2119	K317, R319, and E320 within the proximal C-terminus of the bradykinin B2 receptor form a motif important for phospholipase C and phospholipase A2 but not connective tissue growth factor related signaling. 2004 , 92, 547-59	6
2118	Systematic comparison of force fields for microscopic simulations of NaCl in aqueous solutions: diffusion, free energy of hydration, and structural properties. 2004 , 25, 678-89	187
2117	A fast pairlist-construction algorithm for molecular simulations under periodic boundary conditions. 2004 , 25, 1474-86	45
2116	Solvation forces on biomolecular structures: a comparison of explicit solvent and Poisson-Boltzmann models. 2004 , 25, 1623-9	85
2115	A biomolecular force field based on the free enthalpy of hydration and solvation: the GROMOS force-field parameter sets 53A5 and 53A6. 2004 , 25, 1656-76	2844

2114	Constant pH molecular dynamics in generalized Born implicit solvent. 2004 , 25, 2038-48	368
2113	Cytochrome c: the effect of temperature and pressure from molecular dynamics simulations. 2004 , 65, 1615-1622	12
2112	Auger electron cascades in water and ice. 2004 , 299, 277-283	49
2111	Molecular Dynamics Study of the Effect of the EAbu Insert on the Conformational Behavior of the Glycopeptide Dendrimers Based on the Oligolysine Scaffold in N, N'-dimethylformamide. 2004 , 22, 79-90	5
2110	Existence of specific "folds" in polyproline II ensembles of an "unfolded"alanine peptide detected by molecular dynamics. 2004 , 126, 16332-3	34
2109	Binding modes of two highly potent and nontoxic inhibitors of HIV-1 integrase. 2004 , 2004, 3003-6	
2108	Modeling protonated water networks in bacteriorhodopsin. 2004 , 6, 1848-1859	44
2107	BioSimGrid: towards a worldwide repository for biomolecular simulations. 2004 , 2, 3219-21	34
2106	Hydrophobic collapse in multidomain protein folding. 2004 , 305, 1605-9	441
2105	MOLECULAR DYNAMICS SIMULATIONS OF LIQUID CRYSTAL MOLECULES AT AN AIR-WATER INTERFACE. 2004 , 413, 161-169	4
2104	Angular resolution and range of dipole-dipole correlations in water. 2004 , 120, 4393-403	34
2103	Molecular simulations suggest protein salt bridges are uniquely suited to life at high temperatures. 2004 , 126, 2208-14	73
2102	Structural and Dynamic Properties of the CAGQW Peptide in Water: A Molecular Dynamics Simulation Study Using Different Force Fields. 2004 , 108, 18734-18742	16
2101	Distribution, Orientation, and Dynamics of DPH Probes in DPPC Bilayer. 2004 , 108, 13438-13448	83
2100	Molecular dynamics simulation of the LOV2 domain from Adiantum capillus-veneris. 2004 , 44, 1788-93	14
2099	Coarse-grained model for phospholipid/cholesterol bilayer. 2004 , 121, 9156-65	115
2098	Impact of cholesterol on voids in phospholipid membranes. 2004 , 121, 12676-89	88
2097	Disruption of the LOV-Jalpha helix interaction activates phototropin kinase activity. 2004 , 43, 16184-92	250

2096	How C-terminal carboxyamidation alters the biological activity of peptides from the venom of the eumenine solitary wasp. 2004 , 43, 5608-17	80
2095	Solvent-mediated folding of a doubly charged anion. 2004 , 126, 876-83	39
2094	Molecular Dynamics Simulation of a GM3 Ganglioside Bilayer. 2004 , 108, 20322-20330	23
2093	The Binomial Cell Model of Hydrophobic Solvation. 2004 , 108, 15830-15840	16
2092	Bulk versus interfacial aqueous solvation of dicarboxylate dianions. 2004 , 126, 11691-8	53
2091	Structural stability of wild type and mutated alpha-keratin fragments: molecular dynamics and free energy calculations. 2004 , 5, 2165-75	34
2090	Molecular Dynamics Simulations of Electric Field Poled Nonlinear Optical Chromophores Incorporated in a Polymer Matrix. 2004 , 108, 588-596	49
2089	Simulation of domain formation in DLPC-DSPC mixed bilayers. 2004 , 20, 7686-93	100
2088	All-Atom Folding Simulations of the Villin Headpiece from Stochastically Selected Coarse-Grained Structures. 2004 , 108, 12267-12270	36
2087	The influence of geometry, surface character, and flexibility on the permeation of ions and water through biological pores. 2004 , 1, 42-52	203
2086	Molecular interaction model for the C1B domain of protein kinase C-gamma in the complex with its activator phorbol-12-myristate-13-acetate in water solution and lipid bilayer. 2004 , 47, 6547-55	19
2085	The quaternary structure of the <i>Saccharomyces cerevisiae</i> succinate dehydrogenase. Homology modeling, cofactor docking, and molecular dynamics simulation studies. 2004 , 279, 9424-31	164
2084	An in silico approach to discovering novel inhibitors of human sirtuin type 2. 2004 , 47, 6292-8	96
2083	On the dynamics of water molecules at the protein solute interfaces. 2004 , 93, 199-202	2
2082	Interfacing biological macromolecules with carbon nanotubes and silicon surfaces: a computer modelling and dynamic simulation study. 2004 , 15, S684-S690	14
2081	Size dependent ion hydration, its asymmetry, and convergence to macroscopic behavior. 2004 , 120, 4457-66	133
2080	Adsorption of Atmospherically Relevant Gases at the Air/Water Interface: Free Energy Profiles of Aqueous Solvation of N ₂ , O ₂ , O ₃ , OH, H ₂ O, HO ₂ , and H ₂ O ₂ . 2004 , 108, 11573-11579	162
2079	Photoactivation of the photoactive yellow protein: why photon absorption triggers a trans-to-cis Isomerization of the chromophore in the protein. 2004 , 126, 4228-33	246

2078	Hemoglobin Einstein: semisynthetic deletion in the B-helix of the alpha-chain. 2004 , 13, 1266-75	3
2077	Not ions alone: barriers to ion permeation in nanopores and channels. 2004 , 126, 14694-5	164
2076	Bilayer conformation of fusion peptide of influenza virus hemagglutinin: a molecular dynamics simulation study. 2004 , 87, 14-22	45
2075	Simulations of a membrane-anchored peptide: structure, dynamics, and influence on bilayer properties. 2004 , 86, 3556-75	63
2074	Molecular dynamics simulations of the lipid bilayer edge. 2004 , 87, 182-92	77
2073	A molecular dynamics study of Ca(2+)-calmodulin: evidence of interdomain coupling and structural collapse on the nanosecond timescale. 2004 , 87, 780-91	51
2072	Lipid bilayer pressure profiles and mechanosensitive channel gating. 2004 , 86, 3496-509	287
2071	Computational simulations of interactions of scorpion toxins with the voltage-gated potassium ion channel. 2004 , 86, 3542-55	54
2070	Filter flexibility and distortion in a bacterial inward rectifier K ⁺ channel: simulation studies of KirBac1.1. 2004 , 87, 256-67	56
2069	Lessons of slicing membranes: interplay of packing, free area, and lateral diffusion in phospholipid/cholesterol bilayers. 2004 , 87, 1076-91	249
2068	Sphingomyelin-cholesterol domains in phospholipid membranes: atomistic simulation. 2004 , 87, 1092-100	152
2067	Exterior site occupancy infers chloride-induced proton gating in a prokaryotic homolog of the ClC chloride channel. 2004 , 87, 1686-96	51
2066	The range and shielding of dipole-dipole interactions in phospholipid bilayers. 2004 , 87, 2433-45	79
2065	Direct simulation of transmembrane helix association: role of asparagines. 2004 , 87, 1650-6	36
2064	Simulation of the early stages of nano-domain formation in mixed bilayers of sphingomyelin, cholesterol, and dioleoylphosphatidylcholine. 2004 , 87, 3312-22	154
2063	Nucleotide-dependent conformational changes in HisP: molecular dynamics simulations of an ABC transporter nucleotide-binding domain. 2004 , 87, 3703-15	37
2062	Predicting the three-dimensional structure of the human facilitative glucose transporter glut1 by a novel evolutionary homology strategy: insights on the molecular mechanism of substrate migration, and binding sites for glucose and inhibitory molecules. 2004 , 87, 2990-9	158
2061	Lipid-protein interactions of integral membrane proteins: a comparative simulation study. 2004 , 87, 3737-49	92

2060	Molecular view of hexagonal phase formation in phospholipid membranes. 2004 , 87, 3894-900	167
2059	The active site and substrate-binding mode of 1-aminocyclopropane-1-carboxylate oxidase determined by site-directed mutagenesis and comparative modelling studies. 2004 , 380, 339-46	23
2058	Correlated ab Initio Study of Nucleic Acid Bases and Their Tautomers in the Gas Phase, in a Microhydrated Environment, and in Aqueous Solution. Part 3. Adenine. 2004 , 108, 2087-2097	175
2057	MD simulations of spontaneous membrane protein/detergent micelle formation. 2004 , 126, 15948-9	81
2056	Computational study of imidazolium-based ionic solvents with alkyl substituents of different lengths. 2004 , 102, 829-838	159
2055	Reversible temperature and pressure denaturation of a protein fragment: a replica exchange molecular dynamics simulation study. 2004 , 93, 238105	132
2054	A PELDOR-based nanometer distance ruler for oligonucleotides. 2004 , 126, 5722-9	182
2053	Coarse Grained Model for Semiquantitative Lipid Simulations. 2004 , 108, 750-760	1767
2052	Lipid Bilayers Driven to a Wrong Lane in Molecular Dynamics Simulations by Subtle Changes in Long-Range Electrostatic Interactions. 2004 , 108, 4485-4494	190
2051	Computer modeling of polyleucine-based coiled coil dimers in a realistic membrane environment: insight into helix-helix interactions in membrane proteins. 2004 , 43, 9050-60	20
2050	Analysis of tryptophan surface accessibility in proteins by MALDI-TOF mass spectrometry. 2004 , 323, 1134-8	16
2049	Parmodel: a web server for automated comparative modeling of proteins. 2004 , 325, 1481-6	56
2048	Does common architecture reveal a viral lineage spanning all three domains of life?. 2004 , 16, 673-85	183
2047	A link between sequence conservation and domain motion within the AAA+ family. 2004 , 146, 189-204	21
2046	A conserved arginine plays a role in the catalytic cycle of the protein disulphide isomerases. 2004 , 335, 283-95	109
2045	Influence of proline residues in transmembrane helix packing. 2004 , 335, 631-40	54
2044	Insight into molecular interactions between two PB1 domains. 2004 , 336, 1195-210	13
2043	Does native state topology determine the RNA folding mechanism?. 2004 , 337, 789-97	44

2042	NMR and MD studies on the interaction between ligand peptides and alpha-bungarotoxin. 2004 , 339, 1169-77	5
2041	Mutagenesis and molecular dynamics suggest structural and functional roles for residues in the N-terminal portion of the cytochrome P450 2B1 I helix. 2004 , 423, 266-76	26
2040	Searching for nanostructures of the cubic mesophase of liquid crystal molecules, BABH8. 2004 , 120, 3699-705	9
2039	Molecular dynamics simulation study of the interaction of trehalose with lipid membranes. 2004 , 20, 7844-51	102
2038	Structural basis for octameric ring formation and DNA interaction of the human homologous-pairing protein Dmc1. 2004 , 14, 363-74	94
2037	Computer simulation of the KvAP voltage-gated potassium channel: steered molecular dynamics of the voltage sensor. 2004 , 564, 325-32	47
2036	Cationic DMPC/DMTAP lipid bilayers: molecular dynamics study. 2004 , 86, 3461-72	147
2035	Structure and dynamics of sphingomyelin bilayer: insight gained through systematic comparison to phosphatidylcholine. 2004 , 87, 2976-89	126
2034	Kv channel S6 helix as a molecular switch: simulation studies. 2004 , 151, 17-27	15
2033	Conformational Analysis and Derivation of Molecular Mechanics Parameters for Esters and Thioesters. 2004 , 108, 10173-10185	24
2032	Detailed Hydration Maps of Benzene and Cyclohexane Reveal Distinct Water Structures. 2004 , 108, 13492-13500	90
2031	Distribution of pentachlorophenol in phospholipid bilayers: a molecular dynamics study. 2004 , 86, 337-45	52
2030	Dynamics of water molecules in the bacteriorhodopsin trimer in explicit lipid/water environment. 2004 , 86, 705-17	79
2029	Complexation of phosphatidylcholine lipids with cholesterol. 2004 , 86, 1345-56	130
2028	Molecular dynamics simulation of a palmitoyl-oleoyl phosphatidylserine bilayer with Na ⁺ counterions and NaCl. 2004 , 86, 1601-9	159
2027	Molecular dynamics simulations of hydrophilic pores in lipid bilayers. 2004 , 86, 2156-64	248
2026	Homodimerization of calpain 3 penta-EF-hand domain. 2005 , 388, 585-91	33
2025	Conformational and dynamical properties of the niruricide in aqueous solution: a molecular dynamics approach. 2005 , 714, 189-197	2

2024	A molecular dynamics simulation study of glutamine-binding protein. 2005 , 725, 9-16	12
2023	Molecular dynamics simulation on complex of HPPK and substrate HP. 2005 , 731, 23-28	1
2022	Molecular dynamics simulation of liquid ethylene glycol and its aqueous solution. 2005 , 728, 179-187	47
2021	Computer-aided determination of relative stereochemistry and 3D models of complex organic molecules from 2D NMR spectra. 2005 , 61, 9980-9989	28
2020	Docking studies on monoamine oxidase-B inhibitors: estimation of inhibition constants ($K(i)$) of a series of experimentally tested compounds. 2005 , 15, 4438-46	45
2019	Molecular dynamics investigations of the polysaccharide scleroglucan: first study on the triple helix structure. 2005 , 340, 2154-62	60
2018	Molecular simulations of outersphere reorganization energies for intramolecular electron and hole transfer in polar solvents. 2005 , 319, 4-15	15
2017	Exotic aqueous behavior of synthetic lipids: formation of vesicular nanotubes. 2005 , 136, 23-46	11
2016	Atomistic simulation of KCl transport in charged silicon nanochannels: Interfacial effects. 2005 , 267, 103-109	79
2015	Heme peroxidase clothing and inhibition with polyphenolic substances revealed by molecular modeling. 2005 , 29, 83-90	7
2014	Potential drug targets in Mycobacterium tuberculosis through metabolic pathway analysis. 2005 , 29, 368-78	125
2013	Systematic coarse-graining of atomistic models for simulation of polymeric systems. 2005 , 29, 2380-2385	67
2012	Accounting for polarization in molecular simulation. 2005 , 172, 69-85	195
2011	Calculation of the optical rotatory dispersion of solvated alanine by means of the perturbed matrix method. 2005 , 402, 559-563	6
2010	A severe artifact in simulation of liquid water using a long cut-off length: Appearance of a strange layer structure. 2005 , 406, 49-53	48
2009	Temperature dependence of the transport coefficients of ions from molecular dynamics simulations. 2005 , 408, 84-88	35
2008	Molecular dynamics simulation of the sodium octanoate micelle in aqueous solution. 2005 , 411, 474-478	21
2007	Computer evaluation of protein segments removal effects from naphthalene 1,2-dioxygenase enzyme on polycyclic aromatic hydrocarbons interaction. 2005 , 27, 161-166	9

2006	All are not equal: a benchmark of different homology modeling programs. 2005 , 14, 1315-27	161
2005	Effect of hexafluoroisopropanol alcohol on the structure of melittin: a molecular dynamics simulation study. 2005 , 14, 2582-9	65
2004	Glutathione S-transferase and aluminum toxicity in maize. 2005 , 32, 1045-1055	26
2003	Structure and dynamics of water at the interface with phospholipid bilayers. 2005 , 123, 224702	110
2002	Advanced approaches for the characterization of a de novo designed antiparallel coiled coil peptide. 2005 , 3, 1189-94	22
2001	Virtual screening of novel CB2 ligands using a comparative model of the human cannabinoid CB2 receptor. 2005 , 48, 7166-71	57
2000	Solvation free energies of amino acid side chain analogs for common molecular mechanics water models. 2005 , 122, 134508	329
1999	Why is the partial molar volume of CO ₂ so small when dissolved in a room temperature ionic liquid? Structure and dynamics of CO ₂ dissolved in [Bmim ⁺] [PF ₆ ⁻]. 2005 , 127, 17842-51	307
1998	Modeling Lipid Membranes. 2005 , 929-958	5
1997	Molecular dynamics simulations of the adipocyte lipid binding protein reveal a novel entry site for the ligand. 2005 , 44, 4275-83	32
1996	The electronic structure of liquid water within density-functional theory. 2005 , 123, 014501	89
1995	Connexin-specific cell-to-cell transfer of short interfering RNA by gap junctions. 2005 , 568, 459-68	229
1994	Observation of a dewetting transition in the collapse of the melittin tetramer. 2005 , 437, 159-62	333
1993	Simulating micrometre-scale crystal growth from solution. 2005 , 438, 70-3	177
1992	Solution structure and backbone dynamics of the XPC-binding domain of the human DNA repair protein hHR23B. 2005 , 272, 2467-76	10
1991	A molecular dynamics study of human serum albumin binding sites. 2005 , 60, 485-95	47
1990	The molecular origins of specificity in the assembly of a multienzyme complex. 2005 , 13, 1119-30	53
1989	How pH opens a H ⁺ channel: the gating mechanism of influenza A M2. 2005 , 13, 1789-98	56

1988	Incorporating the effect of ionic strength in free energy calculations using explicit ions. 2005 , 26, 115-22	35
1987	OOPSE: an object-oriented parallel simulation engine for molecular dynamics. 2005 , 26, 252-71	35
1986	Empirical force-field assessment: The interplay between backbone torsions and noncovalent term scaling. 2005 , 26, 682-90	48
1985	A simple method for faster nonbonded force evaluations. 2005 , 26, 691-8	13
1984	MDSIMAID: automatic parameter optimization in fast electrostatic algorithms. 2005 , 26, 1021-31	5
1983	GROMACS: fast, flexible, and free. 2005 , 26, 1701-18	10273
1982	Dual-scale modeling of benzene adsorption onto Ni(111) and Au(111) surfaces in explicit water. 2005 , 6, 1866-71	55
1981	Solvent and protein effects on the structure and dynamics of the rhodopsin chromophore. 2005 , 6, 1836-47	62
1980	Molecular dynamics simulation of water near nanostructured hydrophobic surfaces: interfacial energies. 2005 , 6, 1641-9	20
1979	Simulated folding in polypeptides of diversified molecular tacticity: implications for protein folding and de novo design. 2005 , 78, 96-105	19
1978	Conformation-activity relationship of a novel peptide antibiotic: structural characterization of dermaseptin DS 01 in media that mimic the membrane environment. 2005 , 80, 688-96	9
1977	Structural and dynamic properties of cytochrome P450 BM-3 in pure water and in a dimethylsulfoxide/water mixture. 2005 , 78, 259-67	23
1976	Molecular simulation study of the influence of small molecules on the dynamic and structural properties of phospholipid bilayers. 2005 , 2, 1503-16	7
1975	Stability of SIV gp32 fusion-peptide single-layer protofibrils as monitored by molecular-dynamics simulations. 2005 , 44, 1065-1067	21
1974	Molecular dynamics simulations of protein G challenge NMR-derived correlated backbone motions. 2005 , 44, 3394-9	24
1973	Stability of SIV gp32 Fusion-Peptide Single-Layer Protofibrils as Monitored by Molecular-Dynamics Simulations. 2005 , 117, 1089-1091	4
1972	Molecular Dynamics Simulations of Protein G Challenge NMR-Derived Correlated Backbone Motions. 2005 , 117, 3460-3465	1
1971	Molecular Dynamics Simulations of the Orientation and Reorientational Dynamics of Water and Polypyrrole Rings as a Function of the Oxidation State of the Polymer. 2005 , 14, 40-48	10

1970	Calculation of the redox potential of the protein azurin and some mutants. 2005 , 6, 738-46	46
1969	Influence of protein flexibility on the electrostatic energy landscape in gramicidin A. 2005 , 34, 208-16	16
1968	Lateral pressure profiles in cholesterol-DPPC bilayers. 2005 , 35, 79-88	76
1967	Novel immunoglobulin-like transcripts in teleost fish encode polymorphic receptors with cytoplasmic ITAM or ITIM and a new structural Ig domain similar to the natural cytotoxicity receptor NKp44. 2005 , 57, 77-89	43
1966	Molecular dynamics simulation of barnacle cement. 2005 , 409, 160-166	19
1965	A three-dimensional structure of Plasmodium falciparum serine hydroxymethyltransferase in complex with glycine and 5-formyl-tetrahydrofolate. Homology modeling and molecular dynamics. 2005 , 115, 1-10	25
1964	Simulation of gel phase formation and melting in lipid bilayers using a coarse grained model. 2005 , 135, 223-44	261
1963	Elastic properties, Young's modulus determination and structural stability of the tropocollagen molecule: a computational study by steered molecular dynamics. 2005 , 38, 1527-33	118
1962	Molecular dynamics simulation of PAMAM dendrimer in aqueous solution. 2005 , 46, 3481-3488	83
1961	Identification of a novel gene family, paralogs of inhibitor of apoptosis proteins present in plants, fungi, and animals. 2005 , 10, 471-80	17
1960	Molecular dynamics simulations of bovine rhodopsin: influence of protonation states and different membrane-mimicking environments. <i>Journal of Molecular Modeling</i> , 2005 , 12, 49-64	2 34
1959	Almost all about citrulline in mammals. 2005 , 29, 177-205	387
1958	Describing partially unfolded states of proteins from sparse NMR data. 2005 , 33, 175-86	16
1957	Protein surface dynamics: interaction with water and small solutes. 2005 , 31, 433-52	7
1956	Multiple ligand-binding modes in bacterial R67 dihydrofolate reductase. 2005 , 19, 165-87	11
1955	A Simulative Model for the Analysis of Conduction Properties of Ion Channels Based on First-Principle Approaches. 2005 , 4, 171-174	1
1954	Electro-Chemical Modeling Challenges of Biological Ion Pumps. 2005 , 4, 189-193	4
1953	Molecular dynamics simulations of the periplasmic ferric-hydroxamate binding protein FhuD. 2005 , 18, 375-86	31

1952	Computer simulation of partitioning of ten pentapeptides Ace-WLXLL at the cyclohexane/water and phospholipid/water interfaces. 2005 , 6, 30	36
1951	High-temperature unfolding of a trp-cage mini-protein: a molecular dynamics simulation study. 2005 , 2, 7	18
1950	Investigating interactions of biomembranes and alcohols: A multiscale approach. 2005 , 43, 1025-1032	26
1949	A multibody, whole-residue potential for protein structures, with testing by Monte Carlo simulated annealing. 2005 , 59, 152-69	12
1948	One gene, two diseases and three conformations: molecular dynamics simulations of mutants of human prion protein at room temperature and elevated temperatures. 2005 , 59, 275-90	37
1947	Structure and energy landscape of a photoswitchable peptide: a replica exchange molecular dynamics study. 2005 , 60, 485-94	45
1946	Modeling side-chains using molecular dynamics improve recognition of binding region in CAPRI targets. 2005 , 60, 245-51	33
1945	Incorporation of flexibility into rigid-body docking: applications in rounds 3-5 of CAPRI. 2005 , 60, 263-8	26
1944	Biologically enhanced sampling geometric docking and backbone flexibility treatment with multiconformational superposition. 2005 , 60, 319-23	12
1943	Unwinding the helical linker of calcium-loaded calmodulin: a molecular dynamics study. 2005 , 61, 829-39	24
1942	An assessment of the accuracy of methods for predicting hydrogen positions in protein structures. 2005 , 61, 296-309	32
1941	Comparative molecular dynamics--similar folds and similar motions?. 2005 , 61, 809-22	45
1940	Free energy landscape and folding mechanism of a beta-hairpin in explicit water: a replica exchange molecular dynamics study. 2005 , 61, 795-808	118
1939	Structural differences between allelic variants of the ovine prion protein revealed by molecular dynamics simulations. 2005 , 61, 840-9	18
1938	Characterizing the conformational ensemble of monomeric polyglutamine. 2006 , 63, 297-311	109
1937	Generalized correlation for biomolecular dynamics. 2006 , 62, 1053-61	278
1936	Solution state conformation and degradation of cyclopeptides containing an NGR motif. 2005 , 11, 53-9	6
1935	Evidence of a double-lid movement in Pseudomonas aeruginosa lipase: insights from molecular dynamics simulations. 2005 , 1, e28	45

1934	Membrane-bound ARF1 peptide: interpretation of neutron diffraction data by molecular dynamics simulation methods. 2005 , 22, 379-88	2
1933	The function of the extracellular regions in opioid receptor binding: insights from computational biology. 2005 , 5, 357-67	11
1932	A conformational change in the adeno-associated virus type 2 capsid leads to the exposure of hidden VP1 N termini. 2005 , 79, 5296-303	127
1931	Fluorescence and molecular dynamics studies of the acetylcholine receptor gammaM4 transmembrane peptide in reconstituted systems. 2005 , 22, 471-83	30
1930	THE HELIX-TURN-HELIX AS A SCAFFOLD FOR CHIMERIC NUCLEASE DESIGN. 2005 , 26, 127-164	3
1929	Modeling and experimental validation of the binary complex of the plectin actin-binding domain and the first pair of fibronectin type III (FNIII) domains of the beta4 integrin. 2005 , 280, 22270-7	18
1928	Structural evidence for non-canonical binding of Ca ²⁺ to a canonical EF-hand of a conventional myosin. 2005 , 280, 41458-64	20
1927	Comparative study of generalized Born models: protein dynamics. 2005 , 102, 6760-4	63
1926	Membrane-bound conformation of M13 major coat protein: a structure validation through FRET-derived constraints. 2005 , 280, 38522-7	17
1925	Identification of a novel pharmacophore for peptide toxins interacting with K ⁺ channels. 2005 , 280, 21246-55	25
1924	The N-terminal juxtamembrane segment of the V1a vasopressin receptor provides two independent epitopes required for high-affinity agonist binding and signaling. 2005 , 19, 2871-81	20
1923	Diffusion of water and sodium counter-ions in nanopores of a lactoglobulin crystal: a molecular dynamics study. 2005 , 16, S522-30	19
1922	Conservation and specialization in PAS domain dynamics. 2005 , 18, 127-37	31
1921	Oxidative Bax dimerization promotes its translocation to mitochondria independently of apoptosis. 2005 , 19, 1504-6	110
1920	A G(q/11)-coupled mutant histamine H(1) receptor F435A activated solely by synthetic ligands (RASSL). 2005 , 280, 34741-6	27
1919	The influence of conformational fluctuations on enzymatic activity: modelling the functional motion of secretase. 2005 , 17, S1581-S1593	14
1918	The delta e13 isoform of the calcitonin receptor forms a six-transmembrane domain receptor with dominant-negative effects on receptor surface expression and signaling. 2005 , 19, 2132-44	34
1917	Structure and mechanism of the reversible photoswitch of a fluorescent protein. 2005 , 102, 13070-4	222

1916	Peptides design based on the interfacial helix of integrase dimer. 2005 , 2005, 4743-6	1
1915	Evolution of the structure of amorphous ice: from low-density amorphous through high-density amorphous to very high-density amorphous ice. 2005 , 122, 134501	76
1914	Structural features of the glutamate binding site in recombinant NR1/NR2A N-methyl-D-aspartate receptors determined by site-directed mutagenesis and molecular modeling. 2005 , 67, 1470-84	124
1913	Simulations of transient membrane behavior in cells subjected to a high-intensity ultrashort electric pulse. 2005 , 71, 031914	117
1912	Surface-charge-induced asymmetric electrokinetic transport in confined silicon nanochannels. 2005 , 86, 143105	45
1911	Gaussian split Ewald: A fast Ewald mesh method for molecular simulation. 2005 , 122, 54101	280
1910	Length dependent folding kinetics of phenylacetylene oligomers: structural characterization of a kinetic trap. 2005 , 122, 124908	10
1909	Monte Carlo simulation of a model of water. 2005 , 72, 040201	8
1908	Identification of a hydrophobic residue as a key determinant of fructose transport by the facilitative hexose transporter SLC2A7 (GLUT7). 2005 , 280, 42978-83	43
1907	Mechanism of partial agonism at NMDA receptors for a conformationally restricted glutamate analog. 2005 , 25, 7858-66	64
1906	Unusual compactness of a polyproline type II structure. 2005 , 102, 11698-703	121
1905	The NH2 terminus of RCK1 domain regulates Ca ²⁺ -dependent BK(Ca) channel gating. 2005 , 126, 227-41	27
1904	Conformational transition of amyloid beta-peptide. 2005 , 102, 5403-7	222
1903	Molecular motions of human cyclin-dependent kinase 2. 2005 , 280, 13993-4005	39
1902	Release of long-range tertiary interactions potentiates aggregation of natively unstructured alpha-synuclein. 2005 , 102, 1430-5	612
1901	Cyclophilin A binds to linear peptide motifs containing a consensus that is present in many human proteins. 2005 , 280, 23668-74	55
1900	A true autoactivating enzyme. Structural insight into mannose-binding lectin-associated serine protease-2 activations. 2005 , 280, 33435-44	86
1899	The alpha7 nicotinic acetylcholine receptor: molecular modelling, electrostatics, and energetics. 2005 , 22, 151-62	30

1898	Electrolytic transport through a synthetic nanometer-diameter pore. 2005 , 102, 10445-50	198
1897	Synthesis of spin-labeled RNAs for long range distance measurements by peldor. 2005 , 24, 771-5	38
1896	Possible pathway(s) of testosterone egress from the active site of cytochrome P450 2B1: a steered molecular dynamics simulation. 2005 , 33, 910-9	45
1895	Molecular dynamics study of lignin constituents in water. 2005 , 59, 253-262	8
1894	Functional role of C-terminal sequence elements in the transporter associated with antigen processing. 2005 , 174, 328-39	11
1893	Hydrophobic hydration from small to large lengthscales: Understanding and manipulating the crossover. 2005 , 102, 9475-80	255
1892	Alternative splicing of SNAP-25 regulates secretion through nonconservative substitutions in the SNARE domain. 2005 , 16, 5675-85	56
1891	PROVAT: a tool for Voronoi tessellation analysis of protein structures and complexes. 2005 , 21, 3316-7	13
1890	Unexpected enzyme TEM-126: role of mutation Asp179Glu. 2005 , 49, 4280-7	13
1889	Refinement of docked protein-ligand and protein-DNA structures using low frequency normal mode amplitude optimization. 2005 , 33, 4496-506	56
1888	Synthesis, molecular modeling studies, and selective inhibitory activity against monoamine oxidase of 1-thiocarbamoyl-3,5-diaryl-4,5-dihydro-(1H)- pyrazole derivatives. 2005 , 48, 7113-22	98
1887	Molecular modeling of wild-type and D816V c-Kit inhibition based on ATP-competitive binding of ellipticine derivatives to tyrosine kinases. 2005 , 48, 6194-201	28
1886	Data-driven docking: HADDOCK's adventures in CAPRI. 2005 , 60, 232-8	70
1885	Surfaces affect ion pairing. 2005 , 109, 24056-60	50
1884	Electric-field-induced redox potential shifts of tetraheme cytochromes c3 immobilized on self-assembled monolayers: surface-enhanced resonance Raman spectroscopy and simulation studies. 2005 , 88, 4188-99	56
1883	Binding mode prediction of cytochrome p450 and thymidine kinase protein-ligand complexes by consideration of water and rescoring in automated docking. 2005 , 48, 2308-18	110
1882	Mechanical properties of surfactant bilayer membranes from atomistic and coarse-grained molecular dynamics simulations. 2005 , 109, 19851-8	33
1881	Molecular dynamics simulations of salicylate effects on the micro- and mesoscopic properties of a dipalmitoylphosphatidylcholine bilayer. 2005 , 44, 13425-38	39

1880	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution. Part 4. Uracil and thymine. 2005 , 7, 2006-17	143
1879	Two exchange-correlation functionals compared for first-principles liquid water. 2005 , 31, 361-366	31
1878	From Hydrophobic to Hydrophilic Solvation: An Application to Hydration of Benzene. 2005 , 1, 643-52	60
1877	Properties of p-hydroxybenzoate hydroxylase when stabilized in its open conformation. 2005 , 44, 14807-17	21
1876	Enforcing solution phase nanoscopic aggregation in a palindromic tripeptide. 2005 , 2564-6	12
1875	Molecular dynamics simulations of the cytolytic toxin Cyt1A in solution. 2005 , 4, 235-40	3
1874	On the salt-induced stabilization of pair and many-body hydrophobic interactions. 2005 , 109, 642-51	113
1873	Hydration-induced changes of structure and vibrational frequencies of methylphosphocholine studied as a model of biomembrane lipids. 2005 , 109, 15126-34	32
1872	Effect of the choice of the pressure coupling method on the spontaneous aggregation of DPPC molecules. 2005 , 109, 14667-74	13
1871	Molecular dynamics simulations of helix-forming, amine-functionalized m-poly(phenyleneethynylene)s. 2005 , 109, 7548-56	19
1870	Hydration and dewetting near graphite-CH(3) and graphite-COOH plates. 2005 , 109, 13639-48	67
1869	Characterization of the stereochemical selectivity of beta-hairpin formation by molecular dynamics simulations. 2005 , 109, 1281-8	2
1868	Evolutionarily conserved functional mechanics across pepsin-like and retroviral aspartic proteases. 2005 , 127, 3734-42	71
1867	Novel conotoxins from <i>Conus striatus</i> and <i>Conus kinoshitai</i> selectively block TTX-resistant sodium channels. 2005 , 44, 7259-65	105
1866	Excluded volume effect for large and small solutes in water. 2005 , 109, 6939-46	11
1865	Computational study of the dynamics of mannose disaccharides free in solution and bound to the potent anti-HIV virucidal protein cyanovirin. 2005 , 109, 3639-47	20
1864	Modulating membrane properties: the effect of trehalose and cholesterol on a phospholipid bilayer. 2005 , 109, 24173-81	59
1863	On the performance of molecular dynamics applications on current high-end systems. 2005 , 363, 1987-98	20

1862	Effect of lipid composition on the "membrane response" induced by a fusion peptide. 2005 , 44, 14626-37	27
1861	Molecular dynamics simulation of a perylene-derivative Langmuir film. 2005 , 109, 4032-41	8
1860	Molecular dynamics of a polymer in mixed solvent: atactic polystyrene in a mixture of cyclohexane and N,N-dimethylformamide. 2005 , 109, 15714-23	18
1859	Metabolic regio- and stereoselectivity of cytochrome P450 2D6 towards 3,4-methylenedioxy-N-alkylamphetamines: in silico predictions and experimental validation. 2005 , 48, 6117-27	56
1858	Molecular Dynamics Simulation of a GM3 Ganglioside Bilayer. 2005 , 109, 6036-6036	
1857	The mechanism of proton transfer between adjacent sites exposed to water. 2005 , 109, 11379-88	20
1856	Dynamic mechanism for the autophosphorylation of CheA histidine kinase: molecular dynamics simulations. 2005 , 127, 11709-19	28
1855	Completed three-dimensional model of human coagulation factor va. Molecular dynamics simulations and structural analyses. 2005 , 44, 13082-90	30
1854	Molecular modeling and molecular dynamics simulation of the human A2B adenosine receptor. The study of the possible binding modes of the A2B receptor antagonists. 2005 , 48, 6813-20	26
1853	Supercooled water in PVA matrixes. II. A molecular dynamics simulation study and comparison with QENS results. 2005 , 109, 8091-6	25
1852	Solvophobic and steric effects of side groups on polymer folding: molecular modeling studies of amine-functionalized m-poly(phenyleneethynylene) foldamers in aqueous solution. 2005 , 109, 19952-9	17
1851	Solubility of methane in water: the significance of the methane-water interaction potential. 2005 , 109, 23596-604	26
1850	Rapid Estimation of Solvation Energy for Simulations of Protein-Protein Association. 2005 , 1, 143-52	16
1849	Orientation and dynamics of benzyl alcohol and benzyl alkyl ethers dissolved in nematic lyotropic liquid crystals. 2H NMR and molecular dynamics simulations. 2005 , 109, 6644-51	8
1848	Prediction of the orientations of adsorbed protein using an empirical energy function with implicit solvation. 2005 , 21, 5616-26	38
1847	Scaling of electrokinetic transport in nanometer channels. 2005 , 21, 8972-7	57
1846	Coulombic and hydrophobic interactions in the first intracellular loop are vital for bradykinin B2 receptor ligand binding and consequent signal transduction. 2005 , 44, 5295-306	8
1845	Bench meets bedside: a 10-year-old girl and amino acid residue glycine 75 of the facilitative glucose transporter GLUT1. 2005 , 44, 12621-6	5

