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2	2256	Pterosin Sesquiterpenoids from Pteris cretica as Hypolipidemic Agents via Activating Liver X Receptors.		

- 2255 The N2Furfuryl-deoxyguanosine Adduct Does Not Alter the Structure of BDNA. Quantum Mechanics/Extremely Localized Molecular Orbital Method: A Fully Quantum Mechanical Embedding Approach for Macromolecules. Force Field for Mg2+, Mn2+ Zn2+, and Cd2+ Ions That Have Balanced Interactions with Nucleic 2253 Acids. Atomic Resolution Insights into the Structural Aggregations and Optical Properties of Neat Imidazolium-Based Ionic Liquids. Reaction Path Averaging: Characterizing the Structural Response of the DNA Double Helix to 2251 Electron Transfer. 2250 Structure and Dynamics of Electron Injection and Charge Recombination in iMotif DNA Conjugates. Thermodynamic and Transport Properties of Crown-Ethers: Force Field Development and 2249 Molecular Simulations. 2248 Structural and Dynamic Heterogeneity of Capillary Wave Fronts at Aqueous Interfaces. Protein Hydration Thermodynamics: The Influence of Flexibility and Salt on Hydrophobin II 2247 Hydration. 2246 Role of Polyubiquitin Chain Flexibility in the Catalytic Mechanism of CullinRING Ubiquitin Ligases. Computational Analysis of Sugar Alcohols as Phase-Change Material: Insight into the Molecular 2245 Mechanism of Thermal Energy Storage. Accurate Force Field Parameters and pH Resolved Surface Models for Hydroxyapatite to 2244 Understand Structure, Mechanics, Hydration and Biological Interfaces. 2243 Hydrogen Adsorption in a Zeolitic Imidazolate Framework with Ita Topology. Screening Diffusion of Small Molecules in Flexible Zeolitic Imidazolate Frameworks Using a DFT-Parameterized Force Field. 2241 Amide Rotation Hindrance Predicts Proteolytic Resistance of Cystine-Knot Peptides.
- Repair Rate of Clustered Abasic DNA Lesions by Human Endonuclease: Molecular Bases of Sequence Specificity.

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 Modeling Coordination-Directed Self-Assembly of M2L4 Nanocapsule Featuring Competitive Guest Encapsulation.

Alternative Electron-Transfer Channels Ensure Ultrafast Deactivation of Light-Induced Excited 2237 States in Riboflavin Binding Protein. Impact of Electronic State Mixing on the Photoisomerization Time Scale of the Retinal 2236 Chromophore. Nonconventional CHF Hydrogen Bonds Support a Tetrad Flip in Modified GQuadruplexes. Specific Recognition of GQuadruplexes Over Duplex-DNA by a Macromolecular NIR Two-Photon Fluorescent Probe. Molecular Dynamics Simulations Reveal an Interplay between SHAPE Reagent Binding and RNA 2233 Flexibility. Water in Carbon Nanotubes: Pronounced Anisotropy in Dielectric Dispersion and Its Microscopic Origin. Hofmeister Series for Metal-CationRNA Interactions: The Interplay of Binding Affinity and 2231 Exchange Kinetics. 2230 Theoretical Investigations of CO2 and H2 Sorption in Robust Molecular Porous Materials. Stimuli-Responsive Room-Temperature NHeteroacene Liquid: In Situ Observation of the 2229 Self-Assembling Process and Its Multiple Properties. Integrated Computational Study of the Cu-Catalyzed Hydration of Alkenes in Water Solvent and 2228 into the Context of an Artificial Metallohydratase. How To Break the Janus Effect of H2O2 in Biocatalysis? Understanding Inactivation Mechanisms To 2227 Generate more Robust Enzymes. 2226 Molecular-Scale Interfacial Model for Predicting Electrode Performance in Rechargeable Batteries. Computational Design of Non-natural Sugar Alcohols to Increase Thermal Storage Density: Beyond 2225 Existing Organic Phase Change Materials. Hydration Dynamics of a Peripheral Membrane Protein. 2223 Small Details Matter: The 2-Hydroxyl as a Conformational Switch in RNA. Absorption of Low-Energy UV Radiation by Human Telomere GQuadruplexes Generates Long-Lived 2222 Guanine Radical Cations. Water Sculpts the Distinctive Shapes and Dynamics of the Tumor-Associated Carbohydrate Tn 2221 Antigens: Implications for Their Molecular Recognition. Exploring the Role of the Third Active Site Metal Ion in DNA Polymerase with QM/MM Free Energy 2220 Simulations.

2203 .

Nanoarchitecture through Strained Molecules: Cubane-Derived Scaffolds and the Smallest Carbon 2219 Nanothreads. Molecular Mechanism behind Solvent Concentration-Dependent Optimal Activity of Thermomyces 2218 lanuginosus Lipase in a Biocompatible Ionic Liquid: Interfacial Activation through Arginine Switch. Perfluoropolyethers: Development of an All-Atom Force Field for Molecular Simulations and 2217 Validation with New Experimental Vapor Pressures and Liquid Densities. Density Functional Computations and Molecular Dynamics Simulations of the Triethylammonium 2216 Triflate Protic Ionic Liquid. Identification of the Deprotonated Pyrrole Nitrogen of the Bilin-Based Photoreceptor by Raman 2215 Spectroscopy with an Advanced Computational Analysis. 2214 Computational and Spectroscopic Characterization of the Photocycle of an Artificial Rhodopsin. Excited-State Vibronic Dynamics of Bacteriorhodopsin from Two-Dimensional Electronic Photon 2213 Echo Spectroscopy and Multiconfigurational Quantum Chemistry. 2212 Space and Time Evolution of the Electrostatic Potential During the Activation of a Visual Pigment. 2211 Extending the Nonbonded Cationic Dummy Model to Account for Ion-Induced Dipole Interactions. How Inter- and Intramolecular Processes Dictate Aggregation-Induced Emission in Crystals 2210 Undergoing Excited-State Proton Transfer. Multistate Multiconfiguration Quantum Chemical Computation of the Two-Photon Absorption 2209 Spectra of Bovine Rhodopsin. 2208 Comprehensive Study of Guanine Excited State Relaxation and Photoreactivity in Gquadruplexes. Molecular Bases of DNA Packaging in Bacteria Revealed by All-Atom Molecular Dynamics 2207 Simulations: The Case of Histone-Like Proteins in Borrelia burgdorferi. Potassium Ions Enhance Guanine Radical Generation upon Absorption of Low-Energy Photons by GQuadruplexes and Modify Their Reactivity. 2205 Self-Assembly of Escin Molecules at the AirWater Interface as Studied by Molecular Dynamics. 2204 Vibrational Analysis of Semicrystalline Polyethylene Using Molecular Dynamics Simulation.

2202 Silver-Mediated Double Helix: Structural Parameters for a Robust DNA Building Block.

2201	Smelling Sulfur: Copper and Silver Regulate the Response of Human Odorant Receptor OR2T11 to Low-Molecular-Weight Thiols.	
2200	Resolving the Conformational Dynamics of DNA with Angstrom Resolution by Pulsed ElectronElectron Double Resonance and Molecular Dynamics.	
2199		
2198	Dihedral Angle Calculations To Elucidate the Folding of Peptides through Its Main Mechanical Forces.	
2197	Investigating the Effects of Linker Extension on H2 Sorption in the rht-MetalOrganic Framework NU-111 by Molecular Simulations.	
2196	Investigating CO2 Sorption in SIFSIX-3M (M = Fe, Co, Ni, Cu, Zn) through Computational Studies.	
2195	Cu(II)-Based Paramagnetic Probe to Study RNAProtein Interactions by NMR.	
2194	Molecular Mechanism, Dynamics, and Energetics of Protein-Mediated Dinucleotide Flipping in a Mismatched DNA: A Computational Study of the RAD4-DNA Complex.	
2193	Force Field Benchmark of Amino Acids: I. Hydration and Diffusion in Different Water Models.	
2192	Dynamic and Structural Modeling of the Specificity in ProteinDNA Interactions Guided by Binding Assay and Structure Data.	
2191	Computational Probing of WatsonCrick/Hoogsteen Breathing in a DNA Duplex Containing N1-Methylated Adenine.	
2190	Fitting Corrections to an RNA Force Field Using Experimental Data.	
2189	Constraining Endomorphin1 by ,-Hybrid Dipeptide/Heterocycle Scaffolds: Identification of a Novel Opioid Receptor Selective Partial Agonist.	
2188	Succinimide-Based Conjugates Improve IsoDGR Cyclopeptide Affinity to v3 without Promoting Integrin Allosteric Activation.	
2187	AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules. 1995 , 91, 1-41	2509
2186	Application of the multimolecule and multiconformational RESP methodology to biopolymers: Charge derivation for DNA, RNA, and proteins. 1995 , 16, 1357-1377	820
2185	Applications of free energy derivatives to analog design. 1995 , 3, 106-122	7
2184	Calibration of ring-current effects in proteins and nucleic acids. 1995 , 6, 341-6	80

2183	Potential energy functions. 1995 , 5, 205-10		84
2182	Molecular Dynamics Potential of Mean Force Calculations: A Study of the TolueneAmmonium ECation Interactions. <i>Journal of the American Chemical Society</i> , 1996 , 118, 2998-3005	16.4	85
2181	Performance of the AMBER94, MMFF94, and OPLS-AA Force Fields for Modeling Organic Liquids. 1996 , 100, 18010-18013		220
2180	Electrostatics of a simple membrane model using Green's functions formalism. 1996 , 71, 795-810		23
2179	Bending of DNA by the mitomycin C-induced, GpG intrastrand cross-link. 1996 , 9, 382-9		54
2178	Investigation of the proton-assisted pathway to formation of the catalytically active, ferryl species of P450s by molecular dynamics studies of P450eryF. <i>Journal of the American Chemical Society</i> , 1996 , 118, 6377-87	16.4	45
2177	Time Evolution of NMR Proton Chemical Shifts of an RNA Hairpin during a Molecular Dynamics Simulation. <i>Journal of the American Chemical Society</i> , 1996 , 118, 12812-12820	16.4	13
2176	Structural features of a six-nucleotide RNA hairpin loop found in ribosomal RNA. 1996 , 35, 6539-48		62
2175	Conformations and Dynamics of the Essential Cysteinyl-Cysteine Ring Derived from the Acetylcholine Receptor □ Journal of the American Chemical Society, 1996 , 118, 13031-13039	16.4	15
2174	Investigation of the structural basis for thermodynamic stabilities of tandem GU mismatches: solution structure of (rGAGGUCUC)2 by two-dimensional NMR and simulated annealing. 1996 , 35, 1407	7-89	303
2174		7-89 16.4	
	solution structure of (rGAGGUCUC)2 by two-dimensional NMR and simulated annealing. 1996 , 35, 1407 Benzene Dimer: A Good Model for Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. <i>Journal of the</i>		265
2173	solution structure of (rGAGGUCUC)2 by two-dimensional NMR and simulated annealing. 1996, 35, 1407 Benzene Dimer: A Good Model for Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1996, 118, 11217-11224 Computational Simulations of DNA Distortions by a cis,syn-Cyclobutane Thymine Dimer Lesion	16.4	265 66
2173	solution structure of (rGAGGUCUC)2 by two-dimensional NMR and simulated annealing. 1996, 35, 1407 Benzene Dimer: A Good Model for Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1996, 118, 11217-11224 Computational Simulations of DNA Distortions by a cis,syn-Cyclobutane Thymine Dimer Lesion <i>Journal of the American Chemical Society</i> , 1996, 118, 9156-9163 Identification of Putative Peroxide Intermediates of Peroxidases by Electronic Structure and	16.4	265 66
2173 2172 2171	solution structure of (rGAGGUCUC)2 by two-dimensional NMR and simulated annealing. 1996, 35, 1407 Benzene Dimer: A Good Model for Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1996, 118, 11217-11224 Computational Simulations of DNA Distortions by a cis,syn-Cyclobutane Thymine Dimer Lesion <i>Journal of the American Chemical Society</i> , 1996, 118, 9156-9163 Identification of Putative Peroxide Intermediates of Peroxidases by Electronic Structure and Spectra Calculations. <i>Journal of the American Chemical Society</i> , 1996, 118, 10588-10594 Studies on selectin blocker. 3. Investigation of the carbohydrate ligand sialyl Lewis X recognition	16.4	2656656
2173 2172 2171 2170	Benzene Dimer: A Good Model for Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1996 , 118, 11217-11224 Computational Simulations of DNA Distortions by a cis,syn-Cyclobutane Thymine Dimer Lesion <i>Journal of the American Chemical Society</i> , 1996 , 118, 9156-9163 Identification of Putative Peroxide Intermediates of Peroxidases by Electronic Structure and Spectra Calculations. <i>Journal of the American Chemical Society</i> , 1996 , 118, 10588-10594 Studies on selectin blocker. 3. Investigation of the carbohydrate ligand sialyl Lewis X recognition site of P-selectin. 1996 , 39, 4547-53 Active site of bee venom phospholipase A2: the role of histidine-34, aspartate-64 and tyrosine-87.	16.4	265665620
2173 2172 2171 2170 2169	Benzene Dimer: A Good Model for Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1996 , 118, 11217-11224 Computational Simulations of DNA Distortions by a cis,syn-Cyclobutane Thymine Dimer Lesion <i>Journal of the American Chemical Society</i> , 1996 , 118, 9156-9163 Identification of Putative Peroxide Intermediates of Peroxidases by Electronic Structure and Spectra Calculations. <i>Journal of the American Chemical Society</i> , 1996 , 118, 10588-10594 Studies on selectin blocker. 3. Investigation of the carbohydrate ligand sialyl Lewis X recognition site of P-selectin. 1996 , 39, 4547-53 Active site of bee venom phospholipase A2: the role of histidine-34, aspartate-64 and tyrosine-87. 1996 , 35, 4591-601 Elucidating the Origin of Conformational Energy Differences in Substituted 1,3-Dioxanes: A	16.4	265 66 56 20 45

2165	Observation of the A-DNA to B-DNA transition during unrestrained molecular dynamics in aqueous solution. 1996 , 259, 434-44		269
2164	NMR solution structure of Cu(I) rusticyanin from Thiobacillus ferrooxidans: structural basis for the extreme acid stability and redox potential. 1996 , 263, 752-67		85
2163	Dynamic contributions to the DNA binding entropy of the EcoRI and EcoRV restriction endonucleases. 1996 , 264, 546-55		24
2162	Including Side Chain Flexibility in Continuum Electrostatic Calculations of Protein Titration. 1996, 100, 20156-20163		106
2161	Calculations of nucleic acid conformations. 1996 , 6, 289-98		88
2160	Thermodynamics of base pairing. 1996 , 6, 299-304		82
2159	Organic crystals: engineering and design. 1996 , 1, 501-505		16
2158	Back-Skip of the Growing Chain at Model Complexes for the Metallocene Polymerization Catalysis. 1996 , 29, 4834-4845		82
2157	Solution structure of a naturally-occurring zinc-peptide complex demonstrates that the N-terminal zinc-binding module of the Lasp-1 LIM domain is an independent folding unit. 1996 , 35, 12723-32		49
2156	Hybrid Quantum and Molecular Mechanical Simulations: An Alternative Avenue to Solvent Effects in Organic Chemistry. 1996 , 29, 298-305		467
2155	Hydration of C-H groups in tRNA. 1996 , 151-73		40
2154	Crystal Structures and Properties of Nylon Polymers from Theory. <i>Journal of the American Chemical Society</i> , 1996 , 118, 12291-12301	16.4	180
2153	Geometric Parameters in Nucleic Acids: Nitrogenous Bases. <i>Journal of the American Chemical Society</i> , 1996 , 118, 509-518	16.4	174
2152	Direct evidence for modified solvent structure within the hydration shell of a hydrophobic amino acid. 1996 , 93, 10769-74		78
2151	Individual Reduction Potentials of the Iron Ions in Fe(2)S(2) and High-Potential Fe(4)S(4) Ferredoxins. 1996 , 35, 4248-4253		43
2150	Using molecular modeling and molecular dynamics simulation to predict P450 oxidation products. 1996 , 272, 347-57		7
2149	Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids. <i>Journal of the American Chemical Society</i> , 1996 , 118, 11225-11236	16.4	9849
2148	Solvent and counterion effects on complexation selectivity by conformationally locked calix[4]-bis-crown ligands: Molecular Dynamics and Free Energy Perturbation studies in water and methanol, acetonitrile and chloroform solutions. 1996 , 363, 67-85		37

2147	Probing protein electrostatic interactions through temperature/reduction potential profiles. 1996 , 1, 515-522	20
2146	Molecular Modeling of Host-Guest Inclusion Compounds: Calculations and Practical Application to Chemical Sensors. 1996 , 2, 410-416	6
2145	Chlorinated ethanes in aqueous solution: parameterization based on thermodynamics of hydration. 1996 , 259, 142-145	1
2144	Application of the message-address concept to the docking of naltrexone and selective naltrexone-derived opioid antagonists into opioid receptor models. 1996 , 21, 1287-94	84
2143	Computational tools for structure-based ligand design. 1996 , 66, 197-210	28
2142	Was llisich aus der molekularen Erkennung in Protein-Ligand-Komplexen fildas Design neuer Wirkstoffe lernen?. 1996 , 108, 2750-2778	35
2141	Merck molecular force field. I. Basis, form, scope, parameterization, and performance of MMFF94. 1996 , 17, 490-519	3435
2140	Merck molecular force field. II. MMFF94 van der Waals and electrostatic parameters for intermolecular interactions. 1996 , 17, 520-552	799
2139	Alternative approaches to potential of mean force calculations: Free energy perturbation versus thermodynamic integration. Case study of some representative nonpolar interactions. 1996 , 17, 1112-1131	52
2138	The application of different solvation and electrostatic models in molecular dynamics simulations of ubiquitin: how well is the X-ray structure "maintained"?. 1996 , 25, 315-34	80
2137	Ability of empirical potentials (AMBER, CHARMM, CVFF, OPLS, Poltev) and semi-empirical quantum chemical methods (AM1, MNDO/M, PM3) to describe H-bonding in DNA base pairs; comparison with ab initio results. 1996 , 257, 31-35	35
2136	Oxygen and Nitrogen in Competitive Situations: Which is the Hydrogen-Bond Acceptor?. 1996 , 2, 1509-1513	87
2135	What Can We Learn from Molecular Recognition in ProteinLigand Complexes for the Design of New Drugs?. 1996 , 35, 2588-2614	251
2134	A world-wide web service for calculating approximate AMBER C?C and C?N bond stretching and torsional parameters. 1996 , 20, 483-484	4
2133	Cyclisation of (R)- and (S)-N-allyl-N-(1-phenylethyl) methoxycarbonylacetamide mediated by Mn(III): Preparation and structural assignment of 3-aza-2-oxobicyclo[3.1.0]hexanes. 1996 , 7, 3573-3584	22
2132	The role of the C-4 side chain of kainate and dihydrokainate in EAA receptor and transporter selectivity. 1996 , 6, 1607-1612	23
2131	The new program OPAL for molecular dynamics simulations and energy refinements of biological macromolecules. 1996 , 8, 136-46	174
2130	Improving the quality of NMR and crystallographic protein structures by means of a conformational database potential derived from structure databases. 1996 , 5, 1067-80	180

2129	NMR structure of the mouse prion protein domain PrP(121-231). 1996 , 382, 180-2	1063
2128	Molecular Dynamics Studies of the Properties of Water around Simple Organic Solutes. 1996 , 100, 11460-114	70 45
2127	Design of sequence-specific DNA binding ligands that use a two-stranded peptide motif for DNA sequence recognition. 1996 , 14, 31-47	25
2126	Proposed ligand binding site of the transmembrane receptor for neurotensin(8-13). 1996 , 271, 15060-8	66
2125	Free energy calculations of the mutation of Ile96>Ala in barnase: contributions to the difference in stability. 1996 , 9, 273-81	26
2124	Solvation Free Energies of the Nucleic Acid Bases. 1996 , 100, 8587-8594	69
2123	IR and Raman Spectra, Conformational Flexibility, and Scaled Quantum Mechanical Force Fields of Sodium Dimethyl Phosphate and Dimethyl Phosphate Anion 1996 , 100, 1559-1568	66
2122	HBexplorea new tool for identifying and analysing hydrogen bonding patterns in biological macromolecules. 1996 , 12, 281-9	15
2121	Hydrogen bonding and stacking of DNA bases: a review of quantum-chemical ab initio studies. 1996 , 14, 117-35	202
2120	Modeling DrugReceptor Interactions. 1996 , 235-336	10
2120	Modeling DrugReceptor Interactions. 1996, 235-336 Investigating the Anomalous Solvation Free Energies of Amines with a Polarizable Potential. 1996, 100, 2367-2371	10 52
	Investigating the Anomalous Solvation Free Energies of Amines with a Polarizable Potential. 1996 ,	
2119	Investigating the Anomalous Solvation Free Energies of Amines with a Polarizable Potential. 1996, 100, 2367-2371 Application of Free Energy Perturbation Calculations to the Tennis BallDimer: Why Is CF4 Not	52
2119 2118	Investigating the Anomalous Solvation Free Energies of Amines with a Polarizable Potential. 1996, 100, 2367-2371 Application of Free Energy Perturbation Calculations to the Tennis BallDimer: Why Is CF4 Not Encapsulated by This Host?. 1996, 100, 10779-10783 Generalization of the Molecular Electrostatic Potential for the Study of Noncovalent interactions.	52 15
2119 2118 2117	Investigating the Anomalous Solvation Free Energies of Amines with a Polarizable Potential. 1996, 100, 2367-2371 Application of Free Energy Perturbation Calculations to the Tennis BalliDimer: Why Is CF4 Not Encapsulated by This Host?. 1996, 100, 10779-10783 Generalization of the Molecular Electrostatic Potential for the Study of Noncovalent interactions. 1996, 3, 181-218 Parameterization and Simulation of the Physical Properties of Phosphorothioate Nucleic Acids.	52 15 37
2119211821172116	Investigating the Anomalous Solvation Free Energies of Amines with a Polarizable Potential. 1996, 100, 2367-2371 Application of Free Energy Perturbation Calculations to the Tennis Ball(Dimer: Why Is CF4 Not Encapsulated by This Host?. 1996, 100, 10779-10783 Generalization of the Molecular Electrostatic Potential for the Study of Noncovalent interactions. 1996, 3, 181-218 Parameterization and Simulation of the Physical Properties of Phosphorothioate Nucleic Acids. 1997, 41-54 Nonadiabatic transition and energy relaxation dynamics in the photoisomerization of s-trans	52 15 37 1
2119 2118 2117 2116 2115	Investigating the Anomalous Solvation Free Energies of Amines with a Polarizable Potential. 1996, 100, 2367-2371 Application of Free Energy Perturbation Calculations to the Tennis BallDimer: Why Is CF4 Not Encapsulated by This Host?. 1996, 100, 10779-10783 Generalization of the Molecular Electrostatic Potential for the Study of Noncovalent interactions. 1996, 3, 181-218 Parameterization and Simulation of the Physical Properties of Phosphorothioate Nucleic Acids. 1997, 41-54 Nonadiabatic transition and energy relaxation dynamics in the photoisomerization of s-trans butadiene. 1997, 106, 3159-3173 Molecular Dynamics Simulations Find That 3IPhosphoramidate Modified DNA Duplexes Undergo a B to A Transition and Normal DNA Duplexes an A to B Transition. Journal of the American Chemical 16.4	52 15 37 1

2111	Transition State Structure for the Hydrolysis of NAD Catalyzed by Diphtheria Toxin. <i>Journal of the American Chemical Society</i> , 1997 , 119, 12079-12088	80
2110	How the TATA Box Selects Its Protein Partner. 1997 , 329-345	3
2109	Isoalloxazine derivatives promote photocleavage of natural RNAs at G.U base pairs embedded within helices. 1997 , 25, 4018-27	39
2108	The NMR structure of estrone (Es)-tethered tandem DNA duplex: [d(5'pCAGCp3')-Es] + [Es-d(5'pTCCA3')]: d(5'pTGGAGCTG3'). 1997 , 15, 499-516	3
2107	Density Functional Calculations of Proton Chemical Shifts in Model Peptides. <i>Journal of the American Chemical Society</i> , 1997 , 119, 12262-12273	80
2106	Conversion of prostaglandin G/H synthase-1 into an enzyme sensitive to PGHS-2-selective inhibitors by a double His513> Arg and Ile523> val mutation. 1997 , 272, 9280-6	86
2105	Abstracts: Tenth Conversation. 1997 , 14, 767-930	
2104	Recognition of GC base pairs by triplex forming oligonucleotides containing nucleosides derived from 2-aminopyridine. 1997 , 25, 4891-8	43
2103	A molecular level picture of the stabilization of A-DNA in mixed ethanol-water solutions. 1997 , 94, 9626-30	99
2102	Determination of The Solution Conformation of A Non-Uniformly Deuterium Labelled (Uppsala Mmr-Window) 21Mer Rna Hairpin by Nmr Spectroscopy And Computational Methods 1997 , 16, 743-750	1
2101	Modeling Duplex DNA Oligonucleotides with Modified Pyrimidine Bases. 1997 , 312-328	
2100	Transition State Structure of the Solvolytic Hydrolysis of NAD+ 🛭 Journal of the American Chemical Society, 1997 , 119, 12069-12078	42
2099	Protein Dynamics: A Theoretical Perspective. 1997 , 22, 339-390	1
2098	Effect of warmup protocol and sampling time on convergence of molecular dynamics simulations of a DNA dodecamer using AMBER 4.1 and particle-mesh Ewald method. 1997 , 14, 607-11	33
2097	Theoretical Study of the Electronic Spectrum of Plastocyanin. <i>Journal of the American Chemical Society</i> , 1997 , 119, 218-226	102
2096	Vibrational analysis of phosphorothioate DNA: II. The POS group in the model compound dimethyl phosphorothioate [(CH3O)2(POS)] 1997 , 14, 509-16	12
2095	Hydrogen-bonded trimers of DNA bases and their interaction with metal cations: ab initio quantum-chemical and empirical potential study. 1997 , 14, 613-28	65
2094	Conformational properties of the TATA-box binding sequence of DNA. 1997 , 14, 757-65	40

2093	Thermodynamic Decomposition of Hydration Free Energies by Computer Simulation: Application to Amines, Oxides, and Sulfides. 1997 , 101, 10527-10534		53	
2092	Molecular Dynamics Simulations of DNA with Protein's Consistent GROMOS Force Field and the Role of Counterions' Symmetry. <i>Journal of the American Chemical Society</i> , 1997 , 119, 5934-5938	16.4	23	
2091	Influence of Magnesium Ions on Duplex DNA Structural, Dynamic, and Solvation Properties. 1997 , 101, 646-650		82	
2090	Unrestrained Molecular Dynamics of Photodamaged DNA in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1997 , 119, 7095-7104	16.4	58	
2089	Theoretical Prediction of Vibrational Spectrum of N-Glycylglycine Hydrochloride: ´An ab Initio Study. 1997 , 101, 6964-6969		19	
2088	A Model for the Intermolecular Interactions of the Hydrogen Bond That Incorporates Its Spectroscopic Properties. 1997 , 101, 5825-5827		14	
2087	Intrinsic and Environmental Effects in the Structure and Magnetic Properties of Glycine Radical in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1997 , 119, 12962-12967	16.4	79	
2086	A Simulation of the Catalytic Mechanism of Aspartylglucosaminidase Using ab Initio Quantum Mechanics and Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 1997 , 119, 1189-1196	16.4	48	
2085	Superstructures of Cyclodextrin Derivatives on Au(111): A Combined Random Planting Molecular Dynamics Approach. 1997 , 13, 7092-7098		29	
2084	Selectin-ligand interactions revealed by molecular dynamics simulation in solution. 1997 , 40, 362-9		37	
2083	Kinetic isotope effect characterization of the transition state for oxidized nicotinamide adenine dinucleotide hydrolysis by pertussis toxin. 1997 , 36, 4526-34		43	
2082	Development of a Potential Surface for Simulation of Proton and Hydride Transfer Reactions in Solution: Application to NADH Hydride Transfer. 1997 , 101, 3977-3989		16	
2081	Relationship between Regiospecificity and Type of Stereospecificity in Propene Polymerization with Zirconocene-Based Catalysts 1. <i>Journal of the American Chemical Society</i> , 1997 , 119, 4394-4403	16.4	99	
2080	Pertussis toxin: transition state analysis for ADP-ribosylation of G-protein peptide alphai3C20. 1997 , 36, 8215-23		51	
2079	Modern Computational Methodology Applied to the Simulation of Blocked Trialanine Peptide in Vacuo, Water Clusters, and Bulk Water. 1997 , 101, 7592-7603		21	
2078	Studies on selection blockers. 5. Design, synthesis, and biological profile of sialyl Lewis x mimetics based on modified serine-glutamic acid dipeptides. 1997 , 40, 3534-41		30	
2077	Molecular simulation of dynorphin A-(1-10) binding to extracellular loop 2 of the kappa-opioid receptor. A model for receptor activation. 1997 , 40, 3254-62		74	
2076	Interactions of anesthetics with the water-hexane interface. A molecular dynamics study. 1997 , 101, 782-91		79	

2075	Ligand Binding in the Catalytic Antibody 17E8. A Free Energy Perturbation Calculation Study. Journal of the American Chemical Society, 1997, 119, 11571-11577	35
2074	Structure of an RNA hairpin loop with a 5'-CGUUUCG-3' loop motif by heteronuclear NMR spectroscopy and distance geometry. 1997 , 36, 13989-4002	38
2073	Electrostatic effects on substrate activation in para-hydroxybenzoate hydroxylase: studies of the mutant lysine 297 methionine. 1997 , 36, 7548-56	33
2072	Simulation of a Protein Crystal at Constant Pressure. 1997 , 101, 2105-2108	13
2071	Molecular Dynamics Simulations of the d(TIAIT) Triple Helix. <i>Journal of the American Chemical Society</i> , 1997 , 119, 7463-7469	156
2070	Development of Weiner et al. force field parameters suitable for conformational studies of [1,4]-benzodiazepines and related compounds. 1997 , 37, 951-6	12
2069	What Controls Partitioning of the Nucleic Acid Bases between Chloroform and Water?. 1997, 101, 5084-5088	31
2068	Langevin Dipoles Model for ab Initio Calculations of Chemical Processes in Solution: Parametrization and Application to Hydration Free Energies of Neutral and Ionic Solutes and Conformational Analysis in Aqueous Solution. 1997 , 101, 5583-5595	259
2067	Vibrational Spectroscopy of Peptides and Peptide Water Complexes: Anharmonic Coupled-Mode Calculations. 1997 , 101, 8595-8606	36
2066	Molecular Dynamics Simulations Highlight the Structural Differences among DNA:DNA, RNA:RNA, and DNA:RNA Hybrid Duplexes. <i>Journal of the American Chemical Society</i> , 1997 , 119, 4805-4825	236
2065	Base-base and deoxyribose-base stacking interactions in B-DNA and Z-DNA: a quantum-chemical study. 1997 , 73, 76-87	185
2064	Does TATA matter? A structural exploration of the selectivity determinants in its complexes with TATA box-binding protein. 1997 , 73, 640-52	36
2063	Prediction of solution structures of the Ca2+-bound gamma-carboxyglutamic acid domains of protein S and homolog growth arrest specific protein 6: use of the particle mesh Ewald method. 1997 , 73, 1847-56	18
2062	Differences in hydration structure near hydrophobic and hydrophilic amino acids. 1997 , 73, 2106-15	41
2061	A molecular dynamics study of Fe2S2 putidaredoxin: multiple conformations of the C-terminal region. 1997 , 73, 2138-48	8
2060	A 5-nanosecond molecular dynamics trajectory for B-DNA: analysis of structure, motions, and solvation. 1997 , 73, 2313-36	280
2059	Observation of an A-DNA to B-DNA transition in a nonhelical nucleic acid hairpin molecule using molecular dynamics. 1997 , 73, 2702-10	17
2058	Effect of periodic box size on aqueous molecular dynamics simulation of a DNA dodecamer with particle-mesh Ewald method. 1997 , 72, 2395-7	89

2057	Structure-based drug design: computational advances. 1997 , 37, 71-90		117
2056	Intrusion of Counterions into the Spine of Hydration in the Minor Groove of B-DNA: Fractional Occupancy of Electronegative Pockets. <i>Journal of the American Chemical Society</i> , 1997 , 119, 59-69	16.4	355
2055	Evaluation of the Molecular Configuration Integral in All Degrees of Freedom for the Direct Calculation of Conformational Free Energies: Prediction of the Anomeric Free Energy of Monosaccharides. 1997 , 101, 9900-9905		33
2054	Molecular Modeling of Proteins and Mathematical Prediction of Protein Structure. 1997 , 39, 407-460		120
2053	Accurate ab Initio Quantum Chemical Determination of the Relative Energetics of Peptide Conformations and Assessment of Empirical Force Fields. <i>Journal of the American Chemical Society</i> , 1997 , 119, 5908-5920	16.4	323
2052	A Combined Car P arrinello QM/MM Implementation for ab Initio Molecular Dynamics Simulations of Extended Systems: Application to Transition Metal Catalysis. 1997 , 101, 7877-7880		87
2051	Ab Initio Study of Stacking Interactions in A- and B-DNA. 1997 , 101, 3846-3853		79
2050	Adsorption and solvation of ethanol at the water liquid-vapor interface: a molecular dynamics study. 1997 , 101, 3130-5		95
2049	Derivation of Class II Force Fields. 4. van der Waals Parameters of Alkali Metal Cations and Halide Anions. 1997 , 101, 7243-7252		155
2048	Ab initio quantum mechanics analysis of imidazole C-HO water hydrogen bonding and a molecular mechanics forcefield correction. 1997 , 14, 657-65		33
2047	Calculation of Chloroform/Water Partition Coefficients for the N-Methylated Nucleic Acid Bases. 1997 , 101, 10971-10975		37
2046	Interaction of DNA Base Pairs with Various Metal Cations (Mg2+, Ca2+, Sr2+, Ba2+, Cu+, Ag+, Au+, Zn2+, Cd2+, and Hg2+): Nonempirical ab Initio Calculations on Structures, Energies, and Nonadditivity of the Interaction. 1997 , 101, 9670-9677		208
2045	The Role of Bulky Substituents in Brookhart-Type Ni(II) Diimine Catalyzed Olefin Polymerization: A Combined Density Functional Theory and Molecular Mechanics Study. <i>Journal of the American Chemical Society</i> , 1997 , 119, 6177-6186	16.4	304
2044	The free surface of water: molecular orientation, surface potential and nonlinear susceptibility. 1997 , 92, 625-640		189
2043	DNA base-stacking interactions: a comparison of theoretical calculations with oligonucleotide X-ray crystal structures. 1997 , 265, 603-19		110
2042	Theoretical studies of an exceptionally stable RNA tetraloop: observation of convergence from an incorrect NMR structure to the correct one using unrestrained molecular dynamics. 1997 , 270, 436-50		71
2041	Molecular dynamics simulation study of DNA dodecamer d(CGCGAATTCGCG) in solution: conformation and hydration. 1997 , 272, 553-72		98
2040	Torsion angle dynamics for NMR structure calculation with the new program DYANA. 1997 , 273, 283-98		2561

2039	Solution structure of human p8MTCP1, a cysteine-rich protein encoded by the MTCP1 oncogene, reveals a new alpha-helical assembly motif. 1997 , 274, 801-15	23
2038	Experiment vs Force Fields: DNA Conformation from Molecular Dynamics Simulations. 1997 , 101, 7361-7363	69
2037	Toward a Molecular Orbital Derived Empirical Potential for Liquid Simulations. 1997 , 101, 657-663	189
2036	Empirical free energy calculations: a blind test and further improvements to the method. 1997 , 268, 401-11	73
2035	Structure of oligonucleotides with either a strand break or a bulged nucleotide. 1997 , 79, 593-7	2
2034	Molecular Dynamics Simulation of the Excited-State Dynamics of Bacteriorhodopsin. 1997 , 66, 735-740	10
2033	Insight into the stabilization of A-DNA by specific ion association: spontaneous B-DNA to A-DNA transitions observed in molecular dynamics simulations of d[ACCCGCGGGT]2 in the presence of hexaamminecobalt(III). 1997 , 5, 1297-311	97
2032	Chiral N-substituted glycines can form stable helical conformations. 1997 , 2, 369-75	151
2031	The bioactive conformation of neuropeptide Y analogues at the human Y2-receptor. 1997 , 247, 1019-28	16
2030	A molecular dynamics study in explicit water of the reduced and oxidized forms of yeast iso-1-cytochrome csolvation and dynamic properties of the two oxidation states. 1997 , 249, 716-23	21
2029	Calculations of the structure and spectra of the putative transient peroxide intermediates of peroxidases. 1997 , 398-399, 497-505	4
2028	Structure and dynamics of small peptides at aqueous interfaces a multi-nanosecond molecular dynamics study. 1997 , 398-399, 529-535	10
2027	Proline and hydroxyproline zwitterions ab initio study. 1997 , 417, 255-263	14
2026	A molecular modeling study of the urease active site. 1997 , 419, 33-36	2
2025	The effects of basis set and blocking groups on the conformational energies of glycyl and alanyl dipeptides A Hartree-Fock and MP2 study. 1997 , 392, 101-109	18
2024	Solution structure of alpha-conotoxin MI determined by 1H-NMR spectroscopy and molecular dynamics simulation with the explicit solvent water. 1997 , 1343, 327-34	28
2023	Adventures in Improving the Scaling and Accuracy of a Parallel Molecular Dynamics Program. 1997 , 11, 255-278	79
2022	Automated combined assignment of NOESY spectra and three-dimensional protein structure determination. 1997 , 10, 351-62	128