1844	Structural basis for the enantioselectivity of an epoxide ring opening reaction catalyzed by halo alcohol dehalogenase HheC. 2005 , 127, 13338-43	62
1843	Conformational dynamics of M2 helices in KirBac channels: helix flexibility in relation to gating via molecular dynamics simulations. 2005 , 44, 14586-94	49
1842	Heteroaryl-substituted naphthalenes and structurally modified derivatives: selective inhibitors of CYP11B2 for the treatment of congestive heart failure and myocardial fibrosis. 2005 , 48, 6632-42	65
1841	Molecular structure of the lecithin ripple phase. 2005 , 102, 5392-6	146
1840	Empirical nanotube model for biological applications. 2005 , 109, 11461-7	51
1839	Dimerization of the p53 oligomerization domain: identification of a folding nucleus by molecular dynamics simulations. 2005 , 345, 869-78	35
1838	The relationship between the flexibility of proteins and their conformational states on forming protein-protein complexes with an application to protein-protein docking. 2005 , 347, 1077-101	146
1837	Diversity in hapten recognition: structural study of an anti-cocaine antibody M82G2. 2005 , 349, 570-82	33
1836	Extended intermolecular interactions in a serine protease-canonical inhibitor complex account for strong and highly specific inhibition. 2005 , 350, 156-69	43
1835	X-ray structure of domain I of the proton-pumping membrane protein transhydrogenase from <i>Escherichia coli</i> . 2005 , 352, 299-312	24
1834	How large is an alpha-helix? Studies of the radii of gyration of helical peptides by small-angle X-ray scattering and molecular dynamics. 2005 , 353, 232-41	59
1833	pH-dependent conformational flexibility of the SARS-CoV main proteinase (M(pro)) dimer: molecular dynamics simulations and multiple X-ray structure analyses. 2005 , 354, 25-40	135
1832	The structure of the C5a receptor-blocking domain of chemotaxis inhibitory protein of <i>Staphylococcus aureus</i> is related to a group of immune evasive molecules. 2005 , 353, 859-72	53
1831	Reproducible polypeptide folding and structure prediction using molecular dynamics simulations. 2005 , 354, 173-83	150
1830	Structure and function of the potent cyclic and linear melanocortin analogues. 2005 , 150, 300-8	9
1829	A structural model of a seven-transmembrane helix receptor: the Duffy antigen/receptor for chemokine (DARC). 2005 , 1724, 288-306	55
1828	Molecular cloning, functional expression, and molecular modeling of bothrostatin, a new highly active disintegrin from <i>Bothrops jararaca</i> venom. 2005 , 329, 457-64	25
1827	Miglustat (NB-DNJ) works as a chaperone for mutated acid beta-glucosidase in cells transfected with several Gaucher disease mutations. 2005 , 35, 268-76	105

1826	The conserved residue Phe273(282) of PPARalpha(gamma), beyond the ligand-binding site, functions in binding affinity through solvation effect. 2005 , 87, 539-50	12
1825	Molecular basis of the allosteric mechanism of cAMP in the regulatory PKA subunit. 2005 , 579, 2679-85	9
1824	Nucleotide binding to the homodimeric MJ0796 protein: a computational study of a prokaryotic ABC transporter NBD dimer. 2005 , 579, 4193-9	32
1823	Compact oleic acid in HAMLET. 2005 , 579, 6095-100	30
1822	Protonation state of Asp30 exerts crucial influence over surface loop rearrangements responsible for NO release in nitrophorin 4. 2005 , 579, 5392-8	22
1821	Correlation of temperature induced conformation change with optimum catalytic activity in the recombinant G/11 xylanase A from Bacillus subtilis strain 168 (1A1). 2005 , 579, 6505-10	40
1820	What factor drives the fibrillogenic association of beta-sheets?. 2005 , 579, 6635-40	23
1819	SsNAC23, a member of the NAC domain protein family, is associated with cold, herbivory and water stress in sugarcane. 2005 , 169, 93-106	60
1818	Functional role of residues in the helix B' region of cytochrome P450 2B1. 2005 , 435, 157-65	36
1817	Entropy calculation of HIV-1 Env gp120, its receptor CD4, and their complex: an analysis of configurational entropy changes upon complexation. 2005 , 88, 15-24	55
1816	Exploring the helix-coil transition via all-atom equilibrium ensemble simulations. 2005 , 88, 2472-93	557
1815	Conformational dynamics of the ligand-binding domain of inward rectifier K channels as revealed by molecular dynamics simulations: toward an understanding of Kir channel gating. 2005 , 88, 3310-20	40
1814	The apo and ternary complex structures of a chemotherapeutic target: human glycinamide ribonucleotide transformylase. 2005 , 44, 9841-50	15
1813	Molecular dynamics simulations of ice growth from supercooled water. 2005 , 103, 2957-2967	90
1812	Probing the pH-dependent structural features of alpha-KTx12.1, a potassium channel blocker from the scorpion Tityus serrulatus. 2005 , 14, 1025-38	12
1811	Ligand-binding regulation of LXR/RXR and LXR/PPAR heterodimerizations: SPR technology-based kinetic analysis correlated with molecular dynamics simulation. 2005 , 14, 812-22	42
1810	Molecular dynamics study of the lung surfactant peptide SP-B1-25 with DPPC monolayers: insights into interactions and peptide position and orientation. 2005 , 88, 1577-92	31
1809	2H-NMR study and molecular dynamics simulation of the location, alignment, and mobility of pyrene in POPC bilayers. 2005 , 88, 1818-27	108

1808	Molecular dynamics simulations indicate a possible role of parallel beta-helices in seeded aggregation of poly-Gln. 2005 , 88, 2442-51	62
1807	Mechanically induced titin kinase activation studied by force-probe molecular dynamics simulations. 2005 , 88, 790-804	181
1806	Penetratin-membrane association: W48/R52/W56 shield the peptide from the aqueous phase. 2005 , 88, 939-52	61
1805	Molecular dynamics simulation of the M2 helices within the nicotinic acetylcholine receptor transmembrane domain: structure and collective motions. 2005 , 88, 3321-33	40
1804	The alpha-helical propensity of the cytoplasmic domain of phospholamban: a molecular dynamics simulation of the effect of phosphorylation and mutation. 2005 , 88, 3243-51	35
1803	Molecular dynamics simulations and 2H NMR study of the GalCer/DPPG lipid bilayer. 2005 , 88, 4017-31	34
1802	Hinge-like motions in RNA kink-turns: the role of the second a-minor motif and nominally unpaired bases. 2005 , 88, 3466-85	88
1801	Does water play a structural role in the folding of small nucleic acids?. 2005 , 88, 2516-24	85
1800	Predicting the signaling state of photoactive yellow protein. 2005 , 88, 3525-35	23
1799	Influence of DPH on the structure and dynamics of a DPPC bilayer. 2005 , 88, 3398-410	100
1798	A molecular dynamics study of the formation, stability, and oligomerization state of two designed coiled coils: possibilities and limitations. 2005 , 89, 3701-13	23
1797	Osmolyte trimethylamine-N-oxide does not affect the strength of hydrophobic interactions: origin of osmolyte compatibility. 2005 , 89, 858-66	130
1796	Exploring global motions and correlations in the ribosome. 2005 , 89, 1455-63	115
1795	Molecular dynamics of a protein surface: ion-residues interactions. 2005 , 89, 768-81	62
1794	Probing conformational disorder in neurotensin by two-dimensional solid-state NMR and comparison to molecular dynamics simulations. 2005 , 89, 2113-20	46
1793	Spontaneous formation of detergent micelles around the outer membrane protein OmpX. 2005 , 88, 3191-204	48
1792	Unfolding and extraction of a transmembrane alpha-helical peptide: dynamic force spectroscopy and molecular dynamics simulations. 2005 , 89, 3129-40	27
1791	Interaction of the antimicrobial peptide cyclo(RRWRF) with membranes by molecular dynamics simulations. 2005 , 89, 2296-306	36

1790	Water dependent properties of cutinase in nonaqueous solvents: a computational study of enantioselectivity. 2005 , 89, 999-1008	36
1789	Multi-scale modeling of phase separation in mixed lipid bilayers. 2005 , 89, 2385-94	45
1788	Reorganization and conformational changes in the reduction of tetraheme cytochromes. 2005 , 89, 3919-30	21
1787	Molecular dynamics simulations of the anchoring and tilting of the lung-surfactant peptide SP-B1-25 in palmitic acid monolayers. 2005 , 89, 3807-21	20
1786	A computational study of the closed and open states of the influenza A M2 proton channel. 2005 , 89, 2402-11	41
1785	A salt-bridge motif involved in ligand binding and large-scale domain motions of the maltose-binding protein. 2005 , 89, 3362-71	61
1784	Multiple roles of a conserved GAF domain tyrosine residue in cyanobacterial and plant phytochromes. 2005 , 44, 15203-15	83
1783	Surface tension effect on transmembrane channel stability in a model membrane. 2005 , 109, 19474-83	12
1782	Simulations of nanopore formation and phosphatidylserine externalization in lipid membranes subjected to a high-intensity, ultrashort electric pulse. 2005 , 72, 031902	92
1781	A simple method to predict protein flexibility using secondary chemical shifts. 2005 , 127, 14970-1	325
1780	Application of classical molecular dynamics for evaluation of proton transfer mechanism on a protein. 2005 , 1710, 67-77	21
1779	Rapid computational identification of the targets of protein kinase inhibitors. 2005 , 48, 4138-52	45
1778	Molecular dynamics study of dislocation nucleation from a crack tip. 2005 , 71,	19
1777	Effect of monovalent salt on cationic lipid membranes as revealed by molecular dynamics simulations. 2005 , 109, 21126-34	64
1776	Comparative study of generalized born models: Born radii and peptide folding. 2005 , 109, 3008-22	78
1775	Homology models of the Yersinia pseudotuberculosis and Yersinia pestis general porins and comparative analysis of their functional and antigenic regions. 2005 , 23, 163-74	18
1774	A regularized and renormalized electrostatic coupling Hamiltonian for hybrid quantum-mechanical-molecular-mechanical calculations. 2005 , 123, 164114	44
1773	Covalent cross-links between the gamma subunit (FXD2) and alpha and beta subunits of Na,K-ATPase: modeling the alpha-gamma interaction. 2005 , 280, 18291-301	27

1772	Dielectric permittivity profiles of confined polar fluids. 2005 , 122, 114711	173
1771	Molecular simulation to characterize the adsorption behavior of a fibrinogen gamma-chain fragment. 2005 , 21, 1103-17	127
1770	Pore formation coupled to ion transport through lipid membranes as induced by transmembrane ionic charge imbalance: atomistic molecular dynamics study. 2005 , 127, 17570-1	175
1769	Asymmetry of lipid bilayers induced by monovalent salt: atomistic molecular-dynamics study. 2005 , 122, 244902	99
1768	Direct calculation of the binding free energies of FKBP ligands. 2005 , 123, 084108	165
1767	Can octupolar molecules be poled by an external electric field?. 2005 , 109, 16730-5	19
1766	On the Ewald artifacts in computer simulations. The test-case of the octaalanine peptide with charged termini. 2005 , 23, 135-42	23
1765	Mechanism of helix nucleation and propagation: microscopic view from microsecond time scale MD simulations. 2005 , 109, 20064-7	33
1764	Synthesis and evaluation of imidazolylmethylenetetrahydronaphthalenes and imidazolylmethyleneindanes: potent inhibitors of aldosterone synthase. 2005 , 48, 1796-805	54
1763	Synthesis and evaluation of (pyridylmethylene)tetrahydronaphthalenes/-indanes and structurally modified derivatives: potent and selective inhibitors of aldosterone synthase. 2005 , 48, 1563-75	68
1762	Low-temperature and high-pressure induced swelling of a hydrophobic polymer-chain in aqueous solution. 2005 , 7, 2780-6	38
1761	Molecular dynamics simulations of GlpF in a micelle vs in a bilayer: conformational dynamics of a membrane protein as a function of environment. 2005 , 109, 575-82	35
1760	Association of the cystic fibrosis transmembrane regulator with CAL: structural features and molecular dynamics. 2005 , 44, 16158-66	20
1759	Protein-Ligand Interactions. 2005 ,	31
1758	Conformational dynamics of the nicotinic acetylcholine receptor channel: a 35-ns molecular dynamics simulation study. 2005 , 127, 1291-9	61
1757	The influence of different treatments of electrostatic interactions on the thermodynamics of folding of peptides. 2005 , 109, 21322-8	29
1756	Homology model of human retinoic acid metabolising enzyme cytochrome P450 26A1 (CYP26A1): active site architecture and ligand binding. 2006 , 21, 361-9	19
1755	MD simulations of Mistic: conformational stability in detergent micelles and water. 2006 , 45, 9053-8	16

1754	Preferential solvation of phenol in binary solvent mixtures. A molecular dynamics study. 2006 , 110, 2253-8	6
1753	Control of electroosmotic flow by polymer coating: effects of the electrical double layer. 2006 , 22, 7096-100	37
1752	Solvent Effects and Conformational Stability of a Tripeptide. 2006 , 141-149	1
1751	Molecular dynamics study of methane in water: diffusion and structure. 2006 , 32, 1279-1286	19
1750	Atomistic simulation of structure and dynamics of columnar phases of hexabenzocoronene derivatives. 2006 , 125, 124902	65
1749	Molecular dynamics simulations of water droplets on polymer surfaces. 2006 , 125, 144712	102
1748	Teaching parallel computing to science faculty. 2006 ,	15
1747	Force-induced insulin dimer dissociation: a molecular dynamics study. 2006 , 128, 5330-1	26
1746	The nature of the adsorption of nucleobases on the gold [111] surface. 2006 , 110, 23467-71	106
1745	Adsorption of polycyclic aromatic hydrocarbons at the air-water interface: molecular dynamics simulations and experimental atmospheric observations. 2006 , 8, 4461-7	62
1744	Molecular dynamics simulations applied to electric field induced second harmonic generation in dipolar chromophore solutions. 2006 , 110, 8971-7	17
1743	Collective Langevin dynamics of conformational motions in proteins. 2006 , 124, 214903	89
1742	Anthramycin-DNA binding explored by molecular simulations. 2006 , 110, 24687-95	23
1741	Molecular understanding of osmosis in semipermeable membranes. 2006 , 97, 024501	61
1740	Assisted desolvation as a key kinetic step for crystal growth. 2006 , 128, 13568-74	125
1739	Differential ion transport induced electroosmosis and internal recirculation in heterogeneous osmosis membranes. 2006 , 6, 995-9	31
1738	Cation and anion transport through hydrophilic pores in lipid bilayers. 2006 , 125, 074901	53
1737	Computer simulation of the distribution of hexane in a lipid bilayer: spatially resolved free energy, entropy, and enthalpy profiles. 2006 , 128, 125-30	121

1736	Opening and closing motions in the periplasmic vitamin B12 binding protein BtuF. 2006 , 45, 13284-92	56
1735	Membrane protein simulations with a united-atom lipid and all-atom protein model: lipid-protein interactions, side chain transfer free energies and model proteins. 2006 , 18, S1221-34	138
1734	Running Molecular Dynamics Simulations in a Grid Environment. 2006 ,	4
1733	Effect of quantum partial charges on the structure and dynamics of water in single-walled carbon nanotubes. 2006 , 125, 114701	102
1732	Dielectric response of a polar fluid trapped in a spherical nanocavity. 2006 , 124, 144714	24
1731	Using massively parallel simulation and Markovian models to study protein folding: examining the dynamics of the villin headpiece. 2006 , 124, 164902	137
1730	Simulation of infrared spectra for beta-hairpin peptides stabilized by an Aib-Gly turn sequence: correlation between conformational fluctuation and vibrational coupling. 2006 , 110, 23590-602	29
1729	Homogeneous freezing of water starts in the subsurface. 2006 , 110, 18126-9	99
1728	Synthesis and evaluation of heteroaryl-substituted dihydronaphthalenes and indenenes: potent and selective inhibitors of aldosterone synthase (CYP11B2) for the treatment of congestive heart failure and myocardial fibrosis. 2006 , 49, 2222-31	81
1727	Model of an asymmetric DPPC/DPPS membrane: effect of asymmetry on the lipid properties. A molecular dynamics simulation study. 2006 , 110, 2358-63	43
1726	Vstx1, a modifier of Kv channel gating, localizes to the interfacial region of lipid bilayers. 2006 , 45, 11844-55	33
1725	Diffusion in binary gas mixtures studied by NMR of hyperpolarized gases and molecular dynamics simulations. 2006 , 8, 4182-8	27
1724	Molecular investigation of the interactions of trehalose with lipid bilayers of DPPC, DPPE and their mixture. 2006 , 32, 219-230	30
1723	Full length Vpu from HIV-1: combining molecular dynamics simulations with NMR spectroscopy. 2006 , 23, 485-96	16
1722	Hydrophobic aided replica exchange: an efficient algorithm for protein folding in explicit solvent. 2006 , 110, 19018-22	71
1721	Diversity and functional consequences of germline and somatic PTPN11 mutations in human disease. 2006 , 78, 279-90	292
1720	Molecular dynamics: survey of methods for simulating the activity of proteins. 2006 , 106, 1589-615	818
1719	Under the influence of alcohol: the effect of ethanol and methanol on lipid bilayers. 2006 , 90, 1121-35	275

1718	Molecular Dynamics Simulation of the Glass Transition of Ortho-Terphenyl in Bulk and Thin Films. 2006 , 924, 1	2
1717	Heterogeneity in a room-temperature ionic liquid: persistent local environments and the red-edge effect. 2006 , 103, 831-6	353
1716	Protein-ligand docking: current status and future challenges. 2006 , 65, 15-26	597
1715	Automated Model Reduction for Complex Systems Exhibiting Metastability. 2006 , 5, 802-827	32
1714	The melting point of ice Ih for common water models calculated from direct coexistence of the solid-liquid interface. 2006 , 124, 144506	320
1713	Thermodynamics of hydrogen bonding in hydrophilic and hydrophobic media. 2006 , 110, 4393-8	323
1712	Parallelized-over-parts computation of absolute binding free energy with docking and molecular dynamics. 2006 , 125, 084901	81
1711	Experimental and theoretical investigation of the micellar-assisted solubilization of ibuprofen in aqueous media. 2006 , 22, 1514-25	67
1710	A molecular dynamics study of Lys-Trp-Lys: structure and dynamics in solution following photoexcitation. 2006 , 110, 10497-508	41
1709	Hydration and dewetting near fluorinated superhydrophobic plates. 2006 , 128, 12439-47	60
1708	A molecular dynamics investigation of the influence of hydration and temperature on structural and dynamical properties of a dimyristoylphosphatidylcholine bilayer. 2006 , 110, 14326-36	85
1707	Modulation of amphotericin B membrane interaction by cholesterol and ergosterol--a molecular dynamics study. 2006 , 110, 16743-53	42
1706	Structural and functional diversities among mu-conotoxins targeting TTX-resistant sodium channels. 2006 , 45, 3723-32	56
1705	The influence of amino acid protonation states on molecular dynamics simulations of the bacterial porin OmpF. 2006 , 90, 112-23	55
1704	Influence of chain length and unsaturation on sphingomyelin bilayers. 2006 , 90, 851-63	100
1703	Conformation and environment of channel-forming peptides: a simulation study. 2006 , 90, 1855-64	17
1702	Atomistic simulation studies of cholesteryl oleates: model for the core of lipoprotein particles. 2006 , 90, 2247-57	21
1701	Anionic phospholipid interactions with the potassium channel KcsA: simulation studies. 2006 , 90, 822-30	67

1700	Fatty acid binding proteins: same structure but different binding mechanisms? Molecular dynamics simulations of intestinal fatty acid binding protein. 2006 , 90, 1535-45	35
1699	cAMP Modulation of the cytoplasmic domain in the HCN2 channel investigated by molecular simulations. 2006 , 90, 3428-33	16
1698	The intrinsic flexibility of the Kv voltage sensor and its implications for channel gating. 2006 , 90, 1598-606	28
1697	Molecular dynamics simulations of model trans-membrane peptides in lipid bilayers: a systematic investigation of hydrophobic mismatch. 2006 , 90, 2326-43	148
1696	¹ H and ¹³ C-NMR and molecular dynamics studies of cyclosporin a interacting with magnesium(II) or cerium(III) in acetonitrile. Conformational changes and cis-trans conversion of peptide bonds. 2006 , 90, 1350-61	25
1695	Kinetics and thermodynamics of type VIII beta-turn formation: a CD, NMR, and microsecond explicit molecular dynamics study of the GDNF tetrapeptide. 2006 , 90, 2745-59	38
1694	Folding, misfolding, and amyloid protofibril formation of WW domain FBP28. 2006 , 90, 3983-92	48
1693	Molecular simulation study of structural and dynamic properties of mixed DPPC/DPPE bilayers. 2006 , 90, 3951-65	134
1692	Permeability of psoralen derivatives in lipid membranes. 2006 , 91, 2464-74	26
1691	Interaction of transported drugs with the lipid bilayer and P-glycoprotein through a solvation exchange mechanism. 2006 , 90, 4046-59	68
1690	A molecular dynamics study of the effect of Ca ²⁺ removal on calmodulin structure. 2006 , 90, 3842-50	35
1689	Effects of solvent on the structure of the Alzheimer amyloid-beta(25-35) peptide. 2006 , 91, 1638-47	132
1688	Flexibility in a drug transport accessory protein: molecular dynamics simulations of MexA. 2006 , 91, 558-64	61
1687	A structure-based simulation approach for electron paramagnetic resonance spectra using molecular and stochastic dynamics simulations. 2006 , 91, 2647-64	69
1686	Common mechanism of pore opening shared by five different potassium channels. 2006 , 90, 3929-40	79
1685	Voltage-dependent hydration and conduction properties of the hydrophobic pore of the mechanosensitive channel of small conductance. 2006 , 90, 3555-69	56
1684	Does CO ₂ permeate through aquaporin-1?. 2006 , 91, 842-8	118
1683	Molecular simulation of the binding of nerve growth factor peptide mimics to the receptor tyrosine kinase A. 2006 , 91, 2063-71	13

1682	Molecular dynamics simulations of E. coli MsbA transmembrane domain: formation of a semipore structure. 2006 , 91, 2517-31	22
1681	Pathways of H ₂ toward the active site of [NiFe]-hydrogenase. 2006 , 91, 2035-45	62
1680	Characterization of the structure of RAMP1 by mutagenesis and molecular modeling. 2006 , 91, 662-9	18
1679	Photoinduced conformational dynamics of a photoswitchable peptide: a nonequilibrium molecular dynamics simulation study. 2006 , 91, 1224-34	47
1678	A molecular dynamics study and free energy analysis of complexes between the Mlc1p protein and two IQ motif peptides. 2006 , 91, 2436-50	30
1677	Disease-causing mutations in proteins: structural analysis of the CYP1B1 mutations causing primary congenital glaucoma in humans. 2006 , 91, 4329-39	33
1676	Using metadynamics to understand the mechanism of calmodulin/target recognition at atomic detail. 2006 , 91, 2768-77	39
1675	Stability and structure of oligomers of the Alzheimer peptide Abeta16-22: from the dimer to the 32-mer. 2006 , 91, 3217-29	98
1674	Enantioselective substrate binding in a monooxygenase protein model by molecular dynamics and docking. 2006 , 91, 3206-16	24
1673	Amino-acid solvation structure in transmembrane helices from molecular dynamics simulations. 2006 , 91, 4450-63	66
1672	The Origin of Layer Structure Artifacts in Simulations of Liquid Water. 2006 , 2, 1-11	164
1671	Liquid water simulation: a critical examination of cutoff length. 2006 , 124, 204501	51
1670	Spontaneity in the patellamide biosynthetic pathway. 2006 , 4, 631-8	45
1669	Side chain dynamics and alternative hydrogen bonding in the mechanism of protein thermostabilization. 2006 , 24, 255-62	16
1668	Flexible simple point-charge water model with improved liquid-state properties. 2006 , 124, 024503	742
1667	Dynamics of water at membrane surfaces: Effect of headgroup structure. 2006 , 1, 98-105	76
1666	Glass transition in biomolecules and the liquid-liquid critical point of water. 2006 , 97, 177802	182
1665	Propensity for the air/water interface and ion pairing in magnesium acetate vs magnesium nitrate solutions: molecular dynamics simulations and surface tension measurements. 2006 , 110, 15939-44	75

1664	Lifting a wet glass from a table: a microscopic picture. 2006 , 22, 5666-72	13
1663	Molecular dynamics simulations of PAMAM dendrimer-induced pore formation in DPPC bilayers with a coarse-grained model. 2006 , 110, 18204-11	184
1662	Molecular dynamics studies of the size, shape, and internal structure of 0% and 90% acetylated fifth-generation polyamidoamine dendrimers in water and methanol. 2006 , 110, 4014-9	79
1661	Parametrization of 1-butyl-3-methylimidazolium hexafluorophosphate/nitrate ionic liquid for the GROMOS force field. 2006 , 110, 14444-51	125
1660	Molecular dynamics simulation of nanoparticle self-assembly at a liquid-liquid interface. 2006 , 22, 6385-90	55
1659	Free energy of a trans-membrane pore calculated from atomistic molecular dynamics simulations. 2006 , 124, 154905	123
1658	Evaluation of 3-carboxy-4(1H)-quinolones as inhibitors of human protein kinase CK2. 2006 , 49, 6443-50	53
1657	Aggregation and dispersion of small hydrophobic particles in aqueous electrolyte solutions. 2006 , 110, 22736-41	84
1656	Structural disorder of the CD3zeta transmembrane domain studied with 2D IR spectroscopy and molecular dynamics simulations. 2006 , 110, 24740-9	56
1655	Comparison of NMR and MD NMR bond order parameters: example of HIV-1 protease. 2006 , 32, 1155-1163	2
1654	Antimicrobial peptides in action. 2006 , 128, 12156-61	372
1653	Conformational flexibility of the peptide hormone ghrelin in solution and lipid membrane bound: a molecular dynamics study. 2006 , 23, 357-64	23
1652	Thermodynamic basis for promiscuity and selectivity in protein-protein interactions: PDZ domains, a case study. 2006 , 128, 12766-77	96
1651	Closing of the flaps of HIV-1 protease induced by substrate binding: a model of a flap closing mechanism in retroviral aspartic proteases. 2006 , 45, 6606-14	45
1650	Molecular-dynamics simulation of a ceramide bilayer. 2006 , 124, 14708	45
1649	Complementary use of simulations and molecular-thermodynamic theory to model micellization. 2006 , 22, 1500-13	52
1648	Asymmetric stability among the transmembrane helices of lactose permease. 2006 , 45, 8088-95	21
1647	Loopless Rop: structure and dynamics of an engineered homotetrameric variant of the repressor of primer protein. 2006 , 45, 10905-19	15

1646	Lactobionamide surfactants with hydrogenated, perfluorinated or hemifluorinated tails: physical-chemical and biochemical characterization. 2006 , 22, 8881-90	34
1645	Diverse functional motifs within the three intracellular loops of the CGRP1 receptor. 2006 , 45, 12976-85	29
1644	Phase transition of a DPPC bilayer induced by an external surface pressure: from bilayer to monolayer behavior. a molecular dynamics simulation study. 2006 , 22, 5818-24	20
1643	Entropic folding pathway of human epidermal growth factor explored by disulfide scrambling and amplified collective motion simulations. 2006 , 45, 15269-78	9
1642	Fluorescence correlation spectroscopy simulations of photophysical phenomena and molecular interactions: a molecular dynamics/monte carlo approach. 2006 , 110, 1896-906	42
1641	Direct observation of salt effects on molecular interactions through explicit-solvent molecular dynamics simulations: differential effects on electrostatic and hydrophobic interactions and comparisons to Poisson-Boltzmann theory. 2006 , 128, 7796-806	41
1640	Molecular dynamics study of the properties of capsaicin in an 1-octanol/water system. 2006 , 110, 2351-7	15
1639	Electronic structure, ionization potential, and electron affinity of the enzyme cofactor (6R)-5,6,7,8-tetrahydrobiopterin in the gas phase, solution, and protein environments. 2006 , 110, 22861-71	18
1638	Cation-mediated interplay of loops in chaperonin-10. 2006 , 23, 365-76	1
1637	Proton antenna effect of the gamma-cyclodextrin outer surface, measured by excited state proton transfer. 2006 , 110, 26354-64	30
1636	Reorganization of Nanopatterned Polymer Brushes by the AFM Measurement Process. 2006 , 39, 4540-4546	19
1635	Molecular dynamics study of 2-nitrophenyl octyl ether and nitrobenzene. 2006 , 110, 12530-8	21
1634	Hydrogen bonding pathways in human dihydroorotate dehydrogenase. 2006 , 110, 19704-10	7
1633	Molecular Dynamics Simulation of Iminosugar Inhibitor-Glycosidase Complex: Insight into the Binding Mechanism of 1-Deoxynojirimycin and Isfagomine toward α -Glucosidase. 2006 , 2, 157-65	20
1632	Dynamics of water confined in the interdomain region of a multidomain protein. 2006 , 110, 3704-11	88
1631	Domain motions of the Mip protein from Legionella pneumophila. 2006 , 45, 12303-11	21
1630	Coarse grained protein-lipid model with application to lipoprotein particles. 2006 , 110, 3674-84	226
1629	Equilibrium distributions of dipalmitoyl phosphatidylcholine and dilauroyl phosphatidylcholine in a mixed lipid bilayer: atomistic semigrand canonical ensemble simulations. 2006 , 110, 25875-82	26

1628	Self-assembly of single-walled carbon nanotubes into multiwalled carbon nanotubes in water: molecular dynamics simulations. 2006 , 6, 430-4	69
1627	Shedding light on biomolecule conformational dynamics using fluorescence measurements of trapped ions. 2006 , 110, 12714-27	40
1626	Determination of the interfacial characteristics of a series of bolaamphiphilic poly(fluorooxetane) surfactants through molecular dynamics simulation. 2006 , 110, 19393-405	14
1625	Fatty acid amide hydrolase inhibitors from virtual screening of the endocannabinoid system. 2006 , 49, 4650-6	58
1624	Amyloid fibril structure modeling using protein threading and molecular dynamics simulations. 2006 , 412, 300-14	2
1623	Transmembrane helix-helix interactions: comparative simulations of the glycophorin a dimer. 2006 , 45, 14298-310	62
1622	Systematic Coarse-Graining of a Polymer Blend: Polyisoprene and Polystyrene. 2006 , 2, 607-15	57
1621	Coarse-grained model simulations of mixed-lipid systems: composition and line tension of a stabilized bilayer edge. 2006 , 22, 998-1005	41
1620	Myo1c binds phosphoinositides through a putative pleckstrin homology domain. 2006 , 17, 4856-65	116
1619	Simulations of a protein translocation pore: SecY. 2006 , 45, 13018-24	29
1618	The crystal structure of the ternary complex of phenylalanyl-tRNA synthetase with tRNAPhe and a phenylalanyl-adenylate analogue reveals a conformational switch of the CCA end. 2006 , 45, 10572-83	45
1617	Lipid headgroup superlattice modulates the activity of surface-acting cholesterol oxidase in ternary phospholipid/cholesterol bilayers. 2006 , 45, 10855-64	10
1616	Crossover from Unentangled to Entangled Dynamics in a Systematically Coarse-Grained Polystyrene Melt. 2006 , 39, 812-820	80
1615	Chirally directed formation of nanometer-scale proline clusters. 2006 , 128, 10833-9	30
1614	Influence of Long-Range Electrostatic Treatments on the Folding of the N-Terminal H4 Histone Tail Peptide. 2006 , 2, 246-50	26
1613	Influence of pyrene-labeling on fluid lipid membranes. 2006 , 110, 15403-10	62
1612	What NMR Relaxation Can Tell Us about the Internal Motion of an RNA Hairpin: A Molecular Dynamics Simulation Study. 2006 , 2, 1228-36	34
1611	Synthetic polymers and biomembranes. How do they interact? Atomistic molecular dynamics simulation study of PEO in contact with a DMPC lipid bilayer. 2006 , 110, 26170-9	24

1610	On the accuracy of force fields for predicting the physical properties of dimethylnitramine. 2006 , 110, 16082-8	6
1609	Solvated docking: introducing water into the modelling of biomolecular complexes. 2006 , 22, 2340-7	123
1608	Inverse temperature transition of a biomimetic elastin model: reactive flux analysis of folding/unfolding and its coupling to solvent dielectric relaxation. 2006 , 110, 3576-87	26
1607	Hierarchical multiscale simulation of electrokinetic transport in silica nanochannels at the point of zero charge. 2006 , 22, 9041-51	60
1606	Combination of a modified scoring function with two-dimensional descriptors for calculation of binding affinities of bulky, flexible ligands to proteins. 2006 , 128, 1233-9	28
1605	Natural domain design: enhanced thermal stability of a zinc-lacking ferredoxin isoform shows that a hydrophobic core efficiently replaces the structural metal site. 2006 , 45, 10376-84	12
1604	Gas enrichment at liquid-wall interfaces. 2006 , 96, 206101	108
1603	Can principal components yield a dimension reduced description of protein dynamics on long time scales?. 2006 , 110, 22842-52	78
1602	Molecular simulations of outersphere reorganization energies in polar and quadrupolar solvents. The case of intramolecular electron and hole transfer. 2006 , 110, 14950-5	15
1601	Mechanism of dihydroneopterin aldolase: a molecular dynamics study of the apo enzyme and its product complex. 2006 , 110, 1443-56	3
1600	Blocking of the nicotinic acetylcholine receptor ion channel by chlorpromazine, a noncompetitive inhibitor: A molecular dynamics simulation study. 2006 , 110, 20640-8	16
1599	A trimerizing GxxxG motif is uniquely inserted in the severe acute respiratory syndrome (SARS) coronavirus spike protein transmembrane domain. 2006 , 45, 11349-56	27
1598	A Novel Hamiltonian Replica Exchange MD Protocol to Enhance Protein Conformational Space Sampling. 2006 , 2, 217-28	112
1597	Conformational polymorphism of the PrP106-126 peptide in different environments: a molecular dynamics study. 2006 , 110, 1423-8	34
1596	The link between sequence and conformation in protein structures appears to be stereochemically established. 2006 , 110, 9314-23	42
1595	Molecular dynamics simulation of a phosphatidylglycerol membrane. 2006 , 580, 144-8	66
1594	Purification, cDNA cloning and homology modeling of endo-1,3-beta-D-glucanase from scallop <i>Mizuhopecten yessoensis</i> . 2006 , 143, 473-85	45
1593	Effect of salt on the interactions of antimicrobial peptides with zwitterionic lipid bilayers. 2006 , 1758, 1274-84	54

1592	Electrostatic interactions of colicin E1 with the surface of Escherichia coli total lipid. 2006 , 1758, 693-701	7
1591	Molecular study of the diffusional process of DMSO in double lipid bilayers. 2006 , 1758, 1751-8	16
1590	Structure and dynamics of the N-terminal loop of PsbQ from photosystem II of Spinacia oleracea. 2006 , 345, 287-91	7
1589	Structural features of the reprotolysin atrolysin C and tissue inhibitors of metalloproteinases (TIMPs) interaction. 2006 , 347, 641-8	4
1588	The acidic domain of hnRNPQ (NSAP1) has structural similarity to Barstar and binds to Apobec1. 2006 , 350, 288-97	11
1587	Bayesian model based clustering analysis: application to a molecular dynamics trajectory of the HIV-1 integrase catalytic core. 2006 , 46, 1742-50	18
1586	Molecular basis for nucleotide-binding specificity: role of the exocyclic amino group "N2" in recognition by a guanylyl-ribonuclease. 2006 , 355, 72-84	6
1585	The solvation interface is a determining factor in peptide conformational preferences. 2006 , 356, 248-56	40
1584	Nucleotide channel of RNA-dependent RNA polymerase used for intermolecular uridylylation of protein primer. 2006 , 357, 665-75	26
1583	Kinetic computational alanine scanning: application to p53 oligomerization. 2006 , 357, 1039-49	16
1582	High-resolution structures of Escherichia coli cDsbD in different redox states: A combined crystallographic, biochemical and computational study. 2006 , 358, 829-45	34
1581	Alternate structural conformations of Streptococcus pneumoniae hyaluronan lyase: insights into enzyme flexibility and underlying molecular mechanism of action. 2006 , 358, 1165-78	19
1580	Crystal structure of yeast peroxisomal multifunctional enzyme: structural basis for substrate specificity of (3R)-hydroxyacyl-CoA dehydrogenase units. 2006 , 358, 1286-95	14
1579	Computational sampling of a cryptic drug binding site in a protein receptor: explicit solvent molecular dynamics and inhibitor docking to p38 MAP kinase. 2006 , 359, 202-14	83
1578	Structure-stability-activity relationship in covalently cross-linked N-carbamoyl D-amino acid amidohydrolase and N-acylamino acid racemase. 2006 , 359, 741-53	29
1577	Two-rung model of a left-handed beta-helix for prions explains species barrier and strain variation in transmissible spongiform encephalopathies. 2006 , 360, 907-20	51
1576	The transmembrane domain of the oncogenic mutant ErbB-2 receptor: a structure obtained from site-specific infrared dichroism and molecular dynamics. 2006 , 361, 945-53	21
1575	Folding landscapes of the Alzheimer amyloid-beta(12-28) peptide. 2006 , 362, 567-79	74

1574	Structure-function mapping of BbCRASP-1, the key complement factor H and FHL-1 binding protein of <i>Borrelia burgdorferi</i> . 2006 , 296 Suppl 40, 177-84	21
1573	Role of each residue in catalysis in the active site of pyrimidine nucleoside phosphorylase from <i>Bacillus subtilis</i> : a hybrid QM/MM study. 2006 , 154, 20-6	13
1572	Molecular dynamics analysis of the engrailed homeodomain-DNA recognition. 2006 , 155, 426-37	16
1571	A molecular dynamics analysis of the GCC-box binding domain in ethylene-responsive element binding factors. 2006 , 156, 537-45	3
1570	Lys296 and Arg299 residues in the C-terminus of MD-ACO1 are essential for a 1-aminocyclopropane-1-carboxylate oxidase enzyme activity. 2006 , 156, 407-20	27
1569	Kinetic and mechanistic characterization of the Sphingomyelinases D from <i>Loxosceles intermedia</i> spider venom. 2006 , 47, 380-6	18
1568	. 2006 ,	2
1567	On the art of computing the IR spectra of molecules in the condensed phase. 2006 , 159-177	5
1566	High-Resolution Protein Structure Determination by NMR. 2006 , 59, 235-273	4
1565	Binding of 7-methoxy-4-(aminomethyl)-coumarin to wild-type and W128F mutant cytochrome P450 2D6 studied by time-resolved fluorescence spectroscopy. 2006 , 393, 635-43	10
1564	Molecular Modeling and Simulations of Ion Channels: Applications to Potassium Channels. 2006 , 241-267	
1563	The effect of water structure and surface charge correlations on the hydration force acting between model hydrophilic surfaces. 2006 , 104, 3607-3617	9
1562	Molecular dynamics study of nitrobenzene and 2-nitrophenyloctyl ether saturated with water. 2006 , 104, 3627-3634	6
1561	Normal modes of carbon nanotubes: similarities and differences with their continuum counterpart. 2006 , 26, 131-134	5
1560	Similar folds with different stabilization mechanisms: the cases of Prion and Doppel proteins. 2006 , 6, 17	17
1559	Molecular-dynamic studies of carbon-water-carbon composite nanotubes. 2006 , 2, 1348-55	33
1558	Theoretical studies on waterâ€¦tetracaine interaction. 2006 , 106, 1277-1282	5
1557	Redox regulation of cyclophilin A by glutathionylation. 2006 , 6, 817-25	40

1556	Modeling and simulations of a bacterial outer membrane protein: OprF from <i>Pseudomonas aeruginosa</i> . 2006 , 63, 6-15	24
1555	Molecular dynamics simulations of the hydrophobin SC3 at a hydrophobic/hydrophilic interface. 2006 , 64, 863-73	27
1554	Molecular dynamics study of a calmodulin-like protein with an IQ peptide: spontaneous refolding of the protein around the peptide. 2006 , 64, 133-46	3
1553	Local feature analysis: a statistical theory for reproducible essential dynamics of large macromolecules. 2006 , 64, 391-403	20
1552	Cofactor assisted gating mechanism in the active site of NADH oxidase from <i>Thermus thermophilus</i> . 2006 , 64, 465-76	11
1551	The planar conformation of a strained proline ring: a QM/MM study. 2006 , 64, 700-10	13
1550	Structural and functional effects of disease-causing amino acid substitutions affecting residues Ala72 and Glu76 of the protein tyrosine phosphatase SHP-2. 2007 , 66, 963-74	22
1549	Structural and dynamical properties of manganese catalase and the synthetic protein DF1 and their implication for reactivity from classical molecular dynamics calculations. 2006 , 65, 317-30	19
1548	Aggregating the amyloid Abeta(11-25) peptide into a four-stranded beta-sheet structure. 2006 , 65, 877-88	21
1547	Complexity of free energy landscapes of peptides revealed by nonlinear principal component analysis. 2006 , 65, 898-913	26
1546	A hinge of the endogeneous ATP synthase inhibitor protein: the link between inhibitory and anchoring domains. 2006 , 65, 999-1007	2
1545	Locating missing water molecules in protein cavities by the three-dimensional reference interaction site model theory of molecular solvation. 2007 , 66, 804-13	83
1544	Computer simulations of transport through membranes: passive diffusion, pores, channels and transporters. 2006 , 33, 893-903	40
1543	The natural mutation by deletion of Lys9 in the thrombin A-chain affects the pKa value of catalytic residues, the overall enzyme's stability and conformational transitions linked to Na ⁺ binding. 2006 , 273, 159-69	24
1542	Red fluorescent protein DsRed: parametrization of its chromophore as an amino acid residue for computer modeling in the OPLS-AA force field. 2006 , 71, 1133-52	5
1541	Cloning and structural analysis of an Indian little millet (<i>Panicum sumatrense</i>) zein-like storage protein: implications for molecular assembly. 2006 , 71, 1183-91	7
1540	Phylogenetic analysis of the p53 family. 2006 , 51, 571-580	
1539	Solution of the spatial structure of dimeric transmembrane domains of proteins by heteronuclear NMR spectroscopy and molecular modeling. 2006 , 51, 23-27	1

1538	In silico modelling of the interaction of flavonoids with human P-glycoprotein nucleotide-binding domain. 2006 , 41, 285-95	40
1537	Molecular docking study and development of an empirical binding free energy model for phosphodiesterase 4 inhibitors. 2006 , 14, 6001-11	14
1536	A comparison between two prokaryotic potassium channels (KirBac1.1 and KcsA) in a molecular dynamics (MD) simulation study. 2006 , 120, 1-9	27
1535	The improvement of the algorithm for order parameter calculation (S2) from molecular dynamics simulation using the correlation motion function. 2006 , 123, 25-8	
1534	Interaction of local anesthetics with a peptide encompassing the IV/S4-S5 linker of the Na ⁺ channel. 2006 , 123, 29-39	11
1533	BclV, a new paralyzing peptide obtained from the venom of the sea anemone <i>Bunodosoma caissarum</i> . A comparison with the Na ⁺ channel toxin BclIII. 2006 , 1764, 1592-600	30
1532	Target structure-based discovery of small molecules that block human p53 and CREB binding protein association. 2006 , 13, 81-90	119
1531	All-atom molecular dynamics studies of the full-length β -amyloid peptides. 2006 , 323, 138-147	35
1530	Molecular dynamics simulations of spontaneous bile salt aggregation. 2006 , 280, 182-193	86
1529	ESPResoãan extensible simulation package for research on soft matter systems. 2006 , 174, 704-727	544
1528	Principal component analysis of fast-folding β -repressor mutants. 2006 , 421, 5-10	14
1527	Molecular dynamics study of diffusion of formaldehyde in ice. 2006 , 432, 78-83	19
1526	Nonequilibrium molecular dynamics simulation of a photoswitchable peptide. 2006 , 323, 36-44	60
1525	Investigation on a new scleroglucan/borax hydrogel: structure and drug release. 2006 , 322, 13-21	25
1524	Prediction of N-C bond cleavage frequencies in electron capture dissociation of Trp-cage dications by force-field molecular dynamics simulations. 2006 , 248, 124-135	58
1523	The water molecules orientation around the dipalmitoylphosphatidylcholine head group: A molecular dynamics study. 2006 , 362, 197-203	11
1522	Pressure denaturation of apomyoglobin: a molecular dynamics simulation study. 2006 , 1764, 506-15	12
1521	Prediction of the binding mode between BMS-378806 and HIV-1 gp120 by docking and molecular dynamics simulation. 2006 , 1764, 766-72	36

1520	Beta-hairpins with native-like and non-native hydrogen bonding patterns could form during the refolding of staphylococcal nuclease. 2006 , 25, 103-15	10
1519	Systematic molecular dynamics searching in a lipid bilayer: application to the glycoporphin A and oncogenic ErbB-2 transmembrane domains. 2006 , 25, 226-33	20
1518	Binding mode analysis of the NADH cofactor in nitric oxide reductase: a theoretical study. 2006 , 25, 363-72	4
1517	Distance between a native cofactor and a spin label in the reaction centre of Rhodobacter sphaeroides by a two-frequency pulsed electron paramagnetic resonance method and molecular dynamics simulations. 2006 , 180, 178-85	40
1516	Three-dimensional kinetic Monte Carlo simulation of crystal growth from solution. 2006 , 294, 46-52	36
1515	Al(III)-binding ability of an octapeptide and its phosphorylated derivative. 2006 , 100, 351-61	12
1514	Molecular dynamics simulation of GM1 gangliosides embedded in a phospholipid membrane. 2006 , 129, 86-91	10
1513	Structural identification of a novel thioredoxin SoxS: Prediction of the function in the process of transport of reductants during sulfur oxidation by the novel global sulfur oxidation reaction cycle. 2006 , 758, 113-118	1
1512	Molecular dynamics study on the conformational transition of prion induced by the point mutation: F198S. 2006 , 499, 224-228	11
1511	A hydrophobic gate in an ion channel: the closed state of the nicotinic acetylcholine receptor. 2006 , 3, 147-59	152
1510	X-ray absorption spectra of water from first principles calculations. 2006 , 96, 215502	291
1509	Lipid-carbon nanotube self-assembly in aqueous solution. 2006 , 128, 13656-7	93
1508	Insertion and assembly of membrane proteins via simulation. 2006 , 128, 2697-704	293
1507	Hydration thermodynamic properties of amino acid analogues: a systematic comparison of biomolecular force fields and water models. 2006 , 110, 17616-26	271
1506	Monte Carlo simulations of the properties and structure of hexadecyltrimethylammonium chloride micelles of various shapes in aqueous-salt solutions. 2006 , 80, 1259-1264	
1505	Macroscopic properties and self-organization in mixed solutions of surfactants. 2006 , 80, 1608-1616	1
1504	Characterization of the interaction of hypericin with protein kinase C in U-87 MG human glioma cells. 2006 , 82, 720-8	19
1503	Mimicking the action of GroEL in molecular dynamics simulations: application to the refinement of protein structures. 2006 , 15, 441-8	8

1502	CIRSE: a solvation energy estimator compatible with flexible protein docking and design applications. 2006 , 15, 1579-96		10
1501	Structure of the 21-30 fragment of amyloid beta-protein. 2006 , 15, 1239-47		130
1500	Comparative NMR study on the impact of point mutations on protein stability of Pseudomonas mendocina lipase. 2006 , 15, 1915-27		13
1499	Engineered lanthanide-binding metallohomeodomains: designing folded chimeras by modular turn substitution. 2006 , 15, 2159-65		12
1498	Protein folding kinetics and thermodynamics from atomistic simulations. 2006 , 96, 238102		80
1497	Molecular basis for dimethylsulfoxide (DMSO) action on lipid membranes. 2006 , 128, 13982-3		284
1496	On the use of orientational restraints and symmetry corrections in alchemical free energy calculations. 2006 , 125, 084902		213
1495	Liposomal drug transport: a molecular perspective from molecular dynamics simulations in lipid bilayers. 2006 , 58, 1357-78		126
1494	Molecular modeling and bioinformatical analysis of the antibacterial target enzyme MurA from a drug design perspective. 2006 , 20, 621-8		13
1493	Effects of molecular level surface roughness on electroosmotic flow. 2006 , 3, 33-38		46
1492	The effect of methanol on lipid bilayers: an atomistic investigation. 2006 , 34, 1442-51		23
1491	A fold-recognition approach to loop modeling. <i>Journal of Molecular Modeling</i> , 2006 , 12, 125-39	2	9
1490	Role of hydrophobic interactions and salt-bridges in beta-hairpin folding. <i>Journal of Molecular Modeling</i> , 2006 , 12, 197-204	2	5
1489	Model of the whole rat AT1 receptor and the ligand-binding site. <i>Journal of Molecular Modeling</i> , 2006 , 12, 325-37	2	27
1488	Study on improving the selectivity of compounds that inhibit two PI3Ks (gamma and delta). <i>Journal of Molecular Modeling</i> , 2006 , 12, 445-52	2	10
1487	Conformational stability and three-dimensional model of the delta-opioid pharmacophore for the extended antiparallel dimer structure of Met-enkephalin in water. <i>Journal of Molecular Modeling</i> , 2007 , 13, 171-7	2	4
1486	Probing the interaction between vesicular stomatitis virus and phosphatidylserine. 2006 , 35, 145-54		40
1485	Interaction between K ⁺ channel gate modifier hanatoxin and lipid bilayer membranes analyzed by molecular dynamics simulation. 2006 , 35, 373-81		27

1484	Structural investigation of syringomycin-E using molecular dynamics simulation and NMR. 2006 , 35, 459-67	4
1483	Homology modeling of tubulin: influence predictions for microtubule's biophysical properties. 2006 , 36, 35-43	23
1482	The Thermodynamics of Folding of a Hairpin Peptide Probed Through Replica Exchange Molecular Dynamics Simulations. 2006 , 116, 262-273	13
1481	Peptidomimetic C5a receptor antagonists with hydrophobic substitutions at the C-terminus: increased receptor specificity and in vivo activity. 2006 , 16, 5088-92	31
1480	Structural insight into the interactions of SoxV, SoxW and SoxS in the process of transport of reductants during sulfur oxidation by the novel global sulfur oxidation reaction cycle. 2006 , 119, 7-13	14
1479	On the role of chemical detail in simulating protein folding kinetics. 2006 , 323, 66-77	20
1478	Effect of pressure on the conformation of proteins. A molecular dynamics simulation of lysozyme. 2006 , 24, 254-61	17
1477	Targeting the PDZ domains of molecular scaffolds of transmembrane ion channels. 2006 , 8, E396-401	8
1476	A methyl group at C7 of 11-cis-retinal allows chromophore formation but affects rhodopsin activation. 2006 , 46, 4472-81	4
1475	A highly strained nuclear conformation of the exportin Cse1p revealed by molecular dynamics simulations. 2006 , 14, 1469-78	26
1474	Pheromone discrimination by the pheromone-binding protein of Bombyx mori. 2006 , 14, 1577-86	52
1473	Proline and glycine control protein self-organization into elastomeric or amyloid fibrils. 2006 , 14, 1667-76	274
1472	A multi-scale stochastic drug release model for polymer-coated targeted drug delivery systems. 2006 , 110, 314-322	30
1471	Binding of cationic and neutral phenanthridine intercalators to a DNA oligomer is controlled by dispersion energy: quantum chemical calculations and molecular mechanics simulations. 2005 , 12, 280-90	69
1470	The alpha-to-beta conformational transition of Alzheimer's Abeta-(1-42) peptide in aqueous media is reversible: a step by step conformational analysis suggests the location of beta conformation seeding. 2006 , 7, 257-67	314
1469	Hierarchical mechanochemical switches in angiostatin. 2006 , 7, 1774-82	12
1468	Structure, dynamics, and elasticity of free 16s rRNA helix 44 studied by molecular dynamics simulations. 2006 , 82, 504-20	69
1467	Computational design of proteins stereochemically optimized in size, stability, and folding speed. 2006 , 83, 122-34	7

1466	Toward understanding the inactivation mechanism of monooxygenase P450 BM-3 by organic cosolvents: a molecular dynamics simulation study. 2006 , 83, 467-76	26
1465	Conformational fluctuations versus constraints in amino acid side chains: the evolution of information content from free amino acids to proteins. 2006 , 3, 245-73	7
1464	Molecular dynamics simulation and automated docking of the pro-apoptotic Bax protein and its complex with a peptide designed from the Bax-binding domain of anti-apoptotic Ku70. 2006 , 99, 305-18	27
1463	The effect of box shape on the dynamic properties of proteins simulated under periodic boundary conditions. 2006 , 27, 316-25	28
1462	A multiple time step algorithm compatible with a large number of distance classes and an arbitrary distance dependence of the time step size for the fast evaluation of nonbonded interactions in molecular simulations. 2006 , 27, 1163-76	5
1461	PROFASI: A Monte Carlo simulation package for protein folding and aggregation. 2006 , 27, 1548-55	92
1460	Software news and updates. Carma: a molecular dynamics analysis program. 2006 , 27, 1765-8	318
1459	Solvent effect on optical rotation: A case study of methyloxirane in water. 2006 , 7, 2483-6	82
1458	Combining docking and molecular dynamic simulations in drug design. 2006 , 26, 531-68	453
1457	Detailed molecular simulations to investigate multicomponent diffusion models. 2006 , 52, 1304-1307	4
1456	Proliferating cell nuclear antigen loaded onto double-stranded DNA: dynamics, minor groove interactions and functional implications. 2006 , 34, 6023-33	64
1455	Molecular Dynamics Simulations and Analysis of ABC Transporters. 2006 , 2, 203-214	1
1454	Assessing the influence of electrostatic schemes on molecular dynamics simulations of secondary structure forming peptides. 2006 , 18, S329-S345	18
1453	Significance of sterol structural specificity. Desmosterol cannot replace cholesterol in lipid rafts. 2006 , 281, 348-55	114
1452	Quantifying the protein core flexibility through analysis of cavity formation. 2006 , 124, 74704	16
1451	Molecular dynamics study of charged dendrimers in salt-free solution: effect of counterions. 2006 , 124, 94904	70
1450	A comparative molecular simulation study of the glass former ortho-terphenyl in bulk and freestanding films. 2006 , 125, 44506	13
1449	The behavior of reorientational correlation functions of water at the water-lipid bilayer interface. 2006 , 125, 094713	36

1448	Temperature and structural changes of water clusters in vacuum due to evaporation. 2006 , 125, 154508	55
1447	Molecular dynamics simulations of a bacterial autotransporter: NaIP from <i>Neisseria meningitidis</i> . 2006 , 23, 499-508	33
1446	The structural integrity of anion binding exosite I of thrombin is required and sufficient for timely cleavage and activation of factor V and factor VIII. 2006 , 281, 18569-80	21
1445	Biomolecule large-amplitude motion and solvation dynamics: modelling and probes from THz to X-rays. 2006 , 25, 553-582	73
1444	Membrane protein dynamics and detergent interactions within a crystal: a simulation study of OmpA. 2006 , 103, 9518-23	31
1443	N-methylpurine DNA glycosylase and 8-oxoguanine dna glycosylase metabolize the antiviral nucleoside 2-bromo-5,6-dichloro-1-(beta-D-ribofuranosyl)benzimidazole. 2006 , 34, 1070-7	14
1442	Emulsifying performance of modular beta-sandwich proteins: the hydrophobic moment and conformational stability. 2006 , 19, 537-45	19
1441	Picosecond dynamics of a membrane protein revealed by 2D IR. 2006 , 103, 3528-33	190
1440	Nanopore-facilitated, voltage-driven phosphatidylserine translocation in lipid bilayers--in cells and in silico. 2006 , 3, 233-47	119
1439	Two domains that control prefusion stability and transport competence of the measles virus fusion protein. 2006 , 80, 1524-36	44
1438	Quaternary ammonium compounds as water channel blockers. Specificity, potency, and site of action. 2006 , 281, 14207-14	106
1437	The dynamics of the MgATP-driven closure of MalK, the energy-transducing subunit of the maltose ABC transporter. 2006 , 281, 28397-407	53
1436	Binding site flexibility: molecular simulation of partial and full agonists within a glutamate receptor. 2006 , 69, 11-8	36
1435	Allosteric interactions with muscarinic acetylcholine receptors: complex role of the conserved tryptophan M2422Trp in a critical cluster of amino acids for baseline affinity, subtype selectivity, and cooperativity. 2006 , 70, 181-93	52
1434	Transient ordered domains in single-component phospholipid bilayers. 2006 , 97, 238102	36
1433	Karhunen-Loeve analysis for pattern description in phase separated lipid bilayer systems. 2006 , 124, 234906	5
1432	Bayesian update method for adaptive weighted sampling. 2006 , 74, 066703	19
1431	Nonequilibrium molecular dynamics calculation of the conductance of the KcsA potassium ion channel. 2006 , 74, 030905	5

1430	Aggregation of polyalanine in a hydrophobic environment. 2006 , 124, 134904	26
1429	Molecular Dynamics Analysis of High Electric Pulse Effects on Bilayer Membranes Containing DPPC and DPPS. 2006 , 34, 1405-1411	29
1428	Adding salt to an aqueous solution of t-butanol: is hydrophobic association enhanced or reduced?. 2006 , 124, 154508	14
1427	Solubility of simple, nonpolar compounds in TIP4P-Ew. 2006 , 124, 16102	20
1426	Pressure dependence of local structure in liquid carbon disulfide. 2006 , 124, 144511	11
1425	Equilibration of experimentally determined protein structures for molecular dynamics simulation. 2006 , 74, 061901	27
1424	Hydration dependence of the mass fractal dimension and anomalous diffusion of vibrational energy in proteins. 2006 , 73, 051905	23
1423	Parallel implementation of the replica exchange molecular dynamics algorithm on Blue Gene/L. 2006 ,	4
1422	A minimal model for stabilization of biomolecules by hydrocarbon cross-linking. 2006 , 124, 164907	20
1421	Molecular dynamics simulation of micellar aggregates in aqueous solution of hexadecyl trimethylammonium chloride with different additives. 2006 , 104, 3645-3651	20
1420	Charged extracellular residues, conserved throughout a G-protein-coupled receptor family, are required for ligand binding, receptor activation, and cell-surface expression. 2006 , 281, 38478-88	37
1419	Ion separation using a Y-junction carbon nanotube. 2006 , 17, 895-900	91
1418	Molecular dynamics simulations of the ligand-binding domain of an N-methyl-D-aspartate receptor. 2006 , 281, 12736-42	29
1417	Ensemble molecular dynamics yields submillisecond kinetics and intermediates of membrane fusion. 2006 , 103, 11916-21	124
1416	The second intracellular loop of the calcitonin gene-related peptide receptor provides molecular determinants for signal transduction and cell surface expression. 2006 , 281, 1644-51	20
1415	Only one protomer is active in the dimer of SARS 3C-like proteinase. 2006 , 281, 13894-8	75
1414	Exploring atomistic details of pH-dependent peptide folding. 2006 , 103, 18546-50	79
1413	Handbook of Nature-Inspired and Innovative Computing. 2006 ,	22

1412	Sampling the multiple folding mechanisms of Trp-cage in explicit solvent. 2006 , 103, 15859-64	212
1411	Computer simulations of membrane-lytic peptides: perspectives in drug design. 2007 , 5, 611-26	8
1410	Near-native structure refinement using in vacuo energy minimization. 2007 , 104, 3177-82	123
1409	Convergence and sampling efficiency in replica exchange simulations of peptide folding in explicit solvent. 2007 , 126, 014903	105
1408	Critical role of electrostatic interactions of amino acids at the cytoplasmic region of helices 3 and 6 in rhodopsin conformational properties and activation. 2007 , 282, 14272-82	17
1407	Engineered monomeric human histidine triad nucleotide-binding protein 1 hydrolyzes fluorogenic acyl-adenylate and lysyl-tRNA synthetase-generated lysyl-adenylate. 2007 , 282, 15137-47	28
1406	Hydrophobic association of alpha-helices, steric dewetting, and enthalpic barriers to protein folding. 2007 , 104, 6206-10	74
1405	Mutations as trapdoors to two competing native conformations of the Rop-dimer. 2007 , 104, 17674-9	52
1404	Effects of lengthscales and attractions on the collapse of hydrophobic polymers in water. 2007 , 104, 733-8	105
1403	Reversible gelation and dynamical arrest of dipolar colloids. 2007 , 78, 26002	50
1402	Control of membrane fusion mechanism by lipid composition: predictions from ensemble molecular dynamics. 2007 , 3, e220	91
1401	Molecular modeling-guided site-directed mutagenesis of cytochrome P450 2D6. 2007 , 8, 59-77	39
1400	Conformational analysis of lipid molecules by self-organizing maps. 2007 , 126, 054707	16
1399	Probe particles alter dynamic heterogeneities in simple supercooled systems. 2007 , 126, 104501	20
1398	Coarse-grained model for phospholipid/cholesterol bilayer employing inverse Monte Carlo with thermodynamic constraints. 2007 , 126, 075101	58
1397	Peptide translocators with engineered dehydration-prone hydrogen bonds. 2007 , 126, 061102	
1396	Ab initio simulation of a gadolinium-based magnetic resonance imaging contrast agent in aqueous solution. 2007 , 126, 181102	35
1395	Effect of the surface charge discretization on electric double layers: a Monte Carlo simulation study. 2007 , 126, 234703	29

1394	Molecular dynamics simulations of local field factors. 2007 , 127, 014501	4
1393	Solvent-exposed backbone loosens the hydration shell of soluble folded proteins. 2007 , 126, 245103	12
1392	Interatomic potential-based semiclassical theory for Lennard-Jones fluids. 2007 , 127, 174701	33
1391	Molecular dynamics simulation of nanocolloidal amorphous silica particles: Part I. 2007 , 127, 224711	23
1390	State point dependence of systematically coarse-grained potentials. 2007 , 33, 759-767	51
1389	Assessing the nature of lipid raft membranes. 2007 , 3, e34	231
1388	Deprotonation by dehydration: the origin of ammonium sensing in the AmtB channel. 2007 , 3, e22	38
1387	Prediction of the stability of coiled coils using molecular dynamics simulations. 2007 , 33, 463-473	7
1386	Phase separation in polyisoprene/polystyrene blends by a systematically coarse-grained model. 2007 , 126, 144908	25
1385	Impaired peroxisome proliferator-activated receptor gamma function through mutation of a conserved salt bridge (R425C) in familial partial lipodystrophy. 2007 , 21, 1049-65	35
1384	Understanding the pressure-induced emission enhancement for triple fluorescent compound with excited-state intramolecular proton transfer. 2007 , 111, 11793-800	60
1383	Docking of mu-conotoxin GIIIA in the sodium channel outer vestibule. 2007 , 1, 344-52	45
1382	Dynamic effects of nonequilibrium solvation: potential and free energy surfaces for Z/E isomerization in solvent-solute coordinates. 2007 , 126, 234505	7
1381	Allosteric small molecules unveil a role of an extracellular E2/transmembrane helix 7 junction for G protein-coupled receptor activation. 2007 , 282, 34968-76	39
1380	Policy Based Job Analysis. 2007 ,	1
1379	On the Programming Impact of Multi-Core, Multi-Processor Nodes in MPI Clusters. 2007 ,	6
1378	Solvent effects and hydration of a tripeptide in sodium halide aqueous solutions: an in silico study. 2007 , 9, 5423-35	34
1377	Self-consistent molecular dynamics formulation for electric-field-mediated electrolyte transport through nanochannels. 2007 , 76, 011202	21

1376	Anharmonicity and self-similarity of the free energy landscape of protein G. 2007 , 98, 048102	43
1375	Choosing weights for simulated tempering. 2007 , 76, 016703	61
1374	Porting the GROMACS Molecular Dynamics Code to the Cell Processor. 2007 ,	14
1373	The structure and dynamics of water inside armchair carbon nanotube. 2007 , 16, 335-339	27
1372	Molecular dynamics simulation of polyacrylamides in potassium montmorillonite clay hydrates. 2007 , 40, 545-553	10
1371	Unique dimeric structure of BNip3 transmembrane domain suggests membrane permeabilization as a cell death trigger. 2007 , 282, 16256-66	106
1370	Linking folding with aggregation in Alzheimer's beta-amyloid peptides. 2007 , 104, 16880-5	133
1369	Selective perturbation of the myosin recovery stroke by point mutations at the base of the lever arm affects ATP hydrolysis and phosphate release. 2007 , 282, 17658-64	26
1368	Carbon nanomaterials in biological systems. 2007 , 19, 373101	53
1367	Nucleotide-dependent allostery within the ABC transporter ATP-binding cassette: a computational study of the MJ0796 dimer. 2007 , 282, 22793-803	59
1366	Molecular dynamics studies of AChBP with nicotine and carbamylcholine: the role of water in the binding pocket. 2007 , 20, 353-9	69
1365	Possible pathway(s) of metyrapone egress from the active site of cytochrome P450 3A4: a molecular dynamics simulation. 2007 , 35, 689-96	49
1364	Effective potentials for 1:1 electrolyte solutions incorporating dielectric saturation and repulsive hydration. 2007 , 126, 044509	61
1363	Bilayer deformation by the Kv channel voltage sensor domain revealed by self-assembly simulations. 2007 , 104, 2631-6	95
1362	Structures and spectral signatures of protonated water networks in bacteriorhodopsin. 2007 , 104, 6980-5	131
1361	Water surface is acidic. 2007 , 104, 7342-7	296
1360	An electrostatic/hydrogen bond switch as the basis for the specific interaction of phosphatidic acid with proteins. 2007 , 282, 11356-64	176
1359	Structure of the Ebola fusion peptide in a membrane-mimetic environment and the interaction with lipid rafts. 2007 , 282, 27306-27314	38

1358	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
1357	Phospholemman transmembrane structure reveals potential interactions with Na ⁺ /K ⁺ -ATPase. 2007 , 282, 32742-8	13
1356	Estimation of absolute solvent and solvation shell entropies via permutation reduction. 2007 , 126, 014102	37
1355	Setting up and running molecular dynamics simulations of membrane proteins. 2007 , 41, 475-88	364
1354	Interfacial surface charge and free accessibility to the PLA2-active site-like region are essential requirements for the activity of Lys49 PLA2 homologues. 2007 , 49, 378-87	55
1353	Evidence for a C-terminal structural motif in gastrin and its bioactive fragments in membrane mimetic media. 2007 , 28, 1561-71	13
1352	Further evidence for a C-terminal structural motif in CCK2 receptor active peptide hormones. 2007 , 28, 2211-22	13
1351	Molecular and functional characterization of a new non-hemorrhagic metalloprotease from Bothrops jararacussu snake venom with antiplatelet activity. 2007 , 28, 2328-39	33
1350	Detecting similarities among distant homologous proteins by comparison of domain flexibilities. 2007 , 20, 285-99	19
1349	Structural properties of ionic detergent aggregates: a large-scale molecular dynamics study of sodium dodecyl sulfate. 2007 , 111, 11722-33	153
1348	Dynamics and function in a bacterial ABC transporter: simulation studies of the BtuCDF system and its components. 2007 , 46, 2767-78	56
1347	Thermally driven large-amplitude fluctuations in carbon-nanotube-based devices: Molecular dynamics simulations. 2007 , 75,	26
1346	Modeling 2D and 3D diffusion. 2007 , 400, 295-321	31
1345	Molecular characterization of gel and liquid-crystalline structures of fully hydrated POPC and POPE bilayers. 2007 , 111, 6026-33	100
1344	Mapping von Willebrand factor A domain binding sites on a snake venom metalloproteinase cysteine-rich domain. 2007 , 457, 41-6	31
1343	Does isoprene protect plant membranes from thermal shock? A molecular dynamics study. 2007 , 1768, 198-206	81
1342	Location and dynamics of acyl chain NBD-labeled phosphatidylcholine (NBD-PC) in DPPC bilayers. A molecular dynamics and time-resolved fluorescence anisotropy study. 2007 , 1768, 467-78	74
1341	Molecular studies of the gel to liquid-crystalline phase transition for fully hydrated DPPC and DPPE bilayers. 2007 , 1768, 354-65	133

1340	Phase behavior and dynamic heterogeneities in lipids: a coarse-grained simulation study of DPPC-DPPE mixtures. 2007 , 1768, 620-7	15
1339	Characterization of the conformational and orientational dynamics of ganglioside GM1 in a dipalmitoylphosphatidylcholine bilayer by molecular dynamics simulations. 2007 , 1768, 1628-40	19
1338	Interfacial interactions of glutamate, water and ions with carbon nanopore evaluated by molecular dynamics simulations. 2007 , 1768, 2319-41	5
1337	Interactions of amphotericin B derivatives with lipid membranes--a molecular dynamics study. 2007 , 1768, 2616-26	12
1336	A multidomain outer membrane protein from <i>Pasteurella multocida</i> : modelling and simulation studies of PmOmpA. 2007 , 1768, 2831-40	17
1335	1-Alkanols and membranes: a story of attraction. 2007 , 1768, 2899-913	55
1334	Translocation and interactions of L-arabinose in OmpF porin: A molecular dynamics study. 2007 , 352, 104-10	7
1333	Phage display identification of functional binding peptides against 4-acetamidophenol (Paracetamol): an exemplified approach to target low molecular weight organic molecules. 2007 , 358, 285-91	7
1332	Molecular dynamics simulations of thioredoxin with S-glutathiolated cysteine-73. 2007 , 362, 532-7	13
1331	Molecular dynamics simulation of polarizable carbon nanotubes. 2007 , 40, 460-465	8
1330	Flap opening dynamics in HIV-1 protease explored with a coarse-grained model. 2007 , 157, 606-15	100
1329	Coarse-grained molecular dynamics simulations of membrane proteins and peptides. 2007 , 157, 593-605	275
1328	Electric field effects on membranes: gramicidin A as a test ground. 2007 , 157, 545-56	34
1327	Replica exchange simulation of reversible folding/unfolding of the Trp-cage miniprotein in explicit solvent: on the structure and possible role of internal water. 2007 , 157, 524-33	105
1326	Fluctuations of primary ubiquitin folding intermediates in a force clamp. 2007 , 157, 557-69	27
1325	Homology model of 1alpha,25-dihydroxyvitamin D3 24-hydroxylase cytochrome P450 24A1 (CYP24A1): active site architecture and ligand binding. 2007 , 104, 53-60	20
1324	A three-dimensional model of CYP19 aromatase for structure-based drug design. 2007 , 105, 63-70	31
1323	Insights into molecular plasticity of choline binding proteins (pneumococcal surface proteins) by SAXS. 2007 , 365, 411-24	20

1322	The structure of the Alzheimer amyloid beta 10-35 peptide probed through replica-exchange molecular dynamics simulations in explicit solvent. 2007 , 366, 275-85	125
1321	Propagation of dynamic changes in barnase upon binding of barstar: an NMR and computational study. 2007 , 367, 1079-92	48
1320	The folding mechanics of a knotted protein. 2007 , 368, 884-93	122
1319	The Alzheimer's peptides Abeta40 and 42 adopt distinct conformations in water: a combined MD / NMR study. 2007 , 368, 1448-57	367
1318	Active and exo-site inhibition of human factor Xa: structure of des-Gla factor Xa inhibited by NAP5, a potent nematode anticoagulant protein from <i>Ancylostoma caninum</i> . 2007 , 371, 774-86	21
1317	Probing the flexibility of the DsbA oxidoreductase from <i>Vibrio cholerae</i> --a 15N - 1H heteronuclear NMR relaxation analysis of oxidized and reduced forms of DsbA. 2007 , 371, 703-16	20
1316	Predicting absolute ligand binding free energies to a simple model site. 2007 , 371, 1118-34	234
1315	Structural studies of the final enzyme in the alpha-aminoadipate pathway-saccharopine dehydrogenase from <i>Saccharomyces cerevisiae</i> . 2007 , 373, 745-54	17
1314	Heterogeneity even at the speed limit of folding: large-scale molecular dynamics study of a fast-folding variant of the villin headpiece. 2007 , 374, 806-16	154
1313	Molecular dynamics simulations of palmitate entry into the hydrophobic pocket of the fatty acid binding protein. 2007 , 581, 1243-7	34
1312	Activation of <i>Candida rugosa</i> lipase at alkane-aqueous interfaces: a molecular dynamics study. 2007 , 581, 4377-83	36
1311	Tailoring cutinase activity towards polyethylene terephthalate and polyamide 6,6 fibers. 2007 , 128, 849-57	135
1310	Pressure-area isotherm of a lipid monolayer from molecular dynamics simulations. 2007 , 23, 12617-23	139
1309	Ion transport across transmembrane pores. 2007 , 92, 4209-15	80
1308	Modulating the structure and properties of cell membranes: the molecular mechanism of action of dimethyl sulfoxide. 2007 , 111, 10453-60	281
1307	Polymorphic phase behavior of cardiolipin derivatives studied by coarse-grained molecular dynamics. 2007 , 111, 7194-200	57
1306	Stability and disintegration of ultrathin heptane films in water: molecular dynamics simulations. 2007 , 23, 1792-803	10
1305	Aspartic acid as a crystal growth catalyst. 2007 , 9, 1187	55