2021	Theoretical study of the conformational and electrostatic properties of C4-monosubstituted 2-azetidinones. 1997 , 8, 39-47	11
2020	Simulation of Surface Excess Concentrations for a Binary Hydrocarbon Mixture on Graphite. 1997 , 3, 315-320	15
2019	De novo design of the hydrophobic core of ubiquitin. 1997 , 6, 1167-78	143
2018	Conformational analysis using distance geometry methods. 1997 , 15, 18-36	56
2017	Graphical visualization of mean hydration from molecular dynamics simulations. 1997 , 15, 355-8, 386-8	5
2016	Simulation of alternative binding modes in a structure-based QSAR study of HIV-1 protease inhibitors. 1997 , 15, 364-71, 389	15
2015	Molecular dynamics and tunnelling in supramolecular complexes. 1997 , 234-236, 115-120	6
2014	Ab initio derived spectroscopic quality force fields for molecular modeling and dynamics. 1997 , 53, 1347-1363	3 14
2013	Multi-basin dynamics of a protein in a crystal environment. 1997 , 107, 225-239	76
2012	Cadira: an object-oriented platform for modelling molecules and analyzing simulations. 1997 , 21, 343-345	2
2011	A combined density functional theory/molecular mechanics formalism and its application to small water clusters. 1997 , 412, 121-133	20
2010	The Crystal Polymorphism of Tetrolic Acid (CH3C?CCOOH): A Molecular Dynamics Study of Precursors in Solution, and a Crystal Structure Generation. 1997 , 3, 893-899	62
2009	Free energies of solvation in chloroform and water from a linear response approach. 1997 , 10, 563-576	92
2008	A computational analysis of interaction energies in methane and neopentane dimer systems. 1997 , 18, 70-79	19
2007	Free energies of hydration from thermodynamic integration: Comparison of molecular mechanics force fields and evaluation of calculation accuracy. 1997 , 18, 449-462	32
2006	Internal coordinate modeling of DNA: Force field comparisons. 1997 , 18, 1043-1055	36
2005	Energy components of aqueous solution: Insight from hybrid QM/MM simulations using a polarizable solvent model. 1997 , 18, 1061-1071	102
2004	Performance of empirical potentials (AMBER, CFF95, CVFF, CHARMM, OPLS, POLTEV), semiempirical quantum chemical methods (AM1, MNDO/M, PM3), and ab initio Hartreeflock method for interaction of DNA bases: Comparison with nonempirical beyond Hartreeflock results.	239

2003	Strength of hydrogen bonds in Helices. 1997 , 18, 1245-1252	38
2002	Quasi-Hamiltonian equations of motion for internal coordinate molecular dynamics of polymers. 1997 , 18, 1354-1364	34
2001	Fast and accurate molecular dynamics simulation of a protein using a special-purpose computer. 1997 , 18, 1546-1563	64
2000	Advancing beyond the atom-centered model in additive and nonadditive molecular mechanics. 1997 , 18, 1632-1646	116
1999	Development and validation of force-field parameters for molecular simulations of peptides and proteins containing open-shell residues. 1997 , 18, 1720-1728	10
1998	ORAC: A Molecular dynamics program to simulate complex molecular systems with realistic electrostatic interactions. 1997 , 18, 1848-1862	152
1997	OPLS all-atom force field for carbohydrates. 1997 , 18, 1955-1970	535
1996	Knowledge-based modeling of a bacterial dichloromethane dehalogenase. 1997 , 28, 217-26	23
1995	Pseudocontact shifts as constraints for energy minimization and molecular dynamics calculations on solution structures of paramagnetic metalloproteins. 1997 , 29, 68-76	94
1994	Monte Carlo Simulations of Guanidinium Acetate and Methylammonium Acetate Ion Pairs in Water. 1997 , 25, 11-21	9
1993	Sulfur Aromatic Interactions: A Computational Study of the Dimethyl Sulfide Benzene Complex. 1997, 25, 213-219	26
1992	Common Molecular Dynamics Algorithms Revisited: Accuracy and Optimal Time Steps of Stimer Leapfrog Integrators. 1997 , 136, 354-365	33
1991	Synthesis, molecular and electronic structure of the first homoleptic complex of platinum with a secondary phosphine. 1997 , 264, 185-191	13
1990	A comparison and chemometric analysis of several molecular mechanics force fields and parameter sets applied to carbohydrates. 1998 , 314, 141-155	141
1989	Effect of backbone Itorsion angle on low energy single base opening in B-DNA crystal structures. 1998 , 287, 570-574	11
1988	A selectively enhanced multicanonical molecular dynamics method for conformational sampling of peptides in realistic water molecules. 1998 , 288, 319-326	28
1987	Excited states and electron transfer mechanism in the photosynthetic reaction center of Rhodopseudomonas viridis: SACII study. 1998 , 296, 499-504	35
1986	Conformational analysis of protein and nucleic acid fragments with the new grid search algorithm FOUND. 1998 , 12, 543-8	49

1985	All-atom empirical potential for molecular modeling and dynamics studies of proteins. 1998, 102, 3586-616	11429
1984	A novel mode of DNA recognition by a beta-sheet revealed by the solution structure of the GCC-box binding domain in complex with DNA. 1998 , 17, 5484-96	363
1983	Comparative binding energy analysis. 1998 , 9/11, 19-34	16
1982	Molecular dynamics simulations: a tool for drug design. 1998 , 9/11, 181-209	11
1981	Conformational equilibria of terminally blocked single amino acids at the water-hexane interface. A molecular dynamics study. 1998 , 102, 281-90	43
1980	Proton transport along water chains and NADH hydride transfer in solution. 1998 , 102, 533-543	6
1979	Demixing of Binary Water Thloroform Mixtures Containing Ionophoric Solutes and Ion Recognition at a Liquid Liquid Interface: A Molecular Dynamics Study. 1998 , 102, 10772-10788	72
1978	An HLA-B27 polymorphism (B*2710) that is critical for T-cell recognition has limited effects on peptide specificity. 1998 , 51, 1-9	40
1977	Free energy perturbation studies on binding of the inhibitor 5,6-dihydrobenzo[h]cinnolin-3(2H)one-2-acetic acid and its methoxylated analogs to aldose reductase. 1998 , 54, 9415-9428	11
1976	Molecular dynamics simulation of phospholipid bilayer membrane. 1998 , 144, 387-393	2
1975	Development of an all-atom force field for heterocycles. Properties of liquid pyridine and diazenes. 1998 , 424, 145-155	260
1974	An ab initio study of pyruvic acid. 1998 , 430, 51-56	21
1973	The structure of a methylated tetraloop in 16S ribosomal RNA. 1998 , 6, 747-56	32
1972	The solution structure of an RNA loop-loop complex: the ColE1 inverted loop sequence. 1998 , 6, 993-1005	86
1971	Exploration of metal ion binding sites in RNA folds by Brownian-dynamics simulations. 1998, 6, 1303-14	94
1970	Crystallographic water sites from a theoretical perspective. 1998 , 6, 1351-4	31
1969	The Structures of the EnzymeBubstrate Complex and Transition State Formed in the SN2 Displacement of Clfrom 1,2-Dichloroethane at the Active Site ofXanthobacter autotrophicusHaloalkane Dehalogenase. 1998 , 26, 169-174	2
1968	A molecular simulation picture of DNA hydration around A- and B-DNA. 1998 , 48, 199-209	86

1967	Comparison of methods for deriving atomic charges from the electrostatic potential and moments. 1998 , 19, 377-395	301
1966	Derivation of class II force fields: V. Quantum force field for amides, peptides, and related compounds. 1998 , 19, 430-458	119
1965	Crystal structure predictions for acetic acid. 1998 , 19, 459-474	76
1964	Automated molecular mechanics parameterization with simultaneous utilization of experimental and quantum mechanical data. 1998 , 19, 1146-1166	88
1963	Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function. 1998 , 19, 1639-1662	754 ⁸
1962	Essential spaces defined by NMR structure ensembles and molecular dynamics simulation show significant overlap. 1998 , 31, 370-382	58
1961	Functional conformational changes of endo-1,4-xylanase II from Trichoderma reesei: A molecular dynamics study. 1998 , 31, 434-444	44
1960	Reaction path and free energy calculations of the transition between alternate conformations of HIV-1 protease. 1998 , 32, 7-16	61
1959	Molecular dynamics study of femtosecond events in photoactive yellow protein after photoexcitation of the chromophore. 1998 , 32, 268-75	19
1958	Can one predict protein stability? An attempt to do so for residue 133 of T4 lysozyme using a combination of free energy derivatives, PROFEC, and free energy perturbation methods. 1998 , 32, 438-458	20
1957	A new method for predicting binding free energy between receptor and ligand. 1998, 33, 62-73	20
1956	Accuracy of side-chain prediction upon near-native protein backbones generated by Ab initio folding methods. 1998 , 33, 204-17	39
1955	Molecular dynamics simulations of epidermal growth factor and transforming growth factor-⊞ structures in water. 1998 , 33, 396-407	5
1954	Analysis of domain motions by approximate normal mode calculations. 1998 , 33, 417-29	582
1953	SCORE: A New Empirical Method for Estimating the Binding Affinity of a Protein-Ligand Complex. 1998 , 4, 379-394	248
1952	Molecular dynamics simulations of the oligonucleotide with the modified phosphate/phosphonate internucleotide linkage. 1998 , 48, 409-415	4
1951	Molecular dynamics investigations of hammerhead ribozyme RNA. 1998 , 27, 153-65	60
1950	Molecular mechanics conformational analysis of tylosin. 1998 , 440, 121-130	9

1949	The COMPASS force field: parameterization and validation for phosphazenes. 1998, 8, 229-246	940
1948	Q: a molecular dynamics program for free energy calculations and empirical valence bond simulations in biomolecular systems. 1998 , 16, 213-25, 261	258
1947	A free energy calculation can be used to predict K(+)-binding constants for new macrotetrolide antibiotics. 1998 , 8, 1725-8	8
1946	LIF receptor-gp130 interaction investigated by homology modeling: implications for LIF binding. 1998 , 7, 886-96	13
1945	Engineering of betabellin-15D: a 64 residue beta sheet protein that forms long narrow multimeric fibrils. 1998 , 7, 1545-54	26
1944	Molecular mechanisms of resistance: free energy calculations of mutation effects on inhibitor binding to HIV-1 protease. 1998 , 7, 1750-6	21
1943	Enhancing the relaxivity of paramagnetic coordination complexes through the optimization of the molecular electrostatic potential. 1998 , 16, 811-28	5
1942	Brownian dynamics simulations of DNA-ligand interactions: a theoretical study on the kinetics of DAPI-DNA complexation. 1998 , 77, 157-163	6
1941	On the helical conformation of un-ionized poly(gamma-D-glutamic acid). 1998 , 23, 175-84	52
1940	Application of molecular dynamics calculations in the prediction of dynamical molecular properties. 1998 , 29, 1043-1050	21
1939	The effects of conformational constraints on aspartic acid racemization. 1998 , 29, 1227-1232	43
1938	Use of Locally Enhanced Sampling in Free Energy Calculations: Testing and Application to the ∃> ∄ Anomerization of Glucose. <i>Journal of the American Chemical Society</i> , 1998 , 120, 5771-5782	85
1937	Thermodynamic Properties of the Williams, OPLS-AA, and MMFF94 All-Atom Force Fields for Normal Alkanes. 1998 , 102, 2578-2586	81
1936	Inherent DNA curvature and flexibility correlate with TATA box functionality. 1998 , 46, 403-15	40
1935	Quantum mechanical calculations on biological systems. 1998 , 8, 257-62	106
1934	Solution Structure of a Substrate for the Archaeal Pre-tRNA Splicing Endonucleases: The Bulge-Helix-Bulge Motif. 1998 , 1, 883-894	46
1933	Molecular mechanics study of hydrogen bonded self-assembled adenine monolayers on graphite. 1998 , 417, 201-209	84
1932	Molecular dynamics and continuum solvent studies of the stability of polyG-polyC and polyA-polyT DNA duplexes in solution. 1998 , 16, 265-80	163

1931	Different types of interactions involving cysteine sulfhydryl group in proteins. 1998 , 15, 1059-72		70
1930	Continuum solvent studies of the stability of RNA hairpin loops and helices. 1998 , 16, 671-82		180
1929	Structure and Spectra of Ferrous Dioxygen and Reduced Ferrous Dioxygen Model Cytochrome P450. <i>Journal of the American Chemical Society</i> , 1998 , 120, 4308-4318	16.4	83
1928	Critical Evaluation of Metal Complex Molecular Mechanics. Part 1. Cobalt(III) Hexaamines. 1998 , 37, 479.	5-480	5 18
1927	Investigation of the Anomalous Solvation Free Energies of Amides and Amines: FEP Calculations in Cyclohexane and PS-GVB Calculations on Amide Water Complexes. 1998 , 102, 4004-4010		10
1926	Substituting nonpeptidic spacers for the T cell receptor-binding part of class I major histocompatibility complex-binding peptides. 1998 , 273, 19072-9		21
1925	Molecular Dynamics of Hemiprotonated Intercalated Four-Stranded i-DNA: Stable Trajectories on a Nanosecond Scale. <i>Journal of the American Chemical Society</i> , 1998 , 120, 6147-6151	16.4	74
1924	Potential Catalyst Deactivation Reaction in Homogeneous Ziegler Natta Polymerization of Olefins: Formation of an Allyl Intermediate. 1998 , 17, 4997-5002		47
1923	Combined Locally Enhanced Sampling and Particle Mesh Ewald as a Strategy To Locate the Experimental Structure of a Nonhelical Nucleic Acid. <i>Journal of the American Chemical Society</i> , 1998 , 120, 7149-7155	16.4	66
1922	Folding and translocation of the undecamer of poly-L-leucine across the water-hexane interface. A molecular dynamics study. <i>Journal of the American Chemical Society</i> , 1998 , 120, 11912-24	16.4	68
1921	Assessment of a Combined QM/MM Approach for the Study of Large Nitroxide Systems in Vacuo and in Condensed Phases. <i>Journal of the American Chemical Society</i> , 1998 , 120, 7069-7078	16.4	94
1920	A pseudosquare knot structure of DNA in solution. 1998 , 37, 12715-26		11
1919	Activation energies for dissociation of double strand oligonucleotide anions: evidence for watson-crick base pairing in vacuo. <i>Journal of the American Chemical Society</i> , 1998 , 120, 9605-13	16.4	144
1918	Interactions between DNA polymerase beta and the major covalent adduct of the carcinogen (+)-anti-benzo[a]pyrene diol epoxide with DNA at a primer-template junction. 1998 , 37, 878-84		16
1917	Application of the RESP Methodology in the Parametrization of Organic Solvents. 1998 , 102, 8070-8079		421
1916	Molecular dynamics simulation of interaction of histone-like protein of mycobacterium tuberculosis (Hlpmt) and histone of clostridium pasteurianum (DBHclopa) with 35 based paired GC rich U-bend DNA. 1998 , 16, 223-35		2
1915	Conformations of nicked and gapped DNA structures by NMR and molecular dynamic simulations in water. 1998 , 37, 4059-70		56
1914	Nuclear Dynamics of Benzene∭(Ar)n Clusters. 1998 , 102, 8268-8278		8

1913	Effect of Guanine Stacking on the Oxidation of 8-Oxoguanine in B-DNA. <i>Journal of the American Chemical Society</i> , 1998 , 120, 845-846	260
1912	Helical Nylons 3. Synthesis and Crystal Structure of Poly(組-aspartate)s with Branched Alkyl Side Chains. 1998 , 31, 124-134	24
1911	Accurate DNA Dynamics without Accurate Long-Range Electrostatics. <i>Journal of the American Chemical Society</i> , 1998 , 120, 10928-10937	42
1910	Molecular Mechanics Modeling of the Cobaloximes and Reevaluation of the Parameters for Modeling of the Cobalt Corrins. 1998 , 37, 2578-2581	37
1909	Homology model for oncostatin M based on NMR structural data. 1998 , 37, 10581-8	9
1908	Molecular Dynamics Studies of the Conformational Preferences of a DNA Double Helix in Water and an Ethanol/Water Mixture: Theoretical Considerations of the A <=> B Transition. 1998, 102, 4658-4667	87
1907	Hierarchy of Fast Motions in Protein Dynamics. 1998 , 102, 473-479	32
1906	Oligonucleotides Composed of 2EDeoxy-1DEnhydro-d-mannitol Nucleosides with a Purine Base Moiety. 1998 , 63, 1574-1582	18
1905	Free Energy Analysis of the Conformational Preferences of A and B Forms of DNA in Solution. <i>Journal of the American Chemical Society</i> , 1998 , 120, 10629-10633	177
1904	Nuclear magnetic resonance solution structure of the plasminogen-activator protein staphylokinase. 1998 , 37, 10635-42	22
1903	Stereochemistry of Ruthenium Bis-chelate Disulfoxide Complexes. A Molecular Mechanics Investigation. 1998 , 37, 4094-4103	16
1902	Brownian and essential dynamics studies of the HIV-1 integrase catalytic domain. 1998 , 16, 733-45	16
1901	Proteins in Vacuo. Denaturation of Highly-Charged Lysozyme Studied by Molecular Dynamics Simulations. 1998 , 102, 9344-9352	38
1900	Monte Carlo simulation of DNA fragment hydration in the presence of alkaline cations using novel atom-atom potential functions. 1998 , 16, 289-300	9
1899	Molecular Dynamics Simulation To Investigate Differences in Minor Groove Hydration of HNA/RNA Hybrids As Compared to HNA/DNA Complexes. <i>Journal of the American Chemical Society</i> , 1998 , 120, 5381-539	94 ⁴⁰
1898	Modeling the mechanics of a DNA oligomer. 1998 , 16, 593-604	23
1897	Solvent Effect on Intramolecular Long-Range Electron-Transfer Reactions between Porphyrin and Benzoquinone in an Acetonitrile Solution: Molecular Dynamics Calculations of Reaction Rate Constants. 1998 , 102, 3333-3342	14
1896	Kinetic role of electrostatic interactions in the unfolding of hyperthermophilic and mesophilic rubredoxins. 1998 , 37, 3369-76	104

1895	Designing an Optimum Guest for a Host Using Multimolecule Free Energy Calculations: Predicting the Best Ligand for Rebek's Tennis Ball Journal of the American Chemical Society, 1998 , 120, 7557-7567 16.4	33
1894	Conformational Properties of the Deoxyribose and Ribose Moieties of Nucleic Acids: A Quantum Mechanical Study. 1998 , 102, 6669-6678	71
1893	Charge-Transfer Interactions in Macromolecular Systems: A New View of the Protein/Water Interface. <i>Journal of the American Chemical Society</i> , 1998 , 120, 5593-5594	82
1892	Theoretical Study of the Structural and Spectroscopic Properties of Stellacyanin. 1998 , 102, 4638-4647	35
1891	Mechanism and Unidirectionality of the Electron Transfer in the Photosynthetic Reaction Center of Rhodopseudomonas Viridis: SACII Theoretical Study. 1998 , 102, 10420-10430	58
1890	Molecular Dynamics Simulations in Aqueous Solution of Triple Helices Containing d(GICIC) Trios. Journal of the American Chemical Society, 1998 , 120, 11226-11233	57
1889	Molecular Theories and Simulation of Ions and Polar Molecules in Water. 1998 , 102, 7885-7895	164
1888	Electrostatic Model for the Interaction Force Constants of the Formic Acid Dimer. 1998 , 102, 659-667	23
1887	Insights into the dynamic nature of DNA duplex structure via analysis of nuclear Overhauser effect intensities. 1998 , 37, 11478-87	18
1886	Uracil glycol deoxynucleoside triphosphate is a better substrate for DNA polymerase I Klenow fragment than thymine glycol deoxynucleoside triphosphate. 1998 , 37, 330-8	20
1885	Trans-cis isomerization of proline 22 in bovine prothrombin fragment 1: a surprising result of structural characterization. 1998 , 37, 10920-7	16
1884	Theoretical Studies of Peptide Models. <i>Journal of the American Chemical Society</i> , 1998 , 120, 13485-1349 2 6.4	114
1883	Mixed Quantum/Classical Dynamics of Hydrogen Transfer Reactions. 1998 , 102, 10443-10454	76
1882	Excited States of the Photosynthetic Reaction Center of Rhodopseudomonas viridis: SACII Study. 1998 , 102, 10410-10419	64
1881	Theoretical Studies on the UO22+and Sr2+Complexation by Phosphoryl-Containing OPR3Ligands: ´QM ab Initio Calculations in the Gas Phase and MD FEP Calculations in Aqueous Solution. 1998 , 102, 3773-378	1 ³³
1880	Computer Design of Living Olefin Polymerization Catalysts: A Combined Density Functional Theory and Molecular Mechanics Study. 1998 , 17, 3240-3253	70
1879	Abasic analogues of TSAO-T as the first sugar derivatives that specifically inhibit HIV-1 reverse transcriptase. 1998 , 41, 4636-47	22
1878	Relation between the Structure and Spectroscopic Properties of Blue Copper Proteins. <i>Journal of the American Chemical Society</i> , 1998 , 120, 13156-13166	140

1877	B-DNA's BI-> BIIConformer Substate Dynamics Is Coupled with Water Migration. 1998, 102, 8934-8940	57
1876	Development of an All-Atom Force Field for Heterocycles. Properties of Liquid Pyrrole, Furan, Diazoles, and Oxazoles. 1998 , 102, 8049-8059	270
1875	A role for CHO interactions in protein-DNA recognition. 1998 , 277, 1129-40	162
1874	Ligand-induced domain movement in an antibody Fab: molecular dynamics studies confirm the unique domain movement observed experimentally for Fab NC6.8 upon complexation and reveal its segmental flexibility. 1998 , 278, 301-6	21
1873	Solution structure of a non-palindromic 16 base-pair DNA related to the HIV-1 kappa B site: evidence for BI-BII equilibrium inducing a global dynamic curvature of the duplex. 1998 , 279, 127-42	60
1872	Are there non-trivial dynamic cross-correlations in proteins?. 1998 , 279, 911-20	45
1871	On the potential role of the amino nitrogen atom as a hydrogen bond acceptor in macromolecules. 1998 , 279, 1123-36	105
1870	Sequence-dependent DNA structure: the role of the sugar-phosphate backbone. 1998 , 280, 407-20	87
1869	The NMR solution structure of human glutaredoxin in the fully reduced form. 1998, 280, 687-701	78
1868	Molecular dynamics simulations of an oligonucleotide duplex with adenine tracts phased by a full helix turn. 1998 , 281, 675-87	118
1867	Solution structure of Desulfovibrio vulgaris (Hildenborough) ferrocytochrome c3: structural basis for functional cooperativity. 1998 , 281, 719-39	54
1866	CHO hydrogen bond involving proline residues in alpha-helices. 1998 , 284, 867-73	158
1865	Stacking interactions and intercalative DNA binding. 1998 , 14, 277-92	86
1864	Comparative binding energy analysis of HIV-1 protease inhibitors: incorporation of solvent effects and validation as a powerful tool in receptor-based drug design. 1998 , 41, 836-52	123
1863	Solvation Free Energy of Biomacromolecules: Parameters for a Modified Generalized Born Model Consistent with the AMBER Force Field. 1998 , 102, 9571-9576	222
1862	Ab Initio Study of Hydrogen-Bonded Complexes of Small Organic Molecules with Water. 1998 , 102, 3782-3797	376
1861	Uracil Dimer: Potential Energy and Free Energy Surfaces. Ab Initio beyond Hartreeflock and Empirical Potential Studies. 1998 , 102, 6921-6926	100
1860	Role of hydrogen bonds in protein-DNA recognition: a comparison of generalized born and finite difference Poisson-Boltzmann solvation treatments. 1998 , 16, 237-42	8

1859	COMPASS: An ab Initio Force-Field Optimized for Condensed-Phase ApplicationsOverview with Details on Alkane and Benzene Compounds. 1998 , 102, 7338-7364		3990
1858	Molecular Dynamics Simulation of a PNAÍDNAÍPNA Triple Helix in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1998 , 120, 5895-5904	6.4	94
1857	Continuum Solvent Studies of the Stability of DNA, RNA, and Phosphoramidate D NA Helices. <i>Journal of the American Chemical Society</i> , 1998 , 120, 9401-9409	6.4	1269
1856	The solution conformation of a carbocyclic analog of the Dickerson-Drew dodecamer: comparison with its own X-ray structure and that of the NMR structure of the native counterpart. 1998 , 16, 547-68		22
1855	Validation of molecular dynamics simulation. 1998 , 108, 6109-6116		139
1854	Structural equilibrium of DNA represented with different force fields. 1998 , 75, 134-49		125
1853	Diffusion of solvent around biomolecular solutes: a molecular dynamics simulation study. 1998 , 75, 150-8		143
1852	Sequence-dependent dynamics of TATA-Box binding sites. 1998 , 75, 372-81		54
1851	NMR structure refinement and dynamics of the K+-[d(G3T4G3)]2 quadruplex via particle mesh Ewald molecular dynamics simulations. 1998 , 75, 968-81		93
1850	Selective binding of the TATA box-binding protein to the TATA box-containing promoter: analysis of structural and energetic factors. 1998 , 75, 2411-21		18
1849	Progressive DNA bending is made possible by gradual changes in the torsion angle of the glycosyl bond. 1998 , 74, 2191-8		11
1848	Importance of explicit salt ions for protein stability in molecular dynamics simulation. 1998 , 74, 2906-11		87
1847	Molecular mechanics studies on the conformations of 2',3'-dideoxy-2',3'-didehydroguanine nucleoside, D4G. 1998 , 74, 3131-9		3
1846	Computer simulation study of synthetic 4-helix bundle that binds halothane. 1998 , 100-101, 377-85		1
1845	Structure and Magnetic Properties of Glycine Radical in Aqueous Solution at Different pH Values. Journal of the American Chemical Society, 1998 , 120, 5723-5732	6.4	81
1844	Molecular Dynamics Simulations of Ground and Transition States for the SN2 Displacement of Clfrom 1,2-Dichloroethane at the Active Site of Xanthobacter autotrophicus Haloalkane 1 Dehalogenase Journal of the American Chemical Society, 1998, 120, 5611-5621	6.4	57
1843	Strong Trans Influence Methoxymethyl Ligand in B(12) Cobaloxime and Imine/Oxime Model Complexes: Structural, Spectroscopic, and Molecular Mechanics Investigations. 1998 , 37, 6890-6897		62
1842	Conformational analysis and automated receptor docking of selective arylacetamide-based kappa-opioid agonists. 1998 , 41, 4777-89		53

1841	Computer simulations with explicit solvent: recent progress in the thermodynamic decomposition of free energies and in modeling electrostatic effects. 1998 , 49, 531-67	223
1840	Removal of pressure and free energy artifacts in charged periodic systems via net charge corrections to the Ewald potential. 1998 , 108, 7070-7084	143
1839	Pathways to a protein folding intermediate observed in a 1-microsecond simulation in aqueous solution. 1998 , 282, 740-4	1076
1838	Molecular dynamics simulations of DNA in solutions with different counter-ions. 1998 , 16, 579-92	74
1837	Quantum-Chemistry-Based Force Field for 1,2-Dimethoxyethane and Poly(ethylene oxide) in Aqueous Solution. 1998 , 102, 996-1001	82
1836	Molecular Dynamics Simulation of a Binary Hydrocarbon Mixture near an Adsorbing Wall: Benzene/n-Heptane on Graphite. 1998 , 14, 429-437	8
1835	Studies on selectin blockers. 6. Discovery of homologous fucose sugar unit necessary for E-selectin binding. 1998 , 41, 2302-7	24
1834	Quantitative analysis of the structural requirements for blockade of the N-methyl-D-aspartate receptor at the phencyclidine binding site. 1998 , 41, 393-400	35
1833	Enzymatic processing of uracil glycol, a major oxidative product of DNA cytosine. 1998 , 273, 10026-35	76
1832	The early stage of folding of villin headpiece subdomain observed in a 200-nanosecond fully solvated molecular dynamics simulation. 1998 , 95, 9897-902	139
	Solvated molecular dynamics simulation. 1996, 95, 9691-902	<u> </u>
1831	Atomistic modelling of ferroelectric liquid crystals. 1998 , 212, 45-53	3
1831 1830	Atomistic modelling of ferroelectric liquid crystals. 1998, 212, 45-53	
	Atomistic modelling of ferroelectric liquid crystals. 1998, 212, 45-53 Ab Initio and Hybrid Molecular Dynamics Simulations of the Active Site of Human Carbonic Anhydrase II: A Test Case Study. 1998, 264-274	3
1830	Atomistic modelling of ferroelectric liquid crystals. 1998, 212, 45-53 Ab Initio and Hybrid Molecular Dynamics Simulations of the Active Site of Human Carbonic Anhydrase II: A Test Case Study. 1998, 264-274	3
1830 1829	Atomistic modelling of ferroelectric liquid crystals. 1998, 212, 45-53 Ab Initio and Hybrid Molecular Dynamics Simulations of the Active Site of Human Carbonic Anhydrase II: A Test Case Study. 1998, 264-274 Ion channels: a challenge for computer simulations. 1998, The opening of a single base without perturbations of neighboring nucleotides: a study on crystal B-DNA duplex d(CGCGAATTCGCG)2. 1998, 15, 765-77	3
1830 1829 1828 1827	Atomistic modelling of ferroelectric liquid crystals. 1998, 212, 45-53 Ab Initio and Hybrid Molecular Dynamics Simulations of the Active Site of Human Carbonic Anhydrase II: A Test Case Study. 1998, 264-274 Ion channels: a challenge for computer simulations. 1998, The opening of a single base without perturbations of neighboring nucleotides: a study on crystal B-DNA duplex d(CGCGAATTCGCG)2. 1998, 15, 765-77 Rationalization of the dielectric properties of common three-site water models in terms of their	3 4
1830 1829 1828 1827	Atomistic modelling of ferroelectric liquid crystals. 1998, 212, 45-53 Ab Initio and Hybrid Molecular Dynamics Simulations of the Active Site of Human Carbonic Anhydrase II: A Test Case Study. 1998, 264-274 Ion channels: a challenge for computer simulations. 1998, The opening of a single base without perturbations of neighboring nucleotides: a study on crystal B-DNA duplex d(CGCGAATTCGCG)2. 1998, 15, 765-77 Rationalization of the dielectric properties of common three-site water models in terms of their force field parameters. 1998, 109, 4927-4937 3D QSAR in Drug Design. 1998,	3 4 17 125

1823	Coordinates scaling and multiple time step algorithms for simulation of solvated proteins in the NPT ensemble. 1998 , 109, 5194-5202	88
1822	Use of molecular overlap to predict intermolecular repulsion in N IIIHD hydrogen bonds. 1998 , 95, 525-537	16
1821	Molecular dynamic simulations of environment and sequence dependent DNA conformations: the development of the BMS nucleic acid force field and comparison with experimental results. 1998 , 16, 487-509	100
1820	The GAGA factor of Drosophila binds triple-stranded DNA. 1998, 273, 24640-8	36
1819	Structural characteristics of 2'-O-(2-methoxyethyl)-modified nucleic acids from molecular dynamics simulations. 1998 , 26, 3694-799	29
1818	Quantum Mechanical-Molecular Mechanical Coupled Potentials. 1998, 2-15	14
1817	Design and synthesis of conformationally constrained inhibitors of high-affinity, sodium-dependent glutamate transporters. 1998 , 296, 175-89	9
1816	Energetics of Base Pairs in B-DNA in Solution: An Appraisal of Potential Functions and Dielectric Treatments. 1998 , 102, 6139-6144	55
1815	Exciting Green Flourescent Protein. 1998 , 288-295	3
1814	Conformational Studies on Nucleosides with Furanose Ring Modifications. 1 1998 , 17, 791-814	5
1813	Stability of G,A triple helices. 1999 , 27, 2699-707	13
1812	Anharmonic Vibrational Self-Consistent Field Calculations as an Approach to Improving Force Fields for Monosaccharides. 1999 , 103, 3476-3488	32
1811	Photoluminescence studies of the light-emitting species in new materials for polymer devices. 1999 ,	
1810	Determining transition states from kinetic isotope effects. 1999 , 308, 355-97	37
1809	Modelling Protein-DNA Interactions. 1999 , 8, 441-483	5
1808	An NMR and molecular modelling analysis of d(CTACTGCTTTAG). d(CTAAAGCAGTAG) reveals that the particular behaviour of TpA steps is related to edge-to-edge contacts of their base-pairs in the major groove. 1999 , 27, 4759-67	16
1807	Redesign of the coenzyme specificity in L-lactate dehydrogenase from bacillus stearothermophilus using site-directed mutagenesis and media engineering. 1999 , 12, 851-6	70
1806	Structural properties of DNA:RNA duplexes containing 2'-O-methyl and 2'-S-methyl substitutions: a molecular dynamics investigation. 1999 , 27, 2189-95	39

1805	A structural snapshot of an intermediate on the streptavidin-biotin dissociation pathway. 1999 , 96, 8384-9	57
1804	Theoretical calculations, synthesis and base pairing properties of oligonucleotides containing 8-amino-2'-deoxyadenosine. 1999 , 27, 1991-8	30
1803	The maximal affinity of ligands. 1999 , 96, 9997-10002	709
1802	3D modeling, ligand binding and activation studies of the cloned mouse delta, mu; and kappa opioid receptors. 1999 , 12, 927-42	39
1801	Can G-C Hoogsteen-wobble pairs contribute to the stability of d(G. C-C) triplexes?. 1999 , 27, 2248-55	16
1800	Differential stability of the triple helix of (Pro-Pro-Gly)10 in H2O and D2O: thermodynamic and structural explanations. 1999 , 17, 481-91	8
1799	A molecular-dynamics simulation study of water on NaCl(100) using a polarizable water model. 1999 , 110, 12097-12107	65
1798	Effect of solvent fluctuation on the electronic transitions of formaldehyde in aqueous solution. 1999 , 110, 3484-3492	52
1797	Folding of oligoglutamines: a theoretical approach based upon thermodynamics and molecular mechanics. 1999 , 17, 409-27	30
1796	Symplectic integration of closed chain rigid body dynamics with internal coordinate equations of motion. 1999 , 111, 1407-1414	26
1795	Solvent electronic polarization effect on the electronic transitions in solution: Charge polarizable reference interaction site model self-consistent field approach. 1999 , 111, 481-491	14
1794	Calculation of optical spectra in liquid methanol using molecular dynamics and the chemical potential equalization method. 1999 , 111, 4218-4229	65
1793	Dynamic heterogeneities of translational and rotational motion of a molecular glass former from computer simulations. 1999 , 110, 4514-4522	54
1792	A simplified force field for describing vibrational protein dynamics over the whole frequency range. 1999 , 111, 10766-10769	49
1791	An Empirical Analysis of Proton Chemical Shifts in Nucleic Acids. 1999 , 194-206	13
1790	Modified self-consistent harmonic approach to thermal fluctuational disruption of disulfide bonds in proteins. 1999 , 60, 5938-42	1
1789	Molecular dynamics simulations of a protein-protein dimer: particle-mesh Ewald electrostatic model yields far superior results to standard cutoff model. 1999 , 16, 1205-18	60
1788	Accurate dipole moments from HartreeBock calculations by means of class IV charges. 1999 , 111, 885-892	22

1787 Molecular Dynamics Simulation of the Hin-Recombinase D NA Complex. 1999 , 21, 303-324	10
"RKKH" peptides from the snake venom metalloproteinase of Bothrops jararaca bind near the metal ion-dependent adhesion site of the human integrin alpha(2) I-domain. 1999 , 274, 31493-505	30
Molecular dynamics and free-energy calculations applied to affinity maturation in antibody 48G7. 1999 , 96, 14330-5	235
$_{17}8_{4}$ Self-assembly of chlorophenols in water. 1999 , 96, 6577-80	16
Three-dimensional models of alpha(2A)-adrenergic receptor complexes provide a structural explanation for ligand binding. 1999 , 274, 23405-13	25
New Free Energy Calculation Methods for Structure-Based Drug Design and Prediction of Protein Stability. 1999 , 37-52	1
A World Wide Web-service to aid the development of AMBER parameters using analogy to standard parameters. 1999 , 23, 435-7	4
The influence of electronic and steric factors on chain branching in ethylene polymerization by Brookhart-type Ni(II) diimine catalysts: a combined density functional theory and molecular mechanics study. 1999 , 591, 204-213	42
1779 MD-simulation study of the hydrophobic hydration of nonionic surfactants. 1999 , 156, 489-500	8
Dissociation energies of deoxyribose nucleotide dimer anions measured using blackbody infrared radiative dissociation. 1999 , 10, 1095-104	40
A comparative study of MP2, B3LYP, RHF and SCC-DFTB force fields in predicting the vibrational spectra of N-acetyl-L-alanine-N'-methyl amide: VA and VCD spectra. 1999 , 246, 13-36	72
1776 Implicit solvent models. 1999 , 78, 1-20	708
Towards a better description and understanding of biomolecular solvation. 1999 , 78, 43-68	40
Towards molecular dynamics simulation of large proteins with a hydration shell at constant pressure. 1999 , 78, 157-82	52
Adenine-thymine molecular dynamics simulation. Conformation, hydration and magnetic behaviour. 1999 , 79, 177-186	4
1.8 and 1.9 A resolution structures of the Penicillium amagasakiense and Aspergillus niger glucose oxidases as a basis for modelling substrate complexes. 1999 , 55, 969-77	229
Three-centre C-HO hydrogen bonds in the DNA minor groove: analysis of oligonucleotide crystal structures. 1999 , 55, 2005-12	10
The chimeric peptide [Lys(-2)-Arg(-1)]-sarafotoxin-S6b, composed of the endothelin pro-sequence and sarafotoxin, retains the salt-bridge staple between Arg(-1) and Asp8 previously observed in [Lys(-2)-Arg(-1)]-endothelin. Implications of this salt-bridge in the contractile activity and the	5

1769	Structure and dynamics at the liquid surface of benzyl alcohol. 1999 , 241, 55-73	6
1768	Towards more realistic computational modeling of homogenous catalysis by density functional theory: combined QM/MM and ab initio molecular dynamics. 1999 , 50, 479-500	59
1767	Molecular dynamics study on mobility and dipole ordering of solvent around proteins: effects of periodic-box size and protein charge. 1999 , 306, 395-401	18
1766	Adenine?2,4-difluorotoluene (modified base) pair: potential and free-energy surfaces. 1999 , 313, 393-398	16
1765	Rational design of a GCN4-derived mimetic of interleukin-4. 1999 , 6, 652-6	42
1764	Calculating the electrostatic properties of RNA provides new insights into molecular interactions and function. 1999 , 6, 1055-61	176
1763	A novel loop-loop recognition motif in the yeast ribosomal protein L30 autoregulatory RNA complex. 1999 , 6, 1139-47	99
1762	Simulations of the dynamics at an RNA-protein interface. 1999 , 6, 540-4	35
1761	Stability of hairpin ribozyme tertiary structure is governed by the interdomain junction. 1999 , 6, 544-9	132
1760	The structure of cobalt corrinoids based on molecular mechanics and NOE-restrained molecular mechanics and dynamics simulations. 1999 , 190-192, 127-153	18
1759	Molecular dynamics of a tetrasaccharide subunit of chondroitin 4-sulfate in water. 1999 , 318, 1-9	14
1758	Molecular modelling of the adsorption of aromatic and aromatic sulfonate molecules from aqueous solutions onto graphite. 1999 , 37, 1133-1142	11
1757	A new insight into the structure and stability of Hoogsteen hydrogen-bonded G-tetrad: an ab initio SCF study. 1999 , 311, 209-214	77
1756	The multicanonical weighted histogram analysis method for the free-energy landscape along structural transition paths. 1999 , 312, 247-254	33
1755	Modelling DNA stretching for physics and biology. 1999 , 106, 75-84	27
1754	On Spectral Identification of DNA-Base Pairs Polymorphism. 1999 , 24, 167-84	10
1753	Refined solution structure and backbone dynamics of 15N-labeled C12A-p8MTCP1 studied by NMR relaxation. 1999 , 15, 271-88	32
1752	Calculations of NMR dipolar coupling strengths in model peptides. 1999 , 15, 95-102	93

1751	1999 , 13, 119-31	32
1750	Local water bridges and protein conformational stability. 1999 , 8, 1982-9	58
1749	Study of the stability and unfolding mechanism of BBA1 by molecular dynamics simulations at different temperatures. 1999 , 8, 1292-304	47
1748	The NMR structure of the 5S rRNA E-domain-protein L25 complex shows preformed and induced recognition. 1999 , 18, 6508-21	73
1747	Amino Acid Protonation States Determine Binding Sites of the Secondary Ubiquinone and Its Anion in the Rhodobacter sphaeroides Photosynthetic Reaction Center 1. 1999 , 103, 5380-5387	57
1746	Application of a pairwise generalized Born model to proteins and nucleic acids: inclusion of salt effects. 1999 , 101, 426-434	244
1745	Hydroxyproline interference during the gas chromatographic analysis of D/L aspartic acid in human dentine. 1999 , 112, 124-31	11
1744	Homology Modeling and Molecular Dynamics Simulations of PBCV-1 Glycosylase Complexed with UV-damaged DNA. 1999 , 5, 302-316	8
1743	Computational approaches to structure-based ligand design. 1999 , 84, 179-91	73
1742	Molecular mechanics with QEq-CS (charge equilibration method generalized for charge separation system). 1999 , 461-462, 239-247	13
1741	Force field parametrization of 1,3-dihydroimidazol-2-one. 1999 , 464, 249-255	1
1740	Studies on aliphatic polyesters I: Ab initio, density functional and force field studies of esters with one carboxyl group. 1999 , 488, 247-262	25
1739	Conformational analysis of dimethyl phosphate in aqueous solution: a density functional theory-based molecular dynamics study. 1999 , 489, 237-245	19
1738	NMR structure of the human oncofoetal fibronectin ED-B domain, a specific marker for angiogenesis. 1999 , 7, 381-90	44
1737	Effective Computational Strategies for Determining Structures of Carcinogen-Damaged DNA. 1999 , 151, 313-332	4
1736	Free Energy Analysis of Protein D NA Binding: The EcoRI Endonuclease D NA Complex. 1999 , 151, 333-357	96
1735	Active-site dynamics of ASADHA bacterial biosynthetic enzyme. 1999 , 73, 137-146	12
1734	Ab initio study of preferential interactions between aromatic side chains. 1999 , 73, 175-186	8

1733	Toward an effective and reliable representation of solvent effects in the study of biochemical systems. 1999 , 73, 219-227	11
1732	Computational approaches to the study of some lanthanide (III) polyazamacrocyclic chelates for magnetic resonance imaging. 1999 , 73, 237-248	23
1731	Transfer RNA recognition by aminoacyl-tRNA synthetases. 1999 , 52, 1-28	131
1730	Comparison of the dynamics of bovine and human angiogenin: a molecular dynamics study. 1999 , 49, 131-44	6
1729	Computational investigations of structural changes resulting from point mutations in a collagen-like peptide. 1999 , 49, 167-83	42
1728	Conformation in solution and dynamics of a structurally constrained linear insect kinin pentapeptide analogue. 1999 , 49, 403-13	40
1727	Mouse acetylcholinesterase unliganded and in complex with huperzine A: a comparison of molecular dynamics simulations. 1999 , 50, 35-43	25
1726	A molecular dynamics simulation of the flavin mononucleotide-RNA aptamer complex. 1999 , 50, 287-302	71
1725	Molecular dynamics of mouse acetylcholinesterase complexed with huperzine A. 1999 , 50, 347-59	22
1724	Mode-coupling smoluchowski dynamics of a double-stranded DNA oligomer. 1999 , 50, 613-29	15
1723	Effects of turn residues on beta-hairpin foldinga molecular dynamics study. 1999 , 50, 763-76	14
1722	Prodock: Software package for protein modeling and docking. 1999 , 20, 412-427	91
1721	United atom force field for phospholipid membranes: Constant pressure molecular dynamics simulation of dipalmitoylphosphatidicholine/water system. 1999 , 20, 531-545	136
1720	A 500-ps molecular dynamics simulation trajectory of cardiotoxin II from Taiwan cobra venom in solution: Correlation with NMR and X-ray crystallography data. 1999 , 20, 546-562	1
1719	MMFF VI. MMFF94s option for energy minimization studies. 1999 , 20, 720-729	855
1718	MMFF VII. Characterization of MMFF94, MMFF94s, and other widely available force fields for conformational energies and for intermolecular-interaction energies and geometries. 1999 , 20, 730-748	597
1717	Simple method for locating possible ligand binding sites on protein surfaces. 1999 , 20, 983-988	37
1716	Automatic parameterization of force fields for liquids by simplex optimization. 1999 , 20, 1009-1017	108

1715	New out-of-plane angle and bond angle internal coordinates and related potential energy functions for molecular mechanics and dynamics simulations. 1999 , 20, 1067-1084	16
1714	Improving performance of polarizable continuum model for study of large molecules in solution. 1999 , 20, 1186-1198	23
1713	Consensus bond-charge increments fitted to electrostatic potential or field of many compounds: Application to MMFF94 training set. 1999 , 20, 1495-1516	26
1712	Analysis of domain motions in large proteins. 1999 , 34, 369-382	157
1711	What determines the van der Waals coefficient In the LIE (linear interaction energy) method to estimate binding free energies using molecular dynamics simulations?. 1999 , 34, 395-402	104
1710	Prediction of loop geometries using a generalized born model of solvation effects. 1999 , 35, 173-183	81
1709	Impact of Cland Na+ ions on simulated structure and dynamics of ARK1 PH domain. 1999 , 35, 206-217	21
1708	Correlation between knowledge-based and detailed atomic potentials: Application to the unfolding of the GCN4 leucine zipper. 1999 , 35, 447-452	29
1707	Flexible ligand docking: A multistep strategy approach. 1999 , 36, 1-19	119
1706	Protein strain in blue copper proteins studied by free energy perturbations. 1999 , 36, 157-74	38
1705	Conformational dynamics of cytochrome c: Correlation to hydrogen exchange. 1999 , 36, 175-191	76
1704	Early events in the folding of an amphipathic peptide: A multinanosecond molecular dynamics study. 1999 , 36, 383-399	23
1703	Dynamical properties of fasciculin-2. 1999 , 36, 447-53	12
1702	Protein fold recognition score functions: Unusual construction strategies. 1999 , 36, 454-461	1
1701	The free energies for mutating S27 and W79 to alanine in streptavidin and its biotin complex: The relative size of polar and nonpolar free energies on biotin binding. 1999 , 36, 471-473	12
1700	Enzyme polarization of substrates of dihydrofolate reductase by different theoretical methods. 1999 , 37, 157-165	19
1699	Computational studies of the domain movement and the catalytic mechanism of thymidine phosphorylase. 1999 , 37, 242-52	22
1698	Molecular dynamics simulations of beta-hairpin folding. 1999 , 37, 325-33	26

1697	Serine proteases: An ab initio molecular dynamics study. 1999 , 37, 611-618		29
1696	A Molecular Mechanics Force Field for Alkylcobaloximes, a Model of Vitamin B12 Coenzyme [] Implications of Steric and Electronic Factors in the Coll Bond Cleavage. 1999 , 1999, 981-992		20
1695	Effects of 5-[S-(2,4-dinitrophenyl)-thio]-2'-deoxyuridine analog incorporation on the structure and stability of DNA hybrids: implications for the design of nucleic acid probes. 1999 , 12, 337-45		2
1694	Algorithm Engineering. 1999,		О
1693	Ground State and Transition State Contributions to the Rates of Intramolecular and Enzymatic Reactions. 1999 , 32, 127-136		235
1692	Adjusted Connection Atoms for Combined Quantum Mechanical and Molecular Mechanical Methods. 1999 , 103, 9290-9295		174
1691	A modified version of the Cornell et al. force field with improved sugar pucker phases and helical repeat. 1999 , 16, 845-62		810
1690	Predicting binding affinities of protein ligands from three-dimensional models: application to peptide binding to class I major histocompatibility proteins. 1999 , 42, 4650-8		159
1689	Conformational Control of Intramolecular Electron Transfer in Calix[4]diquinones and Their Cationic Complexes. <i>Journal of the American Chemical Society</i> , 1999 , 121, 14-27	16.4	52
1688	Derivation of Class II Force Fields. 7. Nonbonded Force Field Parameters for Organic Compounds. 1999 , 103, 6998-7014		45
1687	A Quantum Mechanical/Molecular Mechanical Approach to Relaxation Dynamics: Calculation of the Optical Properties of Solvated Bacteriochlorophyll-a. 1999 , 103, 7720-7727		54
1686	Free Energy Calculations of Watson Trick Base Pairing in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1999 , 121, 9503-9508	16.4	67
1685	Theoretical Study of Base-Catalyzed Amide Hydrolysis: 'Gas- and Aqueous-Phase Hydrolysis of Formamide. <i>Journal of the American Chemical Society</i> , 1999 , 121, 5712-5726	16.4	93
1684	Determination of Two Structural Forms of Catalytic Bridging Ligand in ZincPhosphotriesterase by Molecular Dynamics Simulation and Quantum Chemical Calculation. <i>Journal of the American Chemical Society</i> , 1999 , 121, 7279-7282	16.4	76
1683	Binding preferences of hydroxamate inhibitors of the matrix metalloproteinase human fibroblast collagenase. 1999 , 42, 1225-34		42
1682	Rationalization of the Enantioselectivity of Subtilisin in DMF. <i>Journal of the American Chemical Society</i> , 1999 , 121, 3486-3493	16.4	42
1681	Binding Free Energy and Extraction Selectivity Calculations of Anisole and Phenanthroline Spherands. 1999 , 103, 10015-10020		4
1680	Role of sugar re-puckering in the transition of A and B forms of DNA in solution. A molecular dynamics study. 1999 , 17, 89-99		23

1679	On the origin of dynamic heterogeneities in glass-forming liquids. 1999 , 111, 10177-10182	27
1678	Computer simulation of the interaction of non-steroidal anti-inflammatory drugs: indoprofen and NS398 with cyclooxygenase. 1999 , 16, 901-15	6
1677	Experimental and theoretical studies of the conformational perturbations induced by an abasic site. 1999 , 17, 245-57	9
1676	Nonapeptide analogues containing (R)-3-hydroxybutanoate and beta-homoalanine oligomers: synthesis and binding affinity to a class I major histocompatibility complex protein. 1999 , 42, 2318-31	28
1675	DNA bending induced by high mobility group proteins studied by fluorescence resonance energy transfer. 1999 , 38, 12150-8	65
1674	Semiclassical Wave Packet Dynamics with Electronic Structure Computed on the Fly: Application to Photophysics of Electronic Excited States in Condensed Phase. 1999 , 103, 9469-9474	13
1673	Adiabatic bias molecular dynamics: A method to navigate the conformational space of complex molecular systems. 1999 , 110, 3697-3702	102
1672	Pi7, an orphan peptide from the scorpion Pandinus imperator: a 1H-NMR analysis using a nano-NMR Probe. 1999 , 38, 16756-65	29
1671	Helix morphology changes in B-DNA induced by spontaneous B(I)B(II) substrate interconversion. 1999 , 17, 223-35	26
1670	Cationic 5,10,15,20-tetrakis(N-methylpyridinium-4-yl)porphyrin fully intercalates at 5'-CG-3' steps of duplex DNA in solution. 1999 , 38, 15425-37	103
1669	ESI/ion trap/ion mobility/time-of-flight mass spectrometry for rapid and sensitive analysis of biomolecular mixtures. 1999 , 71, 291-301	179
1668	Internal Dynamics of Green Fluorescent Protein. 1999 , 103, 3263-3269	68
1667	The binding mechanism of urea, hydroxamic acid and N-(N-butyl)-phosphoric triamide to the urease active site. A comparative molecular dynamics study. 1999 , 31, 789-796	79
1666	Mapping of putative binding sites on the ectodomain of the type II TGF-beta receptor by scanning-deletion mutagenesis and knowledge-based modeling. 1999 , 456, 79-84	13
1665	Molecular dynamics simulation of a synthetic four-alpha-helix bundle that binds the anesthetic halothane. 1999 , 455, 332-8	8
1664	Propene Polymerization with the Isospecific, Highly Regiospecific rac-Me2C(3-t-Bu-1-Ind)2ZrCl2/MAO Catalyst. 1. Influence of Hydrogen on Initiation and Propagation: Experimental Detection and Theoretical Investigation of 2,1 Propene Insertion into	30
1663	Predicting relative binding free energies of tacrine-huperzine A hybrids as inhibitors of acetylcholinesterase. 1999 , 42, 5110-9	34
1662	Stability and Activity of Mesophilic Subtilisin E and Its Thermophilic Homolog: Insights from Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 1999 , 121, 6895-6903	4 63

1661	1-Benzopyran-4-one antioxidants as aldose reductase inhibitors. 1999 , 42, 1881-93		82
1660	Mechanistic Aspects of Ethylene Polymerization by Iron(II) B isimine Pyridine Catalysts: A Combined Density Functional Theory and Molecular Mechanics Study. <i>Journal of the American Chemical Society</i> , 1999 , 121, 6479-6487	16.4	132
1659	OPLS All-Atom Model for Amines: Resolution of the Amine Hydration Problem. <i>Journal of the American Chemical Society</i> , 1999 , 121, 4827-4836	16.4	528
1658	The Role of Bonded Terms in Free Energy Simulations: 1. Theoretical Analysis. 1999 , 103, 103-118		108
1657	The Role of Bonded Terms in Free Energy Simulations. 2. Calculation of Their Influence on Free Energy Differences of Solvation. 1999 , 103, 119-136		76
1656	Prediction of the binding free energies of new TIBO-like HIV-1 reverse transcriptase inhibitors using a combination of PROFEC, PB/SA, CMC/MD, and free energy calculations. 1999 , 42, 868-81		57
1655	The Role of Polarization and Charge Transfer in the Solvation of Biomolecules. <i>Journal of the American Chemical Society</i> , 1999 , 121, 9182-9190	16.4	91
1654	Solution structure of Syrian hamster prion protein rPrP(90-231). 1999 , 38, 5362-77		172
1653	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. 1999 , 110, 741-754		225
1652	Determining the Role of Hydration Forces in Protein Folding. 1999 , 103, 5413-5426		86
1651	Nanosecond Molecular Dynamics Simulations of Parallel and Antiparallel Guanine Quadruplex DNA Molecules. <i>Journal of the American Chemical Society</i> , 1999 , 121, 5519-5534	16.4	153
1650	Transferable Potentials for Phase Equilibria. 3. Explicit-Hydrogen Description of Normal Alkanes. 1999 , 103, 5370-5379		233
1649	Probing the structural changes in the light chain of human coagulation factor VIIa due to tissue factor association. 1999 , 77, 99-113		11
1648	Change in conformation by DNA-peptide association: molecular dynamics of the Hin-recombinase-hixL complex. 1999 , 77, 123-38		14
1647	Statistical mechanical equilibrium theory of selective ion channels. 1999 , 77, 139-53		116
1646	Sodium and chlorine ions as part of the DNA solvation shell. 1999 , 77, 1769-81		196
1645	Stability of the beta-sheet of the WW domain: A molecular dynamics simulation study. 1999 , 77, 2191-8		46
1644	From atomic to mesoscopic descriptions of the internal dynamics of DNA. 1999 , 77, 2366-76		51

1643	Comparison of the crystal and solution structures of two RNA oligonucleotides. 1999 , 76, 65-75	33
1642	An atomic model for the pleated beta-sheet structure of Abeta amyloid protofilaments. 1999 , 76, 2871-8	110
1641	Ligand binding by antibody IgE Lb4: assessment of binding site preferences using microcalorimetry, docking, and free energy simulations. 1999 , 76, 2966-77	11
1640	Molecular dynamics studies on the HIV-1 integrase catalytic domain. 1999 , 76, 2999-3011	73
1639	Unrestrained stochastic dynamics simulations of the UUCG tetraloop using an implicit solvation model. 1999 , 76, 3192-205	61
1638	The Riddle of Resorcinol Crystal Growth Revisited: Molecular Dynamics Simulations of Resorcinol Crystal Water Interface. <i>Journal of the American Chemical Society</i> , 1999 , 121, 8583-8591	46
1637	Docking of cationic antibiotics to negatively charged pockets in RNA folds. 1999 , 42, 1250-61	117
1636	Atomic Determinants for Aminoacylation of RNA Minihelices and Relationship to Genetic Code. 1999 , 32, 368-375	49
1635	Donor Acceptor-Assisted Diels Alder Reaction of Anthracene and Tetracyanoethylene. 1999 , 103, 8279-8287	34
1634	Potassium and sodium binding to the outer mouth of the K+ channel. 1999 , 38, 8599-604	141
1633	Calculating the Absolute Free Energy of Association of Netropsin and DNA. <i>Journal of the American Chemical Society</i> , 1999 , 121, 3267-3271	41
1632	Molecular Simulation of ⊞lefins Using a New United-Atom Potential Model: Vapor□iquid Equilibria of Pure Compounds and Mixtures. <i>Journal of the American Chemical Society</i> , 1999 , 121, 3407-3463	26
1631	Effects of C2ESubstitution on Arabinonucleic Acid Structure and Conformation. <i>Journal of the American Chemical Society</i> , 1999 , 121, 5609-5610	24
1630	Why Are Copper(II) Amino Acid Complexes Not Planar in Their Crystal Structures? An ab Initio and Molecular Mechanics Study. 1999 , 38, 2764-2774	43
1629	Cation Interactions in Proteins: Can Simple Models Provide an Accurate Description?. <i>Journal of the American Chemical Society</i> , 1999 , 121, 10366-10372	169
1628	NMR solution structure of alpha-conotoxin ImI and comparison to other conotoxins specific for neuronal nicotinic acetylcholine receptors. 1999 , 38, 3874-82	47
1627	Solution structure and energy calculation of bis-intercalation of homodimeric thiazole orange dye derivatives in DNA: effects of modifying the linker. 1999 , 10, 735-44	8
1626	Development and Validation of Effective Computational Strategies for the Study of Metal Nitroxide Complexes. 1999 , 103, 7676-7685	29

1625	Wild-Type RNA MicrohelixAla and 3:70 Variants: Molecular Dynamics Analysis of Local Helical Structure and Tightly Bound Water. <i>Journal of the American Chemical Society</i> , 1999 , 121, 7310-7317	16.4	39
1624	Redox properties of mesophilic and hyperthermophilic rubredoxins as a function of pressure and temperature. 1999 , 38, 7874-80		22
1623	Molecular dynamics simulations of human prion protein: importance of correct treatment of electrostatic interactions. 1999 , 38, 13862-76		87
1622	Ab Initio Quantum Mechanical Study of Metal Substitution in Analogues of Rubredoxin: Implications for Redox Potential Control. 1999 , 103, 8006-8015		12
1621	A pseudobond approach to combining quantum mechanical and molecular mechanical methods. 1999 , 110, 46-54		421
1620	Molecular dynamics simulations of P450 BM3examination of substrate-induced conformational change. 1999 , 16, 1189-203		23
1619	Asymmetry of the Hydrogen Bond of Hydrogen Phthalate Anion in Solution. A QM/MM Study. Journal of the American Chemical Society, 1999 , 121, 9198-9207	16.4	49
1618	Ionic Conduction in Polyphosphazene Solids and Gels: 13C, 31P, and 15N NMR Spectroscopy and Molecular Dynamics Simulations. 1999 , 32, 732-741		44
1617	Min-21 and min-23, the smallest peptides that fold like a cystine-stabilized beta-sheet motif: design, solution structure, and thermal stability. 1999 , 38, 10615-25		50
1616	Computer Simulation Studies of Finite Temperature Conformational Equilibrium in Alanine-Based Peptides. 1999 , 103, 1752-1766		35
1615	Theoretical Study of Peptides Formed by Aminoxy Acids. <i>Journal of the American Chemical Society</i> , 1999 , 121, 11189-11196	16.4	55
1614	Cobalt(II) Imino Pyridine Assisted Ethylene Polymerization: A Quantum-Mechanical/Molecular-Mechanical Density Functional Theory Investigation. 1999 , 18, 5701-570)8	60
1613	Ab Initio Quantum Mechanical Study of the Structures and Energies for the Pseudorotation of 5EDehydroxy Analogues of 2EDeoxyribose and Ribose Sugars. <i>Journal of the American Chemical Society</i> , 1999 , 121, 985-993	16.4	71
1612	Free Energy Perturbation and Molecular Dynamics Studies of [16]Starand with Various Alkali Metal lons. 1999 , 64, 5787-5793		6
1611	Free-Energy Maps of BaseAmino Acid Interactions for DNAProtein Recognition. <i>Journal of the American Chemical Society</i> , 1999 , 121, 6152-6157	16.4	42
1610	Molecular Dynamics Simulations of Ground and Transition States for the Hydride Transfer from Formate to NAD+in the Active Site of Formate Dehydrogenase. <i>Journal of the American Chemical Society</i> , 1999 , 121, 8164-8173	16.4	44
1609	Intercalative G-Tetraplex Stabilization of Telomeric DNA by a Cationic Porphyrin1. <i>Journal of the American Chemical Society</i> , 1999 , 121, 1768-1779	16.4	217
1608	Binding constants of neuraminidase inhibitors: An investigation of the linear interaction energy method. 1999 , 42, 5142-52		77

1607	Solution structure and dynamics of a complex between DNA and the antitumor bisnaphthalimide LU-79553: intercalated ring flipping on the millisecond time scale. 1999 , 38, 15104-15	55
1606	Dimethyl Phosphate: Stereoelectronic versus Environmental Effects. 1999 , 103, 6121-6126	44
1605	Conformational analysis of the major DNA adduct derived from the food mutagen 2-amino-3-methylimidazo[4,5-f]quinoline. 1999 , 12, 895-905	25
1604	Application of a Multiple Time Step Algorithm to Biomolecular Systems. 1999 , 103, 5396-5405	18
1603	Implementation and Testing of a Frozen Density Matrix Divide and Conquer Algorithm. 1999, 103, 1868-1875	22
1602	Ab Initio Quantum Mechanical and Molecular Dynamical Study of Intra- and Intermolecular Anhydride Formation. 1999 , 103, 8067-8074	12
1601	Collisional Activation of Small Peptides. 1999 , 103, 3981-3990	71
1600	Structure and Dynamics of Liquid Diphenyl Carbonate Investigated by Molecular Dynamics Simulations. 1999 , 103, 10591-10598	14
1599	Solvent Dynamics and Mechanism of Proton Transfer in Human Carbonic Anhydrase II. <i>Journal of the American Chemical Society</i> , 1999 , 121, 2290-2302	107
1598	Exploring Multicomponent Phase Equilibria by Monte Carlo Simulations: Toward a Description of Gas-Liquid Chromatography. 1999 , 82-95	4
1597	Binding of Organic Cations to a Cyclophane Host As Studied with Molecular Dynamics Simulations and Free Energy Calculations. 1999 , 103, 4474-4480	13
1596	Reactive Flux Calculations of Methyl Vinyl Ketone Reacting with Cyclopentadiene in Water. 1999 , 103, 925-931	13
1595	Computational and Experimental Studies of (2,2)-Bis(indol-1-yl-methyl)acetate Suggest the Importance of the Hydrophobic Effect in Aromatic Stacking Interactions. <i>Journal of the American Chemical Society</i> , 1999 , 121, 1717-1725	37
1594	Single-turnover analysis of mutant human apurinic/apyrimidinic endonuclease. 1999 , 38, 4958-64	41
1593	Isoxazolo-[3,4-d]-pyridazin-7-(6H)-one as a potential substrate for new aldose reductase inhibitors. 1999 , 42, 1894-900	30
1592	Conformations of trypsin-bound amidine inhibitors of blood coagulant factor Xa by double REDOR NMR and MD simulations. 1999 , 42, 3910-8	22
1591	Structure, energetics, and dynamics of the nucleic Acid base pairs: nonempirical ab initio calculations. 1999 , 99, 3247-76	932
1590	Free Energy Perturbation Study of Octanol/Water Partition Coefficients: Comparison with Continuum GB/SA Calculations. 1999 , 103, 714-726	88

1589	NF-kappa B binding mechanism: a nuclear magnetic resonance and modeling study of a GGG> CTC mutation. 1999 , 38, 3883-94		33
1588	Computational Alanine Scanning To Probe Protein Protein Interactions: A Novel Approach To Evaluate Binding Free Energies. <i>Journal of the American Chemical Society</i> , 1999 , 121, 8133-8143	16.4	636
1587	Molecular dynamics studies of axis bending in d(G5-(GA4T4C)2-C5) and d(G5-(GT4A4C)2-C5): effects of sequence polarity on DNA curvature. 1999 , 285, 1623-32		80
1586	Stabilization of the anticodon stem-loop of tRNALys,3 by an A+-C base-pair and by pseudouridine. 1999 , 285, 115-31		145
1585	Modeling high-resolution hydration patterns in correlation with DNA sequence and conformation. 1999 , 286, 1075-95		108
1584	Functionally important correlated motions in the single-stranded DNA-binding protein encoded by filamentous phage Pf3. 1999 , 287, 569-77		18
1583	Conformational analysis of single-base bulges in A-form DNA and RNA using a hierarchical approach and energetic evaluation with a continuum solvent model. 1999 , 289, 261-75		36
1582	Conformational changes of the BS2 operator DNA upon complex formation with the Antennapedia homeodomain studied by NMR with 13C/15N-labeled DNA. 1999 , 292, 609-17		11
1581	Local folding coupled to RNA binding in the yeast ribosomal protein L30. 1999 , 292, 345-59		28
1580	How NF-kappaB can be attracted by its cognate DNA. 1999 , 293, 139-50		53
1579	The recognition of distorted DNA structures by HMG-D: a footprinting and molecular modelling study. 1999 , 294, 79-91		43
1578	A DNA hairpin with a single residue loop closed by a strongly distorted Watson-Crick G x C base-pair. 1999 , 294, 427-42		18
1577	C-H.O hydrogen bonds in minor groove of A-tracts in DNA double helices. 1999 , 294, 1149-58		70
1576	Solution structure of a beta-neurotoxin from the New World scorpion Centruroides sculpturatus Ewing. 1999 , 254, 406-12		15
1575	Full-length cDNA of human cathepsin F predicts the presence of a cystatin domain at the N-terminus of the cysteine protease zymogen. 1999 , 257, 313-8		64
1574	A general ab initio approach for free energy landscapes of biological molecules around the transition states. 1999 , 75, 291-294		2
1573	Analysis of low-frequency motions in proteins by computer simulation and neutron scattering. 1999 ,		
1572	Treatment of electrostatic interactions in computer simulations and calculation of thermodynamic properties such as free energies and pressures. 1999 ,		8

(2000-1999)

1571	Potential Energy and Free Energy Surfaces of Floppy Systems. Ab initio Calculations and Molecular Dynamics Simulations. 1999 , 7, 829-857	1
1570	Exploring the Structural Repertoire of Guanine-Rich DNA Sequences: Computer Modelling Studies. 1999 , 8, 279-323	4
1569	Requirement for the kinase activity of human DNA-dependent protein kinase catalytic subunit in DNA strand break rejoining. 1999 , 19, 3877-84	242
1568	Dynamics of macromolecules and nuclear magnetic relaxation: Application of mode-coupling diffusion theory to DNA, proteins and their complexes. 1999 , 146, 97-101	
1567	Molecular dynamics investigation of polar diacylglycerolipid monolayers: bond ordering properties. 2000 , 4064, 144	4
1566	Diffusive Dynamics in a Detailed Potential: Application to Biological Macromolecules. 2000 , 24, 307-324	4
1565	Similarities in the HIV-1 and ASV integrase active sites upon metal cofactor binding. 2000 , 53, 308-15	27
1564	One nanosecond molecular dynamics simulation of the N-terminal domain of the lambda repressor protein. 2000 , 53, 596-605	10
1563	All-atom empirical force field for nucleic acids: II. Application to molecular dynamics simulations of DNA and RNA in solution. 2000 , 21, 105-120	648
1562	Fast, efficient generation of high-quality atomic charges. AM1-BCC model: I. Method. 2000 , 21, 132-146	1113
1561	The molecular modeling toolkit: A new approach to molecular simulations. 2000 , 21, 79-85	253
1560	All-atom empirical force field for nucleic acids: I. Parameter optimization based on small molecule and condensed phase macromolecular target data. 2000 , 21, 86-104	1308
1559	Peptide free-energy profile is strongly dependent on the force field: Comparison of C96 and AMBER95. 2000 , 21, 748-762	60
1558	Comparison of enzyme polarization of ligands and charge-transfer effects for dihydrofolate reductase using point-charge embedded ab initio quantum mechanical and linear-scaling semiempirical quantum mechanical methods. 2000 , 21, 788-811	33
1557	Stability analysis for the cavity-filling mutations of the Myb DNA-binding domain utilizing free-energy calculations. 2000 , 38, 197-209	15
1556	Water penetration and escape in proteins. 2000 , 38, 261-272	139
1555	Molecular dynamics of mouse and Syrian hamster PrP: Implications for activity. 2000 , 38, 327-340	29
1554	Molecular dynamics simulation accurately predicts the experimentally-observed distributions of the (C, N, O) protein atoms around water molecules and sodium ions. 2000 , 39, 212-215	4

1553	Use of MM-PB/SA in estimating the free energies of proteins: Application to native, intermediates, and unfolded villin headpiece. 2000 , 39, 309-316	168
1552	BiGGER: A new (soft) docking algorithm for predicting protein interactions. 2000 , 39, 372-384	241
1551	Solvent density and long-range dipole field around a DNA-binding protein studied by molecular dynamics. 2000 , 40, 193-206	36
1550	Charge transfer in biologically important molecules: comparison of high-level ab initio and semiempirical methods. 2000 , 77, 27-43	28
1549	QCMEE study of the reductive half-reaction of glucose oxidase. 2000 , 77, 71-81	2
1548	Molecular dynamics simulation studies of liquid acetonitrile: New six-site model. 2000 , 21, 901-908	125
1547	Multicanonical Monte Carlo calculation of the free-energy map of the baselimino acid interaction. 2000 , 21, 954-962	17
1546	Flexible ligand docking using a robust evolutionary algorithm. 2000 , 21, 988-998	37
1545	How well does a restrained electrostatic potential (RESP) model perform in calculating conformational energies of organic and biological molecules?. 2000 , 21, 1049-1074	3321
1544	Dipole lattice membrane model for protein calculations. 2000 , 41, 211-23	24
1544 1543	Dipole lattice membrane model for protein calculations. 2000 , 41, 211-23 Exhaustive mutagenesis in silico: Multicoordinate free energy calculations on proteins and peptides. 2000 , 41, 385-397	24 58
1543	Exhaustive mutagenesis in silico: Multicoordinate free energy calculations on proteins and	
1543	Exhaustive mutagenesis in silico: Multicoordinate free energy calculations on proteins and peptides. 2000 , 41, 385-397	58
1543 1542 1541	Exhaustive mutagenesis in silico: Multicoordinate free energy calculations on proteins and peptides. 2000 , 41, 385-397 G-quadruplexes as therapeutic targets. 2000 , 56, 195-208	58
1543 1542 1541	Exhaustive mutagenesis in silico: Multicoordinate free energy calculations on proteins and peptides. 2000, 41, 385-397 G-quadruplexes as therapeutic targets. 2000, 56, 195-208 Molecular dynamics simulation of nucleic acids: successes, limitations, and promise. 2000, 56, 232-56	58 190 279
1543 1542 1541 1540	Exhaustive mutagenesis in silico: Multicoordinate free energy calculations on proteins and peptides. 2000, 41, 385-397 G-quadruplexes as therapeutic targets. 2000, 56, 195-208 Molecular dynamics simulation of nucleic acids: successes, limitations, and promise. 2000, 56, 232-56 Development and current status of the CHARMM force field for nucleic acids. 2000, 56, 257-65 ADAPT: a molecular mechanics approach for studying the structural properties of long DNA	58 190 279 795
1543 1542 1541 1540 1539	Exhaustive mutagenesis in silico: Multicoordinate free energy calculations on proteins and peptides. 2000, 41, 385-397 G-quadruplexes as therapeutic targets. 2000, 56, 195-208 Molecular dynamics simulation of nucleic acids: successes, limitations, and promise. 2000, 56, 232-56 Development and current status of the CHARMM force field for nucleic acids. 2000, 56, 257-65 ADAPT: a molecular mechanics approach for studying the structural properties of long DNA sequences. 2000, 56, 292-310 Smoluchowski dynamics of the vnd/NK-2 homeodomain from Drosophila melanogaster:	58 190 279 795 18

1535	Computational studies on carbohydrates: in vacuo studies using a revised AMBER force field, AMB99C, designed for alpha-(1>4) linkages. 2000 , 326, 194-209	66
1534	Computational studies on carbohydrates: solvation studies on maltose and cyclomaltooligosaccharides (cyclodextrins) using a DFT/ab initio-derived empirical force field, AMB99C. 2000 , 326, 210-26	63
1533	Comparison of linear-scaling semiempirical methods and combined quantum mechanical/molecular mechanical methods applied to enzyme reactions. 2000 , 320, 169-176	32
1532	Parallel molecular dynamics using OpenMP on a shared memory machine. 2000 , 124, 49-59	15
1531	A novel method for determining the electron tunneling pathway in protein. 2000, 300-302, 862-868	22
1530	A test of crystal structure prediction of small organic molecules. 2000 , 56, 697-714	338
1529	Interactions of Streptomyces griseus aminopeptidase with a methionine product analogue: a structural study at 1.53 A resolution. 2000 , 56, 551-8	34
1528	Simulation of electrostatic effects in Fab-antigen complex formation. 2000 , 267, 4861-9	10
1527	Molecular dynamics simulation of trp-repressor/operator complex: analysis of hydrogen bond patterns of protein DNA interaction. 2000 , 526, 209-218	13
1526	A new electrostatic model for molecular mechanics force fields. 2000 , 556, 1-21	56
1525	A QM/MM model for O(3 P) reaction with an alkyl thiolate self-assembled monolayer. 2000 , 556, 43-57	53
1524	Molecular structure of bis[(1,3)2-oxaadamantano]-18-crown-6 and its potassium picrato complex. 2000 , 554, 279-287	6
1523	Conformational stability of avarol-type molecules. Crystal structure of 3?-methylaminoavarone, a metabolite from Dysidea avara. 2000 , 516, 31-41	3
1522	A conformational model for poly(dichlorophosphazene) derived from molecular dynamics simulations. 2000 , 41, 3337-3347	18
1521	Clustering of a molecular dynamics trajectory with a Hamming distance. 2000 , 24, 693-8	14
1520	A global optimization strategy for predicting alpha-helical protein tertiary structure. 2000 , 24, 489-97	12
1519	Computational enzymology. 2000 , 4, 540-4	38
1518	Limited plasticity in the recognition of peptide epitope variants by an alloreactive CTL clone correlates directly with conservation of critical residues and inversely with peptide length. 2000 , 55, 289-95	