1304	Picosecond fluctuating protein energy landscape mapped by pressure temperature molecular dynamics simulation. 2007 , 104, 17261-5	63
1303	Metadynamics in essential coordinates: free energy simulation of conformational changes. 2007 , 111, 3073-6	81
1302	Comparison of charge models for fixed-charge force fields: small-molecule hydration free energies in explicit solvent. 2007 , 111, 2242-54	232
1301	Three-dimensional structure of HIV-1 VIF constructed by comparative modeling and the function characterization analyzed by molecular dynamics simulation. 2007 , 5, 617-26	27
1300	The distribution and conformation of very long-chain plant wax components in a lipid bilayer. 2007 , 111, 8702-4	7
1299	A coarse grain model for DNA. 2007 , 126, 084901	242
1298	Molecular dynamics simulations of mixed cationic/anionic wormlike micelles. 2007 , 23, 6588-97	39
1297	Nanosecond field alignment of head group and water dipoles in electroporating phospholipid bilayers. 2007 , 111, 12993-6	69
1296	Domain coupling in the ABC transporter system BtuCD/BtuF: molecular dynamics simulation, normal mode analysis and protein-protein docking. 2007 ,	1
1295	Water and polymer dynamics in chemically cross-linked hydrogels of poly(vinyl alcohol): a molecular dynamics simulation study. 2007 , 111, 2820-7	83
1294	Conformational analysis of L-prolines in water. 2007 , 111, 14034-42	48
1293	Structure and dynamics of the homologous series of alanine peptides: a joint molecular dynamics/NMR study. 2007 , 129, 1179-89	272
1292	Water permeation through a subnanometer boron nitride nanotube. 2007 , 129, 2748-9	169
1291	Effect of double bond position on lipid bilayer properties: insight through atomistic simulations. 2007 , 111, 11162-8	54
1290	Translocation of C60 and its derivatives across a lipid bilayer. 2007 , 7, 614-9	338
1289	Molecular dynamics simulations of hydrophobic associations in aqueous salt solutions indicate a connection between water hydrogen bonding and the Hofmeister effect. 2007 , 129, 14887-98	137
1288	Structure and UV-vis spectrum of C(60) fullerene in ethanol: a sequential molecular dynamics/quantum mechanics study. 2007 , 111, 11935-9	36
1287	Carbon nanotube/detergent interactions via coarse-grained molecular dynamics. 2007 , 7, 1923-8	115

1286	Adsorption processes of Gly and Glu amino acids on hydroxyapatite surfaces at the atomic level. 2007 , 23, 8972-81	109
1285	Pressure dependence of the compressibility of a micelle and a protein: insights from cavity formation analysis. 2007 , 105, 189-199	8
1284	G protein-coupled receptors self-assemble in dynamics simulations of model bilayers. 2007 , 129, 10126-32	275
1283	Molecular aggregates in aqueous solutions of bile acid salts. Molecular dynamics simulation study. 2007 , 111, 9886-96	118
1282	Molecular Dynamics Simulations of Cruzipains 1 and 2 at Different Temperatures. 2007 , 158-162	1
1281	Interaction of urea with amino acids: implications for urea-induced protein denaturation. 2007 , 129, 16126-31	242
1280	Metabolic pathway analysis of <i>S. pneumoniae</i> : an in silico approach towards drug-design. 2007 , 5, 135-53	16
1279	Ion pairing as a possible clue for discriminating between sodium and potassium in biological and other complex environments. 2007 , 111, 14077-9	72
1278	Molecular dynamic simulations of eicosanoic acid and 18-methyleicosanoic acid langmuir monolayers. 2007 , 111, 10849-52	13
1277	Molecular dynamics simulation of pore growth in lipid bilayer membranes in the presence of edge-active agents. 2007 , 91, 204104	21
1276	Base-specific spin-labeling of RNA for structure determination. 2007 , 35, 3128-43	127
1275	Determination of the macroscopic optical properties for composite materials. 2007 , 79, 012030	4
1274	Unravelling the solvent response to neutral and charged solutes. 2007 , 105, 1-16	94
1273	Integrating multi-level molecular simulations across heterogeneous resources. 2007 ,	1
1272	Signatures of hydrophobic collapse in extended proteins captured with force spectroscopy. 2007 , 104, 7916-21	87
1271	Coarse-grained simulations of ABA amphiphilic triblock copolymer solutions in thin films. 2007 , 9, 4662-72	31
1270	Molecular modeling of conformational properties of oligodepsipeptides. 2007 , 8, 3015-24	13
1269	Conformational dynamics of a lipid-interacting protein: MD simulations of saposin B. 2007 , 46, 13573-80	8

1268	A structurally altered D,L-amino acid TCRalpha transmembrane peptide interacts with the TCRalpha and inhibits T-cell activation in vitro and in an animal model. 2007 , 46, 2317-25	25
1267	Fluorescence probe of Trp-cage protein conformation in solution and in gas phase. 2007 , 129, 6726-35	59
1266	Carbohydrate clustering in aqueous solutions and the dynamics of confined water. 2007 , 111, 11948-56	38
1265	A Multiscale Model for Efficient Simulation of a Membrane Bound Viral Fusion Peptide. 2007 ,	
1264	Evaporation from water clusters containing singly charged ions. 2007 , 9, 5105-11	55
1263	Azines: conjugation stoppers or conjugation switches. 2007 , 17, 4304	15
1262	Autoionization at the surface of neat water: is the top layer pH neutral, basic, or acidic?. 2007 , 9, 4736-47	140
1261	Dual roles of borax in kinetics of calcium sulfate dihydrate formation. 2007 , 23, 5070-6	15
1260	The insertion of the antimicrobial peptide dicynthaurin monomer in model membranes: thermodynamics and structural characterization. 2007 , 46, 5678-86	25
1259	Nanoscale dewetting transition in protein complex folding. 2007 , 111, 9069-77	72
1258	A direct comparison of protein structure in the gas and solution phase: the Trp-cage. 2007 , 111, 13147-50	42
1257	A minimal transmembrane beta-barrel platform protein studied by nuclear magnetic resonance. 2007 , 46, 1128-40	29
1256	Cross-strand coupling of a beta-hairpin peptide stabilized with an Aib-Gly turn studied using isotope-edited IR spectroscopy. 2007 , 129, 13592-603	40
1255	Dehydration propensity of order-disorder intermediate regions in soluble proteins. 2007 , 6, 3519-26	41
1254	Molecular dynamics simulations of polycarbonate doped with Lemke chromophores. 2007 , 111, 10645-50	9
1253	Calculation of water-exchange rates on aqueous polynuclear clusters and at oxide-water interfaces. 2007 , 46, 2962-4	56
1252	Aqueous urea solutions: structure, energetics, and urea aggregation. 2007 , 111, 6220-8	177
1251	Specific anion effects on the optical rotation of alpha-amino acids. 2007 , 111, 10510-9	26

1250	Hydration dynamics and time scales of coupled water-protein fluctuations. 2007 , 129, 3376-82	210
1249	Molecular dynamics studies of the molecular structure and interactions of cholesterol superlattices and random domains in an unsaturated phosphatidylcholine bilayer membrane. 2007 , 111, 11021-31	23
1248	How sensitive are nanosecond molecular dynamics simulations of proteins to changes in the force field?. 2007 , 111, 6015-25	16
1247	Optimizing the Poisson Dielectric Boundary with Explicit Solvent Forces and Energies: Lessons Learned with Atom-Centered Dielectric Functions. 2007 , 3, 170-83	39
1246	Enhanced microtubule binding and tubulin assembly properties of conformationally constrained paclitaxel derivatives. 2007 , 46, 11514-27	17
1245	Study of the interaction of human defensins with cell membrane models: relationships between structure and biological activity. 2007 , 111, 11318-29	32
1244	Docking of ATP to Ca-ATPase: considering protein domain motions. 2007 , 47, 1171-81	8
1243	Stearic acid spin labels in lipid bilayers: insight through atomistic simulations. 2007 , 111, 12447-53	22
1242	Effect of membrane environment on proton permeation through gramicidin A channels. 2007 , 111, 9931-9	19
1241	Structure, topology, and tilt of cell-signaling peptides containing nuclear localization sequences in membrane bilayers determined by solid-state NMR and molecular dynamics simulation studies. 2007 , 46, 965-75	60
1240	Protein structures under electrospray conditions. 2007 , 46, 933-45	109
1239	Computational modeling of poly(alkylthiophene) conductive polymer insertion into phospholipid bilayers. 2007 , 23, 10672-81	16
1238	Influence of perfluorinated compounds on the properties of model lipid membranes. 2007 , 111, 9908-18	39
1237	Effects of chain length on the rates of C-C bond dissociation in linear alkanes and polyethylene. 2007 , 111, 3875-83	23
1236	Electric field poled polymeric nonlinear optical systems: molecular dynamics simulations of poly(methyl methacrylate) doped with disperse red chromophores. 2007 , 111, 3591-8	24
1235	Hydrophobic Solvation: Aqueous Methane Solutions. 2007 , 84, 864	5
1234	Catabolite activator protein in aqueous solution: a molecular simulation study. 2007 , 111, 1496-501	14
1233	Microscopic structure of phospholipid bilayers: comparison between molecular dynamics simulations and wide-angle X-ray spectra. 2007 , 111, 2484-9	11

1232	Temperature dependence of looping rates in a short peptide. 2007 , 111, 2639-46	23
1231	Monotopic enzymes and lipid bilayers: a comparative study. 2007 , 46, 3108-15	31
1230	Accurate and efficient corrections for missing dispersion interactions in molecular simulations. 2007 , 111, 13052-63	141
1229	Transient pockets on protein surfaces involved in protein-protein interaction. 2007 , 50, 3457-64	189
1228	Interaction of oleic acid with dipalmitoylphosphatidylcholine (DPPC) bilayers simulated by molecular dynamics. 2007 , 111, 12748-55	33
1227	Energetics of peptide recognition by the second PDZ domain of human protein tyrosine phosphatase 1E. 2007 , 46, 1064-78	18
1226	Molecular dynamics simulations of rhodopsin in different one-component lipid bilayers. 2007 , 111, 7052-63	43
1225	Temperature-induced conformational transition of a model elastin-like peptide GVG(VPGVG)(3) in water. 2007 , 8, 2196-202	34
1224	Structure-activity relationships of alphaS1-casomorphin using AM1 calculations and molecular dynamics simulations. 2007 , 111, 7377-83	3
1223	Molecular Dynamics Study on Diameter Effect in Structure of Ethanol Molecules Confined in Single-Walled Carbon Nanotubes. 2007 , 111, 15677-15685	46
1222	Differential effects of cholesterol, ergosterol and lanosterol on a dipalmitoyl phosphatidylcholine membrane: a molecular dynamics simulation study. 2007 , 111, 1786-801	111
1221	Insight into the radical mechanism of phycocyanobilin-ferredoxin oxidoreductase (PcyA) revealed by X-ray crystallography and biochemical measurements. 2007 , 46, 1484-94	45
1220	Gadolinium acetylacetonate tetraphenyl monoporphyrinate complex and some of its derivatives: EXAFS study and molecular dynamics simulation. 2007 , 46, 6871-9	4
1219	On the orientation of a designed transmembrane peptide: toward the right tilt angle?. 2007 , 129, 15174-81	92
1218	On the response of an ionic liquid to external perturbations and the calculation of shear viscosity. 2007 , 111, 4705-14	41
1217	Intrinsic Structure and Dynamics of the Water/Nitrobenzene Interface. 2007 , 111, 17612-17626	102
1216	Stability and dynamics of the porcine odorant-binding protein. 2007 , 46, 11120-7	25
1215	Role of zinc content on the catalytic efficiency of B1 metallo beta-lactamases. 2007 , 129, 2808-16	77

1214	L-alanine in a droplet of water: a density-functional molecular dynamics study. 2007 , 111, 4227-34	73
1213	Multiscale coarse-graining of monosaccharides. 2007 , 111, 11566-75	78
1212	Solubilization of Paclitaxel (taxol) by peptoid self-assemblies. 2007 , 23, 2308-10	9
1211	Conformational manifold of alpha-aminoisobutyric acid (Aib) containing alanine-based tripeptides in aqueous solution explored by vibrational spectroscopy, electronic circular dichroism spectroscopy, and molecular dynamics simulations. 2007 , 129, 13095-109	48
1210	Myosin V movement: lessons from molecular dynamics studies of IQ peptides in the lever arm. 2007 , 46, 14524-36	2
1209	Protonation of the chromophore in the photoactive yellow protein. 2007 , 111, 3765-73	16
1208	Morphology of bile salt micelles as studied by computer simulation methods. 2007 , 23, 12322-8	68
1207	Counterion and surface density dependence of the adsorption layer of ionic surfactants at the vapor-aqueous solution interface: a computer simulation study. 2007 , 111, 1769-74	41
1206	Molecular conformations in a phospholipid bilayer extracted from dipolar couplings: a computer simulation study. 2007 , 111, 13638-44	5
1205	Effect of the barometric phase transition of a DMPA bilayer on the lipid/water interface. An atomistic description by molecular dynamics simulation. 2007 , 111, 13726-33	1
1204	Molecular dynamics simulations of methane hydrate using polarizable force fields. 2007 , 111, 6486-92	63
1203	Self-Organization in Catalyst Layers of Polymer Electrolyte Fuel Cells. 2007 , 111, 13627-13634	131
1202	Physical Adsorption of Block Copolymers to SWNT and MWNT: A Nonwrapping Mechanism. 2007 , 40, 3676-3685	141
1201	Atomic-scale structure and electrostatics of anionic palmitoyl-oleoyl-phosphatidylglycerol lipid bilayers with Na ⁺ counterions. 2007 , 92, 1114-24	159
1200	Insight into the putative specific interactions between cholesterol, sphingomyelin, and palmitoyl-oleoyl phosphatidylcholine. 2007 , 92, 1125-37	115
1199	Dopamine D1 receptor agonist and D2 receptor antagonist effects of the natural product (-)-stepholidine: molecular modeling and dynamics simulations. 2007 , 93, 1431-41	33
1198	A molecular view of melting in anhydrous phospholipidic membranes. 2007 , 92, 147-61	52
1197	Conformation of a peptide encompassing the proton translocation channel of vacuolar H ⁽⁺⁾ -ATPase. 2007 , 92, 138-46	13

1196	Detailed mechanism for AmtB conducting NH ₄ ⁺ /NH ₃ : molecular dynamics simulations. 2007 , 92, 877-85	36
1195	A molecular dynamics study of slow base flipping in DNA using conformational flooding. 2007 , 93, 770-86	30
1194	The cPLA2 C2alpha domain in solution: structure and dynamics of its Ca ²⁺ -activated and cation-free states. 2007 , 92, 966-76	7
1193	Beta-sheet containment by flanking prolines: molecular dynamic simulations of the inhibition of beta-sheet elongation by proline residues in human prion protein. 2007 , 92, 2080-9	16
1192	The pH-dependent conformational states of kyotorphin: a constant-pH molecular dynamics study. 2007 , 92, 1836-45	44
1191	Structural stabilization and functional improvement of horseradish peroxidase upon modification of accessible lysines: experiments and simulation. 2007 , 92, 1192-203	64
1190	Self-assembling of peptide/membrane complexes by atomistic molecular dynamics simulations. 2007 , 92, 903-12	45
1189	Structural modeling of snow flea antifreeze protein. 2007 , 92, 1717-23	50
1188	Structure and molecular mechanism of Bacillus anthracis cofactor-independent phosphoglycerate mutase: a crucial enzyme for spores and growing cells of Bacillus species. 2007 , 92, 977-88	19
1187	Ion leakage through transient water pores in protein-free lipid membranes driven by transmembrane ionic charge imbalance. 2007 , 92, 1878-90	104
1186	Structural features of parathyroid hormone receptor coupled to Galpha(s)-protein. 2007 , 92, 535-40	6
1185	Cholesterol surrogates: a comparison of cholesterol and 16:0 ceramide in POPC bilayers. 2007 , 92, 920-7	68
1184	What happens if cholesterol is made smoother: importance of methyl substituents in cholesterol ring structure on phosphatidylcholine-sterol interaction. 2007 , 92, 3346-57	88
1183	Charge structure and counterion distribution in hexagonal DNA liquid crystal. 2007 , 92, 947-58	12
1182	Molecular dynamics simulations of SOPS and sphingomyelin bilayers containing cholesterol. 2007 , 92, 1284-95	38
1181	How alcohol chain-length and concentration modulate hydrogen bond formation in a lipid bilayer. 2007 , 92, 2366-76	74
1180	Simulation of the coupling between nucleotide binding and transmembrane domains in the ATP binding cassette transporter BtuCD. 2007 , 92, 2727-34	48
1179	A molecular dynamics study of the ligand release path in yeast cytosine deaminase. 2007 , 92, 2301-10	6

1178	HIV-1 protease substrate binding and product release pathways explored with coarse-grained molecular dynamics. 2007 , 92, 4179-87	67
1177	Molecular dynamics simulations of a stretch-activated channel inhibitor GsMTx4 with lipid membranes: two binding modes and effects of lipid structure. 2007 , 92, 4233-43	42
1176	Invariance of single-file water mobility in gramicidin-like peptidic pores as function of pore length. 2007 , 92, 3930-7	29
1175	Molecular dynamics simulations using temperature-enhanced essential dynamics replica exchange. 2007 , 92, 4262-70	45
1174	Effects of serine-to-cysteine mutations on beta-lactamase folding. 2007 , 93, 1707-18	20
1173	The permeability enhancing mechanism of DMSO in ceramide bilayers simulated by molecular dynamics. 2007 , 93, 2056-68	129
1172	Short-range order and collective dynamics of DMPC bilayers: a comparison between molecular dynamics simulations, X-ray, and neutron scattering experiments. 2007 , 93, 3156-68	72
1171	Structure and aggregation mechanism of beta(2)-microglobulin (83-99) peptides studied by molecular dynamics simulations. 2007 , 93, 3353-62	17
1170	Nucleotide effects on the structure and dynamics of actin. 2007 , 93, 1277-83	67
1169	Molecular dynamics simulations of two tandem octarepeats from the mammalian prion protein: fully Cu ²⁺ -bound and metal-free forms. 2007 , 93, 3762-74	17
1168	Quantitative characterization of intrinsic disorder in polyglutamine: insights from analysis based on polymer theories. 2007 , 93, 1923-37	125
1167	New insights into the mechanism of Alzheimer amyloid-beta fibrillogenesis inhibition by N-methylated peptides. 2007 , 93, 3015-25	68
1166	Effect of lipid peroxidation on the properties of lipid bilayers: a molecular dynamics study. 2007 , 93, 4225-36	407
1165	The dynamic orientation of membrane-bound peptides: bridging simulations and experiments. 2007 , 93, 4278-88	61
1164	The molecular mechanism of monolayer-bilayer transformations of lung surfactant from molecular dynamics simulations. 2007 , 93, 3775-82	86
1163	Structure of hydrophobic hydration of benzene and hexafluorobenzene from first principles. 2007 , 111, 1081-9	49
1162	A peptide dendrimer enzyme model with a single catalytic site at the core. 2007 , 129, 13238-46	66
1161	Glycolipid membranes through atomistic simulations: effect of glucose and galactose head groups on lipid bilayer properties. 2007 , 111, 10146-54	57

1160	Short-range structure of a GM3 ganglioside membrane: comparison between experimental WAXS and computer simulation results. 2007 , 111, 10965-9	14
1159	Effect of ions on the hydrophobic interaction between two plates. 2007 , 129, 4678-86	208
1158	Molecular dynamics simulations of surfactant and nanoparticle self-assembly at liquid-liquid interfaces. 2007 , 19, 375109	47
1157	Transport in Protein Crystals, Part I: Insights from Molecular Simulations. 2007 , 9, 90-95	1217
1156	Transport in Protein Crystals, Part II: Diffusion Simulation and Chiral Recognition. 2007 , 9, 70-75	2
1155	The <i>Saccharomyces cerevisiae</i> succinate dehydrogenase does not require heme for ubiquinone reduction. 2007 , 1767, 1436-45	40
1154	Conformational templates for rational drug design: flexibility of cyclo(D-Pro1-Ala2-Ala3-Ala4-Ala5) in DMSO solution. 2007 , 50, 2921-5	14
1153	Identification of critical residues in novel drug metabolizing mutants of cytochrome P450 BM3 using random mutagenesis. 2007 , 50, 455-61	95
1152	Molecular dynamics simulations of inwardly rectifying (Kir) potassium channels: a comparative study. 2007 , 46, 3643-52	38
1151	Computational Parameters. 2007 , 59-65	2
1150	Method to assess packing quality of transmembrane alpha-helices in proteins. 2. Validation by "correct vs misleading" test. 2007 , 47, 1163-70	4
1149	In silico mutation of cysteine residues in the ligand-binding domain of an N-methyl-D-aspartate receptor. 2007 , 46, 2136-45	7
1148	Simulated surface tensions of common water models. 2007 , 126, 221101	153
1147	On the characterization of host-guest complexes: surface tension, calorimetry, and molecular dynamics of cyclodextrins with a non-ionic surfactant. 2007 , 111, 4383-92	89
1146	Free pyrene probes in gel and fluid membranes: perspective through atomistic simulations. 2007 , 111, 3640-50	52
1145	Clustering of Lennard-Jones particles in water: temperature and pressure effects. 2007 , 127, 104502	4
1144	Computational Analysis of Current and Noise Properties of a Single Open Ion Channel. 2007 , 3, 248-55	4
1143	From mesoscale back to atomistic models: a fast reverse-mapping procedure for vinyl polymer chains. 2007 , 111, 2765-73	85

1142	Lipid transmembrane asymmetry and intrinsic membrane potential: two sides of the same coin. 2007 , 129, 5358-9	70
1141	Molecular mechanism for lipid flip-flops. 2007 , 111, 13554-9	114
1140	Ion transport through chemically induced pores in protein-free phospholipid membranes. 2007 , 111, 13379-82	30
1139	Methods in Membrane Lipids. 2007 ,	16
1138	PcrA Helicase, a Molecular Motor Studied from the Electronic to the Functional Level. 2006 , 319-347	8
1137	Ion Channels: Insights for Drug Design from Structure and Modeling. 2007 , 703-724	
1136	Dispersion interactions govern the strong thermal stability of a protein. 2007 , 13, 9022-7	27
1135	VCD spectroscopic and molecular dynamics analysis of the Trp-cage miniprotein TC5b. 2007 , 88, 427-37	15
1134	Structure-activity relationships of Leu-Enkephalin analog with (4-Carboxamido)phenylalanine substituted for tyrosine: a molecular dynamics study. 2007 , 86, 231-9	2
1133	Merozoite surface protein 2 of Plasmodium falciparum: expression, structure, dynamics, and fibril formation of the conserved N-terminal domain. 2007 , 87, 12-22	40
1132	A mixed-alpha,beta miniprotein stereochemically reprogrammed to high-binding affinity for acetylcholine. 2007 , 87, 231-43	20
1131	Asymmetric crystal growth of alpha-resorcinol from the vapor phase: surface reconstruction and conformational change are the culprits. 2007 , 46, 5537-40	15
1130	Amide-to-ester substitution in coiled coils: the effect of removing hydrogen bonds on protein structure. 2007 , 46, 7766-9	36
1129	Pressure and salt effects in simulated water: two sides of the same coin?. 2007 , 46, 8907-11	76
1128	Asymmetric Crystal Growth of α -Resorcinol from the Vapor Phase: Surface Reconstruction and Conformational Change Are the Culprits. 2007 , 119, 5633-5636	4
1127	Estersubstitutionen in α -helicalen Coiled-Coil-Peptiden: Effekt der Eliminierung von Wasserstoffbrücken auf die Struktur von Proteinen. 2007 , 119, 7912-7916	12
1126	Druck- und Salzeffekte in simuliertem Wasser: zwei Seiten einer Medaille?. 2007 , 119, 9065-9069	10
1125	Effect of different treatments of long-range interactions and sampling conditions in molecular dynamic simulations of rhodopsin embedded in a dipalmitoyl phosphatidylcholine bilayer. 2007 , 28, 1017-30	27

1124	Identification of biomolecular conformations from incomplete torsion angle observations by hidden Markov models. 2007 , 28, 2453-64	13
1123	Speeding up parallel GROMACS on high-latency networks. 2007 , 28, 2075-84	98
1122	Information theoretical measures to analyze trajectories in rational molecular design. 2007 , 28, 2576-80	24
1121	Comparison of thermodynamic properties of coarse-grained and atomic-level simulation models. 2007 , 8, 452-61	92
1120	Understanding Segmental Dynamics in Polymer Electrolytes: A Computer Study. 2007 , 208, 2215-2221	14
1119	Docking and molecular dynamics simulation of the Azurin-Cytochrome c551 electron transfer complex. 2007 , 20, 122-31	24
1118	Molecular dynamics simulations of conserved Hox protein hexapeptides II. Folded structures in water solution. 2007 , 805, 61-70	1
1117	A mechanism for the stabilization of the secondary structure of a peptide by liquid ethylene glycol and its aqueous solutions. 2007 , 808, 93-96	8
1116	Molecular dynamics simulations of conserved Hox protein hexapeptides. I. Folding behavior in water solution. 2007 , 810, 113-120	2
1115	Interfacial activation of snake venom phospholipases A2 (svPLA2) probed by molecular dynamics simulations. 2007 , 818, 31-41	6
1114	Identification of the bioactive conformation for mucin epitope peptides. 2007 , 823, 16-27	2
1113	Molecular dynamics simulation of the room-temperature ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate. 2007 , 847, 93-100	56
1112	Molecular dynamics simulation study of interaction between a class IIa bacteriocin and its immunity protein. 2007 , 1774, 1002-13	7
1111	Computer modeling of binding of diverse weak toxins to nicotinic acetylcholine receptors. 2007 , 31, 72-81	18
1110	Long-range interactions and parallel scalability in molecular simulations. 2007 , 176, 14-22	34
1109	Ions at the ice/vapor interface. 2007 , 436, 99-103	38
1108	Computational study of anion solvation in nitrobenzene. 2007 , 436, 362-367	10
1107	Simulation of micelle of zwitterionic DSB in NaCl aqueous solution. 2007 , 438, 326-329	9

1106	Atomic level description of the protecting effect of osmolytes against thermal denaturation of proteins. 2007 , 438, 298-303	8
1105	Surface diffusion of n-alkanes: Mechanism and anomalous behavior. 2007 , 447, 310-315	14
1104	'Bridged' stilbene derivatives as selective cyclooxygenase-1 inhibitors. 2007 , 15, 6109-18	33
1103	Dynamical and structural properties of charged and uncharged lidocaine in a lipid bilayer. 2007 , 125, 416-24	52
1102	Structural, dynamical and functional aspects of the inner motions in the blue copper protein azurin. 2007 , 125, 532-9	20
1101	Buckling and axially compressive properties of perfect and defective single-walled carbon nanotubes. 2007 , 45, 2486-2495	51
1100	Preferential interaction parameters in biological systems by Kirkwood's Buff theory and computer simulation. 2007 , 256, 14-19	45
1099	Molecular dynamics analysis of the AOT/water/isooctane system: Effect of simulation time, initial configuration, and model salts. 2007 , 262, 264-270	28
1098	Conotoxins containing nonnatural backbone spacers: cladistic-based design, chemical synthesis, and improved analgesic activity. 2007 , 14, 399-407	62
1097	Calculation of absolute free energy of binding for theophylline and its analogs to RNA aptamer using nonequilibrium work values. 2007 , 337, 135-143	18
1096	Self-assembly and structural characterization of Echinococcus granulosus antigen B recombinant subunit oligomers. 2007 , 1774, 278-85	21
1095	Simulations of Biomembranes and Water: Important Technical Aspects. 2007 , 261, 18-25	23
1094	The structure of the zwitterionic headgroups in a DMPC bilayer as seen from Monte Carlo simulation: Comparisons with ionic solutions. 2007 , 131-132, 225-234	4
1093	Molecular dynamics study of structural properties of β -sheet assemblies formed by synthetic de novo oligopeptides. 2007 , 373, 455-476	10
1092	The puzzling unsolved mysteries of liquid water: Some recent progress. 2007 , 386, 729-743	71
1091	Molecular dynamics study of the fibril elongation of the prion protein fragment PrP106-126. 2007 , 245, 238-42	2
1090	Study of the molecular weight dependence of glass transition temperature for amorphous poly(L-lactide) by molecular dynamics simulation. 2007 , 48, 4900-4905	54
1089	Structural and functional behavior of biologically active monomeric melittin. 2007 , 25, 767-72	37

1088	Molecular characterization and phylogenetic analysis of BjuMP-I: a RGD-P-III class hemorrhagic metalloprotease from Bothrops jararacussu snake venom. 2007 , 26, 69-85	25
1087	Synthesis, in vitro and in silico assessment of organometallic Rhenium(I) and Technetium(I) thymidine complexes. 2007 , 692, 1255-1264	20
1086	Theoretical investigations of the dissociation of charged protein complexes in the gas phase. 2007 , 18, 2242-53	38
1085	Counterion and composition effects on discotic nematic lyotropic liquid crystals II. Ion exchange and molecular dynamics. 2007 , 316, 120-5	
1084	A boundary element formulation of protein electrostatics with explicit ions. 2007 , 223, 416-435	9
1083	Generator estimation of Markov jump processes. 2007 , 227, 353-375	32
1082	On the application of molecular-dynamics simulations to validate thermal parameters and to optimize TLS-group selection for macromolecular refinement. 2007 , 63, 705-13	8
1081	Structural and functional definition of the specificity of a novel caspase-3 inhibitor, Ac-DNLD-CHO. 2007 , 7, 8	21
1080	A previously unobserved conformation for the human Pex5p receptor suggests roles for intrinsic flexibility and rigid domain motions in ligand binding. 2007 , 7, 24	21
1079	Structure of the dimeric N-glycosylated form of fungal beta-N-acetylhexosaminidase revealed by computer modeling, vibrational spectroscopy, and biochemical studies. 2007 , 7, 32	22
1078	Characterizing structural features of cuticle-degrading proteases from fungi by molecular modeling. 2007 , 7, 33	29
1077	Water solvent and local anesthetics: A computational study. 2007 , 107, 1642-1649	6
1076	The structural properties of magainin in water, TFE/water, and aqueous urea solutions: molecular dynamics simulations. 2007 , 67, 931-40	21
1075	Dynamical behavior of the vascular endothelial growth factor: biological implications. 2007 , 67, 517-25	8
1074	Conformational states and folding pathways of peptides revealed by principal-independent component analyses. 2007 , 67, 579-92	7
1073	Hydration of a hydrophobic cavity and its functional role: a simulation study of human interleukin-1beta. 2007 , 67, 868-85	17
1072	Free energy landscape of a biomolecule in dihedral principal component space: sampling convergence and correspondence between structures and minima. 2007 , 67, 569-78	78
1071	Molecular modeling of prohibitin domains. 2007 , 68, 353-62	33

1070	Recognition of Cdk2 by Cdk7. 2007 , 67, 1048-59	18
1069	Molecular dynamics simulations from putative transition states of alpha-spectrin SH3 domain. 2007 , 69, 536-50	13
1068	The conformation of the extracellular binding domain of Death Receptor 5 in the presence and absence of the activating ligand TRAIL: a molecular dynamics study. 2008 , 70, 333-43	14
1067	Full correlation analysis of conformational protein dynamics. 2008 , 70, 1294-312	108
1066	Position-resolved free energy of solvation for amino acids in lipid membranes from molecular dynamics simulations. 2008 , 70, 1332-44	56
1065	Correction of âDynamical behavior of the vascular endothelial growth factor: Biological implicationsâ 2007 , 70, 307-308	1
1064	Protein-protein docking: progress in CAPRI rounds 6-12 using a combination of methods: the introduction of steered solvated molecular dynamics. 2007 , 69, 816-22	6
1063	The investigation of interactions of kappa-Hefutoxin1 with the voltage-gated potassium channels: a computational simulation. 2008 , 71, 1441-9	7
1062	Exploring the protein G helix free-energy surface by solute tempering metadynamics. 2008 , 71, 1647-54	56
1061	The sequence TGAAKAVALVL from glyceraldehyde-3-phosphate dehydrogenase displays structural ambivalence and interconverts between alpha-helical and beta-hairpin conformations mediated by collapsed conformational states. 2007 , 13, 314-26	7
1060	Loop propensity of the sequence YKGQP from staphylococcal nuclease: implications for the folding of nuclease. 2007 , 13, 679-92	8
1059	A partially structured region of a largely unstructured protein, Plasmodium falciparum merozoite surface protein 2 (MSP2), forms amyloid-like fibrils. 2007 , 13, 839-48	28
1058	Diameter sorting of carbon nanotubes by gradient centrifugation: role of endohedral water. 2007 , 244, 3896-3900	27
1057	A novel method for packing quality assessment of transmembrane alpha-helical domains in proteins. 2007 , 72, 293-300	
1056	Identification of the PIP2-binding site on Kir6.2 by molecular modelling and functional analysis. 2007 , 26, 3749-59	69
1055	Probing the chemistry of thioredoxin catalysis with force. 2007 , 450, 124-7	224
1054	Pyrazolinone analgesics prevent the antiplatelet effect of aspirin and preserve human platelet thromboxane synthesis. 2008 , 6, 166-73	40
1053	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. 2007 , 274, 2424-36	67

1052	Targeting HIV-1 through molecular modeling and docking studies of CXCR4: leads for therapeutic development. 2007 , 69, 191-203	18
1051	Denaturation and aggregation of β -lactoglobulin preliminary molecular dynamics study. 2007 , 21, 1081-1091	24
1050	How does a voltage sensor interact with a lipid bilayer? Simulations of a potassium channel domain. 2007 , 15, 235-44	89
1049	Gating of HCN channels by cyclic nucleotides: residue contacts that underlie ligand binding, selectivity, and efficacy. 2007 , 15, 655-70	85
1048	Conformational change in an MFS protein: MD simulations of LacY. 2007 , 15, 873-84	63
1047	Geometry-based sampling of conformational transitions in proteins. 2007 , 15, 1482-92	106
1046	An experimental and theoretical study of <i>Coprinus cinereus</i> peroxidase-catalyzed biodegradation of isoelectronic to dioxin recalcitrants. 2007 , 44, 20-26	2
1045	A molecular dynamics simulation of micellar aggregates in aqueous solutions of hexadecyltrimethylammonium chloride with admixtures of low-molecular-weight substances. 2007 , 81, 1256-1262	7
1044	Solvation of transmembrane proteins by isotropic membrane mimetics: a molecular dynamics study. 2007 , 111, 11285-96	8
1043	The ion sensitivity of surface conductive single crystalline diamond. 2007 , 129, 1287-92	71
1042	Structural and functional characterization of the aryl hydrocarbon receptor ligand binding domain by homology modeling and mutational analysis. 2007 , 46, 696-708	97
1041	Quantifying the hydrophobic effect. 1. A computer simulation-molecular-thermodynamic model for the self-assembly of hydrophobic and amphiphilic solutes in aqueous solution. 2007 , 111, 1025-44	34
1040	Quantifying the hydrophobic effect. 2. A computer simulation-molecular-thermodynamic model for the micellization of nonionic surfactants in aqueous solution. 2007 , 111, 1045-62	26
1039	Quantifying the hydrophobic effect. 3. A computer simulation-molecular-thermodynamic model for the micellization of ionic and zwitterionic surfactants in aqueous solution. 2007 , 111, 1063-75	17
1038	A bias-exchange approach to protein folding. 2007 , 111, 4553-9	430
1037	Construction and application of the weighted amino acid network based on energy. 2007 , 75, 051903	29
1036	Close contacts between carbonyl oxygen atoms and aromatic centers in protein structures: π ... π or lone-pair... π interactions?. 2007 , 111, 8680-3	84
1035	Force field of the TMGL ionic liquid and the solubility of SO ₂ and CO ₂ in the TMGL from molecular dynamics simulation. 2007 , 111, 10461-7	88

1034	Subunit-specific agonist activity at NR2A-, NR2B-, NR2C-, and NR2D-containing N-methyl-D-aspartate glutamate receptors. 2007 , 72, 907-20	128
1033	The MARTINI force field: coarse grained model for biomolecular simulations. 2007 , 111, 7812-24	3596
1032	Combining substrate dynamics, binding statistics, and energy barriers to rationalize regioselective hydroxylation of octane and lauric acid by CYP102A1 and mutants. 2007 , 16, 420-31	33
1031	Docking and homology modeling explain inhibition of the human vesicular glutamate transporters. 2007 , 16, 1819-29	42
1030	Spin-labeled photosynthetic reaction centers from <i>Rhodobacter sphaeroides</i> studied by electron paramagnetic resonance spectroscopy and molecular dynamics simulations. 2007 , 31, 167-178	15
1029	Computational approaches to shed light on molecular mechanisms in biological processes. 2007 , 117, 723-741	8
1028	A gate mechanism indicated in the selectivity filter of the potassium channel KscA. 2007 , 117, 1121-1129	5
1027	Acyl chain order parameter profiles in phospholipid bilayers: computation from molecular dynamics simulations and comparison with 2H NMR experiments. 2007 , 36, 919-31	245
1026	Chimeric Protein Engineering. 2007 , 13, 151-160	7
1025	Structural and Functional Mimicry of the Binding Site of hYAP-WW Domain for Proline-rich Ligands. 2007 , 13, 245-250	1
1024	Interaction of omeprazole with a methylated derivative of beta-cyclodextrin: phase solubility, NMR spectroscopy and molecular simulation. 2007 , 24, 377-89	60
1023	Tubulin: from atomistic structure to supramolecular mechanical properties. 2007 , 42, 8864-8872	38
1022	Studying the unfolding kinetics of proteins under pressure using long molecular dynamic simulation runs. 2007 , 33, 515-22	7
1021	Modification of axial fiber contact residues impact sickle hemoglobin polymerization by perturbing a network of coupled interactions. 2007 , 26, 445-55	3
1020	Mechanical response and conformational changes of alpha-actinin domains during unfolding: a molecular dynamics study. 2007 , 6, 399-407	23
1019	Solute transport in orthorhombic lysozyme crystals: a molecular simulation study. 2007 , 29, 1865-73	10
1018	Docking of novel reversible monoamine oxidase-B inhibitors: efficient prediction of ligand binding sites and estimation of inhibitors thermodynamic properties. 2007 , 114, 725-32	20
1017	Dynamic domains and geometrical properties of HIV-1 gp120 during conformational changes induced by CD4 binding. <i>Journal of Molecular Modeling</i> , 2007 , 13, 411-24	2 8

1016	Cold-active enzymes studied by comparative molecular dynamics simulation. <i>Journal of Molecular Modeling</i> , 2007 , 13, 485-97	2	41
1015	Molecular dynamics studies on HIV-1 protease: a comparison of the flap motions between wild type protease and the M46I/G51D double mutant. <i>Journal of Molecular Modeling</i> , 2007 , 13, 1151-6	2	10
1014	Molecular motions and conformational transition between different conformational states of HIV-1 gp120 envelope glycoprotein. 2007 , 52, 3074-3088		4
1013	Molecular simulation of water behaviors on crystal faces of hydroxyapatite. 2007 , 2, 156-163		22
1012	The molecular dynamics of assembly of the ubiquitous aortic medial amyloid medin fragment. 2007 , 25, 903-11		5
1011	Molecular dynamics at the receptor level of immunodominant myelin basic protein epitope 87-99 implicated in multiple sclerosis and its antagonists altered peptide ligands: triggering of immune response. 2007 , 26, 471-81		22
1010	The N-homologue LRR domain adopts a folding which explains the TMV-Cg-induced HR-like response in sensitive tobacco plants. 2008 , 26, 850-60		13
1009	On the structure, interactions, and dynamics of bound VEGF. 2008 , 26, 1091-103		7
1008	How amantadine and rimantadine inhibit proton transport in the M2 protein channel. 2008 , 27, 342-8		58
1007	Molecular dynamics simulations of microstructure and mixing dynamics of cryoprotective solvents in water and in the presence of a lipid membrane. 2008 , 136, 23-31		27
1006	Molecular dynamics simulations of lung surfactant lipid monolayers. 2008 , 138, 67-77		45
1005	Buckling of defective single-walled and double-walled carbon nanotubes under axial compression by molecular dynamics simulation. 2008 , 68, 1809-1814		72
1004	Secondary structure prediction of beta-hairpin peptide tryptophan zipper-I. 2008 , 387, 3537-3545		
1003	Application of the random coil index to studying protein flexibility. 2008 , 40, 31-48		86
1002	Comparison of multiple crystal structures with NMR data for engrailed homeodomain. 2008 , 40, 189-202		16
1001	A tool for the prediction of structures of complex sugars. 2008 , 42, 241-56		21
1000	Model and molecular dynamic simulations of active and inactive endo-beta-1,4-mannanase in tomato fruit. 2008 , 27, 363-70		3
999	An Ergodic Sampling Scheme for Constrained Hamiltonian Systems with Applications to Molecular Dynamics. 2008 , 130, 687-711		9

998	Molecular dynamics studies of alpha-helix stability in fibril-forming peptides. 2008 , 22, 53-8		13
997	New insight into the discrimination between omeprazole enantiomers by cyclodextrins in aqueous solution. 2008 , 62, 345-351		2
996	Outer membrane proteins: comparing X-ray and NMR structures by MD simulations in lipid bilayers. 2008 , 37, 131-41		16
995	Molecular dynamics simulations and membrane protein structure quality. 2008 , 37, 403-9		32
994	Structure and dynamics of the antifungal molecules Syringotoxin-B and Syringopeptin-25A from molecular dynamics simulation. 2008 , 37, 495-502		7
993	Selectivity in the mechanism of action of antimicrobial mastoparan peptide Polybia-MP1. 2008 , 37, 879-91		46
992	Effects of oxidation, pH and lipids on amyloidogenic peptide structure: implications for fibril formation?. 2008 , 38, 99-110		27
991	Efficient and reproducible folding simulations of the Trp-cage protein with multiscale molecular dynamics. 2008 , 53, 1699-1707		1
990	Molecular dynamics simulations of the adsorption of amino acids on the hydroxyapatite {100}-water interface. 2008 , 2, 239-245		9
989	Molecular motions of human HIV-1 gp120 envelope glycoproteins. <i>Journal of Molecular Modeling</i> , 2008 , 14, 857-70	2	23
988	Continuous metadynamics in essential coordinates as a tool for free energy modelling of conformational changes. <i>Journal of Molecular Modeling</i> , 2008 , 14, 995-1002	2	21
987	Receptors for organochlorine pesticides based on calixarenes. 2008 , 163, 195-202		8
986	Diffusion of anionic and neutral GFP derivatives through plasmodesmata in epidermal cells of <i>Nicotiana benthamiana</i> . 2008 , 234, 13-23		21
985	Is TEA an inhibitor for human Aquaporin-1?. 2008 , 456, 663-9		29
984	Solution structure of the <i>Legionella pneumophila</i> Mip-rapamycin complex. 2008 , 8, 17		23
983	Multiple molecular dynamics simulation of the isoforms of human translation elongation factor 1A reveals reversible fluctuations between "open" and "closed" conformations and suggests specific for eEF1A1 affinity for Ca ²⁺ -calmodulin. 2008 , 8, 4		29
982	Residue contact-count potentials are as effective as residue-residue contact-type potentials for ranking protein decoys. 2008 , 8, 53		8
981	Real-time translocation of fullerene reveals cell contraction. 2008 , 4, 1986-92		38

980	Molecular dynamics simulations of HIV-1 protease monomer: Assembly of N-terminus and C-terminus into beta-sheet in water solution. 2008 , 70, 731-8	13
979	Water penetration in the low and high pressure native states of ubiquitin. 2008 , 70, 1175-84	57
978	Electrostatic contribution to the thermodynamic and kinetic stability of the homotrimeric coiled coil Lpp-56: A computational study. 2008 , 70, 810-22	13
977	Computational studies of the structure, dynamics and native content of amyloid-like fibrils of ribonuclease A. 2008 , 70, 863-72	18
976	Hydrophobic interactions and ionic networks play an important role in thermal stability and denaturation mechanism of the porcine odorant-binding protein. 2008 , 71, 35-44	28
975	Structural rationalization of novel drug metabolizing mutants of cytochrome P450 BM3. 2008 , 71, 336-52	37
974	Conformational and dynamics changes induced by bile acids binding to chicken liver bile acid binding protein. 2008 , 71, 1889-98	15
973	Helix formation is a dynamical bottleneck in the recovery reaction of Photoactive Yellow Protein. 2008 , 72, 136-49	6
972	Acidic range titration of HEWL using a constant-pH molecular dynamics method. 2008 , 72, 289-98	66
971	On defining the dynamics of hydrophobic patches on protein surfaces. 2008 , 72, 105-14	5
970	Molecular dynamics study of Pseudomonas aeruginosa lectin-II complexed with monosaccharides. 2008 , 72, 382-92	18
969	Rigid body essential X-ray crystallography: distinguishing the bend and twist of glutamate receptor ligand binding domains. 2008 , 72, 434-46	20
968	Protein thermal stabilization by charged compatible solutes: Computational studies in rubredoxin from Desulfovibrio gigas. 2008 , 72, 580-8	
967	Relationship between energy distribution and fold stability: Insights from molecular dynamics simulations of native and mutant proteins. 2008 , 72, 660-72	45
966	Mutant bovine odorant-binding protein: Temperature affects the protein stability and dynamics as revealed by infrared spectroscopy and molecular dynamics simulations. 2008 , 72, 769-78	13
965	Refining homology models by combining replica-exchange molecular dynamics and statistical potentials. 2008 , 72, 1171-88	65
964	HingeMaster: normal mode hinge prediction approach and integration of complementary predictors. 2008 , 73, 299-319	35
963	Effect of lipid composition on buforin II structure and membrane entry. 2008 , 73, 480-91	23

962	Anti-apoptotic Bcl-XL protein in complex with BH3 peptides of pro-apoptotic Bak, Bad, and Bim proteins: comparative molecular dynamics simulations. 2008 , 73, 492-514	40
961	Molecular strategies for protein stabilization: the case of a trehalose/maltose-binding protein from <i>Thermus thermophilus</i> . 2008 , 73, 839-50	6
960	Effect of altered glycosylation on the structure of the I-like domain of beta1 integrin: a molecular dynamics study. 2008 , 73, 989-1000	29
959	Molecular dynamic simulations of nanomechanic chaperone peptide and effects of in silico His mutations on nanostructured function. 2008 , 14, 1173-82	4
958	Synthesis and immunosuppressive activity of new cyclolinopeptide A analogs modified with beta-prolines. 2008 , 14, 1283-94	16
957	Study of the mechanism of action of anoplin, a helical antimicrobial decapeptide with ion channel-like activity, and the role of the amidated C-terminus. 2008 , 14, 661-9	52
956	Supramolecular structure of perylene tetracarboxdiimides. 2008 , 245, 820-824	34
955	Charge transport parameters of HBC at different temperatures. 2008 , 245, 835-838	15
954	Theoretical and experimental evaluation of a CYP106A2 low homology model and production of mutants with changed activity and selectivity of hydroxylation. 2008 , 9, 1439-49	36
953	Mechanism of binding of fluoroquinolones to the quinolone resistance-determining region of DNA gyrase: towards an understanding of the molecular basis of quinolone resistance. 2008 , 9, 2081-6	29
952	Glutathione transferase: new model for glutathione activation. 2008 , 14, 9591-8	51
951	Identification of putative binding sites of P-glycoprotein based on its homology model. 2008 , 3, 280-95	66
950	A 3D QSAR model of 17beta-HSD1 inhibitors based on a thieno[2,3-d]pyrimidin-4(3H)-one core applying molecular dynamics simulations and ligand-protein docking. 2008 , 3, 461-72	32
949	Ionic liquids: dissecting the enthalpies of vaporization. 2008 , 9, 549-55	117
948	On the validity of Stokes-Einstein and Stokes-Einstein-Debye relations in ionic liquids and ionic-liquid mixtures. 2008 , 9, 1851-8	127
947	Effect of Na ⁺ and Ca ²⁺ ions on a lipid Langmuir monolayer: an atomistic description by molecular dynamics simulations. 2008 , 9, 2538-43	27
946	Potential proton-release channels in bacteriorhodopsin. 2008 , 9, 2751-8	16
945	Spectral signatures of the pentagonal water cluster in bacteriorhodopsin. 2008 , 9, 2703-7	31

944	Conformational dynamics of minimal elastin-like polypeptides: the role of proline revealed by molecular dynamics and nuclear magnetic resonance. 2008 , 9, 2759-65	27
943	The solvent-dependent shift of the amide I band of a fully solvated peptide as a local probe for the solvent composition in the peptide/solvent interface. 2008 , 9, 2742-50	11
942	Temperature and concentration effects on the solvophobic solvation of methane in aqueous salt solutions. 2008 , 9, 2722-30	12
941	Salt effects on the structure of water probed by attenuated total reflection infrared spectroscopy and molecular dynamics simulations. 2008 , 9, 2731-6	23
940	Modeling the hERG potassium channel in a phospholipid bilayer: Molecular dynamics and drug docking studies. 2008 , 29, 795-808	42
939	A new method for determining the interfacial molecules and characterizing the surface roughness in computer simulations. Application to the liquid-vapor interface of water. 2008 , 29, 945-56	155
938	Parameterization of Ca ²⁺ -protein interactions for molecular dynamics simulations. 2008 , 29, 1163-9	37
937	Modification of the CHARMM force field for DMPC lipid bilayer. 2008 , 29, 2359-69	62
936	Insight into Proton Conduction of Immobilised Imidazole Systems Via Simulations and Impedance Spectroscopy. 2008 , 8, 244-253	29
935	Modelling of Proton Diffusion in Immobilised Imidazole Systems for Application in Fuel Cells. 2008 , 8, 236-243	15
934	Coarse Grained Molecular Dynamics Simulation of Electromechanically-Gated DNA Modified Conical Nanopores. 2008 , 20, 301-307	18
933	Time-resolved fluorescence spectroscopy and molecular dynamics simulations point out the effects of pressure on the stability and dynamics of the porcine odorant-binding protein. 2008 , 89, 284-91	6
932	Large scale motions in a biosensor protein glucose oxidase: a combined approach by QENS, normal mode analysis, and molecular dynamics studies. 2008 , 89, 582-94	7
931	Folding propensity and biological activity of peptides: the effect of a single stereochemical isomerization on the conformational properties of bombinins in aqueous solution. 2008 , 89, 769-78	22
930	Mechanical properties of physiological and pathological models of collagen peptides investigated via steered molecular dynamics simulations. 2008 , 41, 3073-7	43
929	Association (micellization) and partitioning of aglycon triterpenoids. 2008 , 325, 324-30	11
928	GSHMC: An efficient method for molecular simulation. 2008 , 227, 4934-4954	40
927	Thermal properties of poly(lactic acid) fumed silica nanocomposites: Experiments and molecular dynamics simulations. 2008 , 49, 2381-2386	62

926	New proton conducting hybrid membranes for HT-PEMFC systems based on polysiloxanes and SO ₃ H-functionalized mesoporous Si-MCM-41 particles. 2008 , 316, 164-175	50
925	Chiral separation in modified silica nanotube membranes: A molecular simulation study. 2008 , 311, 192-199	6
924	Molecular modeling of histamine H ₃ receptor and QSAR studies on arylbenzofuran derived H ₃ antagonists. 2008 , 26, 834-44	34
923	Development and initial testing of an empirical forcefield for simulation of poly(alkylthiophenes). 2008 , 27, 34-44	12
922	Temperature-induced unfolding pathway of a type III antifreeze protein: insight from molecular dynamics simulation. 2008 , 27, 88-94	26
921	Structure-activity relationships of modified C-terminal endomorphin-2 analogues by molecular dynamics simulations. 2008 , 27, 489-96	2
920	Right-handed 14-helix in beta 3-peptides from L-aspartic acid monomers. 2008 , 1784, 658-65	5
919	Towards understanding the structure and capacitance of electrical double layer in ionic liquids. 2008 , 53, 6835-6840	322
918	SMMP v. 3.0—Simulating proteins and protein interactions in Python and Fortran. 2008 , 178, 459-470	19
917	The main factor of the decrease in activity of luciferase on the Si surface. 2008 , 453, 279-282	3
916	Behavior of molecular oxygen at the liquid-liquid interface: A molecular dynamics simulation study. 2008 , 457, 78-81	1
915	Equilibrium exchange enhances the convergence rate of umbrella sampling. 2008 , 460, 375-381	19
914	A water molecule identified as a substrate of enzymatic hydrolysis of cellulose: A statistical-mechanics study. 2008 , 465, 279-284	3
913	Computational modeling study of functional microdomains in cannabinoid receptor type 1. 2008 , 16, 4378-89	21
912	Structure-based discovery of a novel non-peptidic small molecular inhibitor of caspase-3. 2008 , 16, 4854-9	10
911	Comparative molecular dynamics simulations of the potent synthetic classical cannabinoid ligand AMG3 in solution and at binding site of the CB1 and CB2 receptors. 2008 , 16, 7377-87	12
910	Novel insights into GPCR-peptide interactions: mutations in extracellular loop 1, ligand backbone methylations and molecular modeling of neurotensin receptor 1. 2008 , 16, 9359-68	33
909	Computational design of novel fullerene analogues as potential HIV-1 PR inhibitors: Analysis of the binding interactions between fullerene inhibitors and HIV-1 PR residues using 3D QSAR, molecular docking and molecular dynamics simulations. 2008 , 16, 9957-74	77

908	Distribution and favorable binding sites of pyrroloquinoline and its analogues in a lipid bilayer studied by molecular dynamics simulations. 2008 , 136, 128-35	19
907	Ultrafast quenching of tryptophan fluorescence in proteins: Interresidue and intrahelical electron transfer. 2008 , 350, 154-164	72
906	New flexible boundary hybrid solvation models for efficient biomolecular simulations. 2008 , 864, 31-41	2
905	Evaluation of 4,5,6,7-tetrahalogeno-1H-isoindole-1,3(2H)-diones as inhibitors of human protein kinase CK2. 2008 , 1784, 143-9	38
904	3D QSAR CoMFA/CoMSIA, molecular docking and molecular dynamics studies of fullerene-based HIV-1 PR inhibitors. 2008 , 18, 6283-9	56
903	GROMACS 4: Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. 2008 , 4, 435-47	11706
902	Spatial structure and pH-dependent conformational diversity of dimeric transmembrane domain of the receptor tyrosine kinase EphA1. 2008 , 283, 29385-95	86
901	Early events in protein folding: Is there something more than hydrophobic burst?. 2008 , 17, 1424-33	14
900	A buried lysine that titrates with a normal pKa: role of conformational flexibility at the protein-water interface as a determinant of pKa values. 2008 , 17, 833-45	62
899	Induced-fit or preexisting equilibrium dynamics? Lessons from protein crystallography and MD simulations on acetylcholinesterase and implications for structure-based drug design. 2008 , 17, 601-5	48
898	Effect of ions on a dipalmitoyl phosphatidylcholine bilayer. a molecular dynamics simulation study. 2008 , 112, 1397-408	112
897	Vulnerability in Popular Molecular Dynamics Packages Concerning Langevin and Andersen Dynamics. 2008 , 4, 1669-1680	68
896	Crystal structure of the peroxisome proliferator-activated receptor gamma (PPARgamma) ligand binding domain complexed with a novel partial agonist: a new region of the hydrophobic pocket could be exploited for drug design. 2008 , 51, 7768-76	80
895	CGDB: a database of membrane protein/lipid interactions by coarse-grained molecular dynamics simulations. 2008 , 25, 662-9	36
894	DNA and lipid bilayers: self-assembly and insertion. 2008 , 5 Suppl 3, S241-50	59
893	Nanophase segregation and water dynamics in hydrated Nafion: molecular modeling and experimental validation. 2008 , 129, 204702	107
892	Comparison of protein force fields for molecular dynamics simulations. 2008 , 443, 63-88	132
891	Computer simulations of the behavior of arylpropargyl phenol esters. 2008 , 82, 784-788	2

890	Molecular dynamic simulation of micellar solutions: A coarse-grain model. 2008 , 70, 1-5	18
889	Construction of a molecular model of a fragment of a lipid membrane in the gel and liquid crystalline states. 2008 , 63, 405-409	1
888	Bioinformatic analysis and molecular modelling of human ameloblastin suggest a two-domain intrinsically unstructured calcium-binding protein. 2008 , 116, 124-34	37
887	Molecular modeling and docking analysis of <i>Entamoeba histolytica</i> glyceraldehyde-3 phosphate dehydrogenase, a potential target enzyme for anti-protozoal drug development. 2008 , 71, 554-62	12
886	Hydrogen bond residue positioning in the 599-611 loop of thimet oligopeptidase is required for substrate selection. 2008 , 275, 5607-17	9
885	Molecular modeling studies of substrate binding by penicillin acylase. 2008 , 73, 56-64	6
884	Mutants of monomeric red fluorescent protein mRFP1 at residue 66: structure modeling by molecular dynamics and search for correlations with spectral properties. 2008 , 73, 1085-95	4
883	Plasma sputtering of water molecules from the liquid phase by low-energy ions: Molecular dynamics simulation. 2008 , 42, 235-239	18
882	Computer simulation study of fullerene translocation through lipid membranes. 2008 , 3, 363-8	411
881	Cystatin F is a cathepsin C-directed protease inhibitor regulated by proteolysis. 2008 , 27, 499-508	77
880	GPU Computing. 2008 , 96, 879-899	1014
879	The Simbios National Center: Systems Biology in Motion. 2008 , 96, 1266	47
878	GPR17: molecular modeling and dynamics studies of the 3-D structure and purinergic ligand binding features in comparison with P2Y receptors. 2008 , 9, 263	42
877	The meaning of alignment: lessons from structural diversity. 2008 , 9, 556	11
876	TraR auto-inducer enhances protein backbone fluctuations in DNA binding domain. 2008 , 582, 805-9	0
875	A single histidine residue modulates enzymatic activity in acidic mammalian chitinase. 2008 , 582, 931-5	13
874	Ca(2+) dissociation from the C-terminal EF-hand pair in calmodulin: a steered molecular dynamics study. 2008 , 582, 1355-61	8
873	Redox-coupled proton pumping in cytochrome c oxidase: further insights from computer simulation. 2008 , 1777, 196-201	34

872	Multi-scale computational modelling in biology and physiology. 2008 , 96, 60-89	120
871	b-DAZL: A novel gene in bovine spermatogenesis. 2008 , 18, 1209-1218	18
870	A proposed time-resolved X-ray scattering approach to track local and global conformational changes in membrane transport proteins. 2008 , 16, 21-8	18
869	Coarse-grained MD simulations of membrane protein-bilayer self-assembly. 2008 , 16, 621-30	179
868	The molecular mechanism of toxin-induced conformational changes in a potassium channel: relation to C-type inactivation. 2008 , 16, 747-54	43
867	The atomistic mechanism of conformational transition in adenylate kinase: a TEE-REX molecular dynamics study. 2008 , 16, 1175-82	51
866	Molecular dynamics simulations of membrane proteins. 2008 , 443, 147-60	18
865	Computational methods in nanostructure design: replica exchange simulations of self-assembling peptides. 2008 , 474, 133-51	3
864	FOLDING FREE ENERGY LANDSCAPE OF THE DECAPEPTIDE CHIGNOLIN. 2008 , 22, 3087-3098	7
863	Enthalpy-entropy contributions to salt and osmolyte effects on molecular-scale hydrophobic hydration and interactions. 2008 , 112, 5661-70	52
862	Unbinding of nicotine from the acetylcholine binding protein: steered molecular dynamics simulations. 2008 , 112, 4087-93	22
861	Structure and dynamics of surfactant and hydrocarbon aggregates on graphite: a molecular dynamics simulation study. 2008 , 112, 2915-21	41
860	Surfactant and hydrocarbon aggregates on defective graphite surface: structure and dynamics. 2008 , 112, 12954-61	28
859	Ionic liquid near a charged wall: structure and capacitance of electrical double layer. 2008 , 112, 11868-72	336
858	Role of water in mediating the assembly of Alzheimer amyloid-beta Abeta16-22 protofilaments. 2008 , 130, 11066-72	180
857	MD-tracks: a productive solution for the advanced analysis of molecular dynamics and Monte Carlo simulations. 2008 , 48, 2414-24	20
856	Coarse-grained molecular dynamics simulations of the energetics of helix insertion into a lipid bilayer. 2008 , 47, 11321-31	85
855	Molecular dynamics study on the biophysical interactions of seven green tea catechins with lipid bilayers of cell membranes. 2008 , 56, 7750-8	123

854	Complexes Comprised of Charged Dendrimers, Linear Polyelectrolytes, and Counterions: Insight through Coarse-Grained Molecular Dynamics Simulations. 2008 , 41, 4961-4968	48
853	Chemically induced phospholipid translocation across biological membranes. 2008 , 24, 9656-60	33
852	Effect of local anesthetic lidocaine on electrostatic properties of a lipid bilayer. 2008 , 94, 525-31	67
851	Gating of the mechanosensitive channel protein MscL: the interplay of membrane and protein. 2008 , 94, 3497-511	52
850	Distribution of amino acids in a lipid bilayer from computer simulations. 2008 , 94, 3393-404	434
849	Sliding of alkylating anticancer drugs along the minor groove of DNA: new insights on sequence selectivity. 2008 , 94, 550-61	25
848	Coarse-grained molecular dynamics simulations of phase transitions in mixed lipid systems containing LPA, DOPA, and DOPE lipids. 2008 , 94, 878-90	25
847	Comparing experimental and simulated pressure-area isotherms for DPPC. 2008 , 94, 2965-86	163
846	Extending Bell's model: how force transducer stiffness alters measured unbinding forces and kinetics of molecular complexes. 2008 , 94, 2621-30	72
845	Conformational analysis of the carboxy-terminal tails of human beta-tubulin isoforms. 2008 , 94, 1971-82	43
844	Characterization of the protein unfolding processes induced by urea and temperature. 2008 , 94, 2241-51	67
843	Structure of spheroidal HDL particles revealed by combined atomistic and coarse-grained simulations. 2008 , 94, 2306-19	76
842	Effects of surface water on protein dynamics studied by a novel coarse-grained normal mode approach. 2008 , 94, 3461-74	24
841	Predicting thymine dimerization yields from molecular dynamics simulations. 2008 , 94, 3590-600	76
840	End-point targeted molecular dynamics: large-scale conformational changes in potassium channels. 2008 , 94, 4307-19	23
839	Mechanosensitive membrane channels in action. 2008 , 94, 2994-3002	96
838	Experimental and computational studies investigating trehalose protection of HepG2 cells from palmitate-induced toxicity. 2008 , 94, 2869-83	30
837	High temperature unfolding simulations of the TRPZ1 peptide. 2008 , 94, 4444-53	37

836	Interactions between neuronal fusion proteins explored by molecular dynamics. 2008 , 94, 3436-46	22
835	The beta-strand-loop-beta-strand conformation is marginally populated in beta2-microglobulin (20-41) peptide in solution as revealed by replica exchange molecular dynamics simulations. 2008 , 95, 510-7	11
834	Examining the contributions of lipid shape and headgroup charge on bilayer behavior. 2008 , 95, 2636-46	95
833	Coarse-grained simulations of the membrane-active antimicrobial Peptide maculatin 1.1. 2008 , 95, 3802-15	61
832	Kinetics, statistics, and energetics of lipid membrane electroporation studied by molecular dynamics simulations. 2008 , 95, 1837-50	230
831	Flexibility of aromatic residues in the active-site gorge of acetylcholinesterase: X-ray versus molecular dynamics. 2008 , 95, 2500-11	84
830	Not only enthalpy: large entropy contribution to ion permeation barriers in single-file channels. 2008 , 95, 2275-82	11
829	Pathway and endpoint free energy calculations for cyclic nucleotide binding to HCN channels. 2008 , 94, L90-2	10
828	Lipid bilayer deformation and the free energy of interaction of a Kv channel gating-modifier toxin. 2008 , 95, 3816-26	26
827	Self-assembly of a simple membrane protein: coarse-grained molecular dynamics simulations of the influenza M2 channel. 2008 , 95, 3790-801	67
826	Protein-protein interaction investigated by steered molecular dynamics: the TCR-pMHC complex. 2008 , 95, 3575-90	88
825	Bilayer edge and curvature effects on partitioning of lipids by tail length: atomistic simulations. 2008 , 95, 2647-57	41
824	Incorporating dipolar solvents with variable density in Poisson-Boltzmann electrostatics. 2008 , 95, 5587-605	69
823	Structure and dynamics of helix-0 of the N-BAR domain in lipid micelles and bilayers. 2008 , 95, 4315-23	40
822	Mechanical stability of helical beta-peptides and a comparison of explicit and implicit solvent models. 2008 , 95, 3123-36	10
821	Gating at both ends and breathing in the middle: conformational dynamics of TolC. 2008 , 95, 5681-91	50
820	Peptide aggregation in finite systems. 2008 , 95, 3208-21	27
819	Rate constant and reaction coordinate of Trp-cage folding in explicit water. 2008 , 95, 4246-57	120

818	Pore formation induced by an antimicrobial peptide: electrostatic effects. 2008 , 95, 5748-56	78
817	Behavioral differences between phosphatidic acid and phosphatidylcholine in the presence of the nicotinic acetylcholine receptor. 2008 , 95, 5637-47	9
816	Interplay of unsaturated phospholipids and cholesterol in membranes: effect of the double-bond position. 2008 , 95, 3295-305	111
815	Simulations of skin barrier function: free energies of hydrophobic and hydrophilic transmembrane pores in ceramide bilayers. 2008 , 95, 4763-71	39
814	Modeling by assembly and molecular dynamics simulations of the low Cu ²⁺ occupancy form of the mammalian prion protein octarepeat region: gaining insight into Cu ²⁺ -mediated beta-cleavage. 2008 , 95, 5084-91	17
813	The influence of 1-alkanols and external pressure on the lateral pressure profiles of lipid bilayers. 2008 , 95, 5766-78	47
812	Columnar mesophases of hexabenzocoronene derivatives. I. Phase transitions. 2008 , 129, 094505	38
811	Determination of phase diagrams via computer simulation: methodology and applications to water, electrolytes and proteins. 2008 , 20, 153101	180
810	Mechanical model of the tubulin dimer based on molecular dynamics simulations. 2008 , 130, 041008	25
809	Structural studies of melting on the picosecond time scale. 2008 , 10, 6344-9	11
808	Predicting small-molecule solvation free energies: an informal blind test for computational chemistry. 2008 , 51, 769-79	228
807	Highly specific inhibition of leukaemia virus membrane fusion by interaction of peptide antagonists with a conserved region of the coiled coil of envelope. 2008 , 5, 70	11
806	Influences of surfactant and nanoparticle assembly on effective interfacial tensions. 2008 , 10, 2207-13	141
805	Molecular dynamics simulation of the interaction between the complex iron-sulfur flavoprotein glutamate synthase and its substrates. 2004 , 13, 2979-91	7
804	Coarse-grained molecular dynamics studies of the concentration and size dependence of fifth- and seventh-generation PAMAM dendrimers on pore formation in DMPC bilayer. 2008 , 112, 7778-84	146
803	Molecular dynamics simulation of self-assembly of n-decyltrimethylammonium bromide micelles. 2008 , 24, 5714-25	88
802	Molecular modeling of the cytoskeleton. 2008 , 84, 893-910	2
801	Effect of anions on static orientational correlations, hydrogen bonds, and dynamics in ionic liquids: a simulational study. 2008 , 112, 1743-51	105

800	Molecular dynamics simulations. 2008 , 443, 3-23	40
799	Structured water and water-polymer interactions in hydrogels of molecularly imprinted polymers. 2008 , 112, 7515-21	27
798	Improved sampling for simulations of interfacial membrane proteins: application of generalized shadow hybrid Monte Carlo to a peptide toxin/bilayer system. 2008 , 112, 5710-7	20
797	Water phase transition induced by a Stone-Wales defect in a boron nitride nanotube. 2008 , 130, 13649-52	21
796	Targets looking for drugs: a multistep computational protocol for the development of structure-based pharmacophores and their applications for hit discovery. 2008 , 48, 2166-79	55
795	Advances in Bioinformatics and Computational Biology. 2008 ,	1
794	Computational investigation of interaction between nanoparticles and membranes: hydrophobic/hydrophilic effect. 2008 , 112, 16647-53	196
793	Enhanced ion transport in an ether aided super concentrated ionic liquid electrolyte for long-life practical lithium metal battery applications. 2020 , 8, 18826-18839	20
792	Conformational Flexibility of Hybrid [3]- and [4]-Rotaxanes. 2020 , 142, 15941-15949	7
791	Molecular simulation and the collaborative computational projects. 2020 , 45, 259-343	
790	Virtual high-throughput screening and simulation studies of compounds from selected traditionally important medicinal plants for the identification of potential inhibitors of AcrB. 2020 , 1-9	1
789	Casuarictin: A new herbal drug molecule for Alzheimer's disease as inhibitor of presenilin stabilization factor like protein. 2020 , 6, e05546	2
788	Structural insights and evaluation of the potential impact of missense variants on the interactions of SLIT2 with ROBO1/4 in cancer progression. 2020 , 10, 21909	1
787	Modification of lipid membrane compressibility induced by an electric field. 2020 , 102, 062413	1
786	Understanding the pH-Directed Self-Assembly of a Four-Arm Block Copolymer. 2020 , 53, 11065-11076	6
785	Substituent Effect on Porphyrin Film-Gas Interaction by Optical Waveguide: Spectrum Analysis and Molecular Dynamic Simulation. 2020 , 13,	3
784	Structural and biochemical characteristics of two RNase J paralogs RNase J1 and RNase J2. 2020 , 295, 16863-16876	3
783	Molecular Modeling Study of c-KIT/PDGFR β Dual Inhibitors for the Treatment of Gastrointestinal Stromal Tumors. 2020 , 21,	8

782	Solvent Nuances Modulate the Decreasing Effect of a Model Asphaltene on Interfacial Tension. 2020 , 34, 13862-13870	0
781	Entropy Rules: Molecular Dynamics Simulations of Model Oligomers for Thermoresponsive Polymers. 2020 , 22,	4
780	Frequency and water saturation dependency of dielectric properties of clay mineral. 2020 , 198, 105840	5
779	Molecular dynamics simulation of the n-octacosane-water mixture confined in hydrophilic and hydrophobic mesopores: The effect of oxygenates. 2020 , 526, 112816	1
778	Molecular simulation of folding and aggregation of multi-core polycyclic aromatic compounds. 2020 , 310, 113248	2
777	Spontaneous lid closure and substrate-induced lid opening dynamics of human pancreatic lipase-related protein 2: A computational study. 2020 , 1217, 128365	2
776	Engineering high-energy-density sodium battery anodes for improved cycling with superconcentrated ionic-liquid electrolytes. 2020 , 19, 1096-1101	70
775	Computational Study of Pyrimidin-2-Aminopyrazol-Hydroxamate-based JAK2 Inhibitors for the Treatment of Myeloproliferative Neoplasms. 2020 , 41, 542-551	2
774	How to polarise an interface with ions: the discrete Helmholtz model. 2020 , 11, 10807-10813	16
773	Parallel performance of molecular dynamics trajectory analysis. 2020 , 32, e5789	0
772	Simulations of dielectric constants and viscosities of organic electrolytes by quantum mechanics and molecular dynamics. 2020 , 312, 113288	9
771	Molecular assemblies built with the artificial protein Pizza. 2020 , 4, 100027	4
770	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. 2020 , 152, 184107	255
769	A beginner's guide to molecular dynamics simulations and the identification of cross-correlation networks for enzyme engineering. 2020 , 643, 15-49	3
768	Hydrogen bonds in anoplin peptides aid in identification of a structurally stable therapeutic drug scaffold. <i>Journal of Molecular Modeling</i> , 2020 , 26, 155	2 3
767	New insights into bulk and interface properties of [Bmim][Ac]/[Bmim][BF4] ionic liquid/CO2 systems âMolecular dynamics simulation approach. 2020 , 317, 113497	4
766	To unravel the connection between the non-equilibrium and equilibrium solvation dynamics of tryptophan: success and failure of the linear response theory of fluorescence Stokes shift.. 2020 , 10, 18348-18354	
765	The acidic tail of HMGB1 regulates its secondary structure and conformational flexibility: A circular dichroism and molecular dynamics simulation study. 2020 , 18, 1160-1172	7