1517	Molecular simulation of an amorphous poly(methyl methacrylate) poly(tetrafluoroethylene) interface. 2000 , 10, 371-381	41
1516	QM/MM and SCRF studies of the ionization state of 8-methylpterin substrate bound to dihydrofolate reductase: existence of a low-barrier hydrogen bond. 2000 , 18, 42-9	10
1515	A method for including protein flexibility in protein-ligand docking: improving tools for database mining and virtual screening. 2000 , 18, 247-57, 302-4	63
1514	Interaction of pyrimethamine, cycloguanil, WR99210 and their analogues with Plasmodium falciparum dihydrofolate reductase: structural basis of antifolate resistance. 2000 , 8, 1117-28	118
1513	Structural bases for the inhibition of aldose reductase by phenolic compounds. 2000 , 8, 1151-8	30
1512	Domain motions in proteins. 2000 , 84, 53-63	5
1511	The role of water in B-DNAs BI to BII conformer substates interconversion: a combined study by calorimetry, FT-IR spectroscopy and computer simulation. 2000 , 258, 391-404	20
1510	Harmonicity in slow protein dynamics. 2000 , 261, 25-37	178
1509	Self-assembled complexes of oligopeptides and metalloporphyrins: measurements of the reorganization and electronic interaction energies for photoinduced electron-transfer reactions. 2000 , 83, 121-40	20
1508	Selective targeting of lysosomal cysteine proteases with radiolabeled electrophilic substrate analogs. 2000 , 7, 27-38	182
1507	thairpin folds by molecular dynamics simulations. 2000 , 326, 421-429	15
1506	Replica-exchange multicanonical algorithm and multicanonical replica-exchange method for simulating systems with rough energy landscape. 2000 , 329, 261-270	268
1505	Nucleic acids: theory and computer simulation, Y2K. 2000 , 10, 182-96	197
1504	Modeling DNA deformations. 2000 , 10, 286-97	152
1503	The crystal structure of the formiminotransferase domain of formiminotransferase-cyclodeaminase: implications for substrate channeling in a bifunctional enzyme. 2000 , 8, 35-46	37
1502	The design and applications of a recursive molecular modeling framework. 2000 , 4, 159-64	1
1501	A family competition evolutionary algorithm for automated docking of flexible ligands to proteins. 2000 , 4, 225-37	11
1500	About the TATB assumption: effect of charge reversal on transfer of large spherical ions from aqueous to non-aqueous solvents and on their interfacial behaviour. 2000 , 500, 139-155	27

1499	Ab initio hybrid quantum mechanical/molecular mechanical studies of the mechanisms of the enzymes protein kinase and thymidine phosphorylase. 2000 , 506, 35-44		17
1498	Towards solvation simulations with a combined ab initio molecular dynamics and molecular mechanics approach. 2000 , 506, 313-334		20
1497	Dynamic modeling of EDG1 receptor structural changes induced by site-directed mutations. 2000 , 529, 219-224		12
1496	530 ps molecular dynamics simulation of indoprofen and NS398 with COX-1 and COX-2. Study of perturbative changes in the complexes. 2000 , 498, 133-148		5
1495	Importance of the proximity of solvation: molecular dynamics and free energy perturbation studies of [16]starand and its model with various alkali metal ions. 2000 , 499, 111-119		2
1494	Ewald summation and multiple time step methods for molecular dynamics simulation of biological molecules. 2000 , 530, 237-243		20
1493	Atomic charges for molecular dynamics calculations. 2000 , 507, 17-23		9
1492	Identification of selective inhibitors of acetylcholinesterase from a combinatorial library of 2,5-piperazinediones. 2000 , 5, 131-43		8
1491	Backbone dynamics and solution structure refinement of the 15N-labeled human oncogenic protein p13MTCP1: comparison with X-ray data. 2000 , 17, 215-30		20
1490	Discovering high-affinity ligands from the computationally predicted structures and affinities of small molecules bound to a target: A virtual screening approach. 2000 , 20, 209-230		22
1489	Combined molecular mechanical and continuum solvent approach (MM-PBSA/GBSA) to predict ligand binding. 2000 , 18, 113-135		638
1488	Engineering the substrate specificity of Escherichia coli asparaginase. II. Selective reduction of glutaminase activity by amino acid replacements at position 248. 2000 , 9, 2009-17		104
1487	Synthesis and NMR solution structure of an alpha-helical hairpin stapled with two disulfide bridges. 2000 , 9, 942-55		29
1486	Modeling of loops in protein structures. 2000 , 9, 1753-73		1586
1485	Calculating structures and free energies of complex molecules: combining molecular mechanics and continuum models. 2000 , 33, 889-97		3346
1484	Molecular docking reveals a novel binding site model for fentanyl at the mu-opioid receptor. 2000 , 43, 381-91		79
1483	Origins of the Loss of Concertedness in Pericyclic Reactions: Theoretical Prediction and Direct Observation of Stepwise Mechanisms in [3 + 2] Thermal Cycloadditions. <i>Journal of the American Chemical Society</i> , 2000 , 122, 6078-6092	16.4	103
1482	The nonplanarity of the peptide group: Molecular dynamics simulations with a polarizable two-state model for the peptide bond. 2000 , 112, 5230-5241		31

1481	Homology predicted structure and functional interaction of ferredoxin from the eukaryotic alga Chlamydomonas reinhardtii with nitrite reductase and glutamate synthase. 2000 , 5, 713-9	21
1480	B -> A -> B Transitions in a Molecular Dynamics Trajectory of Low Salt DNA Solution. 2000 , 6, 654-658	7
1479	Differential modes of agonist binding to 5-hydroxytryptamine(2A) serotonin receptors revealed by mutation and molecular modeling of conserved residues in transmembrane region 5. 2000 , 58, 877-86	101
1478	Analysis of the free energy landscape of a peptide molecule. 2000 ,	
1477	. 2000,	32
1476	Thermal molecular dynamics simulation of cardiotoxin III from Taiwan cobra venom in solution. 2000 ,	
1475	Allosteric, chiral-selective drug binding to DNA. 2000 , 97, 12032-7	140
1474	Docking of peptide-T onto the D1 domain of the CD4 receptor. 2000 , 17, 725-33	
1473	Identification of Edg1 receptor residues that recognize sphingosine 1-phosphate. 2000 , 275, 39379-84	133
1472	Protein Structure Prediction. 2000 ,	6
1472 1471	Protein Structure Prediction. 2000, Evaluation of protein-protein association energies by free energy perturbation calculations. 2000, 13, 239-45	20
.,	Evaluation of protein-protein association energies by free energy perturbation calculations. 2000 ,	
1471	Evaluation of protein-protein association energies by free energy perturbation calculations. 2000 , 13, 239-45 BALLrapid software prototyping in computational molecular biology. Biochemicals Algorithms	20
1471 1470	Evaluation of protein-protein association energies by free energy perturbation calculations. 2000, 13, 239-45 BALLrapid software prototyping in computational molecular biology. Biochemicals Algorithms Library. 2000, 16, 815-24 Sequence-dependent conformational perturbation in DNA duplexes containing an epsilonA.T	20
1471 1470 1469	Evaluation of protein-protein association energies by free energy perturbation calculations. 2000, 13, 239-45 BALLrapid software prototyping in computational molecular biology. Biochemicals Algorithms Library. 2000, 16, 815-24 Sequence-dependent conformational perturbation in DNA duplexes containing an epsilonA.T mismatch using molecular dynamics simulation. 2000, 21, 1727-36 Functional mapping against Escherichia coli for the broad-spectrum antimicrobial peptide, thanatin,	20 80 13
1471 1470 1469 1468	Evaluation of protein-protein association energies by free energy perturbation calculations. 2000, 13, 239-45 BALLrapid software prototyping in computational molecular biology. Biochemicals Algorithms Library. 2000, 16, 815-24 Sequence-dependent conformational perturbation in DNA duplexes containing an epsilonA.T mismatch using molecular dynamics simulation. 2000, 21, 1727-36 Functional mapping against Escherichia coli for the broad-spectrum antimicrobial peptide, thanatin, based on an in vivo monitoring assay system. 2000, 128, 745-54 Structural basis for uracil DNA glycosylase interaction with uracil: NMR study. 2000, 28, 1906-12	20 80 13
1471 1470 1469 1468	Evaluation of protein-protein association energies by free energy perturbation calculations. 2000, 13, 239-45 BALLrapid software prototyping in computational molecular biology. Biochemicals Algorithms Library. 2000, 16, 815-24 Sequence-dependent conformational perturbation in DNA duplexes containing an epsilonA.T mismatch using molecular dynamics simulation. 2000, 21, 1727-36 Functional mapping against Escherichia coli for the broad-spectrum antimicrobial peptide, thanatin, based on an in vivo monitoring assay system. 2000, 128, 745-54 Structural basis for uracil DNA glycosylase interaction with uracil: NMR study. 2000, 28, 1906-12 Rapid software prototyping in molecular modeling using the biochemical algorithms library (BALL).	20 80 13 18

1463	A combinatorial approach to protein docking with flexible side-chains. 2000 ,	10
1462	Computer simulation of acetonitrile and methanol with ab initio-based pair potentials. 2000 , 113, 5401	26
1461	Modeling ion [bn interaction in proteins: A molecular dynamics free energy calculation of the guanidinium-acetate association. 2000 , 112, 9691-9694	59
1460	Constant pressure path integral molecular dynamics studies of quantum effects in the liquid state properties of n-alkanes. 2000 , 112, 870-880	19
1459	Molecular dynamics study of benzeneBenzene and benzeneβotassium ion interactions using polarizable potential models. 2000 , 113, 266-273	27
1458	Structure of the Sm binding site from human U4 snRNA derived from a 3 ns PME molecular dynamics simulation. 2000 , 18, 335-44	8
1457	Critical assessment of the performance of the semiempirical divide and conquer method for single point calculations and geometry optimizations of large chemical systems. 2000 , 113, 10512-10523	42
1456	Geometry optimization of large biomolecules in redundant internal coordinates. 2000 , 113, 6566-6572	44
1455	Base opening in RNA and DNA duplexes: implication for RNA stability. 2000 , 61, 5640-5	5
1454	A new approach for the calculation of the energy of van der Waals interactions in macromolecules of globular proteins. 2000 , 17, 799-809	5
1453	Spontaneous base flipping in DNA and its possible role in methyltransferase binding. 2000 , 62, 1133-7	16
1452	Digitally filtered molecular dynamics: The frequency specific control of molecular dynamics simulations. 2000 , 112, 2586-2597	18
1451	Vibrational energy transfer in a protein molecule. 2000 , 85, 3970-3	131
1450	Molecular Ornstein dernike approach to the solvent effects on solute electronic structures in solution. 2000 , 113, 4974	34
1449	Development of molecular dynamics programs for proteins with a parallelized Barnes-Hut tree code. 2000 ,	3
1448	Influence of molecular flexibility on DNA radiosensitivity: a simulation study. 2000 , 62, 3986-90	11
1447	Surface of active polarons: A semiexplicit solvation method for biomolecular dynamics. 2000 , 112, 7723-7734	18
1446	Projection Methods for the Analysis of Complex Motions in Macromolecules. 2000 , 23, 275-292	26

1445	Local conformational variations observed in B-DNA crystals do not improve base stacking: computational analysis of base stacking in a d(CATGGGCCCATG)(2) BA intermediate crystal structure. 2000 , 28, 4893-902	51
1444	Molecular dynamics studies of the HIV-1 TAR and its complex with argininamide. 2000 , 28, 4944-55	41
1443	Disulfide recognition in an optimized threading potential. 2000 , 13, 679-89	21
1442	Molecular dynamics simulation of human prion protein including both N-linked oligosaccharides and the GPI anchor. 2000 , 10, 959-74	81
1441	NMR structures of three single-residue variants of the human prion protein. 2000 , 97, 8340-5	92
1440	Sequence-specific binding of counterions to B-DNA. 2000 , 97, 629-33	161
1439	Misincorporation of 2'-deoxyoxanosine into DNA: a molecular basis for NO-induced mutagenesis derived from theoretical calculations. 2000 , 28, 4873-83	15
1438	Importance of discriminator base stacking interactions: molecular dynamics analysis of A73 microhelix(Ala) variants. 2000 , 28, 2527-34	28
1437	Inversion of the roles of the nucleophile and acid/base catalysts in the covalent binding of epoxyalkyl xyloside inhibitor to the catalytic glutamates of endo-1,4-beta-xylanase (XYNII): a molecular dynamics study. 2000 , 13, 247-52	7
1436	Temperature Dependence of Collisional Energy Transfer in Highly Excited Aromatics Studied by Classical Trajectory Calculations. 2000 , 214,	15
1435	How Do Hydrogen Bonds Contribute to Protein-DNA Recognition?. 2000 , 17 Suppl 1, 109-12	7
1434	Homology modeling of human leptin/leptin receptor complex. 2000 , 275, 154-8	27
1433	Sequence-dependent DNA structure: tetranucleotide conformational maps. 2000 , 295, 85-103	165
1432	Free energy landscapes of peptides by enhanced conformational sampling. 2000 , 296, 197-216	54
1431	A dimeric DNA interface stabilized by stacked A.(G.G.G.G).A hexads and coordinated monovalent cations. 2000 , 297, 627-44	117
1430	Experimental and theoretical studies of the effects of deoxyribose substitutions on the stability of the UUCG tetraloop. 2000 , 297, 251-65	34
1429	An A-type double helix of DNA having B-type puckering of the deoxyribose rings. 2000 , 297, 907-22	83
1428	NMR structure of activated CheY. 2000 , 297, 543-51	119

1427	Experimental and computational studies of the G[UUCG]C RNA tetraloop. 2000 , 297, 1045-61		58
1426	Structure and thermodynamics of RNA-protein binding: using molecular dynamics and free energy analyses to calculate the free energies of binding and conformational change. 2000 , 297, 1145-58		153
1425	Molecular modelling study of HIV p17gag (MA) protein shell utilising data from electron microscopy and X-ray crystallography. 2000 , 298, 841-57		42
1424	Sequence-dependent elastic properties of DNA. 2000 , 299, 695-709		132
1423	A-Tract bending: insights into experimental structures by computational models. 2000 , 301, 643-63		114
1422	A thermodynamic and structural analysis of DNA minor-groove complex formation. 2000 , 300, 321-37		127
1421	Water and ion binding around RNA and DNA (C,G) oligomers. 2000, 300, 1113-31		232
1420	Accomodation of S-cis-tamoxifen-N(2)-guanine adduct within a bent and widened DNA minor groove. 2000 , 302, 377-93		2 0
1419	Identification of ENV determinants in V3 that influence the molecular anatomy of CCR5 utilization. 2000 , 302, 359-75		46
1418	DNA structure: what's in charge?. 2000 , 304, 803-20		145
1417	Structure-activity relationships in a peptidic alpha7 nicotinic acetylcholine receptor antagonist. 2000 , 304, 911-26		22
1416	Automated docking of ligands to antibodies: methods and applications. 2000 , 20, 280-91		60
1415	Noncovalent interactions: a challenge for experiment and theory. 2000 , 100, 143-68		1403
1414	Origins of Fluorine NMR Chemical Shifts in Fluorine-Containing Proteins Journal of the American Chemical Society, 2000 , 122, 4408-4417	4	32
1413	Protein-based virtual screening of chemical databases. 1. Evaluation of different docking/scoring combinations. 2000 , 43, 4759-67		648
1412	Proton Transfer in Bacteriorhodopsin: Structure, Excitation, IR Spectra, and Potential Energy Surface Analyses by an ab Initio QM/MM Method. 2000 , 104, 10678-10691		188
1411	Developing a dynamic pharmacophore model for HIV-1 integrase. 2000 , 43, 2100-14		248
1410	Elbow flexibility and ligand-induced domain rearrangements in antibody Fab NC6.8: large effects of a small hapten. 2000 , 79, 614-28		27

1409	Bending and adaptability to proteins of the cAMP DNA-responsive element: molecular dynamics contrasted with NMR. 2000 , 79, 656-69	13
1408	Optimization of nucleic acid sequences. 2000 , 79, 680-5	32
1407	Structure and hydration of BamHI DNA recognition site: a molecular dynamics investigation. 2000 , 79, 1263-72	20
1406	On the truncation of long-range electrostatic interactions in DNA. 2000 , 79, 1537-53	205
1405	Modeling zymogen protein C. 2000 , 79, 2925-43	29
1404	Computer simulation of ion channel gating: the M(2) channel of influenza A virus in a lipid bilayer. 2000 , 78, 150-63	65
1403	Stereochemical requirements for receptor recognition of the mu-opioid peptide endomorphin-1. 2000 , 78, 590-9	72
1402	Molecular dynamics simulations of the d(CCAACGTTGG)(2) decamer: influence of the crystal environment. 2000 , 78, 668-82	47
1401	A designed four-alpha-helix bundle that binds the volatile general anesthetic halothane with high affinity. 2000 , 78, 982-93	67
1400	Binding mechanisms of TATA box-binding proteins: DNA kinking is stabilized by specific hydrogen bonds. 2000 , 78, 1988-96	17
1399	Conformational deformability of RNA: a harmonic mode analysis. 2000 , 78, 2528-42	17
1398	Structure of an oligonucleotide containing a N-(2-deoxy-beta-D-erythro-pentofuranosyl)formamide residue facing a guanine. 2000 , 82, 65-9	2
1397	Molecular dynamics generation of nonarbitrary membrane models reveals lipid orientational correlations. 2000 , 79, 3118-38	62
1396	What can x-ray scattering tell us about the radial distribution functions of water?. 2000 , 113, 9149-9161	351
1395	Free energy calculations on dimer stability of the HIV protease using molecular dynamics and a continuum solvent model. 2000 , 303, 567-82	257
1394	Binding of a diverse set of ligands to avidin and streptavidin: an accurate quantitative prediction of their relative affinities by a combination of molecular mechanics and continuum solvent models. 2000 , 43, 3786-91	441
1393	Hypermodified nucleosides in the anticodon of tRNALys stabilize a canonical U-turn structure. 2000 , 39, 12575-84	103
1392	Synthesis and monitored selection of 5'-nucleobase-capped oligodeoxyribonucleotides. 2000 , 28, 4254-65	13

1391	Monte Carlo methods for phase equilibria of fluids. 2000 , 12, R25-R52	210
1390	Water and potassium dynamics inside the KcsA K(+) channel. 2000 , 477, 37-42	101
1389	Molecular dynamics simulation of four-alpha-helix bundles that bind the anesthetic halothane. 2000 , 478, 61-6	10
1388	Transferable Potentials for Phase Equilibria. 4. United-Atom Description of Linear and Branched Alkenes and Alkylbenzenes. 2000 , 104, 8008-8016	435
1387	Molecular Modeling of Energetic Materials: The Parameterization and Validation of Nitrate Esters in the COMPASS Force Field. 2000 , 104, 2477-2489	354
1386	Flexible Structure of DNA: Ion Dependence of Minor-Groove Structure and Dynamics. <i>Journal of the American Chemical Society</i> , 2000 , 122, 10513-10520	110
1385	Investigations on human immunodeficiency virus type 1 integrase/DNA binding interactions via molecular dynamics and electrostatics calculations. 2000 , 85, 123-31	22
1384	Energy transfer pathways in the collisional activation of peptides. 2000 , 201, 233-244	46
1383	Complexation of M3+ Lanthanide Cations by Calix[4]arene-CMPO Ligands: A Molecular Dynamics Study in Methanol Solution and at a Water/Chloroform Interface. 2000 , 12, 27-51	13
1382	New tacrine-huperzine A hybrids (huprines): highly potent tight-binding acetylcholinesterase inhibitors of interest for the treatment of Alzheimer's disease. 2000 , 43, 4657-66	160
1381	X-ray scattering study and molecular simulation of glass forming liquids: Propylene carbonate and salol. 2000 , 113, 4751-4762	57
1380	A Phototautomerizable Model DNA Base Pair. <i>Journal of the American Chemical Society</i> , 2000 , 122, 9917- 9 9 2 0	71
1379	Theoretical Methods for the Description of the Solvent Effect in Biomolecular Systems. 2000, 100, 4187-4226	538
1378	On the Choice of Dihedral Angle Potential Energy Functions for n-Alkanes. 2000 , 25, 301-319	101
1377	The energy landscape theory of protein folding: insights into folding mechanisms and scenarios. 2000 , 53, 87-152	192
1376	Free energy calculation on enzyme reactions with an efficient iterative procedure to determine minimum energy paths on a combined ab initio QM/MM potential energy surface. 2000 , 112, 3483-3492	398
1375	Structural characterization of a guanine-quadruplex ligand complex. 2000 , 39, 13422-32	95
1374	QMBE and Molecular Dynamics Calculations on Catechol O-Methyltransferase: Free Energy of Activation in the Enzyme and in Aqueous Solution and Regioselectivity of the Enzyme-Catalyzed 16.4 Reaction. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2586-2596	85

1373	RNA polymerasepromoter recognition. Specific features of electrostatic potential of "early" T4 phage DNA promoters. 2000 , 18, 325-34	12
1372	Theoretical Study of Electron Transfer between the Photolyase Catalytic Cofactor FADH- and DNA Thymine Dimer. <i>Journal of the American Chemical Society</i> , 2000 , 122, 1057-1065	4 136
1371	Successful virtual screening of a chemical database for farnesyltransferase inhibitor leads. 2000 , 43, 401-8	124
1370	Interaction between Aromatic Residues. Molecular Dynamics and ab Initio Exploration of the Potential Energy Surface of the Tryptophan Histidine Pair. 2000 , 104, 1108-1114	40
1369	Protein-Ligand Docking. 2000, 31-48	16
1368	Dielectric properties of glucose and maltose solutions. 2000 , 112, 9810-9821	40
1367	NMR solution structure of the human prion protein. 2000 , 97, 145-50	914
1366	Effect of coordinated ions on structure and flexiblity of parallel G-quandruplexes: a molecular dynamics study. 2000 , 18, 11-28	16
1365	Structural differences of matrix metalloproteinases. Homology modeling and energy minimization of enzyme-substrate complexes. 2000 , 17, 933-46	19
1364	Protonation states and pH titration in the photocycle of photoactive yellow protein. 2000 , 39, 1100-13	55
1363	Tilted peptides: a motif for membrane destabilization (hypothesis). 2000 , 17, 31-40	68
1362	Probing the Role of Protein Environment in Compound I Formation of Chloroperoxidase (CPO). Journal of the American Chemical Society, 2000 , 122, 3599-3605	.4 15
1361	Influence of Protonation on Internal Rotation of Dimethyl Ether. 2000 , 104, 3231-3238	9
1360	Free-Energy Perturbation Calculations of DNA Destabilization by Base Substitutions: The Effect of Neutral Guanine Thymine, Adenine Cytosine and Adenine Difluorotoluene Mismatches. 2000 , 104, 10092-1	009 5 ²
1359	Molecular Dynamics Study of Water B enzene Interactions at the Liquid/Vapor Interface of Water. 2000 , 104, 4403-4407	42
1358	Unrestrained Molecular Dynamics Simulations of [d(AT)5]2 Duplex in Aqueous Solution: Hydration and Binding of Sodium Ions in the Minor Groove. <i>Journal of the American Chemical Society</i> , 2000 , 16. 122, 5025-5033	.4 26
1357	B-DNA's BII Conformer Substate Population Increases with Decreasing Water Activity. 1. A Molecular Dynamics Study of d(CGCGAATTCGCG)2. 2000 , 104, 11349-11353	13
1356	Studying the Dielectric Properties of a Protein Solution by Computer Simulation. 2000 , 104, 8743-8752	61

1355	Density Functional Calculation of Structural and Vibrational Properties of Glycerol. 2000, 104, 5351-535	7	57	
1354	Density Functional Study of Neutral Salicylaldiminato Nickel(II) Complexes as Olefin Polymerization Catalysts. 2000 , 19, 2741-2750		100	
1353	Modification of the Generalized Born Model Suitable for Macromolecules. 2000 , 104, 3712-3720		830	
1352	Monomer Capture in Brookhart's Ni(II) Diimine Olefin Polymerization Catalyst: Static and Dynamic Quantum Mechanics/Molecular Mechanics Study. 2000 , 104, 121-129		65	
1351	Folding Studies of a Linear Pentamer Peptide Adopting a Reverse Turn Conformation in Aqueous Solution through Molecular Dynamics Simulation. 2000 , 104, 8023-8034		27	
1350	Cation-Dersus OH-Unteractions in Proteins: A Density Functional Study. 2000 , 104, 10087-10091		27	
1349	How Is the Active Site of Enolase Organized To Catalyze Two Different Reaction Steps?. <i>Journal of the American Chemical Society</i> , 2000 , 122, 6560-6570	16.4	98	
1348	[5]HELOL Phosphite: A Helically Grooved Sensor of Remote Chirality. <i>Journal of the American Chemical Society</i> , 2000 , 122, 10027-10032	16.4	94	
1347	Reply to Comment on Crystal Structure Prediction by Global Optimization as a Tool for Evaluating Potentials: Role of the Dipole Moment Correction Term in Successful Predictions' by B. P. van Eijck and J. Kroon. 2000 , 104, 8090-8092		7	
1346	Modeling of the inhibition of retroviral integrases by styrylquinoline derivatives. 2000 , 43, 1949-57		58	
1345	Potent and selective indolomorphinan antagonists of the kappa-opioid receptor. 2000 , 43, 2759-69		101	
1344	Development of a Knowledge-Based Potential for Crystals of Small Organic Molecules: Calculation of Energy Surfaces for C=0IIIHIN Hydrogen Bonds. 2000 , 104, 7293-7298		37	
1343	Cavity-Filling Mutations Enhance Protein Stability by Lowering the Free Energy of Native State. 2000 , 104, 3705-3711		10	
1342	Synthesis, molecular modeling, and opioid receptor affinity of 9, 10-diazatricyclo[4.2.1.1(2,5)]decanes and 2,7-diazatricyclo[4.4.0. 0(3,8)]decanes structurally related to 3,8-diazabicyclo[3.2. 1]octanes. 2000 , 43, 2115-23		10	
1341	Theoretical Studies of the Possible Origin of Intrinsic Static Bends in Double Helical DNA. <i>Journal of the American Chemical Society</i> , 2000 , 122, 12778-12785	16.4	20	
1340	Molecular Dynamics Simulations of PNAIDNA and PNAIRNA Duplexes in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2000 , 122, 5997-6008	16.4	63	
1339	Bending of DNA upon Binding of Ecteinascidin 743 and Phthalascidin 650 Studied by Unrestrained Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2000 , 122, 7172-7182	16.4	32	
1338	Conformation of Amylose in Aqueous Solution: Small-Angle X-ray Scattering Measurements and Simulations. 2000 , 104, 2136-2147		61	

1337	Structural studies on bioactive compounds. 30. Crystal structure and molecular modeling studies on the Pneumocystis carinii dihydrofolate reductase cofactor complex with TAB, a highly selective antifolate. 2000 , 39, 3556-64		19
1336	A Systematic Nonempirical Method of Deriving Model Intermolecular Potentials for Organic Molecules: Application To Amides. 2000 , 104, 10958-10971		35
1335	Conformational determinants of structures in stereoisomeric cis-opened anti-benzo[a]pyrene diol epoxide adducts to adenine in DNA. 2000 , 13, 811-22		17
1334	Are the Hydrophobic AsPh4+ and BPh4- Ions Equally Solvated? A Theoretical Investigation in Aqueous and Nonaqueous Solutions Using Different Charge Distributions. 2000 , 104, 11159-11168		42
1333	Crystal Structure Prediction by Global Optimization as a Tool for Evaluating Potentials: Role of the Dipole Moment Correction Term in Successful Predictions Journal of the American Chemical 50ciety, 2000, 122, 907-921	-4	35
1332	Derivation of an Optimized Potential Model for Phase Equilibria (OPPE) for Sulfides and Thiols. 2000 , 104, 4745-4753		60
1331	Are Many-Body Effects Important in Protein Folding?. 2000 , 104, 9554-9563		60
1330	Solution structure by NMR and molecular dynamics of a duplex containing a guanine opposite a N-(2-deoxy-beta-D-erythro-pentofuranosyl)formamide lesion. 2000 , 39, 5614-21		11
1329	Solution Conformations of Helix-Forming Amino Acid Homooligomers. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2711-2718	-4	111
1328	Influence of Side Chain Restriction and NHIIIIInteraction on the Frurn Folding Modes of Dipeptides Incorporating Phenylalanine Cyclohexane Derivatives. <i>Journal of the American Chemical Society</i> , 2000 , 122, 5811-5821	-4	55
1327	Role of Protein Environment in Horseradish Peroxidase Compound I Formation: Molecular Dynamics Simulations of Horseradish PeroxidaseHOOH Complex. <i>Journal of the American</i> 16 <i>Chemical Society,</i> 2000 , 122, 18-25	·4	61
1326	Principles Governing Conformations in Stereoisomeric Adducts of Bay Region Benzo[a]pyrene Diol Epoxides to Adenine in DNA: Steric and Hydrophobic Effects Are Dominant. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3021-3032	-4	25
1325	Dynamics of a double stranded DNA oligomer: mode-coupling diffusion approach and reduced rigid fragment models. 2000 , 17, 673-85		7
1324	Nanosecond Molecular Dynamics of Zipper-like DNA Duplex Structures Containing Sheared GIA Mismatch Pairs. <i>Journal of the American Chemical Society</i> , 2000 , 122, 7564-7572	-4	44
1323	Molecular Dynamics Simulations of Three-Strand 断heet Folding. <i>Journal of the American Chemical Society</i> , 2000 , 122, 1999-2009	·4	39
1322	Thermoplastic Molecular Sieves. 2000 , 12, 363-368		112
1321	Why Does Trypsin Cleave BPTI so Slowly?. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3436-34446	-4	33
1320	M3+ Lanthanide Cation Solvation by Acetonitrile: The Role of Cation Size, Counterions, and Polarization Effects Investigated by Molecular Dynamics and Quantum Mechanical Simulations. 2000 104 7659-7671		57

1319	Proton translocation by cytochrome c oxidase can take place without the conserved glutamic acid in subunit I. 2000 , 39, 7863-7		64
1318	Zirconocene Complexes with Cyclopenta[l]phenanthrene Ligands: Syntheses, Structural Dynamics, and Properties as Olefin Polymerization Catalysts. 2000 , 19, 3597-3604		38
1317	Which Functional Form Is Appropriate for Hydrogen Bond of Amides?. 2000 , 104, 8321-8326		41
1316	Nature of Intercalator AmilorideNucelobase Stacking. An Empirical Potential and ab Initio Electron Correlation Study. 2000 , 104, 815-822		40
1315	Modeling metal-catalyzed olefin polymerization. 2000 , 100, 1435-56		239
1314	A molecular dynamics simulation study of coaxial stacking in RNA. 2000 , 18, 345-52		9
1313	Calculation and prediction of binding free energies for the matrix metalloproteinases. 2000 , 43, 4180-8		87
1312	The Mode of Action of Phospholipase A2: Semiempirical MO Calculations Including the Protein Environment. 2000 , 104, 1349-1361		21
1311	QM-FE Calculations of Aliphatic Hydrogen Abstraction in Citrate Synthase and in Solution: Reproduction of the Effect of Enzyme Catalysis and Demonstration that an Enolate Rather than an Enol Is Formed. <i>Journal of the American Chemical Society</i> , 2000 , 122, 12270-12280	16.4	32
1310	Nuclear receptor-DNA binding specificity: A COMBINE and Free-Wilson QSAR analysis. 2000 , 43, 1780-92		45
1310	Optical Switching of JonDipole Interactions in a Gramicidin Channel Analogue. <i>Journal of the</i>	16.4	45 7 ¹
	Optical Switching of IonDipole Interactions in a Gramicidin Channel Analogue. <i>Journal of the</i>		
1309	Optical Switching of IonDipole Interactions in a Gramicidin Channel Analogue. <i>Journal of the American Chemical Society</i> , 2000 , 122, 6364-6370 Calibration of the Quantum/Classical Hamiltonian in Semiempirical QM/MM AM1 and PM3 Methods. 2000 , 104, 10923-10931		71
1309	Optical Switching of IonDipole Interactions in a Gramicidin Channel Analogue. <i>Journal of the American Chemical Society</i> , 2000 , 122, 6364-6370 Calibration of the Quantum/Classical Hamiltonian in Semiempirical QM/MM AM1 and PM3 Methods. 2000 , 104, 10923-10931 A Ligand That Is Predicted to Bind Better to Avidin than Biotin: Insights from Computational Fluorine Scanning. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3909-3916	16.4	71 51 108
1309 1308 1307	Optical Switching of IonDipole Interactions in a Gramicidin Channel Analogue. <i>Journal of the American Chemical Society</i> , 2000 , 122, 6364-6370 Calibration of the Quantum/Classical Hamiltonian in Semiempirical QM/MM AM1 and PM3 Methods. 2000 , 104, 10923-10931 A Ligand That Is Predicted to Bind Better to Avidin than Biotin: Insights from Computational Fluorine Scanning. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3909-3916 Simulation of Ecori Dodecamer Netropsin Complex Confirms Class I Complexation Mode. <i>Journal of</i>	16.4 16.4	71 51 108
1309 1308 1307 1306	Optical Switching of IonDipole Interactions in a Gramicidin Channel Analogue. <i>Journal of the American Chemical Society</i> , 2000 , 122, 6364-6370 Calibration of the Quantum/Classical Hamiltonian in Semiempirical QM/MM AM1 and PM3 Methods. 2000 , 104, 10923-10931 A Ligand That Is Predicted to Bind Better to Avidin than Biotin: Insights from Computational Fluorine Scanning. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3909-3916 Simulation ofEcoRI Dodecamer Netropsin Complex Confirms Class I Complexation Mode. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3927-3931 The cyclohexene ring system as a furanose mimic: synthesis and antiviral activity of both enantiomers of cyclohexenylguanine. 2000 , 43, 736-45	16.4 16.4	71 51 108 30
1309 1308 1307 1306 1305	Optical Switching of IonDipole Interactions in a Gramicidin Channel Analogue. <i>Journal of the American Chemical Society</i> , 2000 , 122, 6364-6370 Calibration of the Quantum/Classical Hamiltonian in Semiempirical QM/MM AM1 and PM3 Methods. 2000 , 104, 10923-10931 A Ligand That Is Predicted to Bind Better to Avidin than Biotin: Insights from Computational Fluorine Scanning. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3909-3916 Simulation of Ecorl Dodecamer Netropsin Complex Confirms Class I Complexation Mode. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3927-3931 The cyclohexene ring system as a furanose mimic: synthesis and antiviral activity of both enantiomers of cyclohexenylguanine. 2000 , 43, 736-45 Molecular Dynamics Study of HIV-1 Protease Bubstrate Complex: Roles of the Water Molecules at	16.4 16.4 16.4	71 51 108 30 78

1301	Modeling of kappa-opioid receptor/agonists interactions using pharmacophore-based and docking simulations. 2000 , 43, 2124-34		46
1300	Energy decomposition analysis of intermolecular interactions using a block-localized wave function approach. 2000 , 112, 5530-5538		312
1299	Structure, energetics, vibrational frequencies and charge transfer of base pairs, nucleoside pairs, nucleotide pairs and B-DNA pairs of trinucleotides: ab initio HF/MINI-1 and empirical force field study. 2000 , 17, 1077-86		8
1298	A reactive potential for hydrocarbons with intermolecular interactions. 2000 , 112, 6472-6486		2917
1297	NMR structures of r(GCAGGCGUGC)2 and determinants of stability for single guanosine-guanosine base pairs. 2000 , 39, 11748-62		60
1296	Global Minimum of the Adenine Thymine Base Pair Corresponds Neither to Watson Crick Nor to Hoogsteen Structures. Molecular Dynamic/Quenching/AMBER and ab Initio beyond Hartree Hock Studies. <i>Journal of the American Chemical Society</i> , 2000 , 122, 3495-3499	16.4	67
1295	Molecular dynamics simulation of nucleic acids. 2000 , 51, 435-71		314
1294	Combined Quantum and Molecular Mechanics (QM/MM) Study of the Ionization State of 8-Methylpterin Substrate Bound to Dihydrofolate Reductase. 2000 , 104, 4503-4510		21
1293	Nuclear Magnetic Resonance Spectroscopy and Molecular Modeling Reveal That Different Hydrogen Bonding Patterns Are Possible for G´IU Pairs: One Hydrogen Bond for Each G´IU Pair in r(GGCGUGCC)2 III 2000, 39, 8970-8982		52
1292	Microscopic model of carbon monoxide binding to myoglobin. 2000 , 113, 6831-6850		74
1292 1291	Microscopic model of carbon monoxide binding to myoglobin. 2000 , 113, 6831-6850 Molecular Dynamics Simulations of Nucleic Acids with a Generalized Born Solvation Model. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2489-2498	16.4	
1291	Molecular Dynamics Simulations of Nucleic Acids with a Generalized Born Solvation Model. <i>Journal</i>	16.4	
1291	Molecular Dynamics Simulations of Nucleic Acids with a Generalized Born Solvation Model. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2489-2498	16.4	374
1291 1290	Molecular Dynamics Simulations of Nucleic Acids with a Generalized Born Solvation Model. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2489-2498 Understanding Modern Molecular Dynamics: Techniques and Applications. 2000 , 104, 159-178 Prediction of Properties from Simulations: Free Energies of Solvation in Hexadecane, Octanol, and	16.4	374 259
1291 1290 1289	Molecular Dynamics Simulations of Nucleic Acids with a Generalized Born Solvation Model. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2489-2498 Understanding Modern Molecular Dynamics: Techniques and Applications. 2000 , 104, 159-178 Prediction of Properties from Simulations: Free Energies of Solvation in Hexadecane, Octanol, and Water. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2878-2888 Molecular determinants of MAO selectivity in a series of indolylmethylamine derivatives: biological	16.4	374 259 370
1291 1290 1289	Molecular Dynamics Simulations of Nucleic Acids with a Generalized Born Solvation Model. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2489-2498 Understanding Modern Molecular Dynamics: Techniques and Applications. 2000 , 104, 159-178 Prediction of Properties from Simulations: Free Energies of Solvation in Hexadecane, Octanol, and Water. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2878-2888 Molecular determinants of MAO selectivity in a series of indolylmethylamine derivatives: biological activities, 3D-QSAR/CoMFA analysis, and computational simulation of ligand recognition. 2000 , 43, 168 Monte Carlo Calculations for Alcohols and Their Mixtures with Alkanes. Transferable Potentials for Phase Equilibria. 5. United-Atom Description of Primary, Secondary, and Tertiary Alcohols. 2001 , 105, 3093-3104 Mobility of the active site bound paraoxon and sarin in zinc-phosphotriesterase by molecular	16.4	374 259 370 62 632
1291 1290 1289 1288	Molecular Dynamics Simulations of Nucleic Acids with a Generalized Born Solvation Model. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2489-2498 Understanding Modern Molecular Dynamics: Techniques and Applications. 2000 , 104, 159-178 Prediction of Properties from Simulations: Free Energies of Solvation in Hexadecane, Octanol, and Water. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2878-2888 Molecular determinants of MAO selectivity in a series of indolylmethylamine derivatives: biological activities, 3D-QSAR/CoMFA analysis, and computational simulation of ligand recognition. 2000 , 43, 168 Monte Carlo Calculations for Alcohols and Their Mixtures with Alkanes. Transferable Potentials for Phase Equilibria. 5. United-Atom Description of Primary, Secondary, and Tertiary Alcohols. 2001 , 105, 3093-3104 Mobility of the active site bound paraoxon and sarin in zinc-phosphotriesterase by molecular dynamics simulation and quantum chemical calculation. <i>Journal of the American Chemical Society</i> ,	16.4 4-91	374 259 370 62 632

1283	Homology modeling using multiple molecular dynamics simulations and docking studies of the human androgen receptor ligand binding domain bound to testosterone and nonsteroidal ligands. 2001 , 44, 1729-40		82
1282	A nanosecond molecular dynamics study of antiparallel d(G)7 quadruplex structures: effect of the coordinated cations. 2001 , 18, 647-69		12
1281	Perfluoroalkanes: Conformational Analysis and Liquid-State Properties from ab Initio and Monte Carlo Calculations. 2001 , 105, 4118-4125		340
1280	Backbone dynamics of DNA containing 8-oxoguanine: importance for substrate recognition by base excision repair glycosylases. 2001 , 487, 93-108		6
1279	Structural dynamics and cation interactions of DNA quadruplex molecules containing mixed guanine/cytosine quartets revealed by large-scale MD simulations. <i>Journal of the American Chemical Society</i> , 2001 , 123, 3295-307	16.4	87
1278	Worm Model for Electron Tunneling in Proteins: Consolidation of the Pathway Model and the Dutton Plot. 2001 , 105, 4424-4435		31
1277	Are free energy calculations useful in practice? A comparison with rapid scoring functions for the p38 MAP kinase protein system. 2001 , 44, 3417-23		196
1276	Solvent Effects on Nuclear Shieldings: ´Continuum or Discrete Solvation Models To Treat Hydrogen Bond and Polarity Effects?. 2001 , 105, 7287-7296		105
1275	Salting-In and Salting-Out of Hydrophobic Solutes in Aqueous Salt Solutions. 2001 , 105, 6380-6386		149
1274	Blue Gene: A vision for protein science using a petaflop supercomputer. 2001 , 40, 310-327		175
1273	Effective hydrogen storage in single-wall carbon nanotubes. 2001 , 63,		89
1272	Bond energies and attachments sites of sodium and potassium cations to DNA and RNA nucleic acid bases in the gas phase. <i>Journal of the American Chemical Society</i> , 2001 , 123, 10272-9	16.4	144
1271	Computational analysis of binding of P1 variants to trypsin. 2001 , 10, 1584-95		47
1270	Molecular Dynamics. 2001,		10
1269	Molecular dynamics study of the IIA binding site in human serum albumin: influence of the protonation state of Lys195 and Lys199. 2001 , 44, 250-60		66
1268	A theoretical study of steric and electronic effects in the rhodium-catalyzed carbonylation reactions. <i>Journal of the American Chemical Society</i> , 2001 , 123, 12294-302	16.4	60
1267	Calculations of the Absolute Free Energies of Binding between RNA and Metal Ions Using Molecular Dynamics Simulations and Continuum Electrostatics. 2001 , 105, 11314-11325		70
1266	Gas-phase conformations and folding energetics of oligonucleotides: dTG- and dGT <i>Journal of the American Chemical Society</i> , 2001 , 123, 5610-1	16.4	71

1265	Development of an All-Atom Force Field for the Simulation of Liquid Crystal Molecules in Condensed Phases (LCFF). 2001 , 357, 149-165		6
1264	Molecular Dynamics Simulations and Spectroscopic Studies of Amorphous Tetraglyme (CH3O(CH2CH2O)4CH3) and Tetraglyme:LiCF3SO3 Structures. 2001 , 105, 3329-3337		37
1263	Thiol/disulfide interconversion in bovine lens aldose reductase induced by intermediates of glutathione turnover. 2001 , 40, 11985-94		16
1262	Polysaccharide recognition by surfactant protein D: novel interactions of a C-type lectin with nonterminal glucosyl residues. 2001 , 40, 7789-98		47
1261	A new concept for multidimensional selection of ligand conformations (MultiSelect) and multidimensional scoring (MultiScore) of protein-ligand binding affinities. 2001 , 44, 2333-43		102
1260	Molecular Clusters: Potential Energy and Free Energy Surfaces. Quantum Chemical ab initio and Computer Simulation Studies. 2001 , 565-584		
1259	Conformation-family Monte Carlo: a new method for crystal structure prediction. 2001 , 98, 12351-6		44
1258	G-Quadruplex Structure Can Be Stable with Only Some Coordination Sites Being Occupied by Cations: A Six-Nanosecond Molecular Dynamics Study. 2001 , 105, 7572-7578		48
1257	Computer Simulation of Protein Protein Interactions. 2001 , 105, 1504-1518		184
1256	Biomolecular simulations: recent developments in force fields, simulations of enzyme catalysis, protein-ligand, protein-protein, and protein-nucleic acid noncovalent interactions. 2001 , 30, 211-43		437
1255	Theoretical study of the mechanisms of substrate recognition by catalase. <i>Journal of the American Chemical Society</i> , 2001 , 123, 9665-72	16.4	41
1254	Theoretical 3D model of histamine N-methyltransferase: insights into the effects of a genetic polymorphism on enzymatic activity and thermal stability. 2001 , 287, 204-8		19
1253	[1,2,4]Triazino[4,3-a]benzimidazole acetic acid derivatives: a new class of selective aldose reductase inhibitors. 2001 , 44, 4359-69		36
1252	Kinase recognition by calmodulin: modeling the interaction with the autoinhibitory region of human cardiac titin kinase. 2001 , 306, 81-95		6
1251	Molecular dynamics simulation reveals conformational switching of water-mediated uracil-cytosine base-pairs in an RNA duplex. 2001 , 305, 659-67		44
1250	Water and ion binding around r(UpA)12 and d(TpA)12 oligomerscomparison with RNA and DNA (CpG)12 duplexes. 2001 , 305, 1057-72		101
1249	Structure and function of the conserved 690 hairpin in Escherichia coli 16 S ribosomal RNA. II. NMR solution structure. 2001 , 307, 197-211		13
1248	A-like guanine-guanine stacking in the aqueous DNA duplex of d(GGGGCCCC). 2001 , 307, 513-24		54

1247	Four loops of the catalytic domain of factor viia mediate the effect of the first EGF-like domain substitution on factor viia catalytic activity. 2001 , 307, 1503-17	20
1246	Dynamic simulations of 13 TATA variants refine kinetic hypotheses of sequence/activity relationships. 2001 , 308, 681-703	28
1245	Quantitative analysis of nucleic acid three-dimensional structures. 2001 , 308, 919-36	129
1244	Spermine: an "invisible" component in the crystals of B-DNA. A grand canonical Monte Carlo and molecular dynamics simulation study. 2001 , 308, 907-17	76
1243	Evading the proofreading machinery of a replicative DNA polymerase: induction of a mutation by an environmental carcinogen. 2001 , 309, 519-36	36
1242	Structure-based analysis of protein-RNA interactions using the program ENTANGLE. 2001 , 311, 75-86	202
1241	Molecular dynamics simulations of B '-DNA: sequence effects on A-tract-induced bending and flexibility. 2001 , 314, 23-40	60
1240	Molecular dynamics in the endgame of protein structure prediction. 2001 , 313, 417-30	123
1239	NMR structure of the Euplotes raikovi pheromone Er-23 and identification of its five disulfide bonds. 2001 , 313, 923-31	32
1238	Molecular dynamics of the frame-shifting pseudoknot from beet western yellows virus: the role of non-Watson-Crick base-pairing, ordered hydration, cation binding and base mutations on stability and unfolding. 2001 , 313, 1073-91	68
1237	Do water molecules mediate protein-DNA recognition?. 2001 , 314, 619-32	127
1236	Stability and structure of RNA duplexes containing isoguanosine and isocytidine. <i>Journal of the American Chemical Society</i> , 2001 , 123, 1267-74	41
1235	Water conduction through the hydrophobic channel of a carbon nanotube. 2001 , 414, 188-90	2744
1234	Solution structure of the squash trypsin inhibitor MCoTI-II. A new family for cyclic knottins. 2001 , 40, 7973-83	152
1233	Evaluation of docking functions for protein-ligand docking. 2001 , 44, 3768-85	70
1232	Conformations of an adenine bulge in a DNA octamer and its influence on DNA structure from molecular dynamics simulations. 2001 , 81, 352-70	29
1231	HIV-1 integrase catalytic core: molecular dynamics and simulated fluorescence decays. 2001 , 81, 473-89	25
1230	Structure and hydration of the DNA-human topoisomerase I covalent complex. 2001 , 81, 490-500	23

1229	Molecular dynamics simulation of the human U2B" protein complex with U2 snRNA hairpin IV in aqueous solution. 2001 , 81, 630-42	17
1228	Analysis of a 10-ns molecular dynamics simulation of mouse acetylcholinesterase. 2001 , 81, 715-24	145
1227	Computer simulation of the rough lipopolysaccharide membrane of Pseudomonas aeruginosa. 2001 , 81, 1037-46	94
1226	Carbohydrate-protein recognition: molecular dynamics simulations and free energy analysis of oligosaccharide binding to concanavalin A. 2001 , 81, 1373-88	90
1225	Significance of ligand tails for interaction with the minor groove of B-DNA. 2001 , 81, 1588-99	23
1224	Dynamical properties of a hydrated lipid bilayer from a multinanosecond molecular dynamics simulation. 2001 , 81, 2484-94	125
1223	Calculation of rigid-body conformational changes using restraint-driven Cartesian transformations. 2001 , 81, 2530-46	20
1222	Theoretical studies of the ATP hydrolysis mechanism of myosin. 2001 , 81, 2786-94	58
1221	Rhodopsin-transducin interface: studies with conformationally constrained peptides. 2001 , 81, 3285-93	33
1220	Molecular dynamics simulations of Gly-12>Val mutant of p21(ras): dynamic inhibition mechanism. 2001 , 81, 3483-8	40
1219	Molecular dynamics of DNA quadruplex molecules containing inosine, 6-thioguanine and 6-thiopurine. 2001 , 80, 455-68	52
1218	Molecular dynamics study of the energetic, mechanistic, and structural implications of a closed phosphate tube in ncd. 2001 , 80, 1151-68	31
1217	Functional dynamics of the hydrophobic cleft in the N-domain of calmodulin. 2001, 80, 2082-92	71
1216	Conformational analysis of DNA-trinucleotide-hairpin-loop structures using a continuum solvent model. 2001 , 80, 2350-63	33
1215	Molecular dynamics and binding specificity analysis of the bovine immunodeficiency virus BIV Tat-TAR complex. 2001 , 80, 2833-42	36
1214	Physico-chemical studies on DNA triplexes containing an alternate third strand with a non-nucleotide linker. 2001 , 28, 387-94	5
1213	Free energy component analysis for drug design: a case study of HIV-1 protease-inhibitor binding. 2001 , 44, 4325-38	37
1212	Influence of the dynamic positions of cations on the structure of the DNA minor groove: sequence-dependent effects. <i>Journal of the American Chemical Society</i> , 2001 , 123, 7745-55	. 90

1211	with an alkyllithium in the presence of a chiral diamine. <i>Journal of the American Chemical Society</i> , 16.4 2001 , 123, 8231-8	63
1210	Conformational entropy in protein folding. A guide to estimating conformational entropy via modeling and computation. 2001 , 168, 117-32	3
1209	Empirical force field for the simulation of a class of chromophores in a photosynthetic center. 2001 , 20, 318-324	3
1208	Electrostatic effects play a central role in cold adaptation of trypsin. 2001 , 499, 171-5	32
1207	The solution structure of the viral binding domain of Tva, the cellular receptor for subgroup A avian leukosis and sarcoma virus. 2001 , 509, 161-8	26
1206	Dynamic coupling between the SH2 and SH3 domains of c-Src and Hck underlies their inactivation by C-terminal tyrosine phosphorylation. 2001 , 105, 115-26	329
1205	Mechanism of Processivity Clamp Opening by the Delta Subunit Wrench of the Clamp Loader Complex of E. coli DNA Polymerase III. 2001 , 106, 417-428	205
1204	Molecular docking: a problem with thousands of degrees of freedom.	11
1203	Aminolimino Tautomerism in Derivatives of Cytosine: Effect on Hydrogen-Bonding and Stacking Properties. 2001 , 105, 6575-6580	32
1202	Structure-based design of selective and potent G quadruplex-mediated telomerase inhibitors. 2001 , 98, 4844-9	403
1201	Quantum-chemical analysis of C-HO and C-HN interactions in RNA base pairsH-bond versus anti-H-bond pattern. 2001 , 18, 545-55	27
1200	Predicted Michaelis-Menten complexes of cocaine-butyrylcholinesterase. Engineering effective butyrylcholinesterase mutants for cocaine detoxication. 2001 , 276, 9330-6	74
1199	DFT-based molecular dynamics as a new tool for computational biology: First applications and perspective. 2001 , 45, 397-407	20
1198	Energy landscapes, global optimization and dynamics of the polyalanine Ac(ala)8NHMe. 2001 , 114, 6443-6454	75
1197	Molecular dynamics simulation of proton transport with quantum mechanically derived proton hopping rates (Q-HOP MD). 2001 , 115, 7993-8005	80
1196	Effect of adsorbed water on perfluoropolyether-lubricated magnetic recording disks. 2001, 90, 6287-6296	17
1195	Molecular dynamics studies of trinucleotide repeat DNA involved in neurodegenerative disorders. 2001 , 19, 479-95	7
1194	Optimization of Parameters in Macromolecular Potential Energy Functions by Conformational Space Annealing. 2001 , 105, 7291-7298	59

1193	Hydrophobic Ions in TIP5P Water and at a Watertholoroform Interface: The Effect of Sign Inversion Investigated by MD and FEP Simulations. 2001 , 105, 10700-10708		33
1192	QM/MM studies show substantial tunneling for the hydrogen-transfer reaction in methylamine dehydrogenase. <i>Journal of the American Chemical Society</i> , 2001 , 123, 8604-5	16.4	59
1191	Stereochemical, structural, and thermodynamic origins of stability differences between stereoisomeric benzo[a]pyrene diol epoxide deoxyadenosine adducts in a DNA mutational hot spot sequence. <i>Journal of the American Chemical Society</i> , 2001 , 123, 7054-66	16.4	50
1190	Hoogsteen and Stacked Structures of the 9-Methyladenine 11-Methylthymine Pair Are Populated Equally at Experimental Conditions: Ab Initio and Molecular Dynamics Study. 2001 , 105, 1197-1202		27
1189	A theoretical study on the origin of cooperativity in the formation of 3(10)- and alpha-helices. Journal of the American Chemical Society, 2001 , 123, 5313-9	16.4	127
1188	Structural characterization of a six-nucleotide RNA hairpin loop found in Escherichia coli, r(UUAAGU). 2001 , 40, 9879-86		15
1187	Structural Flexibility of the d(CCAGTACTGG)2 B-DNA Decamer and Its Complex with Two Polyamides. 2001 , 105, 3135-3142		12
1186	Molecular dynamics simulations of the mononuclear zinc-beta-lactamase from Bacillus cereus. Journal of the American Chemical Society, 2001, 123, 3759-70	16.4	72
1185	Reevaluation of stereoelectronic contributions to the conformational properties of the phosphodiester and N3'-phosphoramidate moieties of nucleic acids. <i>Journal of the American Chemical Society</i> , 2001 , 123, 6747-55	16.4	29
1184	Structural Determinants of Spectral Tuning in Retinal ProteinsBacteriorhodopsin vs Sensory Rhodopsin II#. 2001 , 105, 10124-10131		106
1183	The Potassium Ion Channel: Comparison of Linear Scaling Semiempirical and Molecular Mechanics Representations of the Electrostatic Potential. 2001 , 105, 12674-12679		24
1182	Direct comparison of experimental and calculated folding free energies for hydrophobic deletion mutants of chymotrypsin inhibitor 2: free energy perturbation calculations using transition and denatured states from molecular dynamics simulations of unfolding. 2001 , 40, 2723-31		40
1181	Evidence for large structural fluctuations of the photobleached intermediate of photoactive yellow protein in solution. <i>Journal of the American Chemical Society</i> , 2001 , 123, 7445-6	16.4	19
1180	Complex of B-DNA with polyamides freezes DNA backbone flexibility. <i>Journal of the American Chemical Society</i> , 2001 , 123, 5044-9	16.4	40
1179	Investigation of aromatic-backbone amide interactions in the model peptide acetyl-Phe-Gly-Gly-N-methyl amide using molecular dynamics simulations and protein database search. <i>Journal of the American Chemical Society</i> , 2001 , 123, 11782-90	16.4	41
1178	Optimizing Ligand Charges for Maximum Binding Affinity. A Solvated Interaction Energy Approach. 2001 , 105, 889-899		30
1177	Comparative binding energy analysis of the substrate specificity of haloalkane dehalogenase from Xanthobacter autotrophicus GJ10. 2001 , 40, 8905-17		38
(SAC/SACI Study of the Ground, Excited, and Ionized States of Cytochromes P450CO. 2001 , 105, 7341-73		

1175	5-HT(1a)/alpha(1)-adrenergic receptor affinity by classical hansch analysis, artificial neural networks, and computational simulation of ligand recognition. 2001 , 44, 198-207		65	
1174	High pressure neutron diffraction on fluid propane and a mixture of propane and methane. 2001 , 115, 331-338		2	
1173	Inner-sphere reorganization energy of iron-sulfur clusters studied with theoretical methods. 2001 , 40, 2509-19		92	
1172	BI? BIISubstate Transitions Induce Changes in the Hydration of B-DNA, Potentially Mediating Signal Transduction from the Minor to Major Groove. 2001 , 105, 10379-10387		19	
1171	Molecular dynamics and thermodynamics of protein-RNA interactions: mutation of a conserved aromatic residue modifies stacking interactions and structural adaptation in the U1A-stem loop 2 RNA complex. <i>Journal of the American Chemical Society</i> , 2001 , 123, 2548-51	16.4	51	
1170	Determination of the Potential of Mean Force of Aromatic Amino Acid Complexes in Various Solvents Using Molecular Dynamics Simulations: The Case of the Tryptophan Histidine Pair. 2001 , 105, 7835-7846		28	
1169	One-Step Perturbation Methods for Solvation Free Energies of Polar Solutes. 2001 , 105, 11264-11274		55	
1168	Designing protein energy landscapes. 2001 , 101, 3113-30		46	
1167	Quantitative calculations of antibodyantigen binding: steroidDB3 binding energies by the linear interaction energy method. 2001 , 66, 3021-6		19	
1166	Simulation of Hydrated BPTI at High Pressure: Changes in Hydrogen Bonding and Its Relation with NMR Experiments. 2001 , 105, 711-714		32	
1165	Ordered water and ligand mobility in the HIV-1 integrase-5CITEP complex: a molecular dynamics study. 2001 , 44, 3043-7		65	
1164	Experimental and Simulation Studies on the Transport of Argon in Polycarbonate Membranes. 2001 , 34, 4999-5004		16	
1163	Intramolecular interactions in chemically modified Escherichia coli thioredoxin monitored by hydrogen/deuterium exchange and electrospray ionization mass spectrometry. 2001 , 40, 14413-21		18	
1162	A theoretical study of the aminolysis reaction of lysine 199 of human serum albumin with benzylpenicillin: consequences for immunochemistry of penicillins. <i>Journal of the American Chemical Society</i> , 2001 , 123, 7574-83	16.4	22	
1161	Influence of sodium ions on the dynamics and structure of single-stranded DNA oligomers: a molecular dynamics study. <i>Journal of the American Chemical Society</i> , 2001 , 123, 12279-89	16.4	44	
1160	Potential Energy and Free Energy Surfaces of All Ten Canonical and Methylated Nucleic Acid Base Pairs: Molecular Dynamics and Quantum Chemical ab Initio Studies. 2001 , 105, 5804-5817		92	
1159	Acylation of Class A <code>Hactamases</code> by Penicillins: A Theoretical Examination of the Role of Serine 130 and the <code>Hactam</code> Carboxylate Group. 2001 , 105, 11302-11313		37	
1158	Cyclohexene ring and Fjord region twist inversion in stereoisomeric DNA adducts of enantiomeric benzo[c]phenanthrene diol epoxides. 2001 , 14, 1629-42		13	

1157	Cyclic Adenine-, Cytosine-, Thymine-, and Mixed Guanine Lytosine-Base Tetrads in Nucleic Acids Viewed from a Quantum-Chemical and Force Field Perspective. 2001 , 105, 11560-11573		25
1156	Structural versatility of oxalamide-based compounds: a computational study on the isomerization of the oxalamide group and the structural preferences of the polyoxalamides. 2001 , 66, 8076-85		13
1155	Insights into the Self-Assembly of Small, Organic Molecules: Case Study of 2,4,6-Trichlorophenol. 2001 , 105, 5987-5993		1
1154	Binding Affinities for a Series of Selective Inhibitors of Gelatinase-A Using Molecular Dynamics with a Linear Interaction Energy Approach. 2001 , 105, 5304-5315		35
1153	Molecular dynamics simulations of the mononuclear zinc-beta-lactamase from Bacillus cereus complexed with benzylpenicillin and a quantum chemical study of the reaction mechanism. <i>Journal of the American Chemical Society</i> , 2001 , 123, 9867-79	16.4	64
1152	An analysis of the interactions between the Sem-5 SH3 domain and its ligands using molecular dynamics, free energy calculations, and sequence analysis. <i>Journal of the American Chemical Society</i> , 2001 , 123, 3986-94	16.4	121
1151	Molecular dynamics study on hydrophobic effects in aqueous urea solutions. <i>Journal of the American Chemical Society</i> , 2001 , 123, 677-82	16.4	94
1150	Conformational Behavior of Macromolecules in Solution. Homopolypeptides of Aminoisobutyric Acid as Test Cases. 2001 , 34, 7550-7557		29
1149	15-mer DNA duplexes containing an abasic site are thermodynamically more stable with adjacent purines than with pyrimidines. 2001 , 40, 3859-68		25
1148	Identification of a putative binding site for [2',5'-bis-O-(tert-butyldimethylsilyl)-beta-D-ribofuranosyl]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"- (TSAO) derivatives at the p51-p66 interface of HIV-1 reverse transcriptase. 2001 , 44, 1853-65	dioxide)t⁄b¥mine
1148 1147	[2',5'-bis-O-(tert-butyldimethylsilyl)-beta-D-ribofuranosyl]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-	dioxide)tobymine 38
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1147	[2',5'-bis-O-(tert-butyldimethylsilyl)-beta-D-ribofuranosyl]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-(TSAO) derivatives at the p51-p66 interface of HIV-1 reverse transcriptase. 2001 , 44, 1853-65 Cathepsins X and B can be differentiated through their respective mono- and dipeptidyl carboxypeptidase activities. 2001 , 40, 2702-11		38
1147 1146	[2',5'-bis-O-(tert-butyldimethylsilyl)-beta-D-ribofuranosyl]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-(TSAO) derivatives at the p51-p66 interface of HIV-1 reverse transcriptase. 2001 , 44, 1853-65 Cathepsins X and B can be differentiated through their respective mono- and dipeptidyl carboxypeptidase activities. 2001 , 40, 2702-11 Molecular dynamics simulations on the mycotoxin fumonisin B1. 2001 , 49, 1056-61 An alternative explanation for the catalytic proficiency of orotidine 5'-phosphate decarboxylase.		38
1147 1146 1145	[2',5'-bis-O-(tert-butyldimethylsilyl)-beta-D-ribofuranosyl]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-(TSAO) derivatives at the p51-p66 interface of HIV-1 reverse transcriptase. 2001, 44, 1853-65 Cathepsins X and B can be differentiated through their respective mono- and dipeptidyl carboxypeptidase activities. 2001, 40, 2702-11 Molecular dynamics simulations on the mycotoxin fumonisin B1. 2001, 49, 1056-61 An alternative explanation for the catalytic proficiency of orotidine 5'-phosphate decarboxylase. <i>Journal of the American Chemical Society</i> , 2001, 123, 12837-48 Characterization of Bile Salt/Cyclodextrin Interactions Using Isothermal Titration Calorimetry. 2001		38 10 39
1147 1146 1145	[2',5'-bis-O-(tert-butyldimethylsilyl)-beta-D-ribofuranosyl]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-(TSAO) derivatives at the p51-p66 interface of HIV-1 reverse transcriptase. 2001, 44, 1853-65 Cathepsins X and B can be differentiated through their respective mono- and dipeptidyl carboxypeptidase activities. 2001, 40, 2702-11 Molecular dynamics simulations on the mycotoxin fumonisin B1. 2001, 49, 1056-61 An alternative explanation for the catalytic proficiency of orotidine 5'-phosphate decarboxylase. Journal of the American Chemical Society, 2001, 123, 12837-48 Characterization of Bile Salt/Cyclodextrin Interactions Using Isothermal Titration Calorimetry. 2001, 17, 7107-7111		38 10 39 42
1147 1146 1145 1144	[2',5'-bis-O-(tert-butyldimethylsilyl)-beta-D-ribofuranosyl]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-(TSAO) derivatives at the p51-p66 interface of HIV-1 reverse transcriptase. 2001, 44, 1853-65 Cathepsins X and B can be differentiated through their respective mono- and dipeptidyl carboxypeptidase activities. 2001, 40, 2702-11 Molecular dynamics simulations on the mycotoxin fumonisin B1. 2001, 49, 1056-61 An alternative explanation for the catalytic proficiency of orotidine 5'-phosphate decarboxylase. <i>Journal of the American Chemical Society</i> , 2001, 123, 12837-48 Characterization of Bile Salt/Cyclodextrin Interactions Using Isothermal Titration Calorimetry. 2001, 17, 7107-7111 The investigation of the effects of counterions in protein dynamics simulations. 2001, 14, 747-52 Theoretical studies of d(A:T)-based parallel-stranded DNA duplexes. <i>Journal of the American</i>	16.4	38 10 39 42

1139	A Dynamic Model for Electron Transport in DNA. 2001 , 105, 9345-9354	21
1138	Base sequence effects in bending induced by bulky carcinogen-DNA adducts: experimental and computational analysis. 2001 , 40, 10458-72	13
1137	Molecular models of N-benzyladriamycin-14-valerate (AD 198) in complex with the phorbol ester-binding C1b domain of protein kinase C-delta. 2001 , 44, 1028-34	15
1136	Is the CO adduct of myoglobin bent, and does it matter?. 2001 , 34, 137-44	125
1135	Comparative binding energy (COMBINE) analysis of influenza neuraminidase-inhibitor complexes. 2001 , 44, 961-71	86
1134	Simulated and NMR-derived backbone dynamics of a protein with significant flexibility: a comparison of spectral densities for the betaARK1 PH domain. <i>Journal of the American Chemical</i> 16.4 <i>Society</i> , 2001 , 123, 3021-36	51
1133	Integrating adaptive mutations and family competition with differential evolution for flexible ligand docking.	1
1132	Molecular modeling of nucleic acid structure: energy and sampling. 2001 , Chapter 7, Unit 7.8	2
1131	Refinement of the NMR structures of alpha-conotoxin MI using molecular dynamics simulation with explicit solvent water and a full molecular force field. 2001 , 49, 249-52	5
1130	Comparative Protein Structure Modeling. 2001,	5
1129	Determination, prediction, and understanding of structures, using the energy landscapes of chemical systems [Part II. 2001 , 216, 361-383	50
1128	Simulations of Enzymatic Systems: Perspectives from Car-Parrinello Molecular Dynamics Simulations. 2001 , 215-251	13
1127	MODELLING ENZYME - LIGAND INTERACTIONS. 2001 , 539-595	1
1126	Bioinformatics and receptor mechanisms of psychotropic drugs. 2001 , 7, 165-77	3
1125	Computational Chemistry: Application to Biological Systems. 2001 , 26, 73-83	3
1124	Structure-based computational study of the catalytic and inhibition mechanisms of urease. 2001 , 6, 300-14	105
1123	AmberFFC, a flexible program to convert AMBER and GLYCAM force fields for use with commercial molecular modeling packages. 2001 , 7, 422-432	9
1122	Rabbit indolethylamine N-methyltransferase three-dimensional structure prediction: a model approach to bridge sequence to function in pharmacogenomic studies. 2001 , 7, 324-333	5

1121	GROMACS 3.0: a package for molecular simulation and trajectory analysis. 2001 , 7, 306-317	5502
1120	Molecular models in computer simulation of liquid crystals. 2001 , 92, 21-28	11
1119	Parallel molecular dynamics simulation of a protein. 2001 , 27, 977-987	18
1118	Energetics and structure of glycine and alanine based model peptides: Approximate SCC-DFTB, AM1 and PM3 methods in comparison with DFT, HF and MP2 calculations. 2001 , 263, 203-219	128
1117	Short-strong hydrogen bonds and a low barrier transition state for the proton transfer reaction in RNase A catalysis: a quantum chemical study. 2001 , 89, 105-17	24
1116	Thermodynamic and computational studies of DNA triple helices containing a nucleotide or a non-nucleotide linker in the third strand. 2001 , 94, 23-31	2
1115	Complex of Burkholderia cepacia lipase with transition state analogue of 1-phenoxy-2-acetoxybutane: biocatalytic, structural and modelling study. 2001 , 268, 3964-73	47
1114	Structural model of human IL-13 defines the spatial interactions with the IL-13Ralpha/IL-4Ralpha receptor. 2001 , 79, 332-9	5
1113	The combination of molecular dynamics with crystallography for elucidating protein-ligand interactions: a case study involving peanut lectin complexes with T-antigen and lactose. 2001 , 57, 1584-94	13
1112	A computational chemical study of penetration and displacement of water films near mineral surfaces. 2001 , 2, 1	14
1111	Thermodynamic and conformational properties of DNA triplexes containing 3?,3?-phosphodiester bond. 2001 , 372, 129-136	1
1110	Design, synthesis and cation-binding properties of novel adamantane- and 2-oxaadamantane-containing crown ethers. 2001 , 57, 449-457	22
1109	Oligodeoxynucleotides with extended zwitter-ionic internucleotide linkage. 2001 , 57, 10287-10292	5
1108	Parameters for the amber force field for the molecular mechanics modeling of the cobalt corrinoids. 2001 , 561, 71-91	53
1107	A theoretical and experimental 14N NMR study of association of pyridine. 2001 , 569, 111-119	27
1106	Customized versus universal scoring functions: application to class I MHC-peptide binding free energy predictions. 2001 , 11, 675-9	42
1105	3-D-QSAR/CoMFA and recognition models of benzimidazole derivatives at the 5-HT(4) receptor. 2001 , 11, 2807-11	17
1104	Molecular dynamics of buspirone analogues interacting with the 5-HT1A and 5-HT2A serotonin receptors. 2001 , 9, 881-95	21

1103	Internal coordinate phase space analysis of macromolecular systems. 2001 , 11, 35-47	2
1102	Interaction of new PNA-based molecules with TAR RNA of HIV-1: molecular modelling and biological evaluation. 2001 , 19, 579-85, 614-5	6
1101	Prediction of potential toxicity and side effect protein targets of a small molecule by a ligand-protein inverse docking approach. 2001 , 20, 199-218	118
1100	A rationally designed oligopeptide shows significant conformational changes upon binding to sulphate ions. 2001 , 16, 783-9	8
1099	Study of the conformational profile of the cyclohexane analogs of L-phenylalanine. 2001 , 57, 435-46	12
1098	Near ab initio quality molecular electrostatic potential maps using hybridization displacement charges at PM3 level and effects of geometrical changes in amino groups. 2001 , 82, 299-312	8
1097	Ab initio modeling of competitive drugdrug interactions: 5-fluorouracil dimers in the gas phase and in solution. 2001 , 83, 128-142	10
1096	Quantum mode phonon forces between chainmolecules. 2001 , 84, 249-252	21
1095	Three-dimensional model of the cyclin-dependent kinase 1 (CDK1): Ab initio active site parameters for molecular dynamics studies of CDKS. 2001 , 45, 478-85	26
1094	Optimization of solvation models for predicting the structure of surface loops in proteins. 2001 , 43, 303-14	20
1093	Elucidation of the mode of substrate binding to hydroxynitrile lyase from Hevea brasiliensis. 2001 , 44, 26-31	25
1092	Influence of rotational energy barriers to the conformational search of protein loops in molecular dynamics and ranking the conformations. 2001 , 44, 167-79	18
1091	Molecular dynamics simulations of the conformational changes of the glutamate receptor ligand-binding core in the presence of glutamate and kainate. 2001 , 44, 460-9	32
1090	Quantum mechanics simulation of protein dynamics on long timescale. 2001 , 44, 484-9	127
1089	Interactions of Streptomyces griseus aminopeptidase with amino acid reaction products and their implications toward a catalytic mechanism. 2001 , 44, 490-504	45
1088	Peter Andrew Kollman. 2001 , 45, 2-3	40
1087	Molecular dynamics simulations of a highly charged peptide from an SH3 domain: possible sequence-function relationship. 2001 , 45, 4-15	9
1086	Contribution of Thr29 to the thermodynamic stability of goat alpha-lactalbumin as determined by experimental and theoretical approaches. 2001 , 45, 16-29	10

1085	Molecular dynamics of HIV-1 reverse transcriptase indicates increased flexibility upon DNA binding. 2001 , 45, 176-82	28
1084	Successful molecular dynamics simulation of two zinc complexes bridged by a hydroxide in phosphotriesterase using the cationic dummy atom method. 2001 , 45, 183-9	117
1083	Revisiting the structural flexibility of the complex p21(ras)-GTP: the catalytic conformation of the molecular switch II. 2001 , 45, 297-312	12
1082	The active site of HIV-1 protease. 2001 , 21, 348-53	39
1081	Generalized-ensemble algorithms for molecular simulations of biopolymers. 2001 , 60, 96-123	674
1080	Modeling salt-mediated electrostatics of macromolecules: the discrete surface charge optimization algorithm and its application to the nucleosome. 2001 , 58, 106-15	83
1079	Hydrogen-bond disruption probability in proteins by a modified self-consistent harmonic approach. 2001 , 58, 319-28	6
1078	Molecular dynamics simulation reveals sequence-intrinsic and protein-induced geometrical features of the OL1 DNA operator. 2001 , 59, 205-25	6
1077	Hessian-free low-mode conformational search for large-scale protein loop optimization: application to c-jun N-terminal kinase JNK3. 2001 , 22, 21-30	52
1076	Roles of proteins in the electron transfer in the photosynthetic reaction center of Rhodopseudomonas viridis: bacteriopheophytin to ubiquinone. 2001 , 22, 265-272	12
1075	Molecular dynamics of minimal B-DNA. 2001 , 22, 457-467	9
1074	Electron transfer in the c-type cytochrome subunit of the photosynthetic reaction center of Rhodopseudomonas viridis: ab initio theoretical study. 2001 , 22, 521-527	7
1073	Computer modeling of human angiogenin-dinucleotide substrate interaction. 2001, 42, 125-35	5
1072	Folding-unfolding of goat alpha-lactalbumin studied by stopped-flow circular dichroism and molecular dynamics simulations. 2001 , 42, 49-65	18
1071	Helix nucleation kinetics from molecular simulations in explicit solvent. 2001 , 42, 77-84	94
1070	Protein folding simulation with solvent-induced force field: folding pathway ensemble of three-helix-bundle proteins. 2001 , 42, 85-98	43
1069	Three-dimensional structure of a complex of galanthamine (Nivalin) with acetylcholinesterase from Torpedo californica: implications for the design of new anti-Alzheimer drugs. 2001 , 42, 182-91	111
1068	Design, docking, and evaluation of multiple libraries against multiple targets. 2001 , 42, 296-318	59