764	Origin of orientation-dependent $R (=1/T)$ relaxation in white matter. 2020 , 84, 2713-2723	3
763	Insight into structural properties of polyethylene glycol monolaurate in water and alcohols from molecular dynamics studies.. 2020 , 10, 21760-21771	3
762	Structural Basis of Ca-Dependent Self-Processing Activity of Repeat-in-Toxin Proteins. 2020 , 11,	2
761	Volumetric, Ultrasonic, Spectroscopic, and Molecular Dynamics Simulations Studies of Molecular Interactions in Binary Mixtures of [Emim][NTf ₂] with 2-Propoxyethanol at Temperatures from 298.15 to 318.15 K. 2020 , 65, 3566-3578	1
760	Welding dynamics in an atomistic model of an amorphous polymer blend with polymer-polymer interface. 2020 , 58, 2051-2061	6
759	Beyond p: Experiments and Simulations of Nitrile Vibrational Probes in Staphylococcal Nuclease Show the Importance of Local Interactions. 2020 , 124, 3387-3399	2
758	Delineating elastic properties of kinesin linker and their sensitivity to point mutations. 2020 , 10, 4832	
757	Thermodynamic Investigation of the Mechanism of Heat Production During Membrane Depolarization. 2020 , 124, 2815-2822	1
756	Atomistic Molecular Dynamics Simulations of Surfactant-Induced Wettability Alteration in Crevices of Calcite Nanopores. 2020 , 34, 3135-3143	14
755	Power generation by reverse electrodialysis in a single-layer nanoporous membrane made from core-rim polycyclic aromatic hydrocarbons. 2020 , 15, 307-312	57
754	Effects of cholesterol on bilayers with various degrees of unsaturation of their phospholipid tails under mechanical stress.. 2020 , 10, 11088-11094	1
753	Probing the Accuracy of Explicit Solvent Constant pH Molecular Dynamics Simulations for Peptides. 2020 , 16, 2561-2569	3
752	Examining Tail and Headgroup Effects on Binary and Ternary Gel-Phase Lipid Bilayer Structure. 2020 , 124, 3043-3053	2
751	Self-Assembly of Allomelanin Dimers and the Impact of Poly(ethylene glycol) on the Assembly: A Molecular Dynamics Simulation Study. 2020 , 124, 2702-2714	7
750	Molecular Dynamics Analysis of a Rationally Designed Aldehyde Dehydrogenase Gives Insights into Improved Activity for the Non-Native Cofactor NAD. 2020 , 9, 920-929	6
749	Restructuring a Deep Eutectic Solvent by Water: The Nanostructure of Hydrated Choline Chloride/Urea. 2020 , 16, 3335-3342	36
748	Linear Response Theory for Decomposition Energies of Stokes Shift in Proteins. 2020 , 124, 3540-3547	3
747	Energetics and Structural Behavior of Asphaltene Molecules near Mica Surface: Molecular Simulation Study. 2020 , 34, 4071-4083	3

746	Self-assembly of Pseudo-Dipolar Nanoparticles at Low Densities and Strong Coupling. 2020 , 10, 3971	2
745	The effect of alkyl chain length attached to the diglycolamide and n-paraffin on the aggregation behaviour of diglycolamide and MD simulation of aggregates. 2020 , 1221, 128795	3
744	Ether-Functionalized Sulfonium Ionic Liquid and Its Binary Mixtures with Acetonitrile as Electrolyte for Electrochemical Double Layer Capacitors: A Molecular Dynamics Study. 2020 , 124, 6679-6689	13
743	Asymmetry and Rippling in Mixed Surfactant Bilayers from All-Atom and Coarse-Grained Simulations: Interdigitation and Per Chain Entropy Δ 2020 , 124, 6420-6436	4
742	Exact long-range Coulombic energy calculation for net charged systems neutralized by uniformly distributed background charge using fast multipole method and its application to efficient free energy calculation. 2020 , 152, 244115	2
741	Coating of magnetic nanoparticles affects their interactions with model cell membranes. 2020 , 1864, 129671	3
740	Molecular Dynamics Simulation: Methods and Application. 2020 , 213-238	1
739	Lipid domain formation and membrane shaping by C24-ceramide. 2020 , 1862, 183400	5
738	Mixing states of imidazolium-based ionic liquid, [Cmim][TFSI], with cycloethers studied by SANS, IR, and NMR experiments and MD simulations. 2020 , 22, 5332-5346	1
737	Detection of single DNA mismatches by force spectroscopy in short DNA hairpins. 2020 , 152, 074204	5
736	Mechanisms of peptide and phosphoester hydrolysis catalyzed by two promiscuous metalloenzymes (insulin degrading enzyme and glycerophosphodiesterase) and their synthetic analogues. 2020 , 10, e1466	8
735	A positively charged calcite surface model for molecular dynamics studies of wettability alteration. 2020 , 569, 128-139	18
734	Integrating All-Atom and Coarse-Grained Simulations-Toward Understanding of IDPs at Surfaces. 2020 , 16, 1843-1853	3
733	Algal Toxin Goniodomin A Binds Potassium Ion Selectively to Yield a Conformationally Altered Complex with Potential Biological Consequences. 2020 , 83, 1069-1081	4
732	Probing Early-Stage Aggregation of Low Molecular Weight Gelator in an Organic Solvent. 2020 , 124, 2277-2288	6
731	Interfacial structure in the liquid-liquid extraction of rare earth elements by phosphoric acid ligands: a molecular dynamics study. 2020 , 22, 4177-4192	5
730	Self-assembly of glycerol monooleate with the antimicrobial peptide LL-37: a molecular dynamics study.. 2020 , 10, 8291-8302	4
729	A Chiral Voltammetric Sensor Based on a Paste Electrode Modified by Cyanuric Acid for the Recognition and Determination of Tyrosine Enantiomers. 2020 , 75, 101-110	8

728	Calcitonin Receptor N-Glycosylation Enhances Peptide Hormone Affinity by Controlling Receptor Dynamics. 2020 , 432, 1996-2014		13
727	Key Factors Determining Efficiency of Liquid-Liquid Extraction: Implications from Molecular Dynamics Simulations of Biphasic Behaviors of CyMe-BTPhen and Its Am(III) Complexes. 2020 , 124, 1751-1766	3	
726	Impact of lymphoma-linked Asn11Tyr point mutation on the interaction between Bcl-2 and a BH3 mimetic: Insights from molecular dynamics simulation. 2020 , 95, 435-450		0
725	Rationally designed antimicrobial peptides: Insight into the mechanism of eleven residue peptides against microbial infections. 2020 , 1862, 183177		8
724	Tuning Allostery through Integration of Disorder to Order with a Residue Network. 2020 , 59, 790-801		4
723	Solubility of Nitrogen in Methane, Ethane, and Mixtures of Methane and Ethane at Titan-Like Conditions: A Molecular Dynamics Study. 2020 , 4, 241-248		2
722	Revisiting LiClO ₄ as an electrolyte for Li-ion battery: Effect of aggregation behavior on ion-pairing dynamics and conductance. 2020 , 302, 112536		3
721	Comprehensive Evaluation of the Efficiency of Yeast Cell Wall Extract to Adsorb Ochratoxin A and Mitigate Accumulation of the Toxin in Broiler Chickens. 2020 , 12,		10
720	Exploring the binding modes of cordycepin to human adenosine deaminase 1 (ADA1) compared to adenosine and 2'-deoxyadenosine. <i>Journal of Molecular Modeling</i> , 2020 , 26, 29	2	5
719	Proteome analysis of leaf, stem and callus in <i>Viscum album</i> and identification of lectins and viscotoxins with bioactive properties. 2020 , 141, 167-178		3
718	Biomimetic Design of Peptide Neutralizer of Ebola Virus with Molecular Simulation. 2020 , 36, 1813-1821		11
717	Supramolecular Protein Assembly Retains Its Structural Integrity at Liquid-Liquid Interface. 2020 , 7, 1901674	2	
716	Molecular modeling study concerning the self-assembly capacity of some photosensitive amphiphilic polysiloxanes. 2020 , 300, 112298		4
715	Effects of Nanoparticle Electrostatics and Protein-Protein Interactions on Corona Formation: Conformation and Hydrodynamics. 2020 , 16, e1906598		20
714	Measurement of length distribution of beta-lactoglobulin fibrils by multiwavelength analytical ultracentrifugation. 2020 , 49, 745-760		7
713	Understanding water-mediated DNA damage production by molecular dynamics calculation of solvent accessibility. 2020 , 749, 137441		
712	Exploring how structural and dynamic properties of bovine and canine serum albumins differ from human serum albumin. 2020 , 98, 107601		18
711	Towards Molecular Simulations that are Transparent, Reproducible, Usable By Others, and Extensible (TRUE). 2020 , 118,		12

710	Cross-linking, DEER-spectroscopy and molecular dynamics confirm the inward facing state of P-glycoprotein in a lipid membrane. 2020 , 211, 107513	5
709	Revealing the Role of Surface Co-modification in Boosting the Gas Sensing Performance of Graphene Using Experimental and Theoretical Evidences. 2020 , 316, 128162	4
708	Theoretical Infrared Spectra: Quantitative Similarity Measures and Force Fields. 2020 , 16, 3307-3315	14
707	Dimension-Controlled Dewetting in Hydrophobic Porous Nanocapsules. 2020 , 124, 10201-10208	1
706	Heterodimer and pore formation of magainin 2 and PGLa: The anchoring and tilting of peptides in lipid bilayers. 2020 , 1862, 183305	2
705	Direct and Fast Assessment of Antimicrobial Surface Activity Using Molecular Dynamics Simulation and Time-Lapse Imaging. 2020 , 92, 6795-6800	3
704	Separation of CF/N, CF/N, and SF/N Mixtures in Amorphous Activated Carbons Using Molecular Simulations. 2020 , 12, 20044-20055	9
703	The quasi-irreversible inactivation of cytochrome P450 enzymes by paroxetine: a computational approach. 2020 , 18, 3334-3345	8
702	Unusual behavior of Stokes-Einstein relation in liquid mixtures. 2020 , 10, 045327	2
701	Molecular docking and molecular dynamics simulations of a mutant alkaline-stable lipase against tributyrin. 2021 , 39, 2079-2091	10
700	Non-symmetrical structural behavior of a symmetric protein: the case of homo-trimeric TRAF2 (tumor necrosis factor-receptor associated factor 2). 2021 , 39, 319-329	5
699	DL_POLY - A performance overview analysing, understanding and exploiting available HPC technology. 2021 , 47, 194-227	2
698	Adsorption kinetic of myoglobin on mica and silica - Role of electrostatic interactions. 2021 , 198, 111436	3
697	Stabilization of recombinant d-Lactate dehydrogenase enzyme with trehalose: Response surface methodology and molecular dynamics simulation study. 2021 , 101, 26-35	2
696	Effect of non-ionic surfactants on the adsorption of polycyclic aromatic compounds at water/oil interface: A molecular simulation study. 2021 , 586, 766-777	6
695	Large-Scale Molecular Dynamics Simulations on Modular Supercomputer Architecture with Gromacs. 2021 , 359-367	
694	Topological analysis of single-stranded DNA with an alpha-hederin nanopore. 2021 , 171, 112711	1
693	Dynamic Bonds Mediate π -Interaction via Phase Locking Effect for Enhanced Heat Resistant Thermoplastic Polyurethane. 2021 , 39, 154-163	9

692	A molecular dynamics study of the binding effectiveness between undoped conjugated polymer binders and tetra-sulfides in lithium-sulfur batteries. 2021 , 206, 108531	2
691	Structural dynamics of double-stranded DNA with epigenome modification. 2021 , 49, 1152-1162	2
690	Extended diffusion theory: Recovering dynamics from biased/accelerated molecular simulations. 2021 , 42, 586-599	
689	Supramolecular PFPE gel lubricant with anti-creep capability under irradiation conditions at high vacuum. 2021 , 409, 128120	5
688	A green hybrid microextraction for sensitive determination of bisphenol A in aqueous samples using three different sorbents: Analytical and computational studies. 2021 , 160, 105612	3
687	Revealing the structural dynamics of feline serum albumin. 2021 , 32, 69-77	2
686	Molecular dynamics simulations for genetic interpretation in protein coding regions: where we are, where to go and when. 2021 , 22, 3-19	5
685	Moderate and strong static magnetic fields directly affect EGFR kinase domain orientation to inhibit cancer cell proliferation. 2016 , 7, 41527-41539	3 ¹
684	Coarse-Grained Molecular Dynamics Simulations of Membrane Proteins: A Practical Guide. 2021 , 2302, 253-273	1
683	The Impact of Lipid Digestion on the Dynamic and Structural Properties of Micelles. 2021 , 17, e2004761	2
682	QM/MM Investigation of the Spectroscopic Properties of the Fluorophore of Bacterial Luciferase. 2021 , 17, 605-613	3
681	Dendronized vesicles: formation, self-organization of dendron-grafted amphiphiles and stability. 2021 , 3, 725-737	4
680	Chemical functionality at the liquid surface of pure unsaturated fatty acids.	
679	Modifications on the Tetrahydroquinoline Scaffold Targeting a Phenylalanine Cluster on GPER as Antiproliferative Compounds against Renal, Liver and Pancreatic Cancer Cells. 2021 , 14,	3
678	Computationally grafting an IgE epitope onto a scaffold: Implications for a pan anti-allergy vaccine design. 2021 , 19, 4738-4750	0
677	Asymmetric dynamics of dimeric SARS-CoV-2 and SARS-CoV main proteases in an apo form: Molecular dynamics study on fluctuations of active site, catalytic dyad, and hydration water. 2021 , 1, 100016	2
676	The key role of the central cavity in sodium transport through ligand-gated two-pore channels. 2021 , 23, 18461-18474	2
675	Molecular Dynamics Investigation of Phenolic Oxidative Coupling Protein Hyp-1 Derived from <i>Hypericum perforatum</i> . 2021 , 11, 43	0

674	Organic nanoelectronics inside us: charge transport and localization in RNA could orchestrate ribosome operation. 2021 , 23, 7037-7047	1
673	Development of coarse-grained force field for alcohols: an efficient meta-multilinear interpolation parameterization algorithm. 2021 , 23, 1956-1966	2
672	Aggregation of the Dipeptide Leu-Gly in Alcohol-Water Binary Solvents Elucidated from the Solvation Structure for Each Moiety. 2021 , 125, 240-252	0
671	Increasing resonance energy transfer upon dilution: a counterintuitive observation in CTAB micelles. 2021 , 9, 10952-10964	0
670	Dimeric phosphorylation of glyoxalase I alters its symmetry and substrate binding mechanism: simulation studies. 2021 , 1-15	
669	An ultralow-temperature aqueous zinc-ion battery. 2021 , 9, 7042-7047	36
668	Structural effects in nanotribology of nanoscale films of ionic liquids confined between metallic surfaces. 2021 , 23, 22174-22183	1
667	Interactions Determining the Structural Integrity of the Trimer of Plant Light Harvesting Complex in Lipid Membranes. 2021 , 254, 157-173	0
666	Gold(i) bridged dimeric and trimeric heterometallic {CrNi}-based qubit systems and their characterization. 2021 , 50, 4390-4395	2
665	CompassR-guided recombination unlocks design principles to stabilize lipases in ILs with minimal experimental efforts. 2021 , 23, 3474-3486	10
664	Molecular Insight into Cu-Induced Conformational Transitions of Amyloid β Protein from Fast Kinetic Analysis and Molecular Dynamics Simulations. 2021 , 12, 300-310	0
663	The molecular basis for the pH-dependent calcium affinity of the pattern recognition receptor langerin. 2021 , 296, 100718	3
662	Elucidating Solution Structures of Cyclic Peptides Using Molecular Dynamics Simulations. 2021 , 121, 2292-2324	11
661	Probing the structural properties of the water solvation shell around gold nanoparticles: A computational study. 2021 , 154, 044706	1
660	Design and Discovery of Kinase Inhibitors Using Docking Studies. 2021 , 337-365	
659	Factual insights of the allosteric inhibition mechanism of SARS-CoV-2 main protease by quercetin: an in silico analysis. 2021 , 11, 67	8
658	Protonation states at different pH, conformational changes and impact of glycosylation in synapsin Ia. 2021 , 23, 16718-16729	0
657	Computing Cellulase Kinetics with a Two-Domain Linear Interaction Energy Approach. 2021 , 6, 1547-1555	3

656	Insights into the structure and ionic transport in a water-in-bisalt electrolytes for lithium-ion batteries.	2
655	Investigating the protective effects of carbohydrate coatings on the structure and dynamic of l-asparaginase against heat stress; a molecular dynamic simulation. 2021 , 25, 100689	0
654	Inhibition of tau amyloid formation and disruption of its preformed fibrils by Naphthoquinone-Dopamine hybrid. 2021 , 288, 4267-4290	6
653	Modeling the solid/liquid interfacial properties of methylimidazole confined in hydrophobic silica nanopores. 2021 , 231, 116333	
652	Tetracycline as an inhibitor to the SARS-CoV-2. 2021 , 122, 752-759	3
651	NaCl aggregation in water at elevated temperatures and pressures: Comparison of classical force fields. 2021 , 154, 064503	6
650	Structure and Transport of Solvent Ligated Octahedral Mg-Ion in an Aqueous Battery Electrolyte. 2021 , 66, 1543-1554	2
649	How human serum albumin-selective DNA aptamer binds to bovine and canine serum albumins. 2021 , 112, e23421	6
648	Full structural ensembles of intrinsically disordered proteins from unbiased molecular dynamics simulations. 2021 , 4, 243	14
647	Shedding Light on Miniaturized Dialysis Using MXene 2D Materials: A Computational Chemistry Approach. 2021 , 6, 6312-6325	9
646	A Comparative Study on DMSO-Induced Modulation of the Structural and Dynamical Properties of Model Bilayer Membranes. 2021 , 37, 2065-2078	6
645	G-quadruplex binding properties of a potent PARP-1 inhibitor derived from 7-azaindole-1-carboxamide. 2021 , 11, 3869	4
644	Water-Gas Shift Reaction to Capture Carbon Dioxide and Separate Hydrogen on Single-Walled Carbon Nanotubes. 2021 , 13, 11026-11038	1
643	Molecular Dynamics Simulation of the n-Octacosane-Water Mixture Confined in Graphene Mesopores: Comparison of Atomistic and Coarse-Grained Calculations and the Effect of Catalyst Nanoparticle. 2021 , 35, 4313-4332	2
642	Short peptides as predictors for the structure of polyarginine sequences in disordered proteins. 2021 , 120, 662-676	7
641	Ab initio dynamics of gas-phase and aqueous-phase hydrolysis of adenosine triphosphate. 2021 , 121, e26615	0
640	In silico characterization and differential expression analysis of 1-deoxy-d-xylulose-5-phosphate reductoisomerase (DXR) of. 2021 , 11, 184	0
639	Molecular docking and molecular dynamics simulation identify a novel Radicicol derivative that predicts exclusive binding to Topoisomerase VIB. 2021 , 1-13	1

638	Effect of Protein Corona on Nanoparticle-Lipid Membrane Binding: The Binding Strength and Dynamics. 2021 , 37, 3751-3760	2
637	Combined Density Functional Theory and Molecular Dynamics Simulations To Investigate the Effects of Quantum and Double-Layer Capacitances in Functionalized Graphene as the Electrode Material of Aqueous-Based Supercapacitors. 2021 , 125, 5518-5524	5
636	All-Atom Simulations and Free-Energy Calculations of Antibodies Bound to the Spike Protein of SARS-CoV-2: The Binding Strength and Multivalent Hydrogen-Bond Interactions. 2021 , 4, 2100012	1
635	Black tea bioactives as inhibitors of multiple targets of SARS-CoV-2 (3CLpro, PLpro and RdRp): a virtual screening and molecular dynamic simulation study. 2021 , 1-24	7
634	Drug repositioning to target NSP15 protein on SARS-CoV-2 as possible COVID-19 treatment. 2021 , 42, 897-907	5
633	NMR refinement and peptide folding using the GROMACS software. 2021 , 75, 143-149	0
632	Understanding the Confinement Effects and Dynamics of Methylimidazole in Nanoscale Silica Pores. 2021 , 125, 7421-7430	0
631	In vitro and in silico studies of the larvicidal and anticholinesterase activities of berberine and piperine alkaloids on <i>Rhipicephalus microplus</i> . 2021 , 12, 101643	4
630	Position-Dependent Diffusion from Biased Simulations and Markov State Model Analysis. 2021 , 17, 2022-2033	7
629	Interfacial Polarization and Ionic Structure at the Ionic Liquid-Metal Interface Studied by Vibrational Spectroscopy and Molecular Dynamics Simulations. 2021 , 125, 2741-2753	5
628	Molecular dynamics analysis of stabilities of transitional hydrogen bonds in sulfate aqueous solution.	
627	Temperature Dependence of Peptide Conformational Equilibria from Simulations at a Single Temperature. 2021 , 125, 2374-2384	1
626	Fabrication of porphyrin-based aggregates through modulating hexapeptide secondary conformation. 2021 , 187, 109135	0
625	Reverse Actuation of Polyelectrolyte Effect for Antifouling. 2021 , 15, 6811-6828	7
624	Assessment of Amyloid Forming Tendency of Peptide Sequences from Amyloid Beta and Tau Proteins Using Force-Field, Semi-Empirical, and Density Functional Theory Calculations. 2021 , 22,	1
623	The role of plasmalogens, Forssman lipids, and sphingolipid hydroxylation in modulating the biophysical properties of the epithelial plasma membrane. 2021 , 154, 095101	6
622	Design and proof-of-concept for targeted phage-based COVID-19 vaccination strategies with a streamlined cold-free supply chain. 2021 ,	1
621	Dielectric Behavior near a Spherical Ion. 2021 , 125, 2360-2371	1

620	Molecular strategies for antibody binding and escape of SARS-CoV-2 and its mutations.	1
619	Stability of Engineered Ferritin Nanovaccines Investigated by Combined Molecular Simulation and Experiments. 2021 , 125, 3830-3842	1
618	Macroion molecule properties from slender body hydrodynamics. 2021 , 32, 3900-3908	1
617	Hydrogen and Deuterium Molecular Escape from Clathrate Hydrates: "Leaky" Microsecond-Molecular-Dynamics Predictions. 2021 , 125, 8430-8439	2
616	Identification of potential plant-based inhibitor against viral proteases of SARS-CoV-2 through molecular docking, MM-PBSA binding energy calculations and molecular dynamics simulation. 2021 , 25, 1963-1977	9
615	Synergistic Effect of Binary Surfactant Mixtures in Two-Phase and Three-Phase Systems. 2021 , 125, 3855-3866	2
614	Unsupervised Learning Unravels the Structure of Four-Arm and Linear Block Copolymer Micelles. 2021 , 54, 3755-3768	4
613	Balance Between Contact and Solvent-Separated Ion Pairs in Mixtures of the Protic Ionic Liquid [EtNH][MeSO] with Water Controlled by Water Content and Temperature. 2021 , 125, 4476-4488	3
612	Characterization of the Interface Structure of 1-Ethyl-2,3-alkylimidazolium Bis(trifluoromethylsulfonyl)imide on a Au(111) Surface with Molecular Dynamics Simulations. 2021 , 125, 3677-3689	1
611	Zeta potentials of fluoride anion result in the instability of DNA hairpin. 2021 , 134, 28001	
610	The Botrytis cinerea Crh1 transglycosylase is a cytoplasmic effector triggering plant cell death and defense response. 2021 , 12, 2166	10
609	Comparative Perturbation-Based Modeling of the SARS-CoV-2 Spike Protein Binding with Host Receptor and Neutralizing Antibodies: Structurally Adaptable Allosteric Communication Hotspots Define Spike Sites Targeted by Global Circulating Mutations. 2021 , 60, 1459-1484	17
608	Evaluation of the effects of isoniazid and rifampin on the structure and activity of pepsin enzyme by multi spectroscopy and molecular modeling methods. 2021 , 253, 119523	1
607	Molecular dynamics shows complex interplay and long-range effects of post-translational modifications in yeast protein interactions. 2021 , 17, e1008988	4
606	Virtual screening of curcumin analogues as DYRK2 inhibitor: Pharmacophore analysis, molecular docking and dynamics, and ADME prediction. 10, 394	1
605	Elucidating the structural features of ABCA1 in its heterogeneous membrane environment.	
604	Dehydration induced dynamical heterogeneity and ordering mechanism of lipid bilayers. 2021 , 154, 174904	6
603	Chemical computational approaches for optimization of effective surfactants in enhanced oil recovery. 2021 ,	1

602	The Dynamics of Subunit Rotation in a Eukaryotic Ribosome. 2021 , 1, 204-221	2
601	Wettability Reversal on Dolomite Surfaces by Divalent Ions and Surfactants: An Experimental and Molecular Dynamics Simulation Study. 2021 , 37, 6641-6649	6
600	Redox-active binary eutectics: Preparation and their electrochemical properties. 2021 , 126, 107028	2
599	Investigating the binding affinities of fructose and galactose to human serum albumin: simulation studies. 2021 , 47, 738-747	1
598	Protein Structure Prediction: Conventional and Deep Learning Perspectives. 2021 , 40, 522-544	5
597	Molecular Docking and Dynamics Simulation Study of Isolated Scalarane Sesterterpenes as Potential SARS-CoV-2 Dual Target Inhibitors. 2021 , 10,	11
596	assessment of dehalogenase from H2 in relation to its salinity-stability and pollutants degradation. 2021 , 1-15	4
595	Theoretical study of the vibrational properties of L-alanine and its zwitterionic form in the gas phase and in solution. 2021 , 1-9	1
594	ProteinTools: a toolkit to analyze protein structures. 2021 , 49, W559-W566	6
593	Field-Dependent Dehydration and Optimal Ionic Escape Paths for CN Membranes. 2021 , 125, 7044-7059	1
592	Molecular Mechanism of Ultrasound-Induced Structural Defects in Liposomes: A Nonequilibrium Molecular Dynamics Simulation Study. 2021 , 37, 7945-7954	1
591	Nanodelivery of the Gramicidin Peptide for Enhancing Antimicrobial Activity. 2021 , 123, 2000389	0
590	Exploring the Interaction of Curaxin CBL0137 with G-Quadruplex DNA Oligomers. 2021 , 22,	0
589	Lipid-mediated Association of the Slg1 Transmembrane Domains in Yeast Plasma Membranes.	
588	Xanthine oxidase inhibitory activity of Euphorbia peplus L. phenolics. 2021 ,	1
587	Volumetric Interplay between the Conformational States Adopted by Guanine-Rich DNA from the c-MYC Promoter. 2021 , 125, 7406-7416	5
586	Computational Modeling of Novel Phosphoinositol-3-kinase Inhibitors Using Molecular Docking, Molecular Dynamics, and 3D-QSAR. 2021 , 42, 1093-1111	1
585	Predicting solvation free energies in non-polar solvents using classical density functional theory based on the PC-SAFT equation of state. 2021 , 154, 244106	3

- 584 Soluble State of Villin Headpiece Protein as a Tool in the Assessment of MD Force Fields. **2021**, 125, 6897-6911
- 583 Molecular Dynamics and Emerging Network Graphs of Interactions in Dinitrile-Based Li-Ion Battery Electrolytes. **2021**, 125, 7231-7240 1
- 582 Deep Mutational Scanning of Dynamic Interaction Networks in the SARS-CoV-2 Spike Protein Complexes: Allosteric Hotspots Control Functional Mimicry and Resilience to Mutational Escape.
- 581 The order of PDZ3 and TrpCage in fusion chimeras determines their properties-a biophysical characterization. **2021**, 30, 1653-1666 1
- 580 Wettability alteration by Smart Water multi-ion exchange in carbonates: A molecular dynamics simulation study. **2021**, 332, 115830 11
- 579 Cisplatin uptake and release in pH sensitive zeolitic imidazole frameworks. **2021**, 154, 244703 1
- 578 Molecular Dynamics Study of Conformational Changes of Tankyrase 2 Binding Subsites upon Ligand Binding. **2021**, 6, 17609-17620 2
- 577 Molecular Dynamics Simulations of Complexation of Am(III) with a Preorganized Dicationic Ligand in an Ionic Liquid. **2021**, 125, 8532-8538 1
- 576 A new inhibition mechanism in the multifunctional catalytic hemoglobin dehaloperoxidase as revealed by the DHP A(V59W) mutant: A spectroscopic and crystallographic study. **2021**, 25, 756-771
- 575 Improving Cycle Life through Fast Formation Using a Superconcentrated Phosphonium Based Ionic Liquid Electrolyte for Anode-Free and Lithium Metal Batteries. **2021**, 4, 6399-6407 5
- 574 Solubility Prediction of Organic Molecules with Molecular Dynamics Simulations. **2021**, 21, 5198-5205 4
- 573 Unraveling the Interaction of Water-in-Oil Emulsion Droplets via Molecular Simulations and Surface Force Measurements. **2021**, 125, 7556-7567 1
- 572 Investigation of the reactivity properties of a thiourea derivative with anticancer activity by DFT and MD simulations. *Journal of Molecular Modeling*, **2021**, 27, 217 2 5
- 571 Molecular dynamics simulation for mechanism revelation of the safety and nutrition of lipids and derivatives in food: State of the art. **2021**, 145, 110399 2
- 570 Effect of Cholesterol Versus Ergosterol on DPPC Bilayer Properties: Insights from Atomistic Simulations. **2021**, 125, 7679-7690 0
- 569 Using Molecular Simulations to Understand the Effect of Dodecyl Sulfate on the Calcium-Binding Ability of Polystyrene Sulfonate. **2021**, 125, 7919-7931 1
- 568 Leishmanicidal and cytotoxic activities and 4D-QSAR of 2-arylidene indan-1,3-diones. **2021**, 354, e2100081 0
- 567 Isohemigossypolone: Antiophidic properties of a naphthoquinone isolated from *Pachira aquatica* Aubl. **2021**, 245, 109028 0

566	Size Matters: A Mechanistic Model of Nanoparticle Curvature Effects on Amyloid Fibril Formation.	
565	Identification of potential carboxylic acid-containing drug candidate to design novel competitive NDM inhibitors: An in-silico approach comprising combined virtual screening and molecular dynamics simulation.	1
564	Ionic-Group Dependence of Polyelectrolyte Coacervate Phase Behavior. 2021 , 54, 7572-7581	0
563	Molecular Dynamics of Decane Solubilization and Diffusion of Aggregates Consisting of Surfactant and Decane Molecules in Aqueous Solutions. 2021 , 83, 406-417	0
562	Design and proof of concept for targeted phage-based COVID-19 vaccination strategies with a streamlined cold-free supply chain. 2021 , 118,	13
561	Determining structure and action mechanism of LBF14 by molecular simulation. 2021 , 1-12	0
560	Apropos of Universal Epitope Discovery for COVID-19 Vaccines: A Framework for Targeted Phage Display-Based Delivery and Integration of New Evaluation Tools. 2021 ,	3
559	On the molecular origins of the ferroelectric splay nematic phase. 2021 , 12, 4962	14
558	Competing Roles of Ca and Nonmuscle Myosin IIA on the Dynamics of the Metastasis-Associated Protein S100A4. 2021 , 125, 10059-10071	1
557	Ultrafast dynamics and scattering of protic ionic liquids induced by XFEL pulses. 2021 , 28, 1296-1308	1
556	Structure-based virtual screening and computational study towards identification of novel inhibitors of hypoxanthine-guanine phosphoribosyltransferase of <i>Trypanosoma cruzi</i> . 2021 , 122, 1701-1714	0
555	Molecular Dynamics Simulations to Explore the Structure and Rheological Properties of Normal and Hyperconcentrated Airway Mucus. 2021 , 147, 1369-1387	2
554	Recent advances of molecular dynamics simulations in nanotribology. 2021 , 335, 116154	12
553	Effects of Weak Nonspecific Interactions with ATP on Proteins. 2021 , 143, 11982-11993	6
552	In silico investigation on the inhibitory effect of fungal secondary metabolites on RNA dependent RNA polymerase of SARS-CoV-II: A docking and molecular dynamic simulation study. 2021 , 135, 104613	10
551	Modeling the Adsorption of the miR-29a Cancer Biomarker on a Graphene Quantum Dot. 2021 , 6, 21764-21772	
550	Structural dynamics of <i>Rhipicephalus microplus</i> serpin-3. 2021 , 47, 1209-1216	1
549	DNA Aptamers Block the Receptor Binding Domain at the Spike Protein of SARS-CoV-2. 2021 , 8, 713003	5

548	Inter-pulse delay optimization for dynamical decoupling pulse sequences with up to six refocusing pulses. 2021 , 136, 1	0
547	Low Density Interior in Supercooled Aqueous Nanodroplets Expels Ions to the Subsurface. 2021 , 143, 13113-13123	1
546	Sterically confined rearrangements of SARS-CoV-2 Spike protein control cell invasion. 2021 , 10,	3
545	Relaxation Times of Solid-like Polyelectrolyte Complexes of Varying pH and Water Content. 2021 , 54, 7765-7776	5
544	Markov State Models and Molecular Dynamics Simulations Provide Understanding of the Nucleotide-Dependent Dimerization-Based Activation of LRRK2 ROC Domain. 2021 , 26,	3
543	Differential MMP-14 Targeting by Lumican-Derived Peptides Unraveled by In Silico Approach. 2021 , 13,	0
542	Molecular architecture of SARS-CoV-2 envelope by integrative modeling.	3
541	Interplay of lipid and surfactant: Impact on nanoparticle structure. 2021 , 597, 278-288	6
540	Exploring EZH2-Proteasome Dual-Targeting Drug Discovery through a Computational Strategy to Fight Multiple Myeloma. 2021 , 26,	
539	Thermomechanical enhancement of DPP-4T through purposeful β -conjugation disruption.	0
538	Design and Computational Analysis of a Chimeric Avian Influenza Antigen: A Yeast-displayed, Universal and Cross-protective Vaccine Candidate.	
537	pH-Dependent Conformations of an Antimicrobial Spider Venom Peptide, Cupiennin 1a, from Unbiased HREMD Simulations. 2021 , 6, 24166-24175	0
536	Investigating the Accuracy of Water Models through the Van Hove Correlation Function. 2021 , 17, 5992-6005	3
535	Allosteric Control of Structural Mimicry and Mutational Escape in the SARS-CoV-2 Spike Protein Complexes with the ACE2 Decoys and Miniprotein Inhibitors: A Network-Based Approach for Mutational Profiling of Binding and Signaling. 2021 , 61, 5172-5191	2
534	Alkali Metal- and Acid-Catalyzed Interconversion of Goniodomin A with Congeners B and C. 2021 , 84, 2554-2567	1
533	Subdiffusive-Brownian crossover in membrane proteins: a generalized Langevin equation-based approach. 2021 , 120, 4722-4737	2
532	Flower-like Micelles of Polyethylene Oxide End-Capped with Cholesterol.	3
531	Thermodynamic and MD studies of anion complexation by cyclopentaleucine in acetonitrile and dimethyl sulfoxide. 2021 , 340, 116848	0