1067	Exploring the energy landscape of a beta hairpin in explicit solvent. 2001 , 42, 345-54	330
1066	Computationally accessible method for estimating free energy changes resulting from site-specific mutations of biomolecules: systematic model building and structural/hydropathic analysis of deoxy and oxy hemoglobins. 2001 , 42, 355-77	43
1065	Conformation spaces of proteins. 2001 , 42, 495-511	32
1064	Solvation energy density occlusion approximation for evaluation of desolvation penalties in biomolecular interactions. 2001 , 43, 12-27	17
1063	Ligand-protein inverse docking and its potential use in the computer search of protein targets of a small molecule. 2001 , 43, 217-26	297
1062	DNA repair mechanism by photolyase: electron transfer path from the photolyase catalytic cofactor FADH(-) to DNA thymine dimer. 2001 , 210, 237-48	52
1061	Calculation of sequence-dependent free energies of hydration of dipeptides formed by alanine and glycine. 2001 , 22, 846-860	2
1060	Chemistry with ADF. 2001 , 22, 931-967	7628
1059	Conformational analysis of thiopeptides: derivation of sp2 sulfur parameters for the CFF91 force field. 2001 , 22, 1010-1025	9
1058	Molecular mechanical models for organic and biological systems going beyond the atom centered two body additive approximation: aqueous solution free energies of methanol and N-methyl acetamide, nucleic acid base, and amide hydrogen bonding and chloroform/water partition	338
1057	Repeated-annealing sampling combined with multicanonical algorithm for conformational sampling of bio-molecules. 2001 , 22, 1098-1106	10
1056	An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase. 2001 , 22, 1205-1218	741
1055	Automatic parameterization of force field by systematic search and genetic algorithms. 2001 , 22, 1219-1228	112
1054	Gas-phase and liquid-state properties of esters, nitriles, and nitro compounds with the OPLS-AA force field. 2001 , 22, 1340-1352	380
1053	EUDOC: a computer program for identification of drug interaction sites in macromolecules and drug leads from chemical databases. 2001 , 22, 1750-1771	95
1052	Conformational analysis of the HIV-1 virus reverse transcriptase nonnucleoside inhibitors: TIBO and nevirapine. 2001 , 22, 1817-1829	13
1051	Molecular mechanics and dynamics of biomolecules using a solvent continuum model. 2001 , 22, 1830-1842	23
1050	Hydrophobic Groups Stabilize the Hydration Shell of 2?-O-Methylated RNA Duplexes. 2001 , 113, 4784-4786	5

1049	A possible mechanism for enantioselectivity in the chiral epoxidation of olefins with. 2001, 7, 800-7	86
1048	The energetic and structural effects of steric crowding in phosphate and dithiophosphinate complexes of lanthanide cations M3+: a computational study. 2001 , 7, 1398-407	28
1047	At nonzero temperatures, stacked structures of methylated nucleic acid base pairs and microhydrated nonmethylated nucleic acid base pairs are favored over planar hydrogen-bonded structures: a molecular dynamics simulations study. 2001 , 7, 2067-74	49
1046	Alpha-homo-DNA and RNA form a parallel oriented non-A, non-B-type double helical structure. 2001 , 7, 5183-94	16
1045	Hydrophobic Groups Stabilize the Hydration Shell of 2'-O-Methylated RNA Duplexes. 2001 , 40, 4648-4650	50
1044	RISM-SCF study for the rate constant of SN2 reaction CH3Cl+ClIn aqueous solution. 2001, 348, 75-80	11
1043	Effects of oxygenated sterol on phospholipid bilayer properties: a molecular dynamics simulation. 2001 , 112, 31-9	36
1042	Structure-based design, synthesis, and biological evaluation of conformationally restricted novel 2-alkylthio-6-[1-(2,6-difluorophenyl)alkyl]-3,4-dihydro-5-alkylpyrimidin-4(3H)-ones as non-nucleoside inhibitors of HIV-1 reverse transcriptase. 2001 , 44, 2544-54	76
1041	TBP at the WaterDil Interface: The Effect of TBP Concentration and Water Acidity Investigated by Molecular Dynamics Simulations. 2001 , 105, 11131-11141	107
1040	Metabolism of sirolimus and its derivative everolimus by cytochrome P450 3A4: insights from docking, molecular dynamics, and quantum chemical calculations. 2001 , 44, 2027-34	58
1039	3-Aryl[1,2,4]triazino[4,3-a]benzimidazol-4(10H)-ones: a new class of selective A1 adenosine receptor antagonists. 2001 , 44, 316-27	53
1038	Use of MM-PBSA in reproducing the binding free energies to HIV-1 RT of TIBO derivatives and predicting the binding mode to HIV-1 RT of efavirenz by docking and MM-PBSA. <i>Journal of the American Chemical Society</i> , 2001 , 123, 5221-30	616
1037	Structure prediction of protein complexes by an NMR-based protein docking algorithm. 2001, 20, 15-21	12
1036	Derivation of 13C chemical shift surfaces for the anomeric carbons of oligosaccharides and glycopeptides using ab initio methodology. 2001 , 21, 49-61	27
1035	[Effect of linker length on the photomodification process of tyrosine residues in N-(tyrosyl)-N'-(5-azido-2-nitrobenzoyl)diaminoalkanes]. 2001 , 27, 408-16	1
1034	Simulation of carbohydrate-protein interactions: computer-aided design of a second generation GM1 mimic. 2001 , 15, 117-28	8
1033	Solution nuclear magnetic resonance structure of a protein disulfide oxidoreductase from Methanococcus jannaschii. 2001 , 10, 384-96	13
1032	Energy landscape of a peptide consisting of alpha-helix, 3(10)-helix, beta-turn, beta-hairpin, and other disordered conformations. 2001 , 10, 1160-71	74

1031	Modeling of the bacterial luciferase-flavin mononucleotide complex combining flexible docking with structure-activity data. 2001 , 10, 1563-71	30
1030	Free-energy analysis of enzyme-inhibitor binding: aspartic proteinase-pepstatin complexes. 2001 , 96, 93-108	5
1029	Continuum solvent molecular dynamics study of flexibility in interleukin-8. 2001 , 19, 136-45	24
1028	A putative three-dimensional arrangement of the human serotonin transporter transmembrane helices: a tool to aid experimental studies. 2001 , 20, 133-44	27
1027	Molecular dynamics simulations of wild-type and point mutation human prion protein at normal and elevated temperature. 2001 , 20, 145-54	47
1026	Molecular dynamics simulations and structural comparisons of amorphous poly(ethylene oxide) and poly(ethylenimine) models. 2001 , 42, 7809-7817	28
1025	Modelling of three-dimensional structures of cytochromes P450 11B1 and 11B2. 2001 , 87, 197-207	51
1024	Monte Carlo simulation of biomolecular systems with BIOMCSIM. 2001, 141, 375-402	3
1023	Domain movement in the epidermal growth factor family of peptides. 2001 , 535, 171-182	5
1022	Calibrating nucleic acids torsional energetics in force-field: insights from model compounds. 2001 , 537, 283-305	13
1021	Computational studies on the binding of	7
1020	Molecular dynamics simulations of a complex of HIV-1 protease and substrate: substrate-dependent efficiency of catalytic activity. 2001 , 543, 53-63	7
1019	Atomic charges in conformers of gaseous glycine. 2001 , 544, 237-251	19
1018	Ab initio MO and density functional studies on trans and cis conformers of N-methylacetamide. 2001 , 546, 183-193	92
1017	Predicting relative binding free energies of substrates and inhibitors of acetylcholin- and butyrylcholinesterases. 2001 , 572, 25-34	9
1016	Ligand induced conformational states of the 5-HT(1A) receptor. 2001 , 416, 33-41	36
1015	Free-energy calculations highlight differences in accuracy between X-ray and NMR structures and add value to protein structure prediction. 2001 , 9, 905-16	30
1014	NMR methodology for the study of nucleic acids. 2001 , 11, 275-81	60

1013	Reverse transcriptase incorporation of 1,5-anhydrohexitol nucleotides. 2001 , 29, 3154-63	46
1012	The arginine finger of RasGAP helps Gln-61 align the nucleophilic water in GAP-stimulated hydrolysis of GTP. 2001 , 98, 6033-8	41
1011	A thermodynamic framework for Mg2+ binding to RNA. 2001 , 98, 12456-61	151
1010	Impact of CpG methylation on structure, dynamics and solvation of cAMP DNA responsive element. 2001 , 29, 2314-26	72
1009	The ORF3 protein of hepatitis E virus binds to Src homology 3 domains and activates MAPK. 2001 , 276, 42389-400	115
1008	Exocyclic groups in the minor groove influence the backbone conformation of DNA. 2001 , 29, 5036-43	12
1007	NMR structure of the calreticulin P-domain. 2001 , 98, 3133-8	154
1006	Computational study of protein specificity: the molecular basis of HIV-1 protease drug resistance. 2001 , 98, 14937-42	215
1005	Molecular modeling of drug-DNA complexes: an update. 2001 , 340, 290-326	11
1004	Molecular modeling of nucleic acid structure: setup and analysis. 2001 , Chapter 7, Unit 7.10	4
1004	Molecular modeling of nucleic acid structure: setup and analysis. 2001 , Chapter 7, Unit 7.10 Sheep prion protein synthetic peptide spanning helix 1 and beta-strand 2 (residues 142-166) shows beta-hairpin structure in solution. 2001 , 276, 46364-70	31
	Sheep prion protein synthetic peptide spanning helix 1 and beta-strand 2 (residues 142-166) shows	
1003	Sheep prion protein synthetic peptide spanning helix 1 and beta-strand 2 (residues 142-166) shows beta-hairpin structure in solution. 2001 , 276, 46364-70 A conserved alpha-helix at the amino terminus of prosomatostatin serves as a sorting signal for the	31
1003	Sheep prion protein synthetic peptide spanning helix 1 and beta-strand 2 (residues 142-166) shows beta-hairpin structure in solution. 2001, 276, 46364-70 A conserved alpha-helix at the amino terminus of prosomatostatin serves as a sorting signal for the regulated secretory pathway. 2001, 276, 26308-16 Constitutive activation of extracellular signal-regulated kinase 2 by synergistic point mutations.	31
1003	Sheep prion protein synthetic peptide spanning helix 1 and beta-strand 2 (residues 142-166) shows beta-hairpin structure in solution. 2001, 276, 46364-70 A conserved alpha-helix at the amino terminus of prosomatostatin serves as a sorting signal for the regulated secretory pathway. 2001, 276, 26308-16 Constitutive activation of extracellular signal-regulated kinase 2 by synergistic point mutations. 2001, 276, 46469-79 The disordered mobile loop of GroES folds into a defined beta-hairpin upon binding GroEL. 2001,	31 28 56
1003 1002 1001	Sheep prion protein synthetic peptide spanning helix 1 and beta-strand 2 (residues 142-166) shows beta-hairpin structure in solution. 2001, 276, 46364-70 A conserved alpha-helix at the amino terminus of prosomatostatin serves as a sorting signal for the regulated secretory pathway. 2001, 276, 26308-16 Constitutive activation of extracellular signal-regulated kinase 2 by synergistic point mutations. 2001, 276, 46469-79 The disordered mobile loop of GroES folds into a defined beta-hairpin upon binding GroEL. 2001, 276, 31257-64	31 28 56 31
1003 1002 1001 1000	Sheep prion protein synthetic peptide spanning helix 1 and beta-strand 2 (residues 142-166) shows beta-hairpin structure in solution. 2001, 276, 46364-70 A conserved alpha-helix at the amino terminus of prosomatostatin serves as a sorting signal for the regulated secretory pathway. 2001, 276, 26308-16 Constitutive activation of extracellular signal-regulated kinase 2 by synergistic point mutations. 2001, 276, 46469-79 The disordered mobile loop of GroES folds into a defined beta-hairpin upon binding GroEL. 2001, 276, 31257-64 Definition of the extended substrate specificity determinants for beta-tryptases I and II. 2001, 276, 34941-7 The effect of amino groups on the stability of DNA duplexes and triplexes based on purines derived	31 28 56 31 50

(2001-2001)

995	Thermodynamics of RNA internal loops with a guanosine-guanosine pair adjacent to another noncanonical pair. 2001 , 40, 2478-83	23
994	-CH2- lengthening of the internucleotide linkage in the ApA dimer can improve its conformational compatibility with its natural polynucleotide counterpart. 2001 , 29, 5182-94	22
993	Molecular dynamics simulations of unsaturated lipid bilayers. 2001 , 4348, 215	6
992	Exploring the unique pharmacology of a novel opioid receptor, ZFOR1, using molecular modeling and the 'message-address' concept. 2001 , 14, 953-60	6
991	Modelling ion binding to AA platform motifs in RNA: a continuum solvent study including conformational adaptation. 2001 , 29, 3910-8	18
990	The TXP motif in the second transmembrane helix of CCR5. A structural determinant of chemokine-induced activation. 2001 , 276, 13217-25	111
989	A conserved Asn in transmembrane helix 7 is an on/off switch in the activation of the thyrotropin receptor. 2001 , 276, 22991-9	94
988	Energetic analysis of binding of progesterone and 5 beta-androstane-3,17-dione to anti-progesterone antibody DB3 using molecular dynamics and free energy calculations. 2001 , 14, 753-8	14
987	A single amino acid determines lysophospholipid specificity of the S1P1 (EDG1) and LPA1 (EDG2) phospholipid growth factor receptors. 2001 , 276, 49213-20	85
986	A NMR-spectra-based scoring function for protein docking. 2001,	1
986 985	A NMR-spectra-based scoring function for protein docking. 2001 , Solution structure of the dodecamer d-(CATGGGCC-CATG)2 is B-DNA. Experimental and molecular dynamics study. 2001 , 19, 159-74	9
	Solution structure of the dodecamer d-(CATGGGCC-CATG)2 is B-DNA. Experimental and molecular	
985	Solution structure of the dodecamer d-(CATGGGCC-CATG)2 is B-DNA. Experimental and molecular dynamics study. 2001 , 19, 159-74	9
985 984	Solution structure of the dodecamer d-(CATGGGCC-CATG)2 is B-DNA. Experimental and molecular dynamics study. 2001 , 19, 159-74 FACILE SYNTHESIS OF SATURATED EIGHT-MEMBERED RING LACTONES. 2001 , 31, 1781-1791	9 22
985 984 983	Solution structure of the dodecamer d-(CATGGGCC-CATG)2 is B-DNA. Experimental and molecular dynamics study. 2001, 19, 159-74 FACILE SYNTHESIS OF SATURATED EIGHT-MEMBERED RING LACTONES. 2001, 31, 1781-1791 Deducing hydration sites of a protein from molecular dynamics simulations. 2001, 19, 105-14	9 22
985 984 983 982	Solution structure of the dodecamer d-(CATGGGCC-CATG)2 is B-DNA. Experimental and molecular dynamics study. 2001, 19, 159-74 FACILE SYNTHESIS OF SATURATED EIGHT-MEMBERED RING LACTONES. 2001, 31, 1781-1791 Deducing hydration sites of a protein from molecular dynamics simulations. 2001, 19, 105-14 The dielectric self-consistent field method. I. Highways, byways, and illustrative results. 2001, 115, 10780-10 Hydrogen bonding and collective proton modes in clusters and periodic layers of squaric acid: A	9 22 9 792 6
985 984 983 982	Solution structure of the dodecamer d-(CATGGGCC-CATG)2 is B-DNA. Experimental and molecular dynamics study. 2001, 19, 159-74 FACILE SYNTHESIS OF SATURATED EIGHT-MEMBERED RING LACTONES. 2001, 31, 1781-1791 Deducing hydration sites of a protein from molecular dynamics simulations. 2001, 19, 105-14 The dielectric self-consistent field method. I. Highways, byways, and illustrative results. 2001, 115, 10780-10 Hydrogen bonding and collective proton modes in clusters and periodic layers of squaric acid: A density functional study. 2001, 115, 6406-6417 Special stability advantages of position-Verlet over velocity-Verlet in multiple-time step	9 22 9 792 6

977	Conformational dynamics of an alanine dipeptide analog: an ab initio molecular dynamics study. 2001 , 64, 011907	34
976	Green fluorescent proteins as optically controllable elements in bioelectronics. 2001, 79, 3353-3355	64
975	Molecular dynamics studies of sequence-directed curvature in bending locus of trypanosome kinetoplast DNA. 2001 , 18, 832-43	3
974	Conformational space comparison of GnRH and lGnRH-III using molecular dynamics, cluster analysis and Monte Carlo thermodynamic integration. 2001 , 18, 733-48	14
973	Optimized particle-mesh Ewald/multiple-time step integration for molecular dynamics simulations. 2001 , 115, 4003-4018	162
972	Atomic charges in molecular mechanical force fields: a theoretical insight. 2001 , 64, 026703	11
971	Electronic structure of overstretched DNA. 2002, 66,	39
970	Generalized form of the conserved quantity in constant-temperature molecular dynamics. 2002 , 116, 33	18
969	Partial optimization of molecular geometry in normal coordinates and use as a tool for simulation of vibrational spectra. 2002 , 117, 4126-4132	101
968	TTD: Therapeutic Target Database. 2002 , 30, 412-5	381
967	MOLECULAR MORPHOLOGY AND CRYSTALLIZATION IN THE QUANTUM LIMIT. 2002, 41, 787-795	1
966	A theoretical study on decomposition of formic acid in sub- and supercritical water. 2002 , 117, 7631-7639	29
965	Energy landscapes of model polyalanines. 2002, 117, 1363-1376	78
964	Predicting the solubility of xenon in n-hexane and n-perfluorohexane: a simulation and theoretical study. 2002 , 100, 2547-2553	38
963	A combined quantum chemistry and classical molecular interaction energy method for the determination of crystal geometries and energies. 2002 , 116, 747-754	3
962	Macroscopic modeling and simulations of supercoiled DNA with bound proteins. 2002, 117, 8573-8586	30
961	A combinatorial approach to protein docking with flexible side chains. 2002 , 9, 597-612	49
960	Application of the local self-consistent-field method to core-ionized and core-excited molecules, polymers, and proteins: True orthogonality between ground and excited states. 2002 , 117, 4119-4125	49

959	Molecular modeling of opioid receptor-ligand complexes. 2002 , 40, 107-35	7
958	SDS-resistant active and thermostable dimers are obtained from the dissociation of homotetrameric beta-glycosidase from hyperthermophilic Sulfolobus solfataricus in SDS. Stabilizing role of the A-C intermonomeric interface. 2002 , 277, 44050-60	43
957	Homology modeling of the cation binding sites of Na+K+-ATPase. 2002, 99, 15977-82	162
956	The molecular dynamics thermocycler. A new approach to sample conformational space, as exemplified by the RNA hairpin. 2002 , 57-8	1
955	PATHWAY ANALYSIS ON ELECTRON TRANSFER IN RUTHENIUM MODIFIED CYTOCHROME c. 2002 , 01, 93-107	
954	Prediction of Conformational Free Energy Differences of Solutes in Solution: An MC-MST Study. 2002 , 28, 153-171	5
953	Dynamics and binding modes of free cdk2 and its two complexes with inhibitors studied by computer simulations. 2002 , 20, 141-54	24
952	COMPUTATIONAL METHOD FOR DRUG TARGET SEARCH AND APPLICATION IN DRUG DISCOVERY. 2002 , 01, 213-224	2
951	Molecular modelling and site-directed mutagenesis of human GALR1 galanin receptor defines determinants of receptor subtype specificity. 2002 , 15, 313-23	26
950	Oxidative modification of aldose reductase induced by copper ion. Definition of the metal-protein interaction mechanism. 2002 , 277, 42017-27	51
949	Structural models of osteogenesis imperfecta-associated variants in the COL1A1 gene. 2002 , 1, 868-75	15
948	Proton shuttle in green fluorescent protein studied by dynamic simulations. 2002 , 99, 2778-81	131
947	FIMM, a database of functional molecular immunology: update 2002. 2002 , 30, 226-9	29
946	Properties of triple helices formed by parallel-stranded hairpins containing 8-aminopurines. 2002 , 30, 2609-19	36
945	Relating repair susceptibility of carcinogen-damaged DNA with structural distortion and thermodynamic stability. 2002 , 30, 3422-32	36
944	Intercalating nucleic acids containing insertions of 1-O-(1-pyrenylmethyl)glycerol: stabilisation of dsDNA and discrimination of DNA over RNA. 2002 , 30, 4918-25	111
943	The structures of the active center in dark-adapted bacteriorhodopsin by solution-state NMR spectroscopy. 2002 , 99, 9765-70	44
942	Distinct interactions of GTP, UTP, and CTP with G(s) proteins. 2002 , 277, 34434-42	13

941	The solution structure of an oligonucleotide duplex containing a 2'-deoxyadenosine-3-(2-hydroxyethyl)- 2'-deoxyuridine base pair determined by NMR and molecular dynamics studies. 2002 , 30, 1371-8	2
940	Brownian-dynamics simulations of metal-ion binding to four-way junctions. 2002 , 30, 507-14	22
939	SYNTHESIS AND CONFORMATIONAL ANALYSIS OF PSEUDOSUGAR ANALOGUES OF CHITOTRIOSE 1*. 2002 , 21, 471-489	7
938	NMR structure of a parallel-stranded DNA duplex at atomic resolution. 2002, 30, 1500-11	62
937	A Hoogsteen base pair embedded in undistorted B-DNA. 2002 , 30, 5244-52	59
936	DIFFERENT PROTONATION STATES OF THE BACILLUS CEREUS BINUCLEAR ZINC METALLO-LACTAMASE ACTIVE SITE STUDIED BY COMBINED QUANTUM MECHANICAL AND MOLECULAR MECHANICAL SIMULATIONS. 2002 , 01, 69-80	4
935	Lysine 183 and glutamic acid 157 of the TSH receptor: two interacting residues with a key role in determining specificity toward TSH and human CG. 2002 , 16, 722-35	49
934	Molecular dynamics characterization of the C2 domain of protein kinase Cbeta. 2002 , 277, 12988-97	40
933	Molecular mimicry of an HLA-B27-derived ligand of arthritis-linked subtypes with chlamydial proteins. 2002 , 277, 37573-81	63
932	Discrimination of C1:G72 MicrohelixAla by AlaRS Is Based on Specific Atomic Groups Rather Than Conformational Effects: An NMR and MD Analysis. 2002 , 106, 8878-8884	2
931	The Reaction Mechanism of Bovine Lens Leucine Aminopeptidase. 2002, 106, 8815-30	21
930	A dimensionality reduction approach to modeling protein flexibility. 2002,	11
929	Effect of a neutralized phosphate backbone on the minor groove of B-DNA: molecular dynamics simulation studies. 2002 , 30, 3615-23	39
928	Discovering high-affinity ligands from the computationally predicted structures and affinities of small molecules bound to a target: A virtual screening approach. 2000 , 209-230	
927	Ligand-induced changes in the binding sites of proteins. 2002 , 18, 939-48	45
926	Photo-control of peptide helix content by an azobenzene cross-linker: steric interactions with underlying residues are not critical. 2002 , 15, 561-9	30
925	Molecular dynamics investigation of the double stranded oligonucleotide d(AT)6d(AT)6. 2002, 175-6	
924	Analysis of membrane stereochemistry with homology modeling of sn-glycerol-1-phosphate dehydrogenase. 2002 , 15, 987-95	26

923	Tiny telomere DNA. 2002 , 30, 2307-15		66
922	Complex pattern of membrane type 1 matrix metalloproteinase shedding. Regulation by autocatalytic cells surface inactivation of active enzyme. 2002 , 277, 26340-50		98
921	Theoretical and experimental studies of biotin analogues that bind almost as tightly to streptavidin as biotin. 2002 , 67, 1827-37		22
920	Evidence for a model of agonist-induced activation of 5-hydroxytryptamine 2A serotonin receptors that involves the disruption of a strong ionic interaction between helices 3 and 6. 2002 , 277, 11441-9		142
919	Discrimination between agonists and antagonists by the alpha-amino-3-hydroxy-5-methyl-4-isoxazole propionic acid-selective glutamate receptor. A mutation analysis of the ligand-binding domain of GluR-D subunit. 2002 , 277, 41940-7		9
918	A novel class of peptides with facilitating action on neuronal nicotinic receptors of rat chromaffin cells in vitro: functional and molecular dynamics studies. 2002 , 61, 43-54		17
917	Design, synthesis and pharmacological evaluation of 5-hydroxytryptamine(1a) receptor ligands to explore the three-dimensional structure of the receptor. 2002 , 62, 15-21		47
916	Rigidity Theory and Applications. 2002,		5
915	Molecular Dynamics and Normal Mode Analysis of Biomolecular Rigidity. 2002, 329-344		2
914	Conformational dynamics in a dipeptide after single-mode vibrational excitation. 2002 , 296, 2369-73		171
913	RNA canonical and non-canonical base pairing types: a recognition method and complete repertoire. 2002 , 30, 4250-63		101
912	The influence of the thymine C5 methyl group on spontaneous base pair breathing in DNA. 2002 , 277, 28491-7		45
911	Drugs that inhibit mycolic acid biosynthesis in Mycobacterium tuberculosis. 2002 , 3, 197-225		109
910	Molecular Dynamics Studies of Ion Distributions around DNA Duplexes and Duplex Dimers: Salt Effects and the Connection to Cooperative DNA Melting. 2002 , 735, 1011		1
909	A single WW domain is the predominant mediator of the interaction between the human ubiquitin-protein ligase Nedd4 and the human epithelial sodium channel. 2002 , 361, 481-8		26
908	A single WW domain is the predominant mediator of the interaction between the human ubiquitin-protein ligase Nedd4 and the human epithelial sodium channel. 2002 , 361, 481-488		40
907	Charge transfer in small hydrogen bonded clusters. 2002 , 116, 7380-7388		58
906	Binding of aminoglycoside antibiotics to the small ribosomal subunit: a continuum electrostatics investigation. <i>Journal of the American Chemical Society</i> , 2002 , 124, 1438-42	6.4	49

905	Evolution and physics in comparative protein structure modeling. 2002, 35, 413-21		97
904	Theoretical Investigation of the Binding Free Energies and Key Substrate-Recognition Components of the Replication Fidelity of Human DNA Polymerase 2002 , 106, 5739-5753		68
903	Internal Loop⊞elix Coupling in the Dynamics of the RNA Duplex (GC*C*AGUUCGCUGGC)2. 2002 , 106, 5075-5085		7
902	Hydrophobicity maps of the N-peptide coiled coil of HIV-1 gp41. 2002 , 41, 2956-61		24
901	From knowledge-based potentials to combinatorial lead design in silico. 2002 , 35, 261-9		48
900	Comparative bending dynamics in DNA with and without regularly repeated adenine tracts. 2002 , 66, 011917		11
899	Structural basis for understanding structure-activity relationships for the glutamate binding site of the NMDA receptor. 2002 , 45, 3836-43		29
898	The Structural Characteristics of Bombyx mori Silk Fibroin before Spinning As Studied with Molecular Dynamics Simulation. 2002 , 35, 8831-8838		39
897	Destructive Interference in the Electron Tunneling through Protein Media. 2002 , 106, 11356-11366		47
896	Conformational heterogeneity observed in simulations of a pyrene-substituted DNA. <i>Journal of the American Chemical Society</i> , 2002 , 124, 12154-64	16.4	19
895	Insights into the structure and dynamics of the dinuclear zinc beta-lactamase site from Bacteroides fragilis. 2002 , 41, 6615-30		69
894	Molecular dynamics simulation study of the negative correlation in antibody AZ28-catalyzed oxy-cope rearrangement. <i>Journal of the American Chemical Society</i> , 2002 , 124, 12535-42	16.4	14
893	Protein Conformational Gate Controlling Binding Site Preference and Migration for Ubiquinone-B in the Photosynthetic Reaction Center of Rhodobacter sphaeroides. 2002 , 106, 3001-3006		28
892	Probing Inter- and Intramolecular Interactions of Six New p-tert-Butylcalix[4]arene-Based Bipyridyl Podands with Langmuir Monolayers. 2002 , 18, 8854-8861		21
891	Long-Range Effects of Mutating R248 to Q/W in the p53 Core Domain. 2002, 106, 13047-13057		7
890	Hoogsteen-based parallel-stranded duplexes of DNA. Effect of 8-amino-purine derivatives. <i>Journal of the American Chemical Society</i> , 2002 , 124, 3133-42	16.4	37
889	Hydration structure and conformational dynamics of urocanic acid: a computer simulation study. 2002 , 100, 1873-1886		4
888	D-RESP: Dynamically Generated Electrostatic Potential Derived Charges from Quantum Mechanics/Molecular Mechanics Simulations. 2002 , 106, 7300-7307		174

887	Protein Folding as Biased Conformational Diffusion. 2002 , 106, 3255-3262	29
886	Studies on the mechanism of hypoxic selectivity in copper bis(thiosemicarbazone) radiopharmaceuticals. 2002 , 45, 1420-31	162
885	Hydronium ion complex of 18-crown-6: where are the protons? A density functional study of static and dynamic properties. <i>Journal of the American Chemical Society</i> , 2002 , 124, 4473-80	35
884	The Effect of the Neglect of Electronic Polarization in Peptide Folding Simulations. 2002 , 106, 12830-12833	16
883	Bending of DNA by asymmetric charge neutralization: all-atom energy simulations. <i>Journal of the American Chemical Society</i> , 2002 , 124, 4838-47	55
882	Molecular Dynamics Simulations ofp-Sulfonatocalix[4]arene Complexes with Inorganic and Organic Cations in Water: A Structural and Thermodynamic Study. 2002 , 106, 4516-4524	47
881	Comparative binding energy (COMBINE) analysis of OppA-peptide complexes to relate structure to binding thermodynamics. 2002 , 45, 4828-37	46
880	Atomic Radii for Continuum Electrostatics Calculations on Nucleic Acids. 2002 , 106, 11026-11035	64
879	Hole Size and Energetics in Double Helical DNA: Competition between Quantum Delocalization and Solvation Localization. 2002 , 106, 7-10	97
878	Antitumor agents. 1. Synthesis, biological evaluation, and molecular modeling of 5H-pyrido[3,2-a]phenoxazin-5-one, a compound with potent antiproliferative activity. 2002 , 45, 5205-16	37
877	DNA dynamics in a water drop without counterions. <i>Journal of the American Chemical Society</i> , 2002 , 124, 14707-15	24
876	The [Lys(-2)-Arg(-1)-des(17-21)]-endothelin-1 peptide retains the specific Arg(-1)-Asp8 salt bridge but reveals discrepancies between NMR data and molecular dynamics simulations. 2002 , 41, 11099-108	4
875	Molecular Dynamics of the tRNAAla Acceptor Stem: Comparison between Continuum Reaction Field and Particle-Mesh Ewald Electrostatic Treatments. 2002 , 106, 3696-3705	40
874	Thermal Degradation and Solution Properties of Poly(2,2Edioxybiphenyl phosphazene). 2002 , 35, 7505-7515	38
873	A 3.(ET743)-DNA complex that both resembles an RNA-DNA hybrid and mimicks zinc finger-induced DNA structural distortions. 2002 , 45, 871-80	26
872	Enzymatic GTP hydrolysis: insights from an ab initio molecular dynamics study. <i>Journal of the American Chemical Society</i> , 2002 , 124, 3763-8	44
871	Human topoisomerase I inhibition: docking camptothecin and derivatives into a structure-based active site model. 2002 , 41, 1428-35	82
870	Aggregation in Dilute Solutions of 1-Hexanol in n-Hexane: A Monte Carlo Simulation Study. 2002 , 106, 3968-3978	53

869	Molecular dynamics at the root of expansion of function in the M69L inhibitor-resistant TEM beta-lactamase from Escherichia coli. <i>Journal of the American Chemical Society</i> , 2002 , 124, 9422-30	16.4	46
868	Molecular Dynamics Simulation with the Charge Response Kernel: Vibrational Spectra of Liquid Water and N-Methylacetamide in Aqueous Solution. 2002 , 106, 3466-3476		67
867	Refolding molecular dynamics simulations of small- and middle-sized proteins in an explicit solvent. 2002 , 28, 337-357		5
866	Indirect readout of the trp-repressor-operator complex by B-DNA's backbone conformation transitions. 2002 , 41, 4088-95		25
865	Polarization of cinnamoyl-CoA substrates bound to enoyl-CoA hydratase: correlation of (13)C NMR with quantum mechanical calculations and calculation of electronic strain energy. 2002 , 41, 2630-40		10
864	Mechanism of acetylcholinesterase inhibition by fasciculin: a 5-ns molecular dynamics simulation. Journal of the American Chemical Society, 2002 , 124, 6153-61	16.4	68
863	Molecular Dynamics Simulations and Vibrational Spectroscopic Studies of Local Structure in Tetraglyme:Sodium Triflate (CH3O(CH2CH2O)4CH3:NaCF3SO3) Solutions. 2002 , 106, 4878-4885		20
862	Computational Methods for the Study of Enzymic Reaction Mechanisms. 1. Application to the Hydride Transfer Step in the Catalysis of Dihydrofolate Reductase. 2002 , 106, 9934-9944		25
861	Crenarchaeol: the characteristic core glycerol dibiphytanyl glycerol tetraether membrane lipid of cosmopolitan pelagic crenarchaeota. 2002 , 43, 1641-51		474
860	Comparison of Simulated and Experimental Transport of Gases in Commercial Poly(vinyl chloride). 2002 , 35, 4167-4174		17
860 859		01	17 201
	2002 , 35, 4167-4174	01	
859	2002, 35, 4167-4174 Hole Migration in DNA: 'a Theoretical Analysis of the Role of Structural Fluctuations. 2002, 106, 2093-21	01	201
859 858	2002, 35, 4167-4174 Hole Migration in DNA: 'a Theoretical Analysis of the Role of Structural Fluctuations. 2002, 106, 2093-21 Quantum mechanical methods for enzyme kinetics. 2002, 53, 467-505 A polarizable mixed Hamiltonian model of electronic structure for solvated excited states. II.	01	201 679
859 858 857	Hole Migration in DNA: 'a Theoretical Analysis of the Role of Structural Fluctuations. 2002, 106, 2093-21 Quantum mechanical methods for enzyme kinetics. 2002, 53, 467-505 A polarizable mixed Hamiltonian model of electronic structure for solvated excited states. II. Application to the blue shift of the H2CO 1(M<-n) excitation in water. 2002, 117, 1256-1268 Solution-state conformational study of the hevamine inhibitor allosamidin and six potential	01	20167924
859 858 857 856	Hole Migration in DNA: 'a Theoretical Analysis of the Role of Structural Fluctuations. 2002, 106, 2093-21 Quantum mechanical methods for enzyme kinetics. 2002, 53, 467-505 A polarizable mixed Hamiltonian model of electronic structure for solvated excited states. II. Application to the blue shift of the H2CO 1(H<-n) excitation in water. 2002, 117, 1256-1268 Solution-state conformational study of the hevamine inhibitor allosamidin and six potential inhibitor analogues by NMR spectroscopy and molecular modeling. 2002, 67, 6328-38 Parametrization and validation of a force field for liquid-crystal forming molecules. 2002, 65, 051709	16.4	201679241350
859 858 857 856	Hole Migration in DNA: 'a Theoretical Analysis of the Role of Structural Fluctuations. 2002, 106, 2093-21 Quantum mechanical methods for enzyme kinetics. 2002, 53, 467-505 A polarizable mixed Hamiltonian model of electronic structure for solvated excited states. II. Application to the blue shift of the H2CO 1(%n) excitation in water. 2002, 117, 1256-1268 Solution-state conformational study of the hevamine inhibitor allosamidin and six potential inhibitor analogues by NMR spectroscopy and molecular modeling. 2002, 67, 6328-38 Parametrization and validation of a force field for liquid-crystal forming molecules. 2002, 65, 051709 Peptide loop-closure kinetics from microsecond molecular dynamics simulations in explicit solvent. Journal of the American Chemical Society, 2002, 124, 6563-8		201 679 24 13 50

851	Comparative thermodynamics for monomer and dimer sequence-dependent binding of a heterocyclic dication in the DNA minor groove. 2002 , 317, 361-74	46
850	RNA simulations: probing hairpin unfolding and the dynamics of a GNRA tetraloop. 2002 , 317, 493-506	97
849	Molecular dynamics and free energy analyses of cathepsin D-inhibitor interactions: insight into structure-based ligand design. 2002 , 45, 1412-9	155
848	Intercalators. 1. Nature of stacking interactions between intercalators (ethidium, daunomycin, ellipticine, and 4',6-diaminide-2-phenylindole) and DNA base pairs. Ab initio quantum chemical, density functional theory, and empirical potential study. <i>Journal of the American Chemical Society</i> ,	275
847	Modeling enzyme reactivity in organic solvents and water through computer simulations. 2002 , 96, 23-33	21
846	Large and Fast Relaxations inside a Protein: Calculation and Measurement of Reorganization Energies in Alcohol Dehydrogenase. 2002 , 106, 11658-11665	69
845	Probing the cysteine-34 position of endogenous serum albumin with thiol-binding doxorubicin derivatives. Improved efficacy of an acid-sensitive doxorubicin derivative with specific albumin-binding properties compared to that of the parent compound. 2002 , 45, 5523-33	227
844	Stereoselective synthesis and antiviral activity of D-2',3'-didehydro-2',3'-dideoxy-2'-fluoro-4'-thionucleosides. 2002 , 45, 4888-98	33
843	A Force Field for Liquid State Simulations on Room Temperature Molten Salts: 1-Ethyl-3-methylimidazolium Tetrachloroaluminate. 2002 , 106, 3546-3548	143
842	The active site of cellobiohydrolase Cel6A from Trichoderma reesei: the roles of aspartic acids D221 and D175. <i>Journal of the American Chemical Society</i> , 2002 , 124, 10015-24	116
841	Site-specific OH attack to the sugar moiety of DNA: a comparison of experimental data and computational simulation. 2002 , 157, 38-44	41
840	Theoretical study of anion binding to calix[4]pyrrole: the effects of solvent, fluorine substitution, cosolute, and water traces. <i>Journal of the American Chemical Society</i> , 2002 , 124, 12796-805	63
839	Understanding the role of stereoelectronic effects in determining collagen stability. 2. A quantum mechanical/molecular mechanical study of (Proline-Proline-Glycine)(n) polypeptides. <i>Journal of the American Chemical Society</i> , 2002 , 124, 7857-65	63
838	Ligand binding affinities from MD simulations. 2002 , 35, 358-65	307
837	Ab initiomolecular dynamics: basic concepts, current trends and novel applications. 2002 , 14, R1297-R1355	187
836	Explicit solvent molecular dynamics simulation of duplex formed by the modified oligonucleotide with alternating phosphate/phosphonate internucleoside linkages and its natural counterpart. 2002, 19, 863-75	8
835	Water structure from scattering experiments and simulation. 2002 , 102, 2651-70	435
834	Benzimidazole derivatives. 3. 3D-QSAR/CoMFA model and computational simulation for the recognition of 5-HT(4) receptor antagonists. 2002 , 45, 4806-15	32

833	Structural determinants of A(3) adenosine receptor activation: nucleoside ligands at the agonist/antagonist boundary. 2002 , 45, 4471-84	139
832	3D structure of Torpedo californica acetylcholinesterase complexed with huprine X at 2.1 A resolution: kinetic and molecular dynamic correlates. 2002 , 41, 2970-81	112
831	Role of the catalytic triad and oxyanion hole in acetylcholinesterase catalysis: an ab initio QM/MM study. <i>Journal of the American Chemical Society</i> , 2002 , 124, 10572-7	211
830	Effects of the protein environment on the structure and energetics of active sites of metalloenzymes. ONIOM study of methane monooxygenase and ribonucleotide reductase. <i>Journal</i> 16.4 of the American Chemical Society, 2002 , 124, 192-3	115
829	Hydrogen storage capacity in single-walled carbon nanotubes. 2002 , 65,	25
828	Electronic structure of wet DNA. 2002 , 89, 108102	148
827	Sheared Aanti. Aanti base pairs in a destabilizing 2 \times 2 internal loop: the NMR structure of 5'(rGGCAAGCCU)2. 2002 , 41, 14969-77	15
826	Tensile strength of single-walled carbon nanotubes with defects under hydrostatic pressure. 2002 , 65,	38
825	Structural refinement of the 8,9-dihydro-8-(N7-guanyl)-9-hydroxy-aflatoxin B(1) adduct in a 5'-Cp(AFB)G-3' sequence. 2002 , 15, 638-47	20
824	Atomistic simulations of complex materials: ground-state and excited-state properties. 2002 , 14, 3015-3047	384
823	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a	175
	microhydrated environment and in aqueous solution. 2002 , 4, 4192-4203	-73
822	Predictions of Binding of a Diverse Set of Ligands to Gelatinase-A by a Combination of Molecular Dynamics and Continuum Solvent Models. 2002 , 106, 5527-5535	76
822	Predictions of Binding of a Diverse Set of Ligands to Gelatinase-A by a Combination of Molecular	
	Predictions of Binding of a Diverse Set of Ligands to Gelatinase-A by a Combination of Molecular Dynamics and Continuum Solvent Models. 2002 , 106, 5527-5535	76
821	Predictions of Binding of a Diverse Set of Ligands to Gelatinase-A by a Combination of Molecular Dynamics and Continuum Solvent Models. 2002, 106, 5527-5535 Free Energy Calculations. The Long and Winding Gilded Road. 2002, 28, 1-12	76 79
821	Predictions of Binding of a Diverse Set of Ligands to Gelatinase-A by a Combination of Molecular Dynamics and Continuum Solvent Models. 2002, 106, 5527-5535 Free Energy Calculations. The Long and Winding Gilded Road. 2002, 28, 1-12 Is the T-Shaped Toluene Dimer a Stable Intermolecular Complex?. 2002, 106, 2945-2948 Optimization of quantum mechanical molecular mechanical partitioning schemes: Gaussian	76 79 36
821 820 819	Predictions of Binding of a Diverse Set of Ligands to Gelatinase-A by a Combination of Molecular Dynamics and Continuum Solvent Models. 2002, 106, 5527-5535 Free Energy Calculations. The Long and Winding Gilded Road. 2002, 28, 1-12 Is the T-Shaped Toluene Dimer a Stable Intermolecular Complex?. 2002, 106, 2945-2948 Optimization of quantum mechanical molecular mechanical partitioning schemes: Gaussian delocalization of molecular mechanical charges and the double link atom method. 2002, 117, 10534-10547 Ab Initio and Improved Empirical Potentials for the Calculation of the Anharmonic Vibrational	76 79 36 162

(2002-2002)

815	An ab Initio Quantum Mechanical Study of Hydrogen-Bonded Complexes of Biological Interest. 2002 , 106, 7820-7827		48
814	Structure and intermolecular potentials in molecular crystals. 2002 , 10, R1-R29		52
813	SMall Molecule Growth 2001 (SMoG2001): an improved knowledge-based scoring function for protein-ligand interactions. 2002 , 45, 2770-80		131
812	Structure and properties of the dendron-encapsulated polyoxometalate (C(52)H(60)NO(12))(12)[(Mn(H(2)O))(3)(SbW(9)O(33))(2)], a first generation dendrizyme. <i>Journal of the American Chemical Society</i> , 2002 , 124, 10489-96	16.4	112
811	Design of noncovalent inhibitors of human cathepsin L. From the 96-residue proregion to optimized tripeptides. 2002 , 45, 5321-9		63
810	Model for the catalytic domain of the proofreading epsilon subunit of Escherichia coli DNA polymerase III based on NMR structural data. 2002 , 41, 94-110		30
809	The infrared and ultraviolet spectra of single conformations of methyl-capped dipeptides: N-acetyl tryptophan amide and N-acetyl tryptophan methyl amide. 2002 , 117, 10688-10702		115
808	Molecular Modeling and Simulation. 2002,		318
807	Ab Initio-Quality Electrostatic Potentials for Proteins: An Application of the ADMA Approach. 2002 , 106, 11791-11800		100
806	Azapeptides structurally based upon inhibitory sites of cystatins as potent and selective inhibitors of cysteine proteases. 2002 , 45, 4202-11		39
805	Escaping free-energy minima. 2002 , 99, 12562-6		3706
804	Interaction of bifunctional carbonyl and phosphoryl ligands with M3+ lanthanide cations: how strong is the bidentate effect? The role of ligand size and counterions investigated by quantum mechanics. 2002 , 4, 5716-5729		31
803	Dynamics of energy transfer in peptide-surface collisions. <i>Journal of the American Chemical Society</i> , 2002 , 124, 1524-31	16.4	81
802	Direct observation of the folding and unfolding of a beta-hairpin in explicit water through computer simulation. <i>Journal of the American Chemical Society</i> , 2002 , 124, 5282-3	16.4	62
801	NMR structure of alpha-bungarotoxin free and bound to a mimotope of the nicotinic acetylcholine receptor. 2002 , 41, 1457-63		21
800	Ab initio pair potential and phase equilibria predictions for the refrigerant methyl fluoride. 2002 , 100, 2433-2447		10
799	Synthesis, X-ray structure and molecular modelling analysis of cobalt(II), nickel(II), zinc(II) and cadmium(II) complexes of the widely used anti-inflammatory drug meloxicam. 2002 , 1888		48
798	Docking ligands to vasopressin and oxytocin receptors via genetic algorithm. 2002 , 22, 393-409		2

797	Tetraethylammonium binding to the outer mouth of the KcsA potassium channel: implications for ion permeation. 2002 , 22, 315-31	17
796	Application of the Free Energy Calculations to Study Drug-enzyme and Drug-dna Complexes. 2002 , 28, 173-186	2
795	Filling and emptying kinetics of carbon nanotubes in water. 2002 , 117, 10789-10795	210
794	Structural analysis of the inhibition of Cdk4 and Cdk6 by p16(INK4a) through molecular dynamics simulations. 2002 , 20, 347-58	22
793	Application of computer assisted combinatorial chemistry in antivirial, antimalarial and anticancer agents design. 2002 , 100, 3187-3198	2
79 ²	Molecular dynamics simulation of 7, 8-dihydro-8-oxoguanine DNA. 2002 , 19, 839-51	11
791	A transferable polarizable electrostatic force field for molecular mechanics based on the chemical potential equalization principle. 2002 , 117, 9175-9189	119
790	Identification of a functional site on the type I TGF-beta receptor by mutational analysis of its ectodomain. 2002 , 513, 147-52	7
789	Molecular dynamics simulations revealed Ca(2+)-dependent conformational change of Calmodulin. 2002 , 521, 133-9	51
788	Solvent environment conducive to protein aggregation. 2002 , 529, 298-301	16
787	Interaction of Kazal-type inhibitor domains with serine proteinases: biochemical and structural studies. 2002 , 318, 533-46	44
786	A compact RNA tertiary structure contains a buried backbone-K+ complex. 2002 , 318, 963-73	115
785	Amino acid modification in the HIV-1 Tat basic domain: insights from molecular dynamics and in vivo functional studies. 2002 , 318, 1331-9	13
7 ⁸ 4	Role of conformational fluctuations in the enzymatic reaction of HIV-1 protease. 2002 , 319, 567-83	122
783	Thermodynamic consequences of burial of polar and non-polar amino acid residues in the protein interior. 2002 , 320, 343-57	97
782	Toward understanding the mutagenicity of an environmental carcinogen: structural insights into nucleotide incorporation preferences. 2002 , 322, 291-309	31
781	A model binding site for testing scoring functions in molecular docking. 2002 , 322, 339-55	178
780	NMR structures of 36 and 73-residue fragments of the calreticulin P-domain. 2002 , 322, 773-84	49

(2016-2002)

779	Pvull-endonuclease induces structural alterations at the scissile phosphate group of its cognate DNA. 2002 , 324, 491-500	7
778	Structural changes during the formation of early intermediates in the bacteriorhodopsin photocycle. 2002 , 83, 1281-97	124
777	Continuum electrostatics fails to describe ion permeation in the gramicidin channel. 2002, 83, 1348-60	101
776	Molecular dynamics simulation of proton transport through the influenza A virus M2 channel. 2002 , 83, 1987-96	104
775	Accurate representation of B-DNA double helical structure with implicit solvent and counterions. 2002 , 83, 382-406	33
774	Structure modeling of the chemokine receptor CCR5: implications for ligand binding and selectivity. 2002 , 83, 3012-31	66
773	Molecular dynamics simulation of the RNA complex of a double-stranded RNA-binding domain reveals dynamic features of the intermolecular interface and its hydration. 2002 , 83, 3542-52	23
772	In silico analysis identifies a C3HC4-RING finger domain of a putative E3 ubiquitin-protein ligase located at the C-terminus of a polyglutamine-containing protein. 2007 , 40, 293-299	1
771	Aplicaciones de los mEodos computacionales al estudio de la estructura y propiedades de polEheros. 2003 , 13, 250-264	2
770	Retention of local conformational compactness in unfolding of barnase; Contribution of end-to-end interactions within quasi-modules. 2007 , 3, 1-12	3
769	Applications of Molecular Simulation in the Discovery of Antituberculosis Drugs: A Review. 2019 , 26, 648-663	5
768	Molecular Dynamics Simulations of Adenosine Receptors: Advances, Applications and Trends. 2019 , 25, 783-816	17
767	Towards a Better Understanding of Computational Models for Predicting DNA Methylation Effects at the Molecular Level. 2020 , 20, 901-909	1
766	Recent Trends in Drug Design and Discovery. 2020 , 20, 1761-1770	4
765	Molecular Docking in Formulation and Development. 2019 , 16, 30-39	22
764	Macroscopic No-Slip Boundary Condition Confirmed in Full Atomistic Simulation of Oil Film. 2014 , 9, 45-50	11
763	Development of an Atomistic Brownian Dynamics Algorithm with Implicit Solvent Model for Long Time Simulation 2002 , 1, 115-122	6
762	Structural Analysis of Molecular Cavity Using a 3D Printer. 2016 , 15, 97-104	6

761	Molecular Dynamics Simulation of 4-n-alkyl-4'-cyanobiphenyl (nCB) Using a Full-atom Model. 2016 , 14, 211-212	1
760	A New Implicit Solvent Model for Brownian Dynamics Simulation: Solvent-Accessible Surface Area Dependent Effective Charge Model. 2004 , 3, 129-136	5
759	A Data Base for Transition States. Ranking of Synthesis Routes by using a System Combined Computational with Information Chemistry 2001 , 2, 37-44	7
758	Binding energy between lactose repressor protein and DNA: semiempirical molecular orbital calculations. 2003 , 4, 35-41	3
757	Semiempirical MO calculations for double-strand DNA and its base-mismatched ones. 2003, 4, 42-51	1
756	Electronic Properties for Medicine Inhibiting Cancer Metastasis (1): Molecular Orbital Calculations for Physiological Substance Bikunin. 2004 , 5, 62-69	4
755	Electronic Properties for Medicine Inhibiting Cancer Metastasis (2): Molecular Mechanics and Molecular Orbital Calculations for Urokinase. 2004 , 5, 70-78	4
754	Molecular Mechanics and Molecular Orbital Simulations on The Specific Interactions between Lactose Repressor Protein and Its Inducer and Anti-Inducer Molecules. 2008 , 9, 17-29	2
753	Putative Dynamics of Vasopressin in its V1a Receptor Binding Site. 2003 , 9, 93-106	4
75 ²	Beyond the Canonical Endocannabinoid System. A Screening of PPAR Ligands as FAAH Inhibitors. 2020 , 21,	6
75 ¹	Mechanical Characterization of Multiwalled Carbon Nanotubes: Numerical Simulation Study. 2020 , 13,	4
75°	Pharmacological Characterization of μ-Opioid Receptor Agonists with Biased G Protein or ΒArrestin Signaling, and Computational Study of Conformational Changes during Receptor Activation. 2020 , 26,	3
749	Computational Study of Binding Mode for N-substituted Pyrrole Derivatives to HIV-1 gp41*. 2010 , 37, 904-915	7
748	Molecular Dynamics Simulation of Deformation of Polymer Resist in Nanoimpirnt Lithography. 2005 , 29, 852-859	4
747	Theoretical study of chitosan-graphene and other chitosan-based nanocomposites stability. 2017 , 4, 317-327	1
746	Molecular modeling studies of peptoid polymers. 2017 , 4, 1029-1051	13
745	Functionalization of the Ring A in Some Benzo[g]pyridazino[1,2-b]- phthalazine-6,13-dione Derivatives Related to Anthracyclinones. 2004 , 63, 1299	4
744	Molecular Docking of Biologically Active Substances to Double Helical Nucleic Acids. 2016, 127-157	1

743	Protein-Ligand Docking Methodologies and Its Application in Drug Discovery. 2017, 891-914	1
742	Multi-Agent Systems in Three-Dimensional Protein Structure Prediction. 2017 , 241-278	1
741	Drug Discovery. 2019 , 1-46	1
740	Molecular dynamics simulations of a DNA photolyase protein: High-mobility and conformational changes of the FAD molecule at low temperatures. 2012 , 03, 169-180	4
739	<i>In Silico</i> Approach for the Identification of Potential Targets and Specific Antimicrobials for <i>Streptococcus mutans</i>. 2014 , 05, 373-385	3
738	Comparative Study of the Chemical Reactivity of Helical Peptide Models for Protein Glycation. 2017 , 05, 65-73	1
737	Computational and Experimental Analyses of Detachment Force at the Interface between Carbon Fibers and Epoxy Resin. 2017 , 07, 179-184	4
736	Molecular Dynamics Study on the Binding of S- and R-Ofloxacin to [d(ATAGCGCTAT)]2Oligonucleotide: Effects of Protonation States. 2008 , 29, 2103-2108	3
735	Protein Structure Prediction Using an Associated Memory Hamiltonian and All-Atom Molecular Dynamics Simulations. 2008 , 29, 2172-2182	4
734	Molecular dynamics simulations on DNA flexibility: a comparative study of Amber bsc1 and bsc0 force fields. 2018 , 67, 108701	2
733	The kinase LYK5 is a major chitin receptor in Arabidopsis and forms a chitin-induced complex with related kinase CERK1. 2014 , 3,	298
732	Verifiability in computer-aided research: the role of digital scientific notations at the human-computer interface. 2018 , 4, e158	4
731	Single mutations in the $\bar{\mu}$ subunit from thermophilic PS3 generate a high binding affinity site for ATP. 2018 , 6, e5505	3
730	Molecular simulations of IDPs: From ensemble generation to IDP interactions leading to disorder-to-order transitions. 2021 , 183, 135-185	1
729	DNA sequence and methylation prescribe the inside-out conformational dynamics and bending energetics of DNA minicircles. 2021 , 49, 11459-11475	2
728	Exploring the Molecular Basis of Substrate and Product Selectivities of Nocardicin Bifunctional Thioesterase. 2021 , 1	O
727	Regulation of Molecular Orientations of ADA Nonfullerene Acceptors for Organic Photovoltaics: The Role of End-Group latacking. 2108551	5
726	Molecular Dynamics Simulations of the Aptamer Domain of Guanidinium Ion Binding Riboswitch -III: Structural Insights into the Discrimination of Cognate and Alternate Ligands. 2021 , 61, 5243-5255	1

Machine Learning of First-Principles Force-Fields for Alkane and Polyene Hydrocarbons. **2021**, 125, 9414-9420 $_3$

724	How to strike a conformational balance in protein force fields for molecular dynamics simulations?. e1578	O
723	Intrinsic voltage plateau of a Nb2CTx MXene cathode in an aqueous electrolyte induced by high-voltage scanning. 2021 ,	20
722	Molecular Dynamics Modeling of Epoxy Resins Using the Reactive Interface Force Field.	2
721	Revisiting OD-stretching dynamics of methanol-d4, ethanol-d6 and dilute HOD/H2O mixture with predefined potentials and wavelet transform spectra. 2021 , 553, 111385	4
720	Cryo-EM structure of a tetrameric photosystem I from TS-821, a thermophilic, unicellular, non-heterocyst-forming cyanobacterium 2022 , 3, 100248	2
719	Modeling Spectral Tuning in Red Fluorescent Proteins Using the Dipole Moment Variation upon Excitation. 2021 , 61, 5125-5132	О
718	An Insight of Protein Structure Predictions Using Homology Modeling. 2021 , 265-277	
717	Temperature and Guanidine Hydrochloride Effects on the Folding Thermodynamics of WW Domain and Variants. 2021 , 125, 11386-11391	0
716	Accelerated Molecular Dynamics to Explore the Binding of Transition Metals to Amyloid- #2021 , 12, 4065-4075	O
715	Comparing Dimerization Free Energies and Binding Modes of Small Aromatic Molecules with Different Force Fields. 2021 , 26,	1
714	A comprehensive review on the significant tools of asphaltene investigation. Analysis and characterization techniques and computational methods. 2021 , 109611	2
713	Synthesis, biological evaluation, and molecular docking studies of deoxygenated C-glycosides as LpxC inhibitors. 2021 , 117, 105403	0
712	Stable electrodellectrolyte interfaces constructed by fluorine- and nitrogen-donating ionic additives for high-performance lithium metal batteries. 2021 , 45, 1-1	4
711	Machine learning applications in macromolecular X-ray crystallography. 1-48	1
710	Photochemistry of Thymine in Protic Polar Nanomeric Droplets Using Electrostatic Embeding TD-DFT/MM. 2021 , 26,	1
709	Atomistic Modelling of Liquid Crystal Phases. 2000 , 251-262	1
708	Self Atom-Atom Empirical Potentials for the Static and Dynamic Simulation of Condensed Phases. 2000 , 235-250	

707	Molecular Dynamics Simulation of Biological Molecules. (1). Methods 2000, 6, 1-36	2
706	MD Simulation of a Phospholipid Bilayer. 2000 , 212-228	
7 ⁰ 5	Modelling of Enzyme Properties in Organic Solvents. 2000 , 1-21	1
704	Multiple Time Steps Algorithms for the Atomistic Simulations of Complex Molecular Systems. 2000 , 333-387	
703	Study on the Force Field for Molecular Dynamics Simulations. 2000 , 40, 266-269	1
702	Protein Interactions. 2001 , 87-108	
701	Peach-Grape system-a high performance simulator for biomolecules. 2002 , 2, 102-118	
700	New Structure Deformation Algorithm for Monte Carlo Simulation of Protein Folding 2002 , 1, 9-22	1
699	Molecular Dynamics Simulations: A Tool for Drug Design. 2002 , 181-209	
698	Mathematics and Molecular Neurobiology. 2002 , 31-60	
697	Molecular Dynamics: DNA.	
696	Free Energy Changes in Solution.	
695	Force Fields: A General Discussion.	
694	Nucleic Acid Force Fields.	
693	Free Energy Calculations: Methods and Applications.	
692	Charge Distribution Calculations: Alternative Approaches.	
691	Protein Force Fields.	1
690	Nucleic Acid Conformation and Flexibility: Modeling Using Molecular Mechanics.	

689	Conformational Analysis: 1.
688	Protein Nucleic Acid Interactions.
687	Quantum Mechanical/Molecular Mechanical (QM/MM) Coupled Potentials.
686	Monte Carlo Simulations for Liquids.
685	DNA Bases and Base Pairs: Ab Initio Calculations.
684	Structural studies on metallobleomycins: The interaction of Pt(II) and Pd(II) with bleomycin. 2003 , 68, 339-348
683	Development of Multifunctional Object-Oriented Program Library for Molecular Simulation and Structure Analysis 2003 , 2, 7-16
682	Drug-Target Binding Forces: Advances in Force Field Approaches. 2003 , 169-185
681	Protonation States of Methionine Aminopeptidase Studied by QM/MM Car-Parrinello Molecular Dynamics Simulations. 2003 , 393-402
680	Structure, Energetics, and Spectroscopy of Models for Enzyme Cofactors. 2003 , 163-175
679	MPI/OpenMP hybrid parallel molecular dynamics simulation of a protein structure on SMP cluster architecture. 2003 , 1826-1828
678	Studies of the Monodipole-macrodipole Interactions within Helices Using the Point-charge Systems for Alanine. 2003 , 24, 824-828
677	Hybrid Quantum Mechanical/Molecular Mechanical Methods. 2003,
676	Accuracy and Applicability of Quantum Chemical Methods in Computational Medicinal Chemistry. 2003 ,
675	Solvent Simulation. 2003,
674	Molecular Mechanics and Comparison of Force Fields. 2003,
673	Stable Structure for the Complex of Catabolite Activator Protein and Cyclic AMP: Molecular Mechanics Optimization by AMBER. 2004 , 5, 19-25
672	Charge Transfer through Single and Double-strand DNAs : Theoretical Analysis Based on Molecular Orbital Calculations. 2004 , 5, 52-61

(2008-2004)

671	Canonical Sampling Method for Initial Conditions for Reactive Flux Calculations Using Nose-Hoover Chains. 2004 , 25, 533-538
670	DNA-Protein Interactions. 2004 , 241-278
669	Empirical Potential Energy Function.
668	Conformational Energy. 2004 ,
667	Conformational Energy.
666	Empirical Potential Energy Function. 2004,
665	AMBER.
664	Specific Interaction between Catabolite Activator Protein and Cyclic AMP: Molecular Mechanics and Molecular Orbital Calculations. 2005 , 6, 67-82
663	Structural Aspects of Polycyclic Aromatic Carcinogen-Damaged DNA and Its Recognition by NER Proteins. 2005 ,
662	Enzymatic Binding Isotope Effects and the Interaction of Glucose with Hexokinase. 2005 , 1019-1053
661	Structures and Electronic Properties of Calcium Binding Proteins with EF-hand Motif :Semiempirical Molecular Orbital Calculations. 2006 , 7, 78-86
660	Quantum-Chemical Investigations of 5-Bromo-2'-Deoxyuridine Derivatives with Antiviral Activity. 2006 , 71, 691-697
659	Density Functional Studies on ATP, ADP, AMP, GTP and Their Mg2+ Complexes in Solvated States. 2006 , 7, 178-189
658	Density Functional Molecular Orbital Calculations on Longer DNA D NA and PNA D NA Double Strands. 2007 , 299-303
657	Molecular Mechanics and Molecular Orbital Simulations on Specific Interactions between Peroxisome Proliferator-Activated Receptor PPAR and Plasticizers. 2007 , 8, 1-11
656	Theoretical Analysis and Prediction of Catalysts for Oxidative Decarboxylation of Melanin-Concentrating Hormone. 2007 , 28, 1151-1155
655	Models of Molecular Structure: Hybrid Perspective. 2008 , 95-204
654	Combined QM/MM methods for the simulation of condensed phase processes using an approximate DFT approach. 2008 , 381-405

653	Density Functional Theory and Car-Parrinello Molecular Dynamics Methods. 2008, 487-499	
652	DFS Based Partial Pathways in GA for Protein Structure Prediction. 2008, 41-53	2
651	Multiscale Modeling and Simulation for Fluid Mechanics at the Nanoscale. 2008, 229-290	
650	Protein Interactions. 87-108	
649	Molecular Mechanics. 920-946	
648	Coarse-Grained Modeling of the HIVII Protease Binding Mechanisms: I. Targeting Structural Flexibility of the Protease Flaps and Implications for Drug Design. 2009 , 1-12	
647	The EDML Format to Exchange Energy Profiles of Protein Molecular Structures. 2009, 146-157	2
646	Neural Network Pairwise Interaction Fields for Protein Model Quality Assessment. 2009 , 235-248	
645	Fragment MO Calculations on Specific Interactions between AhR and TCDD for Beluga and Tern. 2009 , 10, 63-75	
644	Molecular Modelling. 2009 , 225-237	
643	Chapter 10:Computational Simulations of Tunnelling Reactions in Enzymes. 2009 , 219-241	
642	Protein Comparison by the Alignment of Fuzzy Energy Signatures. 2009 , 289-296	
	- rocein companion by the rangimient of rocky line gy organical est 2005 , 200 200	2
641	Simulation Study of the Molecular Mechanism of Intercalation of the Anti-Cancer Drug Daunomycin into DNA. 2009 , 165-180	2
641	Simulation Study of the Molecular Mechanism of Intercalation of the Anti-Cancer Drug Daunomycin	1
ŕ	Simulation Study of the Molecular Mechanism of Intercalation of the Anti-Cancer Drug Daunomycin into DNA. 2009 , 165-180	
640	Simulation Study of the Molecular Mechanism of Intercalation of the Anti-Cancer Drug Daunomycin into DNA. 2009 , 165-180 Agent-Supported Protein Structure Similarity Searching. 2009 , 49-61	
640	Simulation Study of the Molecular Mechanism of Intercalation of the Anti-Cancer Drug Daunomycin into DNA. 2009, 165-180 Agent-Supported Protein Structure Similarity Searching. 2009, 49-61 Predictive Modeling. 2009, 247-289	

(2013-2010)

635	Catalysis. 2010 , 331-353	
634	10.1007/s11497-008-2011-9. 2010 , 5, 131	
633	Theoretical Studies of Polymerisation Reactions. 2010 , 157-186	
632	Derivation of Peptide and Protein Structure using NMR Spectroscopy. 2010 , 14-49	
631	Bioinformatics. 2010 , 151-157	
630	Homology Modeling of 5-HT2C Receptors. 2011 , 97-127	
629	Carbon-Nanotube-Based Composites and Damage Sensing. 2010 , 159-281	2
628	Introduction to Molecular Dynamics Simulation. 2011 , 161-197	O
627	Accelerated molecular dynamics simulation using multi-core CPU and GPU. 2011, 31, 843-847	
626	Recent Advances inDe NovoProtein Design. 207-232	
625	Kinematics Study of Protein Chains and Protein Motion Simulation. 2012, 85-99	
624	Protein Folding Pathways Implementing Dihedral Angle Variable Speed. 2012 , 277-284	
623	A Computational Perspective on the Photochemistry of Photosensory Proteins: Phytochromes and Anabaena Sensory Rhodopsin. 2012 , 169-194	
622	Toward ab initio refinement of protein X-ray crystal structures: interpreting and correlating structural fluctuations. 2012 , 21-36	
621	Molecular Modeling and Conformational Analysis of MuSK Protein. 2012 , 642-650	
620	References. 575-608	
619	Conformational Analysis. 2012 , 91-124	
618	Statistical Mechanical Theory of Protein Folding in Water Environment. 2013 , 493-508	

617	Calculating Energies and Forces. 91-103
616	RBF-POD reduced-order modeling of DNA molecules under stretching and bending. 2013 , 6, 395-409
615	Strictly Localised Molecular Orbitals in QM/MM Methods. 2014 , 71-89
614	Computational Evaluation of Protein Energy Functions. 2014 , 288-299
613	Formal Model of 3D Protein Structures for Functional Genomics, Comparative Bioinformatics, and Molecular Modeling. 2014 , 1-23
612	Graphical Interfaces and Virtual Reality for Molecular Sciences. 2014,
611	Quantum Chemical Approaches in Modeling the Structure of DNA Quadruplexes and Their Interaction with Metal Ions and Small Molecules. 2014 , 181-206
610	DNA Counterion Distributions: Molecular Simulations. 2014 , 1193-1204
609	Metal Cations in Biological Systems: Modeling Metal Ions in Ionophores and DNA. 1997 , 161-166
608	Typische Modelle und Programme. 1997 , 85-206
607	Quantum Mechanical Modeling of Active Sites in Metalloproteins. Electrostatic Coupling to the Protein/Solvent Environment. 1997 , 279-306
606	Molecular Dynamics Calculations on Metalloproteins. 1997 , 191-216
605	The Interplay Between Quantum Chemistry and Molecular Dynamics Simulations. 1997 , 195-223
604	Autonomous Folding and Three-Dimensional Structure of the Carboxy-Terminal Domain of the Mouse Prion Protein, PrP(121 1 31). 1998 , 203-216
603	Molecular Dynamics Simulation of the Excited-State Dynamics of Bacteriorhodopsin. 1998, 1771-1774
602	Recursive, object-oriented structures for molecular modeling. 1998 , 18, 2-8
601	Modelling DNA Stretching for Physics and Biology. 1999 , 115-131
600	Molecular Modeling of Polymers. 1999 , 90-97

599	A New Automated Method for Modeling Non-Covalent Macro-Molecular Interactions. 1999 , 205-223	
598	Computer modeling of protein, nucleic acid, and drug structures. 1999 , 475-505	
597	Effects of force fields for refining protein NMR structures with atomistic force fields and generalized-Born implicit solvent model. 2014 , 18, 24-29	1
596	Proteins: Ssp DnaE Intein. 2015 , 3-12	
595	Research and implementation of Hybrid Parallel Computing for force field calculation. 2015, 21-24	
594	Side Chain Kinematics Simulation on Protein Conformational Changes. 2015 , 121-132	
593	Molecular Dynamics Simulation: From Ab Initiolto Coarse Grained (2015, 1-61	
592	Computational Techniques. 2015 , 19-77	
591	Virtual fragment preparation for computational fragment-based drug design. 2015, 1289, 31-41	
590	MODELAGEM MOLECULAR APLICADA A NANOBIOSSISTEMAS. 2015 , 219-267	
589	On the Mechanical Properties of Functionalized CNT Reinforced Polymer. 2015 , 610-627	
588	Long Timescale Molecular Simulations for Understanding Ion Channel Function. 411-441	
587	Current Trends in Docking Methodologies. 2016 , 320-338	1
586	Protein Structure Prediction using Homology Modeling. 2016 , 339-359	2
585	Using Information about DNA Structure and Dynamics from Experiment and Simulation to Give Insight into Genome-Wide Association Studies. 2016 , 83-98	
584	Protein-Ligand Docking Methodologies and Its Application in Drug Discovery. 2016 , 196-219	
583	Comparative Molecular Mechanics and Quantum Mechanics Study of Monohydration of Nucleic Acid Bases. 2016 , 07, 49-59	
582	Role of Molecular Docking in Computer-Aided Drug Design and Development. 2016 , 1-28	1

Metal Interactions with Nucleobases, Base Pairs, and Oligomer Sequences; Computational 581 Approach. 2016, 1-48 Isolation and Computational Characterization of Glutathione Peroxidase Gene from an Aquatic 580 Fern - Salvinia molesta . 51, 58-62 Explicit Inclusion of Induced Polarization in Atomistic Force Fields Based on the Classical Drude 579 Oscillator Model. 2016, 191-232 - Molecular Thermodynamic Modeling of Fluctuation Solution Theory Properties. 2016, 252-283 578 FF12MC: A revised AMBER forcefield and new protein simulation protocol. 577 Comparison of Empirical Force Fields for Bacteriochlorophyll: an Influence on Hydration and 576 Long-Time Dynamics of Bacterial Photoreaction Centers. 2016, 61, 886-892 Small Oscillations. 2017, 155-187 575 Protein Structure Prediction Using Homology Modeling. 2017, 877-897 574 Molecular Dynamics Simulation of Membrane Free Energy Profiles Using Accurate Force Field for 573 Ionic Liquids. 2017, 265-284 Role of Molecular Docking in Computer-Aided Drug Design and Development. 2017, 683-710 572 Current Trends in Docking Methodologies. 2017, 829-847 571 O General Introduction. 2017, 1-41 570 Salt-bridge Networks within Globular and Disordered Proteins Characterizing Trends for 569 Designable Interactions. Mechanical Properties and Eigenfrequencies of Graphene Sheets. 2017, 21, 26-32 568 567 Shape and Structural Design Optimization of Graphene Sheets in Natural Vibration Problem. 2018, 1719-1725 566 Cloud Services for Efficient Ab Initio Predictions of 3D Protein Structures. 2018, 103-134 Determination of the total energy of a many-particle system. 2018, 28-37 565 Formal Model of 3D Protein Structures for Functional Genomics, Comparative Bioinformatics, and 564 Molecular Modeling. 2018, 3-27

563	Chapter 11:Molecular Modelling Approaches for Assessing Quadruplex Small Molecule Interactions. 2018 , 265-297	
562	Fast and Flexible GPU Accelerated Binding Free Energy Calculations within the AMBER Molecular Dynamics Package.	
561	Protein NMR Structure Refinement Based on Bayesian Inference for Dynamical Ordering of Biomacromolecules. 2018 , 17, 65-75	
560	Buckling Analysis of Hetero-Junction Carbon Nanotubes. 2018 , 68, 9-16	3
559	Molecular Dynamics. 301-319	
558	PLUG (Pruning of Local Unrealistic Geometries) removes restrictions on biophysical modeling for protein design.	
557	A new lipid force field (FUJI).	
556	Simulations of the Folding of Proteins: A Historical Perspective. 2019 , 3-24	
555	Optimizations of Protein Force Fields. 2019 , 203-256	
554	Computer Modelling of the Lipid Matrix of Biomembranes. 2019 , 331-370	1
553	Introduction. 2019 , 1-17	
552	Multi-Agent Systems in Three-Dimensional Protein Structure Prediction. 2019 , 1031-1068	
551	Molecular Modeling and Drug Design Techniques in Microbial Drug Discovery. 2019 , 185-231	
550	Surface-active substance monolayer stability after its formation. 2019,	
549	Induction of Rare Conformation of Oligosaccharide by Binding to Calcium-dependent Bacterial Lectin: X-ray Crystallography and Modelling Study.	
548	In vivo optical clearing of human skin under the effect of aqueous solutions of some monosaccharides. 2019 ,	
547	Adaptive landscape flattening allows the design of both enzyme:substrate binding and catalytic power.	1
546	A physics-based energy function allows the computational redesign of a PDZ domain.	1

545	Protein structure featurization via standard image classification neural networks.	
544	Local Algorithms for Minimizing the Force Field for 3D Representation of Macromolecules. 2019 , 59, 1994-2008	
543	A solvation induced ring puckering effect in fluorinated prolines and its inclusion in classical force-fields.	
542	Molecular Dynamics. 1-18	
541	Primitive RNA-catalysis with guanine-rich oligonucleotide sequences Ithe case of a (GGC)3 nonamer.	
540	A Deep Dive into DNA Base Pairing Interactions Under Water.	
539	Diffusive dynamics of AspartateEdecarboxylase (ADC) liganded with D-serine in aqueous solution.	
538	Base Pairing and Functional Insights intoN3-methylcytidine (m3C) in RNA.	1
537	Organic nanoelectronics inside us: charge transport and localization in RNA could orchestrate ribosome operation.	
536	Ligand-induced unfolding mechanism of an RNA G-quadruplex.	
535	In-silico Pharmacokinetic and Affinity Studies of Piperazine/Morpholine Substituted Quinolines in complex with GAK as promising anti-HCV agent.	О
534	Molecular analysis of out-plane displacement effect on temperature dependent properties of carbon nanotubes. 2021 , 1250, 131835	
533	Tumuc1: A New Accurate DNA Force Field Consistent with High-Level Quantum Chemistry. 2021 , 17, 7096-7105	4
532	Docking and scoring for nucleic acid-ligand interactions: Principles and current status. 2021 ,	3
531	Enabling Magnesium Anodes by Tuning the Electrode/Electrolyte Interfacial Structure. 2021,	3
530	Development and Testing of Force Field Parameters for Phenylalanine and Tyrosine Derivatives. 2020 , 7, 608931	O
529	Structural basis of the protochromic green/red photocycle of the chromatic acclimation sensor RcaE.	
528	Absolute chemical potentials for complex molecules in fluid phases: A centroid reference for predicting phase equilibria. 2020 , 153, 214504	O

527	Molecular dynamics simulation of evaporation of R32 on the solid surface. 2021 , 35, 2150133	O
526	Interactive regulation between aliphatic hydroxylation and aromatic hydroxylation of thaxtomin D in TxtC: a theoretical investigation.	
525	Characterization of the Clathrate Hydrate Formed with Fluoromethane and Pinacolone: The Thermodynamic Stability and Volumetric Behavior of the Structure H Binary Hydrate. 2021 , 125, 328-337	1
524	Methods for studying nucleic acid structure. 2022 , 1-28	
523	Molecular structure and transport of ionic liquid confined in asymmetric graphene-coated silica nanochannel. 2022 , 345, 117869	7
522	Stability of Two-quartet G-quadruplexes and Their Dimers in Atomistic Simulations.	1
521	Developing Kinase Inhibitors Using Computer-Aided Drug Design Approaches. 2020 , 81-108	
520	Plasma and Plasmatell Interaction Simulations. 2020 , 169-208	
519	CHAPTER 3:Computational Methods for the Discovery of Chemical Probes. 2020 , 39-68	
518	Molecular Mechanics. 2020, 281-312	
517	Current Problems in Computer Simulation of Variability of Three-Dimensional Structure of DNA. 2020 , 233-253	
516	Improved Parameterization of Protein ${f D}$ NA Interactions for Molecular Dynamics Simulations of PCNA Diffusion on DNA.	
515	Structure-guided DNA-DNA attraction mediated by divalent cations.	
514	Short-Range Imbalances in the AMBER Lennard-Jones Potential for (Deoxy)Ribose III Nucleobase Lone-Pair IIII Contacts in Nucleic Acids. 2021 , 61, 5644-5657	2
513	The Ad-MD method to calculate NMR shift including effects due to conformational dynamics: The P NMR shift in DNA. 2022 , 43, 132-143	O
512	Thermal transport in organic semiconductors. 2021 , 130, 170902	5
512	Thermal transport in organic semiconductors. 2021, 130, 170902 The Young's modulus of triangle-like three-dimensional graphene under uniaxial tension: Finite element method and theoretical model. 2021, 161, 110473	5 0

509	UNCG RNA tetraloop as a formidable force-field challenge for MD simulations.	O
508	In silico structural homology modelling of EST073 motif coding protein of tea Camellia sinensis (L). 2020 , 18, 32	1
507	Proteus software for physics-based protein design.	1
506	Molecular dynamics simulation of epidermal growth factors in aqueous solution. 2002 , 412-413	
505	Solution structure of 毗onotoxin MI determined by 1H-NMR spectroscopy and molecular dynamics simulation with the explicit solvent water. 1999 , 282-283	
504	Clues from Three-Dimensional Structure Analysis and Molecular Modelling. 2006, 30-38	
503	PoissonNernstPlanck Theory of Ion Permeation Through Biological Channels. 2007, 449-484	2
502	A Mesoscopic Microscopic Perspective on Ion Channel Permeation Energetics: The Semi-Microscopic Approach1. 2007 , 485-505	
501	A Novel Definition of the Local and Instantaneous Liquid-Vapor Interface. 2006 , 131-140	1
500	On Using Energy Signatures in Protein Structure Similarity Searching. 2008 , 939-950	4
499	Comparison of the Incorporation of Watson-Crick Complementary and Mismatched Nucleotides Catalyzed by DNA Polymerase I. 2008 , 187-199	
498	Molecular Mechanics. 2008, 205-227	
498 497	Molecular Mechanics. 2008, 205-227 Parameterization of a Dioxygen Binding Metal Site Using the MCPB.py Program. 2021, 2199, 257-275	
		2
497	Parameterization of a Dioxygen Binding Metal Site Using the MCPB.py Program. 2021 , 2199, 257-275 On the Automatic Construction of QM/MM Models for Biological Photoreceptors: Rhodopsins as	2 O
497 496	Parameterization of a Dioxygen Binding Metal Site Using the MCPB.py Program. 2021, 2199, 257-275 On the Automatic Construction of QM/MM Models for Biological Photoreceptors: Rhodopsins as Model Systems. 2021, 1-75 Photo-Active Biological Molecular Materials: From Photoinduced Dynamics to Transient Electronic	
497 496 495	Parameterization of a Dioxygen Binding Metal Site Using the MCPB.py Program. 2021, 2199, 257-275 On the Automatic Construction of QM/MM Models for Biological Photoreceptors: Rhodopsins as Model Systems. 2021, 1-75 Photo-Active Biological Molecular Materials: From Photoinduced Dynamics to Transient Electronic Spectroscopies. 2021, 77-142 Pro-drug peptide and its metabolites disrupt amyloid fibrils by destabilizing salt bridge interaction	

 $491\,$ $\,$ On The Effect of Methylation on DNA Structure and Dynamics.