530	Titratable transmembrane residues and a hydrophobic plug are essential for manganese import via the Bacillus anthracis ABC transporter MntBC-A. 2021 , 297, 101087	
529	In silico and in vitro analysis of an Aspergillus niger chitin deacetylase to decipher its subsite sugar preferences. 2021 , 297, 101129	1
528	New short cationic antibacterial peptides. Synthesis, biological activity and mechanism of action. 2021 , 1863, 183665	2
527	The cooperative effect between cyclic naphthenic acids and surfactant enhances the separation efficiency. 2021 , 342, 117577	0
526	Expression, solubility monitoring, and purification of the co-folded LUBAC LTM domain by structure-guided tandem folding in autoinducing cultures. 2021 , 187, 105953	1
525	High-viscosity Pickering emulsion stabilized by amphiphilic alginate/SiO via multiscale methodology for crude oil-spill remediation. 2021 , 273, 118492	3
524	3CL and PL affinity, a docking study to fight COVID19 based on 900 compounds from PubChem and literature. Are there new drugs to be found?. 2021 , 1245, 130968	4
523	Deciphering the curved profile of uranyl ions at the aqueous-organic interface by atomistic simulations. 2021 , 343, 117599	0
522	Binding parameters and molecular dynamics of β -lactoglobulin-vanillic acid complexation as a function of pH - part B: Neutral pH. 2022 , 367, 130655	1
521	Molecular Dynamics and Statics. 2022 , 510-520	
520	Development of accurate coarse-grained force fields for weakly polar groups by an indirect parameterization strategy. 2021 , 23, 6763-6774	1
519	Water in biodegradable glucose-water-urea deep eutectic solvent: modifications of structure and dynamics in a crowded environment. 2021 , 23, 12191-12203	3
518	Testing automatic methods to predict free binding energy of host-guest complexes in SAMPL7 challenge. 2021 , 35, 209-222	5
517	An Implementation of Replica Exchange with Dynamical Scaling for Efficient Large-Scale Simulations. 2021 , 61, 810-818	4
516	Concepts, Practices, and Interactive Tutorial for Allosteric Network Analysis of Molecular Dynamics Simulations. 2021 , 2302, 311-334	0
515	Identification of novel potential cyclooxygenase-2 inhibitors using ligand- and structure-based virtual screening approaches. 2021 , 1-23	3
514	Advancements in Cancer Therapeutics. 2021 , 89-115	2
513	Ligand Affinities within the Open-Boundary Ligand Molecular Mechanics/Coarse-Grained Framework (I): Alchemical Transformations within the Hamiltonian Adaptive Resolution Scheme. 2021 , 125, 789-797	2

512	Self-Assembly of Silk-like Protein into Nanoscale Bicontinuous Networks under Phase-Separation Conditions. 2021 , 22, 690-700	3
511	Water and Biological Macromolecules. 263-308	5
510	Cluster Computing: High-Performance, High-Availability, and High-Throughput Processing on a Network of Computers. 2006 , 521-551	14
509	Atomistic Molecular Modeling of Electric Field Poling of Nonlinear Optical Polymers. 2006 , 337-357	2
508	The Targeted Shadowing Hybrid Monte Carlo (TSHMC) Method. 2006 , 141-153	9
507	Sampling Kinetic Protein Folding Pathways using All-Atom Models. 2006 , 393-433	2
506	Structure of Bilayer Membranes of Gemini Surfactants with Rigid and Flexible Spacers from MD Simulations. 2003 , 668-677	1
505	Protein Structure Prediction. 2009 , 225-242	3
504	Basic Molecular Dynamics. 2005 , 565-588	19
503	Molecular dynamics simulations. 2015 , 1215, 3-26	23
502	Molecular dynamics simulations of membrane proteins. 2015 , 1215, 91-108	11
501	Membrane-associated proteins and peptides. 2008 , 443, 161-79	4
500	Atomistic and coarse-grained computer simulations of raft-like lipid mixtures. 2007 , 398, 283-302	3
499	Molecular simulations of peptides: a useful tool for the development of new drugs and for the study of molecular recognition. 2009 , 570, 77-153	6
498	Molecular dynamics applied in drug discovery: the case of HIV-1 protease. 2012 , 819, 527-49	7
497	Distributed Density Peak Clustering of Trajectory Data on Spark. 2020 , 792-804	1
496	Application of Markov State Models to simulate long timescale dynamics of biological macromolecules. 2014 , 805, 29-66	22
495	Modeling of Membrane Proteins. 2019 , 371-451	2

494	Protein Folding Properties from Molecular Dynamics Simulations. 2007 , 109-115	2
493	Dynamics of Water at Low Temperatures and Implications for Biomolecules. 2009 , 3-22	7
492	Molecular Models to Emulate Confinement Effects on the Internal Dynamics of Organophosphorous Hydrolase. 2008 , 68-78	1
491	Optimizations of Protein Force Fields. 2014 , 195-247	1
490	An application of QM/MM simulation: the second protonation of cytochrome P450. 2015 , 827, 311-24	1
489	Ab Initio Protein Structure Prediction. 2017 , 3-35	34
488	CORRFUNC: Blazing Fast Correlation Functions with AVX512FSIMD Intrinsic. 2019 , 3-20	13
487	Interaction modes between nanosized graphene flakes and liposomes: Adsorption, insertion and membrane fusion. 2019 , 1863, 723-731	8
486	Structural Studies of Overlapping Dinucleosomes in Solution. 2020 , 118, 2209-2219	7
485	Computational studies of fibrillation induced selective cytotoxicity of cross-βmyloid αPhenol Soluble Modulin B. 2020 , 535, 110777	1
484	The role of the quaternary structure in the activation of human L-asparaginase. 2020 , 224, 103818	2
483	Solvation Structures of Tetraethylammonium Bromide and Tetrafluoroborate in Aqueous Binary Solvents with Ethanol, Trifluoroethanol, and Acetonitrile. 2020 , 124, 5009-5020	3
482	Intrinsic Conformational Dynamics of Alanine in Water/Ethanol Mixtures: An Experiment-Driven Molecular Dynamics Study. 2020 , 124, 11600-11616	3
481	The Effects of Chain Length on the Structural Properties of Intrinsically Disordered Proteins in Concentrated Solutions. 2020 , 124, 11843-11853	9
480	A conserved histidine in switch-II of EF-G moderates release of inorganic phosphate. 2015 , 5, 12970	19
479	Chapter 20:Computer Simulation Studies of Heat Capacity Effects Associated with Hydrophobic Effects. 2010 , 436-456	6
478	Chapter 2:Lateral Pressure Profiles in Lipid Membranes: Dependence on Molecular Composition. 2010 , 26-55	9
477	Myoglobin molecule charging in electrolyte solutions. 2020 , 22, 26764-26775	3

476	Gating of Water Flow Induced by Bending of a Carbon Nanotube. 2009 , 26, 068702	12
475	Experimental and Computational Investigation of the Structure of Peptide Monolayers on Gold Nanoparticles.	1
474	PBxplorer: a tool to analyze local protein structure and deformability with protein Blocks.	1
473	Heparin as an Anti-Inflammatory Agent.	2
472	Dependence of triboelectric charging behavior on material microstructure. 2017 , 1,	23
471	Propagation of uncertainty in physicochemical data to force field predictions. 2020 , 2,	2
470	A Key Role for Transmembrane Prolines in Calcitonin Receptor-Like Receptor Agonist Binding and Signalling: Implications for Family B G-Protein-Coupled Receptors. 2005 , 67, 20-31	49
469	Hydration Gibbs Energies of Nucleic Acid Bases Determined by Gibbs Energy Perturbation, Continuous and Hybrid Approaches. 2005 , 70, 1756-1768	3
468	A parallel and distributed discrete event approach for spatial cell-biological simulations. 2008 , 35, 22-31	8
467	Molecular Dynamics Simulation of VEGFR2 with Sorafenib and Other Urea-Substituted Aryloxy Compounds. 2013 , 2013, 1-7	7
466	Quantum chemical studies of the myosin ATPase mechanism. 2007 , 74, 4-10	2
465	Ensembler: Enabling High-Throughput Molecular Simulations at the Superfamily Scale. 2016 , 12, e1004728	14
464	Methionine sulfoxides on prion protein Helix-3 switch on the alpha-fold destabilization required for conversion. 2009 , 4, e4296	49
463	Regulation of bestrophins by Ca ²⁺ : a theoretical and experimental study. 2009 , 4, e4672	16
462	HAAD: A quick algorithm for accurate prediction of hydrogen atoms in protein structures. 2009 , 4, e6701	20
461	Cholesterol induces specific spatial and orientational order in cholesterol/phospholipid membranes. 2010 , 5, e11162	94
460	Sub-nanoscale surface ruggedness provides a water-tight seal for exposed regions in soluble protein structure. 2010 , 5, e12844	17
459	Acidic extracellular pH promotes activation of integrin α 5 β 1. 2011 , 6, e15746	94

458	Strength of hydrogen bond network takes crucial roles in the dissociation process of inhibitors from the HIV-1 protease binding pocket. 2011 , 6, e19268	27
457	Visualization of early events in acetic acid denaturation of HIV-1 protease: a molecular dynamics study. 2011 , 6, e19830	7
456	Detailed regulatory mechanism of the interaction between ZO-1 PDZ2 and connexin43 revealed by MD simulations. 2011 , 6, e21527	14
455	Molecular dynamics analysis reveals structural insights into mechanism of nicotine N-demethylation catalyzed by tobacco cytochrome P450 mono-oxygenase. 2011 , 6, e23342	7
454	Structural analysis of prolyl oligopeptidases using molecular docking and dynamics: insights into conformational changes and ligand binding. 2011 , 6, e26251	22
453	The Plasmodium falciparum malaria M1 alanyl aminopeptidase (PfA-M1): insights of catalytic mechanism and function from MD simulations. 2011 , 6, e28589	17
452	Computational predictions of volatile anesthetic interactions with the microtubule cytoskeleton: implications for side effects of general anesthesia. 2012 , 7, e37251	39
451	Lipid interaction and membrane perturbation of human islet amyloid polypeptide monomer and dimer by molecular dynamics simulations. 2012 , 7, e38191	35
450	Weak glycolipid binding of a microdomain-tracer peptide correlates with aggregation and slow diffusion on cell membranes. 2012 , 7, e51222	6
449	Structure and stability of human telomeric G-quadruplex with preclinical 9-amino acridines. 2013 , 8, e57701	17
448	A single disulfide bond disruption in the β integrin subunit promotes thiol/disulfide exchange, a molecular dynamics study. 2013 , 8, e59175	12
447	Molecular dynamics simulations of the cardiac troponin complex performed with FRET distances as restraints. 2014 , 9, e87135	26
446	Formulation optimization and in vivo proof-of-concept study of thermosensitive liposomes balanced by phospholipid, elastin-like polypeptide, and cholesterol. 2014 , 9, e103116	17
445	In silico screening, genotyping, molecular dynamics simulation and activity studies of SNPs in pyruvate kinase M2. 2015 , 10, e0120469	15
444	An S188V mutation alters substrate specificity of non-stereospecific β -haloalkanoic acid dehalogenase E (DehE). 2015 , 10, e0121687	11
443	Phosphorylation Regulates the Bound Structure of an Intrinsically Disordered Protein: The p53-TAZ2 Case. 2016 , 11, e0144284	11
442	Hydrophobic Interactions Are a Key to MDM2 Inhibition by Polyphenols as Revealed by Molecular Dynamics Simulations and MM/PBSA Free Energy Calculations. 2016 , 11, e0149014	43
441	Biological Membranes in Extreme Conditions: Simulations of Anionic Archaeal Tetraether Lipid Membranes. 2016 , 11, e0155287	13

440	An accurate coarse-grained model for chitosan polysaccharides in aqueous solution. 2017 , 12, e0180938	18
439	Free energy profile of permeation of Entecavir through Hepatitis B virus capsid studied by molecular dynamics calculation. 2020 , 92, 1585-1594	2
438	Modelling and computer simulation of food structures. 2007 , 334-386	2
437	and Investigation of a Likely Pathway for Anti-Cancerous Effect of Thrombocidin-1 as a Novel Anticancer Peptide. 2020 , 27, 751-762	2
436	Design and Biological Evaluation of Novel Imidazolyl Flavonoids as Potent and Selective Protein Tyrosine Phosphatase Inhibitors. 2020 , 16, 563-574	2
435	A Comparative Study to Explore the Effect of Different Compounds in Immune Proteins of Human Beings Against Tuberculosis: An In-silico Approach. 2020 , 15, 155-164	4
434	Investigating the Conformation of S100P Protein Under Physiological Parameters Using Computational Modeling: A Clue for Rational Drug Design. 2018 , 12, 36-50	2
433	Hydrogen Inter-Cage Hopping and Cage Occupancies inside Hydrogen Hydrate: Molecular-Dynamics Analysis. 2021 , 11, 282	3
432	Pharmacological Characterization of μ -Opioid Receptor Agonists with Biased G Protein or Arrestin Signaling, and Computational Study of Conformational Changes during Receptor Activation. 2020 , 26,	3
431	Study of HSA interactions with arachidonic acid using spectroscopic methods revealing molecular dynamics of HSA-AA interactions. 2020 , 12, 125-133	2
430	Homology Modeling and Molecular Dynamics Study of the Interactions of SoxY and SoxZ: The Central Player of Biochemical Oxidation of Sulfur Anions in Pseudaminobacter salicylatoxidans. 2007 , 2, 569-576	3
429	Genetic polymorphism at the candidate gene in Iranian Sistani cattle (<i>Bos indicus</i>). 2007 , 10, 3368-73	1
428	Peptide Inhibition of Topoisomerase IB from Plasmodium falciparum. 2011 , 2011, 854626	6
427	A possible therapeutic potential of quercetin through inhibition of β -catenin in hypoxia induced neuronal injury: a molecular dynamics simulation study. 2016 , 11, 1247-53	10
426	A criterion to identify the equilibration time in lipid bilayer simulations. 2012 , 4,	18
425	Pharmacophore Modeling and Molecular Dynamics Simulation to Find the Potent Leads for Aurora Kinase B. 2012 , 33, 869-880	3
424	Evaluation of 4H-4-chromenone derivatives as inhibitors of protein kinase CK2. 2005 , 21, 287-292	4
423	Protein signatures using electrostatic molecular surfaces in harmonic space. 2013 , 1, e185	9

422	Computer modelling reveals new conformers of the ATP binding loop of Na/K-ATPase involved in the transphosphorylation process of the sodium pump. 2017 , 5, e3087	2
421	PBxplore: a tool to analyze local protein structure and deformability with Protein Blocks. 2017 , 5, e4013	18
420	Assessment of the UCST-type liquid-liquid phase separation mechanism of imidazolium-based ionic liquid, [Cmim][TFSI], and 1,4-dioxane by SANS, NMR, IR, and MD simulations. 2021 , 23, 24449-24463	0
419	Site of Cholesterol Oxidation Impacts Its Localization and Domain Formation in the Neuronal Plasma Membrane. 2021 , 12, 3873-3884	0
418	A simple strategy for signal enhancement in lateral flow assays using superabsorbent polymers. 2021 , 188, 364	
417	Ionic distribution of MgCl ₂ near the alcohol/water interface. 2021 , 344, 117902	
416	Enhanced Molecular Dynamics Method to Efficiently Increase the Discrimination Capability of Computational Protein-Protein Docking. 2021 , 17, 7271-7280	1
415	SMOG 2 and OpenSMOG: Extending the limits of structure-based models. 2021 ,	3
414	Pyrrolidinium-PEG Ionic Copolyester: Li-Ion Accelerator in Polymer Network Solid-State Electrolytes. 2021 , 11, 2102660	0
413	Molecular Mechanism of the Anti-Inflammatory Action of Heparin. 2021 , 22,	4
412	Conformational changes in HIV-1 protease: molecular dynamic simulation study in picosecond and nanosecond timescales. 2002 , 18, 117-123	1
411	Homology modeling of structure of NH ₂ -terminal module of mammalian (<i>Bos taurus</i>) tyrosyl-tRNA synthetase. 2002 , 18, 547-550	2
410	Structural Identification of the Interactions of SoxA and SoxX During the Oxidation of Sulfur Anions via the Novel Global Sulfur Oxidizing (Sox) Operon. 2006 , 1, 172-182	
409	Conformational flexibility of interdomain linker in bovine tyrosyl-tRNA synthetase studied by molecular dynamics simulation. 2006 , 22, 433-438	1
408	In Silico Molecular Homology Modeling of Neurotransmitter Receptors. 2007 , 293-304	
407	Structural and Conformational Studies on 5-[1- ¹⁴ C-methylpyrrolidin-2-yl]-1,3-oxazolidin-2-one Free Base and Hydrochloride Form. 2007 , 71, 105	
406	Modeling hydration mechanisms of enzymes in nonpolar and polar organic solvents. 2007 , 070410020306006-???	
405	Conformational mobility of human translation elongation factor A1. 2007 , 23, 307-317	1

- 404 Targeting the PDZ Domains of Molecular Scaffolds of Transmembrane Ion Channels. **2008**, 139-148
- 403 Transmembrane protein models based on high-throughput molecular dynamics simulations with experimental constraints. **2008**, 443, 213-27 1
- 402 Molecular Dynamics Simulations of Proteins and Peptides. 1170
- 401 Receptor-Ligand Interactions in Biological Systems. 1 1
- 400 State-Point Dependence and Transferability of Potentials in Systematic Structural Coarse-Graining. **2008**, 69-82
- 399 Molecular modeling approach to achieving erythropoietin mimetic peptides. **2009**, 611, 51-3
- 398 The LIBI Grid Platform for Bioinformatics. **2009**, 577-613 2
- 397 BioSimGrid Biomolecular Simulation Database. **2009**, 307-326
- 396 Permeability of lipid membranes. A molecular dynamic study. **2009**, 1, 423-436
- 395 Wrapping Deficiencies and De-wetting Patterns in Soluble Proteins: A Blueprint for Drug Design. **2010**, 49-58
- 394 Atomistic Molecular Simulation of Gating Modifier Venom Peptides - Two Binding Modes and Effects of Lipid Structure. **2010**, 167-190
- 393 Under-Wrapped Proteins in the Order-Disorder Twilight: Unraveling the Molecular Etiology of Aberrant Aggregation. **2010**, 59-78
- 392 Molecular dynamics simulation of promotion mechanism of store hydrogen of clathrate hydrate. **2011**, 60, 128801 1
- 391 The influence of the structure of the organic ultra-film on friction. **2012**, 61, 028701 3
- 390 Detecting Protein Conformational Changes in Interactions via Scaling Known Structures. **2013**, 58-74 2
- 389 Relations between the structure, symmetry and the energy mechanism of the polar-organic molecule ultra-films during the tribology. **2013**, 62, 158701 2
- 388 Software. **2013**, 403-429
- 387 Redox specificity of 2-hydroxyacid-coupled NAD(+)/NADH dehydrogenases: a study exploiting "reactive" arginine as a reporter of protein electrostatics. **2013**, 8, e83505 0

- 386 The Effect of Temperature and Pressure on the Self-assembly of Dipalmitoylphosphatidylcholine Using Coarse-Grained Molecular Dynamics. **2014**, 3, 122-127 3
- 385 A Stereochemically-Bent β -Hairpin: Scrutiny of Folding by Comparing a Heteropolypeptide and Cognate Oligoalanine. **2014**, 04, 81-97
- 384 Molecular Dynamics Simulations of Lipid Bilayers with Incorporated Peptides. **2014**, 241-270
- 383 Cloning, Homology Modeling and Active Site Prediction of Secreted Serine Proteinase (PrDI) and Carboxylesterase (CaDI) Gene from Nematophagous Fungi *Dactylellina cionopaga*. **2014**, 7, 76-110
- 382 Computational Methods in SNP Analysis.
- 381 A Combined Pharmacophore-Based Virtual Screening, Docking Study and Molecular Dynamics (MD) Simulation Approach to Identify Inhibitors with Novel Scaffolds for Myeloid cell leukemia (Mcl-1). **2014**, 35, 2097-2108
- 380 - Polymer Electrolyte Membranes. **2014**, 100-195
- 379 Simulations and experiments in protein folding. **2015**, 1215, 289-306
- 378 Proteins in the Order-Disorder Twilight: Unstable Interfaces Promote Protein Aggregation. **2015**, 97-126
- 377 Molecular Dynamics Simulation: From $\alpha\beta$ Initio to α Coarse Grained **2015**, 1-61
- 376 Packing Defects and Protein Hydration: Dynamics of the Aqueous Interface. **2015**, 83-96
- 375 Efficient Implementation of the Force Calculation in MD Simulations. **2015**, 45-58
- 374 Dehydron-Rich Proteins in the Order-Disorder Twilight Zone. **2016**, 121-150
- 373 Biomediated Atomic Metal Nanoclusters: Synthesis and Theory. **2016**, 1397-1426
- 372 In-Cell Biochemistry Using NMR Spectroscopy. **2016**, 167-183
- 371 Approaches for calculating solvation free energies and enthalpies demonstrated with an update of the FreeSolv database.
- 370 Bibliography. **2017**, 349-358
- 369 Simulaç o por din mica molecular da enzima cruzada do trypanosoma cruzi. **2018**, 227-244

- 368 Mechanical evolution of DNA double-strand breaks in the nucleosome.
- 367 Structural plasticity of CENP-A regulated by H4 influences cellular levels and kinetochore assembly.
- 366 Large-scale docking predicts that sORF-encoded peptides may function through protein-peptide interactions in *Arabidopsis thaliana*.
- 365 Conformational dynamics of active site loops 5, 6 and 7 of enzyme Triosephosphate Isomerase: A molecular dynamics study. ○
- 364 Raman and Infrared Spectra of Acoustical, Functional Modes of Proteins from All-Atom and Coarse-Grained Normal Mode Analysis. **2019**, 501-539
- 363 Optimizations of Protein Force Fields. **2019**, 203-256
- 362 Interactions of Heavy Ions with DNA and Radiative Aspects in Physics of Liquid Matter. **2019**, 275-299
- 361 Using SMOG 2 to Simulate Complex Biomolecular Assemblies. **2019**, 2022, 129-151 2
- 360 Molecular dynamic simulation of cellulose nanofiber to determine its nano-mechanical properties. **2019**,
- 359 Distribuci3n del 1-butanol y 2-butanol en los sistemas agua/n-octano y agua/Dodecil Sulfato de Sodio (SDS)/n-octano usando din3mica molecular. Parte II. Uso de las herramientas gmx-density y gmx-densmap. **2019**, 11,
- 358 A structural model of the human serotonin transporter in an outward-occluded state. ○
- 357 Structural Studies of Overlapping Dinucleosomes in Solution.
- 356 Implicit modeling of the impact of adsorption on solid surfaces for protein mechanics and activity with a coarse-grain representation.
- 355 Embedded Mean-Field Theory for Solution-Phase Transition-Metal Polyolefin Catalysis. **2020**, 16, 4226-4237 ○
- 354 Full structural ensembles of intrinsically disordered proteins from unbiased molecular dynamics simulations.
- 353 Allosteric inhibition of adenylyl cyclase type 5 by G-protein: a molecular dynamics study.
- 352 MODELLING OF 3D-STRUCTURES OF THE RARE MELANOCORTIN-1-RECEPTOR MUTATIONS ASSOCIATED TO MELANISM IN THE BANANAQUIT. **2020**, 26, 30-41
- 351 Organic nanoelectronics inside us: charge transport and localization in RNA could orchestrate ribosome operation.

350	Natural Products-Based Drug Design against SARS-CoV-2 Mpro 3CLpro. 2021 , 22,	7
349	Droplet trajectories and collisions in gas forced vortexes: A molecular dynamics study. 2021 , 248, 117242	2
348	Whole Genome Sequencing for Revealing the Point Mutations of SARS-CoV-2 Genome in Bangladeshi Isolates and their Structural Effects on Viral Proteins.	
347	Influence of Lipid Composition on the Insertion Process of Glyphosate into Membranes: A Thermodynamic Study. 2021 , 125, 184-192	0
346	Description of Transport Tunnel in Haloalkane Dehalogenase Variant LinB D147C+L177C from <i>Sphingobium japonicum</i> . 2021 , 11, 5	0
345	Molecular recognition in the product site of cellobiohydrolase Cel7A regulates processive step length. 2020 , 477, 99-110	2
344	The penetration and movement of nanoparticles on membrane. 2020 ,	
343	Molecular mechanism of the pH-dependent calcium affinity in langerin.	1
342	Blockers bearing hydroxyethylamine and hydroxyethylene as potential SARS-CoV-2 Mpro inhibitors: rational based design, , , and SAR studies for lead optimization.. 2021 , 11, 35536-35558	19
341	Understanding the binding mechanism for potential inhibition of SARS-CoV-2 Mpro and exploring the modes of ACE2 inhibition by hydroxychloroquine. 2021 ,	2
340	Membrane Structure of Aquaporin Observed with Combined Experimental and Theoretical Sum Frequency Generation Spectroscopy. 2021 , 37, 13452-13459	1
339	Molecular strategies for antibody binding and escape of SARS-CoV-2 and its mutations. 2021 , 11, 21735	2
338	Effect of Cholesterol vs. Ergosterol on DPPC Bilayer Properties: Insights from Atomistic Simulations.	
337	BioSimGrid Biomolecular Simulation Database. 628-644	
336	Membrane Protein Simulations: Modelling a Complex Environment. 2006 , 3-20	
335	Docking and Molecular Dynamics Simulation of Complexes of High and Low Reactive Substrates with Peroxidases. 2009 , 263-271	
334	Computationally Grafting an IgE Epitope onto a Scaffold: Implications for a Pan Anti-Allergy Vaccine Design.	
333	Structural and dynamic insights into MnCa cluster-depleted Photosystem II. 2021 ,	1

332	Structural and functional analysis of protein. 2022 , 189-206	
331	Conformational exploration of RbgA using molecular dynamics: Possible implications in ribosome maturation and GTPase activity in different nucleotide bound states. 2021 , 111, 108087	1
330	Gating of Substrate Access and Long-Range Proton Transfer in Escherichia coli Nitrate Reductase A: The Essential Role of a Remote Glutamate Residue. 2021 , 11, 14303-14318	0
329	Bioinspired hierarchical porous membrane for efficient uranium extraction from seawater.	11
328	Solutions and Condensed Phases of PEG from All-Atom Molecular Dynamics. 2021 , 125, 12892-12901	2
327	Comparative binding studies of bacosine with human serum albumin and β -acid glycoprotein biophysical evaluation and computational approach. 2021 , 209, 114478	0
326	The Influence of Anion Structure on the Ionic Liquids/Au (100) Interface by Molecular Dynamics Simulations. 2021 , 37, 14059-14071	3
325	The copper-linked E. coli AZY operon: Structure, metal binding, and a possible physiological role in copper delivery. 2021 , 101445	0
324	Hydrophobicity of Self-Assembled Monolayers of Alkanes: Fluorination, Density, Roughness, and Lennard-Jones Cutoffs. 2021 , 37, 13846-13858	1
323	Ionic screening in bulk and under confinement. 2021 , 155, 204501	2
322	Modelling cetrimonium micelles as 4-OH cinnamate carriers targeting a hydrated iron oxide surface. 2021 , 610, 785-785	1
321	Molecular Dynamics Simulation of CO ₂ Adsorption and Diffusion in UTSA-16. 2021 , 24, 57-62	0
320	analysis of a putative dehalogenase from the genome of halophilic bacterium AAD6T. 2021 , 1-17	0
319	Structural modulation of dual oxidase (Duox) in Drosophila melanogaster by phyto-elicitors: A free energy study with molecular dynamics approach. 2021 , 27, 100811	
318	Whole genome sequencing for revealing the point mutations of SARS-CoV-2 genome in Bangladeshi isolates and their structural effects on viral proteins.. 2021 , 11, 38868-38879	2
317	A hybrid coarse-grained model for structure, solvation and assembly of lipid-like peptides.. 2021 ,	1
316	PEA-15 engages in allosteric interactions using a common scaffold in a phosphorylation-dependent manner.. 2022 , 12, 116	
315	What make malarial adenosine deaminase from PLASMODIUM VIVAX recognise adenosine and 5'-methylthioadenosine: simulation studies.. 2022 , 1-8	

314	Pharmaceutical profiling and molecular dynamics simulations reveal crystallization effects in amorphous formulations.. 2021 , 613, 121360	1
313	Biomimetic design of inhibitors of immune checkpoint LILRB4.. 2021 , 282, 106746	1
312	Gas transport and diffusion coefficients in a coupling coal system of matrix and nano-fracture: A molecular simulation study. 2022 , 99, 104407	0
311	Alanine scanning mutagenesis in Cys-His boxes of human immunodeficiency virus type 1 Nucleocapsid protein P7: Insight from an in silico investigation. 2022 , 38, 100828	
310	Atomic-scale insights into allosteric inhibition and evolutionary rescue mechanism of Cas9 by the anti-CRISPR protein AcrIIA6.. 2021 , 19, 6108-6124	10
309	Influence of Oligopeptide Length and Distribution on Polyisoprene Properties.. 2021 , 13,	0
308	The Role of Triazole and Glucose Moieties in Alkali Metal Cation Complexation by Lower-Rim Tertiary-Amide Calix[4]arene Derivatives.. 2022 , 27,	
307	Non-monotonic variation of flow strength in nanochannels grafted with end-charged polyelectrolyte layers.. 2022 , 12, 4061-4071	
306	Molecular modeling of indazole-3-carboxylic acid and its metal complexes (Zn, Ni, Co, Fe and Mn) as NO synthase inhibitors: DFT calculations, docking studies and molecular dynamics simulations. 2022 , 135, 109120	2
305	Do molecular dynamics force fields accurately model Ramachandran distributions of amino acid residues in water?. 2022 ,	2
304	Elucidating the Structural Features of ABCA1 in its Heterogeneous Membrane Environment.. 2021 , 8, 803078	0
303	Exploring Structural Mechanism of COVID-19 Treatment with Glutathione as a Potential Peptide Inhibitor to the Main Protease: Molecular Dynamics Simulation and MM/PBSA Free Energy Calculations Study.. 2022 , 28, 55	3
302	Immuno-Affinity Study of Oxidative Tyrosine Containing Peptides. 2022 , 28, 1	0
301	Simple evaluation of dynamic disorder effects on exciton transport.. 2022 , 156, 044112	
300	In vitro and In silico Assessment of Human Serum Albumin Interactions with Omega 3-6-9 Fatty Acids. 2022 , 88, 1291-1303	0
299	Sub-layer rationale of anomalous layer-shrinkage from atomistic simulations of a fluorinated mesogen. 2022 , 3, 1212-1223	1
298	Self-Diffusive Properties of the Intrinsically Disordered Protein Histatin 5 and the Impact of Crowding Thereon: A Combined Neutron Spectroscopy and Molecular Dynamics Simulation Study.. 2022 ,	1
297	The Structure and Function of Modular Escherichia coli O157:H7 Bacteriophage FTBEc1 endolysin, LysT84: Defining a New Endolysin Catalytic Subfamily.. 2021 ,	1

296	Complex nanoemulsion for vitamin delivery: droplet organization and interaction with skin membranes.. 2021 ,	1
295	Peptide framework for screening the effects of amino acids on assembly.. 2022 , 8, eabj0305	3
294	Deciphering the role of aquaporin 1 in the adaptation of the stinging catfish to environmental hypertonicity by molecular dynamics simulation studies.. 2022 , 1-15	0
293	Delineating the activation mechanism and conformational landscape of a class B G protein-coupled receptor glucagon receptor.. 2022 , 20, 628-639	7
292	Molecular Dynamics Simulation of an β Carrageenan Hexamer as Single and Double Helices. 2022 , 82,	
291	Ultrahigh-flux Nanoporous Graphene Membrane for Sustainable Seawater Desalination Using Low-grade Heat.. 2022 , e2109718	1
290	Structural and molecular dynamics of ammonia transport in Staphylococcus aureus NH-dependent NAD synthetase.. 2022 , 203, 593-600	2
289	Molecular dynamics simulations of aqueous systems of inhibitor candidates for adenosine-5'-phosphosufate reductase.. 2022 , 1-12	1
288	Molecular dynamics study of uranyl adsorption from aqueous solution to smectite. 2022 , 218, 106361	2
287	Insect protease inhibitors; promising inhibitory compounds against SARS-CoV-2 main protease.. 2022 , 142, 105228	1
286	A comparative study of the interaction of naringenin with lysozyme by multi-spectroscopic methods, activity comparisons, and molecular modeling procedures.. 2022 , 271, 120931	1
285	Carnitine palmitoyl transferase I: Conformational changes induced by long-chain fatty acyl CoA ligands.. 2022 , 112, 108125	0
284	Modulation of DNA conformation in electrolytic nanodroplets.. 2022 ,	0
283	Simultaneous parametrization of torsional and third-neighbor interaction terms in force-field development: The LLS-SC algorithm.. 2022 ,	0
282	Meeting Experiments at the Diffraction Barrier with In Silico Fluorescence Microscopy.	0
281	Martini 3 Coarse-Grained Model for Type III Deep Eutectic Solvents: Thermodynamic, Structural, and Extraction Properties. 2021 , 9, 17338-17350	1
280	Interphase control for high performance lithium metal batteries using ether aided ionic liquid electrolyte.	9
279	Elucidation of the conformational dynamics and assembly of Argonaute-RNA complexes by distinct yet coordinated actions of the supplementary microRNA.. 2022 , 20, 1352-1365	1

278	Towards solvent regulated self-activation of N-terminal disulfide bond oxidoreductase-D.. 2022,	0
277	Computational Modeling of the Bio-nanocomposites. 2022, 217-235	
276	Computational characterization of charge transport resiliency in molecular solids.	
275	Elastic moduli of normal and cancer cell membranes revealed by molecular dynamics simulations.. 2022,	2
274	Lipid bilayers as potential ice nucleating agents.. 2022,	
273	Polar/apolar interfaces modulate the conformational behavior of cyclic peptides with impact on their passive membrane permeability.. 2022, 12, 5782-5796	3
272	Length scale effect on the buckling behavior of a graphene sheets using modified couple stress theory and molecular dynamics method. 2022, 233, 943-960	0
271	Molecular dynamics simulations of the Spike trimeric ectodomain of the SARS-CoV-2 Omicron variant: structural relationships with infectivity, evasion to immune system and transmissibility.	
270	Direct Detection of Bound Ammonium Ions in the Selectivity Filter of Ion Channels by Solid-State NMR.. 2022,	0
269	In silico drug design of benzothiadiazine derivatives interacting with bilayer cell membranes.	0
268	Effect of Ionic Strength on Ibuprofenate Adsorption on a Lipid Bilayer of Dipalmitoylphosphatidylcholine from Molecular Dynamics Simulations.. 2022,	0
267	COVID-19: A systematic review and update on prevention, diagnosis, and treatment.. 2022, 3, e115	2
266	Carbon nanotube supported oriented metal organic framework membrane for effective ethylene/ethane separation.. 2022, 8, eabm6741	6
265	High-Dimensional Parameter Search Method to Determine Force Field Mixing Terms in Molecular Simulations.. 2022, 38, 2840-2851	2
264	How Does Surface Charge Engineering of Bacillus subtilis Lipase A Improve Ionic Liquid Resistance? Lessons Learned from Molecular Dynamics Simulations. 2022, 10, 2689-2698	3
263	Effect of Additives on Preferential Crystallization for the Chiral Resolution of Citrulline: Experimental, Statistical, and Molecular Dynamics Simulation Studies. 2022, 22, 2392-2406	0
262	Driving Forces underlying Selectivity Filter Gating in the MthK Potassium Channel.	0
261	Poly-L-Arginine Molecule Properties in Simple Electrolytes: Molecular Dynamic Modeling and Experiments.. 2022, 19,	1

- 260 Mechanistic Pathway of Lipid Phase-Dependent Lipid Corona Formation on Phenylalanine-Functionalized Gold Nanoparticles: A Combined Experimental and Molecular Dynamics Simulation Study.. **2022**, 126, 2241-2255 2
- 259 A Privileged Dual Action Alzheimer's Disease Therapeutic Platform Targeting Immunopathic and Proteopathic Mechanisms: (E)-3-Styrylindoles as Inhibitors of Indoleamine 2,3-Dioxygenase-Mediated Tryptophan Metabolism and β -Amyloid Aggregation.
- 258 Quantifying biomolecular diffusion with a spherical cow model. **2022**, 90, 225-238
- 257 Exploring binding stability of hydroxy-3-(4-hydroxyphenyl)-5-(4-nitrophenyl)-5,5a,7,8,9,9a-hexahydrothiazolo[2,3-b]quinazolin-6-one with T790M/L858R EGFR-TKD.. **2022**, 1-15 1
- 256 Simulation-based inference with approximately correct parameters via maximum entropy. 0
- 255 Bioinformatic Mining and Structure-Activity Profiling of Baeyer-Villiger Monooxygenases from *Mycobacterium tuberculosis*.. **2022**, e0048221 0
- 254 Exploring the potentials of phytochemicals for targeting coronavirus.. **2022**, 12,
- 253 Molecular Dynamics Calculations of Partial Molar Volumes of Amino Acids in Aqueous Solutions.
- 252 Dynamical Anomaly of Aqueous Amphiphilic Solutions: Connection to Solution H-Bond Fluctuation Dynamics?. **2022**, 7, 10970-10984 0
- 251 Metallic Effects on p-Hydroxyphenyl Porphyrin Thin-Film-Based Planar Optical Waveguide Gas Sensor: Experimental and Computational Studies.. **2022**, 12, 1
- 250 Computational Methods for Understanding the Selectivity and Signal Transduction Mechanism of Aminomethyl Tetrahydronaphthalene to Opioid Receptors.. **2022**, 27,
- 249 The effect of explicit counterion binding on the transference number of polyelectrolyte solutions.. **2022**, 156, 104901 0
- 248 In Silico Drug Design of Benzothiadiazine Derivatives Interacting with Phospholipid Cell Membranes.. **2022**, 12, 1
- 247 Overall structure of fully assembled cyanobacterial KaiABC circadian clock complex by an integrated experimental-computational approach.. **2022**, 5, 184 2
- 246 The importance of atomic partial charges in the reproduction of intermolecular interactions for the triacetin - a model of glycerol backbone.. **2022**, 105203
- 245 Research on the phase structure of Styrene-Butadiene-Styrene modified asphalt based on molecular dynamics. **2022**, 326, 126933 0
- 244 Freestanding non-covalent thin films of the propeller-shaped polycyclic aromatic hydrocarbon decacyclene.. **2022**, 13, 1920
- 243 Encapsulating Cas9 into extracellular vesicles by protein myristoylation.. **2022**, 11, e12196 3

242	Landscape-Based Protein Stability Analysis and Network Modeling of Multiple Conformational States of the SARS-CoV-2 Spike D614G Mutant: Conformational Plasticity and Frustration-Induced Allosteric as Energetic Drivers of Highly Transmissible Spike Variants.. 2022 ,	0
241	Structure-Based Discovery of Potent Staphylococcus aureus Thymidylate Kinase Inhibitors by Virtual Screening.. 2022 ,	
240	Binary droplet coalescence in shear gas flow: A molecular dynamics study. 2022 , 354, 118841	0
239	A D-peptide ligand of neuropeptide Y receptor Y1 serves as nanocarrier traversing of the blood brain barrier and targets glioma. 2022 , 44, 101465	1
238	Increasing the surface hydrophobicity of silicone rubber by electron beam irradiation in the presence of a glycerol layer. 2022 , 591, 153097	3
237	Molecular Dynamics Study on the Thermal Aspects of the Effect of Water Molecules at the Adhesive Interface on an Adhesive Structure. 2021 ,	3
236	Anion Effects on the Mixing States of 1-Methyl-3-octylimidazolium Tetrafluoroborate and Bis(trifluoromethylsulfonyl)amide with Methanol, Acetonitrile, and Dimethyl Sulfoxide on the Meso- and Microscopic Scales.. 2021 , 125, 13896-13907	0
235	Molecular Dynamics Study on Regimes of Head-on Droplet Collision.. 2021 ,	0
234	Influence of Methylene Fluorination and Chain Length on the Hydration Shell Structure and Thermodynamics of Linear Diols. 2021 ,	0
233	Computational Simulation of Conjugated Cholera Toxin Protein. 2021 , 36, S13-S22	0
232	The Landscape-Based Protein Stability Analysis and Network Modeling of Multiple Conformational States of the SARS-CoV-2 Spike D614 Mutant: Conformational Plasticity and Frustration-Driven Allosteric as Energetic Drivers of Highly Transmissible Spike Variant.	
231	Interaction of KRSR Peptide with Titanium Dioxide Anatase (100) Surface: A Molecular Dynamics Simulation Study.. 2021 , 22,	0
230	Stable and Efficient Lithium Metal Anode Cycling through Understanding the Effects of Electrolyte Composition and Electrode Preconditioning. 2022 , 34, 165-177	3
229	Virtual Screening with Gnina 1.0. 2021 , 26,	3
228	What Happens When a Complementary DNA Meets miR-29a Cancer Biomarker in Complex with a Graphene Quantum Dot.. 2021 , 4, 8368-8376	0
227	Structural Study on the Impact of S239D/I332E Mutations in the Binding of Fc and Fc β IIIa. 2021 , 26, 985-992	0
226	Effect of Ethanol and Urea as Solvent Additives on PSS-PDADMA Polyelectrolyte Complexation.. 2022 , 55, 3140-3150	0
225	Fundamental Aspects of Lipid-Based Excipients in Lipid-Based Product Development.. 2022 , 14,	2

224	A new insight into the relationship between molecular morphology and water/ion diffusion in cation exchange membranes: Case of partially sulfonated polyether sulfone. 2022 , 120561	0
223	Cooperative catalysis by a single-atom enzyme-metal complex.. 2022 , 13, 2189	2
222	Data_Sheet_1.docx. 2019 ,	
221	Image_1.tif. 2019 ,	
220	Table_1.pdf. 2019 ,	
219	Table_2.pdf. 2019 ,	
218	Data_Sheet_1.pdf. 2019 ,	
217	Video_1.MP4. 2019 ,	
216	Video_2.MP4. 2019 ,	
215	Lipid-Mediated Association of the Slg1 Transmembrane Domains in Yeast Plasma Membranes.. 2022 ,	0
214	Molecular Insights into the Effect of Salinity on the Stability of Water/Oil Interface with Model Asphaltene and Non-Ionic Surfactants.	
213	Effects of the self-hydrogen bonding among formamide molecules on UCST-type liquid-liquid phase separation of binary solutions with imidazolium-based ionic liquid, [Cnmim][TFSI], studied by NMR, IR, MD simulations, and SANS.	1
212	Multiple Poses and Thermodynamics of Ligands Targeting Protein Surfaces: The Case of Furosemide Binding to mitoNEET in Aqueous Solution.. 2022 , 10, 886568	0
211	Characteristic parameter to predict the lubricant outflow from porous polyimide retainer material. 2022 , 107596	0
210	Molecular Interactions between an Enzyme and Its Inhibitor for Selective Detection of Limonene.. 2022 ,	1
209	Substantially Promoted Energy Density of Li CFx Primary Battery Enabled by Li+-DMP Coordinated Structure.	0
208	Protposer: the web server that readily proposes protein stabilizing mutations with high PPV. 2022 ,	0
207	Mechanistic insights into the size-dependent effects of nanoparticles on inhibiting and accelerating amyloid fibril formation.. 2022 , 622, 804-818	3

206	Diclofenac Ion Hydration: Experimental and Theoretical Search for Anion Pairs. 2022 , 27, 3350	1
205	Binding behavior of ibuprofen-based ionic liquids with bovine serum albumin: Thermodynamic and molecular modeling studies. 2022 , 360, 119367	2
204	Molecular Modeling of Nanoparticles. 2022 , 681-703	
203	Computationally Decoding NudF Residues To Enhance the Yield of the DXP Pathway.	
202	Electrolytes with Micelle-Assisted Formation of Directional Ion Transport Channels for Aqueous Rechargeable Batteries with Impressive Performance. 2022 , 12, 1920	0
201	Molecular Dynamics Study of the Thermodynamics of Integer Charge Transfer vs Charge-Transfer Complex Formation in Doped Conjugated Polymers.	1
200	Direct Crystallization Resolution of Racemates Enhanced by Chiral Nanorods: Experimental, Statistical, and Quantum Mechanics/Molecular Dynamics Simulation Studies.	0
199	Molecular models for O2 and N2 from the second virial coefficient. 2022 , 360, 119419	
198	Mapping the deformability of natural and designed cellulosomes in solution. 2022 , 15,	1
197	Structural and inhibitory effects of fulvic and humic acids against tyrosinase.	2
196	Liquid-Liquid Criticality in the WAIL Water Model.	6
195	Water network in the binding pocket of fluorinated BPTI-Trypsin complexes - insights from simulation and experiment.	
194	Micelle Dynamic Reconstruction to Effectively Modulate the Transmission of Smart Windows.	
193	Disulfide Isomerization in nDsbD-DsbC Complex - Exploring an Internal Nucleophile Mediated Reaction Pathway.	
192	Mixed Ligand Mononuclear Copper(II) Complex as a Promising Anticancer Agent: Interaction Studies with DNA/HSA, Molecular Docking, and In Vitro Cytotoxicity Studies.	0
191	Anion-Sensing Properties of Cyclopentaphenylalanine. 2022 , 27, 3918	
190	Insights into the Phase Diagram of Pluronic L64 Using Coarse-Grained Molecular Dynamics Simulations.	0
189	Spectroscopic, electronic structure, molecular docking, and molecular dynamics simulation study of 7-Trifluoromethyl-1H-indole-2-carboxylic acid as an aromatase inhibitor. 2022 , 280, 121530	

- 188 Phenyl glycine incorporated glitazones as promising novel antidiabetic agents through PPAR α agonism: Design, synthesis and preclinical studies. **2022**, 6, 100067
- 187 Synthesis of New Hydrazones using a biodegradable catalyst, their Biological Evaluations and Molecular Modeling Studies (Part-II). 2
- 186 Engineered Design of the E-Helix Structure on Ferritin Nanoparticles. **2022**, 5, 3167-3179
- 185 Structure and Property of Alkylated Graphene Oxide Depending on the Chain Length: Grand Canonical Monte Carlo-Molecular Dynamics Approach.
- 184 Conductance Switching in Liquid Crystal-Inspired Self-Assembled Monolayer Junctions. **2022**, 14, 31044-31053 o
- 183 Solubility of Organic Salts in Solvent Δ Antisolvent Mixtures: A Combined Experimental and Molecular Dynamics Simulations Approach.
- 182 Fusion of two unrelated protein domains in a chimera protein and its 3D prediction. Justification of the X-ray reference structures as a prediction benchmark.
- 181 Binary droplet interactions in shear water-in-oil emulsion: A molecular dynamics study. **2022**, 119823
- 180 Insights from Incorporating Quantum Computing into Drug Design Workflows. o
- 179 Induction of 2-hydroxycatecholestrogens O-methylation: A missing puzzle piece in diagnostics and treatment of lung cancer. **2022**, 55, 102395 o
- 178 Molecular docking and machine learning affinity prediction of compounds identified upon softwood bark extraction to the main protease of the SARS-CoV-2 virus. **2022**, 288, 106854 o
- 177 In silico analysis of SARS-CoV-2 spike protein N501Y and N501T mutation effects on human ACE2 binding. **2022**, 116, 108260
- 176 Effects of Lipid Shape and Interactions on the Conformation, Dynamics, and Curvature of Ultrasound-Responsive Liposomes. **2022**, 14, 1512 o
- 175 Artificial jelly channel inspired by the shark for sensing specific ions and environmental perturbation. **2022**, 26, 101047
- 174 Understanding ion diffusion in anion exchange membranes; effects of morphology and mobility of pendant cationic groups. 1
- 173 Structure and Diffusion of Ionic PDMS Melts. **2022**, 14, 3070 o
- 172 Computer Simulation of the interaction between SARS-CoV-2 Spike Protein and the Surface of Coinage Metals. o
- 171 Impact of bilayer composition on the dimerization properties of the Slg1 stress sensor TMD from a multiscale analysis $\hat{\Delta}$

- 170 Molecular dynamics simulations reveal the inhibitory mechanism of Withanolide A against β -glucosidase and α -amylase. 1-16 1
- 169 The Complexation between Siloxane Species and Methylsiloxane: Electronic Structure, Thermodynamic, and Interaction Characteristics. **2022**, 7,
- 168 Neurospecific fabrication and toxicity assessment of a PNIPAM nanogel encapsulated with trans-tephrostachin for blood-brain-barrier permeability in zebrafish model. **2022**, 8, e10237
- 167 Polymyxins induce lipid scrambling and disrupt the homeostasis of Gram-negative bacteria membrane. **2022**, 0
- 166 Mechanistic insights into the clinical Y96D mutation with acquired resistance to AMG510 in the KRASG12C. 12, 0
- 165 JM-20, a Benzodiazepine-Dihydropyridine Hybrid Molecule, Inhibits the Formation of Alpha-Synuclein-Aggregated Species. 0
- 164 Impact of Polydopamine Nanoparticle Surface Pattern and Roughness on Interactions with Poly(ethylene glycol) in Aqueous Solution: A Multiscale Modeling and Simulation Study. **2022**, 126, 6301-6313
- 163 Using Metadynamics To Explore the Free Energy of Dewetting in Biologically Relevant Nanopores. 0
- 162 Explaining the interaction of mangiferin with MMP-9 and NF- κ B: a computational study. **2022**, 28,
- 161 Observation of strong synergy in the interfacial water response of binary ionic and non-ionic surfactant mixtures.
- 160 Identification of new small molecule monoamine oxidase-B inhibitors through pharmacophore-based virtual screening, molecular docking and molecular dynamics simulation studies. 1-22 0
- 159 Exploring the Dynamics of Shikimate Kinase through Molecular Mechanics. **2022**, 2, 194-202
- 158 Molecular Dynamics Study of the Aggregation Behavior of N,N,N',N'-Tetraoctyl Diglycolamide. **2022**, 126, 6290-6300 0
- 157 Coarse-Grained Molecular Dynamics Simulation of Cobalt Nanoparticle in the n-Octacosane/Water Mixture: The Effect of Water Concentration and Nanoparticle Size. **2022**, 126, 13975-13985
- 156 Molecular Dynamics Simulations of Adsorption of SARS-CoV-2 Spike Protein on Polystyrene Surface. **2022**, 62, 3814-3824 4
- 155 Mechanistic Insights into the Long-range Allosteric Regulation of KRAS Via Neurofibromatosis Type 1 (NF1) Scaffold Upon SPRED1 Loading. **2022**, 434, 167730 2
- 154 Nanoscale tribological aspects of chemical mechanical polishing: A review. **2022**, 11, 100286 0
- 153 Remote communication between unstructured and structured regions of Bcl-2 tunes its ligand binding capacity: Mechanistic insights. **2022**, 100, 107736

- 152 Solvation properties of silver ions in ionic liquids using attenuated total reflectance ultraviolet spectroscopy. **2022**, 364, 119998
- 151 Superhydrophilicity of alumina surfaces results from tight binding of interfacial waters to specific aluminols. **2022**, 628, 943-954
- 150 Elucidating structure and dynamics of glutathione S-transferase from *Rhipicephalus (Boophilus) microplus*. 1-9
- 149 Understanding CO₂ absorption by an ammonium-based ionic liquid confined in porous carbon material under applied voltage. **2022**, 366, 120227
- 148 Nicotinonitrile-derived apoptotic inducers: Design, synthesis, X-ray crystal structure and Pim kinase inhibition. **2022**, 129, 106126
- 147 Structural elucidation of a novel polysaccharide from *Ophiopogonis Radix* and its self-assembly mechanism in aqueous solution. **2023**, 402, 134165
- 146 Fragment-based design of cyanoacrylates and cyanoacrylamides targeting Dengue and Zika NS2B/NS3 proteases.
- 145 Deciphering the effect of mutations in MMAA protein causing methylmalonic acidemia: a computational approach. **2022**, 199-220
- 144 Noncovalent Modification of Single Wall Carbon Nanotubes (SWCNTs) by Thienothiophene Derivatives.
- 143 QM/MM Simulations for the Broken-Symmetry Catalytic Reaction Mechanism of Human Arginase I. **2022**, 7, 32536-32548
- 142 Competitive formation of molecular inclusion complexes of chlordecone and hexachlorocyclohexane with natural cyclodextrins: DFT and Molecular Dynamics study.
- 141 Sitosterol could serve as a dual inhibitor of *Trypanosoma congolense* sialidase and phospholipase A₂: in vitro kinetic analyses and molecular dynamic simulations.
- 140 Chirality Discrimination at Binary Organic|Water Interfaces Monitored by Interfacial Tension Measurements With Preliminary Comparison With MD Simulations.
- 139 Molecular Dynamics Simulations on the Elastic Properties of Polypropylene Bionanocomposite Reinforced with Cellulose Nanofibrils. **2022**, 12, 3379
- 138 Identification of Potential New *Aedes aegypti* Juvenile Hormone Inhibitors from N-Acyl Piperidine Derivatives: A Bioinformatics Approach. **2022**, 23, 9927
- 137 Empagliflozin induces apoptotic-signaling pathway in embryonic vasculature: In vivo and in silico approaches via chick yolk sac membrane model. 13,
- 136 Conformational Heterogeneity and Interchain Percolation Revealed in an Amorphous Conjugated Polymer. **2022**, 16, 14432-14442
- 135 Adsorption of Hexavalent Chromium Using Activated Carbon Produced from *Sargassum* ssp.: Comparison between Lab Experiments and Molecular Dynamics Simulations. **2022**, 27, 6040

- 134 Effect of Tacticity and Degree of Sulfonation of Polystyrene Sulfonate on Calcium-Binding Behavior in the Presence of Dodecyl Sulfate. **2022**, 61, 13442-13452 0
- 133 Nanostructuring with Surfactants: The Self-Assembly of a New Poly(thiophene-phenylene) Conjugated Polymer Bearing Azacrown Ether Pendant Groups. **2022**, 38, 11845-11859 0
- 132 Modeling Absorption and Emission Spectroscopies of Symmetric and Asymmetric Azaoxahelicenes in Vacuum and Solution. **2022**, 126, 6467-6472 1
- 131 Effects of the pH Value on the Electrodeposition of Fe²⁺ Alloy as a Magnetic Film Material. **2022**, 126, 15472-15484 1
- 130 Competitive Photoisomerization and Energy Transfer Processes in Fluorescent Multichromophoric Systems. 0
- 129 Expanding the Substrate Scope of Native Amine Dehydrogenases through In Silico Structural Exploration and Targeted Protein Engineering. 0
- 128 Study on Lubricant Release-Recycle Performance of Porous Polyimide Retainer Materials. **2022**, 38, 11440-11450 0
- 127 Shear and cooling induced regulation of mechanical properties and glass transition temperature of isotactic polypropylene. **2022**, 0
- 126 Directed Self-Assembly of Conducting Polymer Nanofilms on Single-Crystalline Ice Facets. 1
- 125 Hydrogen Bond Thermodynamics in Aqueous Acid Solutions: A Combined DFT and Classical Force-Field Approach. 1
- 124 A dynamical view of protein-protein complexes: Studies by molecular dynamics simulations. 9, 1
- 123 A whole genome sequencing approach to anterior cruciate ligament rupture—twin study in two unrelated families. **2022**, 17, e0274354 0
- 122 Curvature model for nanoparticle size effects on peptide fibril stability and molecular dynamics simulation data. **2022**, 45, 108598 1
- 121 Partial peptide dissociation and binding groove plasticity in two major histocompatibility complex class I alleles—differences between alleles versus force field and sampling effects. **2022**, 12, 29908-29914 0
- 120 Conformational Preferences of Pyridone Adenine Dinucleotides from Molecular Dynamics Simulations. **2022**, 23, 11866 0
- 119 In silico investigation of endoglucanase produced by *Bacillus inaquosorum* KCTC 13429 for valorisation of lignocellulosic biomass. 0
- 118 Hierarchical Virtual Screening and Binding Free Energy Prediction of Potential Modulators of *Aedes Aegypti* Odorant-Binding Protein 1. **2022**, 27, 6777 0
- 117 Molecular insights into the binding of carnosine and anserine to human serum carnosinase 1 (CN1). 4, e25 0

- 116 Crystal structure determination, molecular docking and dynamics of arylidene cyanoacetates as potential JNK-3 inhibitors for Ischemia reperfusion injury. 1-9 0
- 115 Hydrophobicity Determines the Bacterial Killing Rate of α -Helical Antimicrobial Peptides and Influences the Bacterial Resistance Development. 2
- 114 Quantum-based machine learning and AI models to generate force field parameters for drug-like small molecules. 9, 0
- 113 Short-Range Cooperative Slow-down of Water Solvation Dynamics Around $\text{SO}_4^{2-}\text{Mg}^{2+}$ Ion Pairs. 0
- 112 Observing How Glutathione and S-Hexyl Glutathione Bind to Glutathione S-Transferase from *Rhipicephalus (Boophilus) microplus*. **2022**, 23, 12775 0
- 111 Kinetics of Acid-Catalyzed Dehydration of Alcohols in Mixed Solvent Modeled by Multiscale DFT/MD. 13193-13206 0
- 110 Evaluation of a Novel Synthetic Peptide Derived from Cytolytic Mycotoxin Candidalysin. **2022**, 14, 696 0
- 109 Evaluating Allosteric Perturbations in Cannabinoid Receptor 1 by In Silico Single-Point Mutation. **2022**, 7, 37873-37884 0
- 108 Identifying Strategies to Experimentally Probe Multidimensional Dynamics in the Ribosome. **2022**, 126, 8460-8471 0
- 107 High-Throughput Molecular Dynamics-Based Alchemical Free Energy Calculations for Predicting the Binding Free Energy Change Associated with the Selected Omicron Mutations in the Spike Receptor-Binding Domain of SARS-CoV-2. **2022**, 10, 2779 0
- 106 Comparative analyses and molecular videography of MD simulations on WT human SOD1. **2022**, 1217, 113929 0
- 105 Structural insights into conformational stability and binding of thiazolo-[2,3-b] quinazolinone derivatives with EGFR-TKD and in-vitro study. **2022**, 29, 103478 0
- 104 Three birds with one stone: Microphase separation induced by densely grafted short chains in ion conducting membranes. **2022**, 664, 121119 0
- 103 Molecular study of endo and phytocannabinoids on lipid membranes of different composition. **2023**, 221, 113020 0
- 102 Mechanistic Insights into the Protection Effect of Argonaute α BNA Complex on the HCV Genome. **2022**, 12, 1631 0
- 101 Topological origin of the protein folding transition. **2022**, 106, 0
- 100 Hydrogen-bonded networks in alcohol-acetone binary mixtures: molecular dynamics study. **2022**, 28, 0
- 99 Molecular dynamics simulations of the spike trimeric ectodomain of the SARS-CoV-2 Omicron variant: structural relationships with infectivity, evasion to immune system and transmissibility. 1-18 1

- 98 Sesquiterpenoids from the rhizomes of *Homalomena pendula* (Blume) Bakh.f showing acetylcholinesterase inhibitory activity: in vitro and in silico studies. 1
- 97 Insights into the binding interaction of Reactive Yellow 145 with human serum albumin from a biophysics point of view. **2022**, 120800 0
- 96 Explicit Projection of Stokes Shifts onto Solvent Motion in an Aqueous Liquid and Linear Response Theory. **2022**, 126, 9168-9175 0
- 95 Explicit Models of Motion to Understand Protein Side-Chain Dynamics. **2022**, 129, 0
- 94 Modelling diffusive transport of particles interacting with slit nanopore walls: The case of fullerenes in toluene filled alumina pores. **2022**, 120636 0
- 93 In silico designed microtubule-stabilizer drugs against tauopathy in Alzheimer's disease. 1-21 0
- 92 Aggregation Behavior of Nitrilotriacetamide (NTAmide) Ligands in Thorium(IV) Extraction from Acidic Medium: Small-Angle Neutron Scattering, Fourier Transform Infrared, and Theoretical Studies. 0
- 91 The impact of bilayer composition on the dimerization properties of the Slg1 stress sensor TMD from a multiscale analysis. 0
- 90 The tailoring of nanofiltration membrane structure for mono/divalent anions separation via precisely adjusting the reaction site distance. **2023**, 668, 121252 0
- 89 Insights into pathways and solvent effects of fructose dehydration to 5-hydroxymethylfurfural in acetone-water solvent. **2023**, 267, 118352 0
- 88 How Do Salt and Lipids Affect Conformational Dynamics of A β 42 Monomers in Water?. 0
- 87 An In-silico Comparative study of Curcumin and 2-deoxy Uridine Nucleoside Derivatives: Reveals the Role of Angiogenin in ER Stress Induced Apoptosis Signaling. 0
- 86 Molecular dynamics simulation study on *Bacillus subtilis* EngA: the presence of Mg²⁺ at the active-sites promotes the functionally important conformation. 1-13 0
- 85 Sampling the Bulk Viscosity of Water with Molecular Dynamics Simulation in the Canonical Ensemble. **2022**, 126, 10172-10184 0
- 84 In Silico and Structure-Based Assessment of Similar Variants Discovered in Tandem Repeats of BRCT Domains of BRCA1 and BARD1 To Characterize the Folding Pattern. **2022**, 7, 44772-44785 1
- 83 Water Network in the Binding Pocket of Fluorinated BPTI-Trypsin Complexes-Insights from Simulation and Experiment. **2022**, 126, 9985-9999 0
- 82 Computational Study of Helicase from SARS-CoV-2 in RNA-Free and Engaged Form. **2022**, 23, 14721 0
- 81 Targeted photodynamic neutralization of SARS-CoV-2 mediated by singlet oxygen. 0

80	Computer Simulation of the Interaction between SARS-CoV-2 Spike Protein and the Surface of Coinage Metals. 2022 , 38, 14673-14685	1
79	Thermodynamic Driving Forces for Divalent Cations Binding to Zwitterionic Phospholipid Membranes. 2022 , 13, 11237-11244	0
78	Discovery of octahydropyrrolo [3,2-b] pyridin derivative as a highly selective Type I inhibitor of FGFR3 over VEGFR2 by high-throughput virtual screening.	1
77	NEK7 activates the NLRP1 Inflammasome.	0
76	Environmentally Friendly Strategy for Treating In Situ Leaching Solutions of Ion-Adsorption Type Yttrium-Rich Heavy Rare-Earth Ore by a Bubble-Supported Organic Liquid Membrane. 2022 , 10, 17094-17106	0
75	Internal Normal Mode Analysis applied to RNA flexibility and conformational changes.	0
74	Complete Structural Predictions of the Proteome of African Swine Fever Virus Strain Georgia 2007. 2022 , 11,	2
73	Discovery and Characterization of a Functional scFv for CCR2 Inhibition via an Extracellular Loop. 2022 , 122547	0
72	Design, Synthesis, and Characterization of a Novel 2 β -Linked Amikacin-Binding Aptamer: An Experimental and MD Simulation Study. 2022 , 17, 3478-3488	0
71	Repurposing antibiotics as potent multi-drug candidates for SARS-CoV-2 delta and omicron variants: molecular docking and dynamics. 1-11	0
70	Structural characterization of an intrinsically disordered protein complex using integrated small-angle neutron scattering and computing.	0
69	Effect of salinity on water/oil interface with model asphaltene and non-ionic surfactant: Insights from molecular simulations. 2022 , 126944	0
68	Molecular dynamics simulation of cancer cell membrane perforated by shockwave induced bubble collapse. 2022 , 157, 225102	0
67	Molecular characterization of glutor-GLUT interaction and prediction of glutor β drug-likeness: implications for its utility as an antineoplastic agent. 1-12	0
66	Adsorption kinetics investigation of surfactant molecules at the short-chain alkane-water interface. 2022 , 130867	0
65	Insights from incorporating quantum computing into drug design workflows.	0
64	Force Probe Molecular Dynamics Simulations. 2005 , 493-515	6
63	Ligands-Induced Open-Close Conformational Change during DapE Catalysis: Insights from Molecular Dynamics Simulations.	0

- 62 Exploring the structural and dynamic differences between human carnosinase I (CN1) and II (CN2).
- 61 A molecular insight into the dehydration of metal-organic framework and its impact on the CO₂ capture.
- 60 On the Propensity of Excess Hydroxide Ions at the Alcohol MonolayerâWater Interface.
- 59 gmak: A Parameter-Space Mapping Strategy for Force-Field Calibration.
- 58 Drug Design, Molecular Docking and Dynamics Studies on the Interaction of Voxelotor, L-Glutamine and Hydroxy Urea with Human Carbonmonoxy Hemoglobin S.
- 57 Effect of microwave electric field on asphaltene aggregation in a heavy oil system: MD and DFT investigation. **2023**, 372, 121212
- 56 Role of distal sites in enzyme engineering. **2023**, 63, 108094
- 55 Polyelectrolyte Influence on Beta-Hairpin Peptide Stability: A Simulation Study. **2023**, 127, 359-370
- 54 Scalability and efficiency challenges for the exascale supercomputing system: practice of a parallel supporting environment on the Sunway exascale prototype system. **2023**, 24, 41-58
- 53 Molecular Simulation of CO₂ and H₂ Encapsulation in a Nanoscale Porous Liquid. **2023**, 13, 409
- 52 A Top-down and Bottom-up Combined Strategy for Parameterization of Coarse-grained Force Fields for Phospholipids.
- 51 Molecular docking and simulation studies against nucleoside diphosphate kinase (NDK) of *Pseudomonas aeruginosa* with secondary metabolite identified by genome mining from *paenibacillusehimensis*. 1-10
- 50 Trimeric Architecture Ensures the Stability and Biological Activity of the Calf Purine Nucleoside Phosphorylase: In Silico and In Vitro Studies of Monomeric and Trimeric Forms of the Enzyme. **2023**, 24, 2157
- 49 Effect of Charge State on the Equilibrium and Kinetic Properties of Mechanically Interlocked [5]Rotaxane: A Molecular Dynamics Study. **2023**, 127, 1254-1263
- 48 Coevolution and smFRET Enhances Conformation Sampling and FRET Experimental Design in Tandem PDZ1â2 Proteins. **2023**, 127, 884-898
- 47 Druggable sites identification in *Streptococcus mutans* VicRK system evaluated by catechols. 1-16
- 46 Long-Lived States Provide Insights from NMR into the β -Cyclodextrin Drug Assemblies. **2023**, 127, 1158-1167
- 45 Molecular Simulations on the Coalescence of Water-in-Oil Emulsion Droplets with Non-ionic Surfactant and Model Asphaltene.

- 44 Impact and structure of water in aqueous octanol mixtures: Hz-GHz dielectric relaxation measurements and computer simulations. **2023**, 439, 114600
- 43 Antiviral activity and molecular modeling studies on 1H-indole-2,3-diones carrying a naphthalene moiety. **2023**, 1281, 135100
- 42 Coumarin-based derivatives targeting Trypanosoma cruzi cruzain and Trypanosoma brucei cathepsin L-like proteases.
- 41 Bridging Thermodynamics, Antimicrobial Activity, and pH Sensitivity of Cationic Membranolytic Heptapeptides—Computational and Experimental Study.
- 40 Synthesis of benzylidene-indandione derivatives as quantification of amyloid fibrils. **2023**, 296, 106982
- 39 Identification and structure-activity modeling of ACE inhibitory peptides demonstrating anti-inflammatory effects: Extracted from Antheraea assama and Philosomia ricnii pupae. **2023**, 53, 102625
- 38 Molecular dynamics simulation study on interfacial behaviors of betaines and extended surfactants. **2023**, 666, 131323
- 37 Hierarchical Self-Assembly of Organic-Inorganic Hybrid Nanosheets to Construct Tubular Superstructures for Photocatalytic Degradation. **2023**, 6, 6270-6278
- 36 On the Behavior of the Ethylene Glycol Components of Polydisperse Polyethylene Glycol PEG200. **2023**, 127, 1178-1196
- 35 Instigating the in vitro antidiabetic activity of new tridentate Schiff base ligand appended M(II) complexes: From synthesis, structural characterization, quantum computational calculations to molecular docking, and molecular dynamics simulation studies. **2023**, 37,
- 34 Engineering the kinetic stability of a trefoil protein by tuning its topological complexity. 10,
- 33 Targeted photodynamic neutralization of SARS-CoV-2 mediated by singlet oxygen.
- 32 Lessons for Oral Bioavailability: How Conformationally Flexible Cyclic Peptides Enter and Cross Lipid Membranes. **2023**, 66, 2773-2788
- 31 Pseudouridimycin-A Potent Nucleoside Inhibitor of the RNA Polymerase Beta Prime Subunit of Streptococcus pyogenes. **2023**, 8, 7989-8000
- 30 Evaluation of the affinity of asphaltene molecular models A1 and A2 by the water/oil interfaces based on a novel concept of solubility parameter profiles obtained from MD simulations. **2023**, 376, 121430
- 29 How ractopamine binds to bovine serum albumin at the drug site 1. **2023**, 49, 599-607
- 28 Differences in protein distribution, conformation, and dynamics in hard and soft coronas: dependence on protein and particle electrostatics. **2023**, 25, 7496-7507
- 27 Systematic investigation of the mechanism of herbal medicines for the treatment of prostate cancer.

- 26 Hierarchical Aggregation in a Complex Fluid-The Role of Isomeric Interconversion. **2023**, 127, 2052-2065 ○
- 25 Solid phase extraction with rotating cigarette filter for determination of bisphenol A in source and drinking water: computational and analytical studies. **2023**, 39, 607-617 ○
- 24 New insights into the inhibitory effect of phenol carboxylic acid antioxidants on mushroom tyrosinase by molecular dynamic studies and experimental assessment. 1-11 ○
- 23 Molecular architecture and dynamics of SARS-CoV-2 envelope by integrative modeling. **2023**, 31, 492-503.e7 ○
- 22 Effects of Terahertz Radiation on the Aggregation of Alzheimer's A β 2 Peptide. **2023**, 24, 5039 ○
- 21 Effect of cetyl trimethyl ammonium bromide as an electrolyte additive on secondary discharge performance of aluminum-air battery. **2023**, 29, 1887-1899 ○
- 20 Cooperative and structural relationships of the trimeric Spike with infectivity and antibody escape of the strains Delta (B.1.617.2) and Omicron (BA.2, BA.5, and BQ.1). ○
- 19 Quantification and Distribution of Three Types of Hydrogen Bonds in Mixtures of an Ionic Liquid with the Hydrogen-Bond-Accepting Molecular Solvent DMSO Explored by Neutron Diffraction and Molecular Dynamics Simulations. **2023**, 14, 2684-2691 ○
- 18 Synergism for lowering interfacial tensions between betaines and extended surfactants: The role of self-regulating molecular size. **2023**, 378, 121605 ○
- 17 Investigations on molecular interactions of memantine hydrochloride in aqueous solutions by thermophysical methods and molecular dynamics simulations at different temperatures. **2023**, 100, 100967 ○
- 16 Synthesis of vanillin derivatives with 1,2,3-triazole fragments and evaluation of their fungicide and fungistatic activities. ○
- 15 In vivo characterization of the bacterial intramembrane-cleaving protease RseP using the heme binding tag-based assay iCliPSpy. **2023**, 6, ○
- 14 Internal Normal Mode Analysis Applied to RNA Flexibility and Conformational Changes. ○
- 13 Design and Pharmacological Characterization of α 5 β 1 Integrin Cyclopeptide Agonists: Computational Investigation of Ligand Determinants for Agonism versus Antagonism. **2023**, 66, 5021-5040 ○
- 12 Investigation of the Entry Pathway and Molecular Nature of β Receptor Ligands. **2023**, 24, 6367 ○
- 11 Classical Force Field Parameters for InP and InAs Quantum Dots with Various Surface Passivations. **2023**, 127, 3427-3436 ○
- 10 Interfacial water molecules contribute to antibody binding to the receptor-binding domain of SARS-CoV-2 spike protein. 1-10 ○
- 9 Identification and mechanistic exploration of structural and conformational dynamics of NF- κ B inhibitors: rationale insights from in silico and in vitro studies. 1-21 ○

- 8 Unpolarized laser method for infrared spectrum calculation of amide I C O bonds in proteins using molecular dynamics simulation. **2023**, 159, 106902
- 7 Towards Computational Modeling of Ligand Binding to the ILPR G-Quadruplex. **2023**, 28, 3447
- 6 Dynamic and structural properties of porcine serum albumins. 1-8
- 5 Molecular Dynamics Simulations Suggest SARS-CoV-2 3CLpro Mutations in Beta and Omicron Variants Do Not Alter Binding Affinities for Cleavage Sites of Non-Structural Proteins. **2023**, 3, 622-636
- 4 Micro- and Nanoplastics Breach the BloodâBrain Barrier (BBB): Biomolecular CoronaâRole Revealed. **2023**, 13, 1404
- 3 Molecular modeling and DFT studies on the antioxidant activity of Centaurea scoparia flavonoids and molecular dynamics simulation of their interaction with Î²-lactoglobulin. **2023**, 13, 12361-12374
- 2 Effect of double chain anionic surfactant on the dynamic interfacial tensions of betaine solutions. **2023**, 121866
- 1 Radial distribution and hydrogen bonded network graphs of alcohol-aniline binary mixture. **2023**, 29,