,,		
490	Computational NMR Study of Ion Pairing of 1-Decyl-3-methyl-imidazolium Chloride in Molecular Solvents. 2020 , 124, 10776-10786	3
489	Sequence-dependent twist-bend coupling in DNA minicircles. 2021,	1
488	Multidimensional redox potential/p coupling in multicopper oxidases from molecular dynamics: implications for the proton transfer mechanism. 2021 ,	
487	Structural and functional analysis of protein. 2022 , 189-206	
486	Discussion on molecular dynamics (MD) simulations of the asphalt materials. 2021 , 299, 102565	7
485	Molecular dynamics simulations of A-DNA in bivalent metal ions salt solution.	O
484	Structure and Function of the Refined C-Terminal Loop in Imidazole Glycerol Phosphate Dehydratase from Different Homologs. 2021 , 69, 13871-13880	
483	A Coupled Morillanaka model and FEM RVE approach for the geometrical nonlinear dynamic response of the FG-CNTRC plate based on a novel shear strain function using isogeometric finite element procedure. 2021 , 114947	1
482	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	O
481	Accurate modeling of RNA hairpins through the explicit treatment of electronic polarizability with the classical Drude oscillator force field.	2
480	Interaction Analysis on the SARS-CoV-2 Spike Protein Receptor Binding Domain Using Visualization of the Interfacial Electrostatic Complementarity. 2021 , 12, 11267-11272	4
479	Atomistic Simulations of Thermal Unfolding. 2022, 2376, 331-341	1
478	Amphiphilic small molecular mates match hydrophobic drugs to form nanoassemblies based on drug-mate strategy 2022 , 17, 129-138	O
477	Elucidating important structural features for the binding affinity of spike - SARS-CoV-2 neutralizing antibody complexes. 2021 ,	8
476	Advanced descriptors for long-range noncovalent interactions between SARS-CoV-2 spikes and polymer surfaces. 2021 , 120125	1
475	Combinatorial screening of ionic liquid extractant for removal of methanol from methylal. 2021 , 117317	3
474	Molecular Methods for Assessing the Morphology, Topology, and Performance of Polyamide Membranes 2022 , 644, 120110-120110	O

473	Discovery of SARS-CoV-2 Nsp14 and Nsp16 Methyltransferase Inhibitors by High-Throughput Virtual Screening 2021 , 14,	2
472	Mutational signatures in GATA3 transcription factor and its DNA binding domain that stimulate breast cancer and HDR syndrome. 2021 , 11, 22762	
471	Membrane Fouling: Microscopic Insights into the Effects of Surface Chemistry and Roughness. 2100395	1
470	Early steps of oxidative damage in DNA quadruplexes are position-dependent: Quantum mechanical and molecular dynamics analysis of human telomeric sequence containing ionized guanine. 2021 , 194, 882-882	1
469	The Crystal Structure of Cysteamine Dioxygenase Reveals the Origin of the Large Substrate Scope of This Vital Mammalian Enzyme. 2021 , 60, 3728-3737	2
468	Structure and Undulations of Escin Adsorption Layer at Water Surface Studied by Molecular Dynamics. 2021 , 26,	O
467	Modeling galvanostatic chargedischarge of nanoporous supercapacitors. 2021, 1, 725-731	7
466	Learning neural network potentials from experimental data via Differentiable Trajectory Reweighting. 2021 , 12, 6884	4
465	Computational Study of the Structure and Transport in Pyrrolidinium-Li-TFSI-Silica Ionogels. 2021 , 125, 13003-13014	O
464	Structure and Capacitance of Electrical Double Layers in Tricationic Ionic Liquids with Organic Solvents. 2021 , 125, 12753-12762	O
463	Reaction-Controlled Phase-Transfer Process of Polyoxometalate-Based Catalyst for Cellulose Esterification: A Molecular Dynamics Study. 2021 , 125, 25478-25487	O
462	Parallel-slipped Helectron-donor-acceptor in adsorption process: Molecular dynamics simulation. 2021 , 111, 108100	
461	The role of hydrogen bond in catalytic triad of serine proteases.	
460	Molecular Dynamics Study of Fluid- Fluid and Solid- Fluid Interactions in Mixed-Wet Shale Pores.	
459	Exploring structural dynamics and optical properties of UnaG fluorescent protein upon N57 mutations 2022 ,	
458	Molecule in Soft-Crystal at Ground and Excited States: Theoretical Approach. 2022 , 51, 100482	1
457	Characterizing protein protonation microstates using Monte Carlo sampling.	
456	Recent progress in general force fields of small molecules 2021 , 72, 187-193	Ο

455	Nanomodified Cement-Based Materials: Review (2015\(\bar{\textsf{0}} 020 \)) of Molecular Dynamics Studies. 2022 , 34,	1
454	Computational risk assessment framework for the hazard analysis of bisphenols and quinone metabolites 2021 , 426, 128031	О
453	Molecular dynamics simulations of the flexibility and inhibition of SARS-CoV-2 NSP 13 helicase 2022 , 112, 108122	
452	Force-Field Simulations of a Hydrated Lanreotide-Based Derivative: Hydration, Dynamics, and Numerical Evidence of Self-Assembly in Dimers. 2020 , 5, 25423-25431	
451	Dynamical Methods to Study Interaction in Proteins Facilitating Molecular Understanding of Cancer. 2021 , 1-17	0
450	Conformational Particularities of the Tachykinin-Like Decapeptide Sialokinin I. 2021 , 66, 746-752	
449	Inosine and its methyl derivatives: Occurrence, biogenesis, and function in RNA 2022,	0
448	RNA-Specific Force Field Optimization with CMAP and Reweighting 2022, 62, 372-385	2
447	Dynamical Methods to Study Interaction in Proteins Facilitating Molecular Understanding of Cancer. 2022 , 2231-2247	
446	Computational Investigations of the Reactivity of Metalloporphyrins for Ammonia Oxidation. 2022 , 65, 341-353	1
445	Geometric Analysis of Shapes in Ion Mobility-Mass Spectrometry 2022,	1
444	Investigation of Charge-State-Dependent Compaction of Protein Ions with Native Ion Mobility-Mass Spectrometry and Theory 2022 ,	5
443	Integral equation models for solvent in macromolecular crystals 2022, 156, 014801	1
442	Artificial Intelligence Resolves Kinetic Pathways of Magnesium Binding to RNA 2022,	2
441	Raman Spectroscopy of an Atypical C15-, Bilin Chromophore in Cyanobacteriochrome RcaE 2022,	
440	Atomistic Simulations of Functionalized Nano-Materials for Biosensors Applications 2022 , 23,	1
439	State-of-the-art of computational green chemistry in leading universities in Russia. 2022, 55-77	
438	Synthesis and evaluation of potent yaku'amide A analogs 2022 , 13, 1899-1905	O

437	Continuous B- to A-Transition in Protein-DNA Binding - How Well Is It Described by Current AMBER Force Fields?.	
436	A New Series of Aryloxyacetic Acids Endowed with Multi-Target Activity towards Peroxisome Proliferator-Activated Receptors (PPARs), Fatty Acid Amide Hydrolase (FAAH), and Acetylcholinesterase (AChE) 2022 , 27,	2
435	Extended ensemble simulations of a SARS-CoV-2 nsp1-5'-UTR complex 2022 , 18, e1009804	1
434	Nuclear Magnetic Resonance reveals a two hairpin equilibrium near the 3'-splice site of Influenza A segment 7 mRNA that can be shifted by oligonucleotides 2022 ,	O
433	Emission Quenching in Tetraphenylfuran Crystal: Why This Propeller-Shaped Molecule Does Not Emit in the Condensed Phase 2022 , 27,	1
432	Mechanistic Insights into the Ligand-Induced Unfolding of an RNA G-Quadruplex <i>Journal of the American Chemical Society</i> , 2022 ,	6.4 2
431	Dynamics of a DNA minicircle: Poloidal rotation and in-plane circular vibration.	O
430	Modeling the MreB-CbtA Interaction to Facilitate the Prediction and Design of Candidate Antibacterial Peptides 2021 , 8, 814935	
429	Capturing non-local through-bond effects in molecular mechanics force fields: II. Using fractional bond orders to fit torsion parameters.	1
428	The structural pathway from its solvated molecular state to the solution crystallisation of the \Box and \Box polymorphic forms of amino benzoic acid 2022 ,	1
427	Ionophobicity of carbon sub-nanometer pores enables efficient desalination at high salinity. 2022 , 3, 100689	2
426	Comparing Antibody Interfaces to Inform Rational Design of New Antibody Formats 2022 , 9, 812750	О
425	Energetics and -coupling constants for Ala, Gly, and Val peptides demonstrated using ABEEM polarizable force field and an aqueous solution 2022 ,	
424	Oxidation Enhances Binding of Extrahelical 5-Methyl-Cytosines by Thymine DNA Glycosylase 2022 ,	
423	Spontaneous Local Membrane Curvature Induced by Transmembrane Proteins 2022,	1
422	Reliable Prediction of the Protein-Ligand Binding Affinity Using a Charge Penetration Corrected AMOEBA Force Field: A Case Study of Drug Resistance Mutations in Abl Kinase 2022 ,	1
421	Density, excess volume, thermal expansion coefficient and intermolecular hydrogen bonding of binary mixtures of morpholine '+ 'isobutanol: A combined experimental and computational study. 2022 , 348, 118417	
420	Oxygen Ion Implantation Improving Cell Adhesion on Titanium Surfaces through Increased Attraction of Fibronectin PHSRN Domain 2022 , e2101983	1

419	Structural Characterization of a New Collagen Biomimetic Octapeptide with Nanoscale Self-Assembly Potential: Experimental and Theoretical Approaches 2022 , 87, e202100462	2
418	Effective and efficient transport mechanism of CO2 in subnano-porous crystalline membrane of syndiotactic polystyrene. 2022 , 646, 120202	Ο
417	Regulating structure and flow of ionic liquid confined in nanochannel using water and electric field. 2022 , 351, 118612	2
416	Ether tails make a large difference for the structural dynamics of imidazolium-based ionic liquids. 2022 , 2, 100012	O
415	Stabilization and fluorescence light-up of G-quadruplex nucleic acids using indolyl-quinolinium based probes 2022 ,	2
414	Potential energy functions. 2022 , 41-65	
413	Demystifying DPP III Catalyzed Peptide Hydrolysis-Computational Study of the Complete Catalytic Cycle of Human DPP III Catalyzed Tynorphin Hydrolysis 2022 , 23,	2
412	Physical Chemistry of a Single tRNA-Modified Nucleoside Regulates Decoding of the Synonymous Lysine Wobble Codon and Affects Type 2 Diabetes 2022 ,	O
411	Simultaneous parametrization of torsional and third-neighbor interaction terms in force-field development: The LLS-SC algorithm 2022 ,	0
410	Theoretical Modeling of Redox Potentials of Biomolecules 2022 , 27,	2
410	Theoretical Modeling of Redox Potentials of Biomolecules 2022, 27, Property Map Collective Variable as a Useful Tool for a Force Field Correction 2022,	1
409	Property Map Collective Variable as a Useful Tool for a Force Field Correction 2022 , Magnolol and Luteolin Inhibition of Educosidase Activity: Kinetics and Type of Interaction	1
409	Property Map Collective Variable as a Useful Tool for a Force Field Correction 2022, Magnolol and Luteolin Inhibition of EGlucosidase Activity: Kinetics and Type of Interaction Detected by In Vitro and In Silico Studies 2022, 15, Nucleoside Analogues with a Seven-Membered Sugar Ring: Synthesis and Structural Compatibility	1
409 408 407	Property Map Collective Variable as a Useful Tool for a Force Field Correction 2022, Magnolol and Luteolin Inhibition of EGlucosidase Activity: Kinetics and Type of Interaction Detected by In Vitro and In Silico Studies 2022, 15, Nucleoside Analogues with a Seven-Membered Sugar Ring: Synthesis and Structural Compatibility in DNA-RNA Hybrids 2022,	1 2
409 408 407 406	Property Map Collective Variable as a Useful Tool for a Force Field Correction 2022, Magnolol and Luteolin Inhibition of EGlucosidase Activity: Kinetics and Type of Interaction Detected by In Vitro and In Silico Studies 2022, 15, Nucleoside Analogues with a Seven-Membered Sugar Ring: Synthesis and Structural Compatibility in DNA-RNA Hybrids 2022, Extended Strands Contribute to Reversible Amyloid Formation 2022, Structural dynamics of the cooperative binding of small inhibitors in human cytochrome P450 2C9	1 1 2 2
409 408 407 406 405	Property Map Collective Variable as a Useful Tool for a Force Field Correction 2022, Magnolol and Luteolin Inhibition of EGlucosidase Activity: Kinetics and Type of Interaction Detected by In Vitro and In Silico Studies 2022, 15, Nucleoside Analogues with a Seven-Membered Sugar Ring: Synthesis and Structural Compatibility in DNA-RNA Hybrids 2022, Extended Estrands Contribute to Reversible Amyloid Formation 2022, Structural dynamics of the cooperative binding of small inhibitors in human cytochrome P450 2C9 2022, 113, 108151	1 1 2 2

401	A combined crystallography and DFT study on ring-shaped Cucurbit[]urils: structures, surface character, and host-guest recognition 2022 , 12, 10014-10019	1
400	On the effects of induced polarizability at the water-graphene interface classical charge-on-spring models 2022 ,	1
399	Molecular Dynamics Studies of the Physicochemical Properties and Structure of the 1 M LiClO4 Solution in Sulfolane. 2022 , 96, 115-124	1
398	Can the Jigsaw Puzzle Model of Protein Folding Re-assemble a Hydrophobic Core?. 2022,	O
397	Sparse Gaussian Process Regression-Based Machine Learned First-Principles Force-Fields for Saturated, Olefinic, and Aromatic Hydrocarbons.	2
396	Theoretical Calculations and Experiments on the Thermal Properties of Fluorinated Graphene and Its Effects on the Thermal Decomposition of Nitrate Esters 2022 , 12,	1
395	рршрршш2 022, 56, 37	1
394	Free-Energy Profile Analysis of the Catalytic Reaction of Glycinamide Ribonucleotide Synthetase 2022 , 12,	1
393	Emerging Methods and Applications to Decrypt Allostery in Proteins and Nucleic Acids 2022, 167518	1
392	QM/MM Energy Decomposition Using the Interacting Quantum Atoms Approach 2022,	1
391	Discovery of 3H-pyrrolo[2,3-c]quinolines with activity against Mycobacterium tuberculosis by allosteric inhibition of the glutamate-5-kinase enzyme 2022 , 232, 114206	O
390	QM/MM Study of the H2 Formation on the Surface of a Water Ice Grain Doped With Formaldehyde: Molecular Dynamics and Reaction Kinetics. 2022 , 9,	O
389	Investigation of Multilayered Structures of Ionic Liquids on Graphite and Platinum Using Atomic Force Microscopy and Molecular Simulations 2022 ,	1
388	Design, Synthesis, Biological Evaluation, and Computational Studies of Novel Ureidopropanamides as Formyl Peptide Receptor 2 (FPR2) Agonists to Target the Resolution of Inflammation in Central Nervous System Disorders 2022 ,	1
387	Simulating Met-Enkephalin With Population Annealing Molecular Dynamics. 2022, 2241, 012006	2
386	Systematic QM Region Construction in QM/MM Calculations Based on Uncertainty Quantification 2022 ,	2
385	The effect of off-center -hole on the atom-centered partial charges in halogenated molecules 2022 ,	
384	Antibody Mutations Favouring pH-dependent Binding in Solid Tumour Microenvironments: Insights from Large-scale Structure-based Calculations 2022 ,	O

383	Integration of Experimental Data and Use of Automated Fitting Methods in Developing Protein Force Fields 2022 , 5,	1
382	Challenges with Simulating Modified RNA: Insights into Role and Reciprocity of Experimental and Computational Approaches 2022 , 13,	O
381	Characterizing Protein Protonation Microstates Using Monte Carlo Sampling 2022,	О
380	How Photoactivation Triggers Protochlorophyllide Reduction: Computational Evidence of a Stepwise Hydride Transfer during Chlorophyll Biosynthesis 2022 , 12, 4141-4148	Ο
379	Structure-based dual affinity optimization of a SARS-CoV-1/2 cross-reactive single-domain antibody 2022 , 17, e0266250	О
378	Multi-center decomposition of molecular densities: A mathematical perspective 2022, 156, 164107	
377	A structural model of the human plasminogen and Aspergillus fumigatus enolase complex 2022,	
376	Vibrational spectroscopy by means of first-principles molecular dynamics simulations.	5
375	Investigation of cholera toxin interaction mechanism for structure-based drug design. 2022, 13,	
374	Simultaneous Detection of Mixed-Gas Components by Ionic-Gel Sensors with Multiple Electrodes 2022 , 7, 716-721	1
373	Review of Molecular Dynamics Simulations of Phosphonium Ionic Liquid Lubricants. 2022 , 70, 1	1
372	Harnessing Deep Learning for Optimization of Lennard-Jones Parameters for the Polarizable Classical Drude Oscillator Force Field 2022 ,	1
371	A Database of Solution Additives Promoting Mg Dehydration and the Onset of MgCO Nucleation 2022 , 22, 3080-3089	Ο
370	Microscopic Simulations of Electrochemical Double-Layer Capacitors 2022,	5
369	Architecture of the Two Metal Binding Sites in Prolactin 2022,	
368	Advanced Theory and Simulation to Guide the Development of CO Capture Solvents 2022 , 7, 12453-12466	
367	Molecular structure based study on the elastic properties of carbon nanotubes in a thermal environment. 2022 , 133013	О
366	The Pfizer Crystal Structure Database: An essential tool for structure-based design at Pfizer 2022,	

365	Pore-Size-Dependent Capacitance and Charging Dynamics of Nanoporous Carbons in Aqueous Electrolytes.	Ο
364	Lattice inversion potential with neural network corrections for metallic systems. 2022 , 207, 111311	
363	The NMR structure of the engineered halophilic DnaE intein for segmental isotopic labeling using conditional protein splicing 2022 , 338, 107195	
362	Are all-atom any better than united-atom force fields for the description of liquid properties of alkanes? 2. A systematic study considering different chain lengths. 2022 , 354, 118829	O
361	Small angle symmetry splitting of helicene-based molecular wires on pyrolytic graphite. 2022 , 193, 171-181	O
3 60	Molecular dynamics study of fluid-fluid and solid-fluid interactions in mixed-wet shale pores. 2022 , 319, 123587	O
359	Computational Design of Peptides with Improved Recognition of the Focal Adhesion Kinase FAT Domain 2022 , 2405, 383-402	
358	Optical Clearing of Biological Tissues with a Number of Disaccharides. 2021 , 129, 763-769	1
357	Knowledge-Based Unfolded State Model for Protein Design 2022 , 2405, 403-424	
356	Role of the Protein Environment in Photoisomerization of Type I and Type II Rhodopsins: a Theoretical Perspective. 2021 , 76, 407-416	
355	Graphene Field Effect Transistors: A Sensitive Platform for Detecting Sarin 2021 , 13, 61751-61757	1
354	Reductive inactivation of the hemiaminal pharmacophore for resistance against tetrahydroisoquinoline antibiotics. 2021 , 12, 7085	1
353	Electron Holes in G-Quadruplexes: The Role of Adenine Ending Groups 2021 , 22,	0
352	Evolutionary conservation of protein dynamics: insights from all-atom molecular dynamics simulations of 'peptidase' domain of Spt16 2021 , 1-13	О
351	A Computational Study of RNA Tetraloop Thermodynamics, Including Misfolded States. 2021 ,	0
350	Conformation and Metal Cation Binding of Zwitterionic Alanine Tripeptide in Saline Solutions by Infrared Vibrational Spectroscopy and Molecular Dynamics Simulations 2021 ,	О
349	Design of a protein-targeted DNA aptamer using atomistic simulation 2021 , 1-9	1
348	An investigation of some H2S thermodynamical properties at the water interface under pressurised conditions through molecular dynamics.	1

347	Structural analysis and potential extraction from diffraction data of disordered systems by least-biased feature matching 2021 , 155, 234501	2
346	Computational study of the pK a values of a modified GIC base pair in duplex DNA. 2022 , 43, 201-209	
345	Evaluation of the binding effect and cytotoxicity assay of 2-Ethyle-5-(4-methylphenyl) pyrimido pyrazol ophthalazine trione on the calf thymus DNA: spectroscopic, calorimetric and molecular dynamics approaches. 2021 ,	10
344	Rational Design of Nonbonded Point Charge Models for Monovalent Ions with Lennard-Jones 12-6 Potential. 2021 ,	2
343	Accessibility of Grafted Functional Groups Limits Reactivity of Covalent Graphene Derivatives.	
342	Ultra-high permeable phenine nanotube membranes for water desalination 2022,	О
341	Atomistic modeling of Li- and post-Li-ion batteries. 2022 , 6,	1
340	Computational Investigation of Bending Properties of RNA AUUCU, CCUG, CAG, and CUG Repeat Expansions Associated With Neuromuscular Disorders 2022 , 9, 830161	O
339	ABEEM Polarizable Force Field. 2022 , 587-601	
338	Refining the RNA Force Field with Small-Angle X-ray Scattering of Helix-Junction-Helix RNA 2022, 3400	0-3408 1
338	Refining the RNA Force Field with Small-Angle X-ray Scattering of Helix-Junction-Helix RNA 2022, 3400 Reorganization free energy of copper proteins in solution, in vacuum, and on metal surfaces 2022, 156, 175101	2
	Reorganization free energy of copper proteins in solution, in vacuum, and on metal surfaces 2022 ,	
337	Reorganization free energy of copper proteins in solution, in vacuum, and on metal surfaces 2022, 156, 175101 Role of Water in Proton-Coupled Electron Transfer between Tyrosine and Cysteine in	2
337	Reorganization free energy of copper proteins in solution, in vacuum, and on metal surfaces 2022, 156, 175101 Role of Water in Proton-Coupled Electron Transfer between Tyrosine and Cysteine in Ribonucleotide Reductase Journal of the American Chemical Society, 2022, Current State and Perspectives of Simulation and Modeling of Aliphatic Isocyanates and	2 16.4 1
337 336 335	Reorganization free energy of copper proteins in solution, in vacuum, and on metal surfaces 2022, 156, 175101 Role of Water in Proton-Coupled Electron Transfer between Tyrosine and Cysteine in Ribonucleotide Reductase <i>Journal of the American Chemical Society</i> , 2022, Current State and Perspectives of Simulation and Modeling of Aliphatic Isocyanates and Polyisocyanates 2022, 14, Structure-based design of novel donepezil-like hybrids for a multi-target approach to the therapy	2 16.4 1
337 336 335 334	Reorganization free energy of copper proteins in solution, in vacuum, and on metal surfaces 2022, 156, 175101 Role of Water in Proton-Coupled Electron Transfer between Tyrosine and Cysteine in Ribonucleotide Reductase <i>Journal of the American Chemical Society</i> , 2022, Current State and Perspectives of Simulation and Modeling of Aliphatic Isocyanates and Polyisocyanates 2022, 14, Structure-based design of novel donepezil-like hybrids for a multi-target approach to the therapy of Alzheimer's disease 2022, 237, 114358 Unraveling the binding mechanism of the active form of Remdesivir to RdRp of SARS-CoV-2 and	2 16.4 1 0
337 336 335 334 333	Reorganization free energy of copper proteins in solution, in vacuum, and on metal surfaces 2022, 156, 175101 Role of Water in Proton-Coupled Electron Transfer between Tyrosine and Cysteine in Ribonucleotide Reductase <i>Journal of the American Chemical Society</i> , 2022, Current State and Perspectives of Simulation and Modeling of Aliphatic Isocyanates and Polyisocyanates 2022, 14, Structure-based design of novel donepezil-like hybrids for a multi-target approach to the therapy of Alzheimer's disease 2022, 237, 114358 Unraveling the binding mechanism of the active form of Remdesivir to RdRp of SARS-CoV-2 and designing new potential analogues: Insights from molecular dynamics simulations 2022, 799, 139638	2 16.4 1 0

Chapter 12. Molecular Modelling and Simulations Applied to Challenging Drug Discovery Targets. 317-348 329 328 Simulations of Protein Aggregation. 2006, 47-77 Atomistic Potentials for Polymers and Organic Materials. 2005, 2561-2573 327 Protein Folding: Detailed Models. 2005, 1837-1848 326 Distance Dependent Protein Force Field via Linear Optimization. 2008, 787-792 325 Data_Sheet_1.pdf. 2020, 324 Data_Sheet_1.DOCX. 2018, 323 Data_Sheet_1.PDF. 2020, 322 Table_1.XLSX. 2020, 321 320 Table_2.XLSX. 2020, Table_3.XLSX. 2020, 319 318 Table_4.XLSX. 2020, Table_5.XLSX. 2020, 317 DataSheet_1.pdf. 2019, 316 Data_Sheet_1.PDF. 2019, 315 Data_Sheet_1.PDF. 2020, 314 Data_Sheet_1.PDF. 2020, 313 DataSheet_1.pdf. 2019, 312

311	Gliding on Ice in Search of Accurate and Cost-Effective Computational Methods for Astrochemistry on Grains: The Puzzling Case of the HCN Isomerization 2022 ,	
310	Binding of polar and hydrophobic molecules at the LiCoO (001)-water interface: force field development and molecular dynamics simulations 2022 ,	
309	Solid with infused reactive liquid (SWIRL): A novel liquid-based separation approach for effective CO capture 2022 , 8, eabm0144	О
308	A Computational Model for the PLP-Dependent Enzyme Methionine -Lyase 2022 , 9, 886358	
307	CENT2: Improved charge equilibration via neural network technique. 2022 , 105,	1
306	Self-Consistent Parameterization of DNA Residues for the Non-Polarizable AMBER Force Fields. 2022 , 12, 666	
305	Effect of the Cations (Na+, Ca2+, Fe2+, and Fe3+) on the Partially Hydrolyzed Polyacrylamide Shrinking by Molecular Dynamics Simulations.	О
304	Comparing the Performances of Force Fields in Conformational Searching of Hydrogen-Bond-Donating Catalysts 2022 ,	
303	DFT studies on the physicochemical properties of a new potential drug carrier containing cellobiose units and its complex with paracetamol.	О
302	Improving Force Field Accuracy by Training against Condensed-Phase Mixture Properties 2022,	O
301	Nearest-Neighbor dsDNA Stability Analysis Using Alchemical Free-Energy Simulations 2022,	
300	Adsorption, Structure, and Dynamics of Short- and Long-Chain PFAS Molecules in Kaolinite: Molecular-Level Insights 2022 ,	4
299	Accelerating the Ensemble Convergence of RNA Hairpin Simulations with a Replica Exchange Structure Reservoir 2022 ,	О
298	Species Surface Distribution and Surface Tension of Aqueous Solutions of MIBC and NaCl Using Molecular Dynamics Simulations. 2022 , 14, 1967	
297	Improving the Accuracy of Atomistic Simulations of the Electrochemical Interface 2022,	3
296	: A Program for Electrostatic Parameterizations of Additive and Induced Dipole Polarizable Force Fields 2022 ,	1
295	Force Field Parameterization of Actinyl Molecular Cations Using the 12-6-4 Model 2022,	O
294	Unveiling the mechanism of the triethyl phosphate hydrolysis reaction in the synthesis of the sol-gel-derived 58S bioactive glass. 2022 , 24, 100929	

293	Influence of Interface in Structure, Stability and Electronic Properties of Dimeric Gold Nanoclusters.	
292	Design and fabrication of biodegradable electrospun nanofibers loaded with biocidal agents. 1-27	2
291	Applying Classical, , and Machine-Learning Molecular Dynamics Simulations to the Liquid Electrolyte for Rechargeable Batteries 2022 ,	9
290	Transferable Classical Force Field for Pure and Mixed Metal Halide Perovskites Parameterized from First-Principles 2022 ,	2
289	FebRNA: an automated fragment-ensemble-based model for building RNA 3D structures.	
288	Diclofenac Ion Hydration: Experimental and Theoretical Search for Anion Pairs. 2022 , 27, 3350	1
287	The effect of ethanol on B-DNA in salt solution through Molecular Dynamics Simulations. 2022,	
286	Structure and Ɗynamics of Ɓio- and Macromolecules. 2022 , 137-199	
285	Wettability of Graphite Under 2d Confinement.	О
284	Combining classical molecular docking with self-consistent charge density-functional tight-binding computations for the efficient and quality prediction of ligand binding structure. 2022 , 46, 174751982217	1019
284		0
· ·	computations for the efficient and quality prediction of ligand binding structure. 2022 , 46, 174751982217 Evaluating the conformational space of the active site of D 2 dopamine receptor. Scope and	
283	computations for the efficient and quality prediction of ligand binding structure. 2022, 46, 174751982217 Evaluating the conformational space of the active site of D 2 dopamine receptor. Scope and limitations of the standard docking methods. The Streptomyces viridochromogenes product template domain represents an evolutionary	O
283	computations for the efficient and quality prediction of ligand binding structure. 2022, 46, 174751982217 Evaluating the conformational space of the active site of D 2 dopamine receptor. Scope and limitations of the standard docking methods. The Streptomyces viridochromogenes product template domain represents an evolutionary intermediate between dehydratase and aldol cyclase of type I polyketide synthases. 2022, 5,	O
283	computations for the efficient and quality prediction of ligand binding structure. 2022, 46, 174751982217 Evaluating the conformational space of the active site of D 2 dopamine receptor. Scope and limitations of the standard docking methods. The Streptomyces viridochromogenes product template domain represents an evolutionary intermediate between dehydratase and aldol cyclase of type I polyketide synthases. 2022, 5, Inhibition of Arenaviridae nucleoprotein exonuclease by bisphosphonate. 2022, 9,	0
283 282 281 280	Evaluating the conformational space of the active site of D 2 dopamine receptor. Scope and limitations of the standard docking methods. The Streptomyces viridochromogenes product template domain represents an evolutionary intermediate between dehydratase and aldol cyclase of type I polyketide synthases. 2022, 5, Inhibition of Arenaviridae nucleoprotein exonuclease by bisphosphonate. 2022, 9, Structural Basis for the Regiospecificity of a Lipase from Streptomyces sp. W007. 2022, 23, 5822 Atomistic-Level Description of the Covalent Inhibition of SARS-CoV-2 Papain-like Protease. 2022,	0
283 282 281 280	Evaluating the conformational space of the active site of D 2 dopamine receptor. Scope and limitations of the standard docking methods. The Streptomyces viridochromogenes product template domain represents an evolutionary intermediate between dehydratase and aldol cyclase of type I polyketide synthases. 2022, 5, Inhibition of Arenaviridae nucleoprotein exonuclease by bisphosphonate. 2022, 9, Structural Basis for the Regiospecificity of a Lipase from Streptomyces sp. W007. 2022, 23, 5822 Atomistic-Level Description of the Covalent Inhibition of SARS-CoV-2 Papain-like Protease. 2022, 23, 5855 Evaluating Geometric Definitions of Stacking for RNA Dinucleoside Monophosphates Using	o o o

275	Molecular Dynamics Simulation of Association Processes in Aqueous Solutions of Maleate Salts of Drug-Like Compounds: The Role of Counterion. 2022 , 23, 6302	1
274	Fast prediction of methane adsorption in shale nanopores using kinetic theory and machine learning algorithm. 2022 , 446, 137221	3
273	Free Energy Methods in Drug Discovery[htroduction. 1-38	3
272	Impacts of targeting different hydration free energy references in the development of ion potentials.	
271	Methodology-Centered Review of Molecular Modeling, Simulation, and Prediction of SARS-CoV-2.	7
270	Gain and loss of TASK3 channel function and its regulation by novel variation cause KCNK9 imprinting syndrome. 2022 , 14,	1
269	A Unified Approach to Derive Atomic Partial Charges and Polarizabilities of Ionic Liquids.	
268	Water network in the binding pocket of fluorinated BPTI-Trypsin complexes - insights from simulation and experiment.	
267	Spontaneously Restoring Specific Bioaffinity of RGD in Linear RGD-containing Peptides by Conjugation with Zwitterionic Dendrimers. 2022 ,	0
266	Phenylpropanoids on the Inhibition of Mamyloid Aggregation and the Movement of These Molecules through the POPC Lipid Bilayer.	1
265	G-quadruplex recognition by DARPIns through epitope/paratope analogy.	
264	Interactions between S100A9 and Alpha-Synuclein: Insight from NMR Spectroscopy. 2022 , 23, 6781	O
263	Computational Prediction and Experimental Validation of the Unique Molecular Mode of Action of Scoulerine. 2022 , 27, 3991	
262	Universal optothermal micro/nanoscale rotors. 2022 , 8,	3
261	Boosting Near-Infrared Photothermal Conversion by Intermolecular Interactions in Isomeric Cocrystals.	1
260	Generalized Born Implicit Solvent Models Do Not Reproduce Secondary Structures of De Novo Designed Glu/Lys Peptides.	2
259	Desalination Potential of Aquaporin-Inspired Functionalization of Carbon Nanotubes: Bridging Between Simulation and Experiment. 2022 , 14, 28174-28185	0
258	Nonpolarizable Force Fields through the Self-Consistent Modeling Scheme with MD and DFT Methods: From Ionic Liquids to Self-Assembled Ionic Liquid Crystals. 2022 , 126, 4611-4622	2

 $_{\rm 257}$ $\,$ Solvent effects on the NMR shieldings of stacked DNA base pairs.

256	Molecular electronic refrigeration against parallel phonon heat leakage channels.	1
255	Identification and Mechanistic Basis of non-ACE2 Blocking Neutralizing Antibodies from COVID-19 Patients with Deep RNA Sequencing and Molecular Dynamics Simulations.	
254	Interplay between the Enamine and Imine Forms of the Hydrolyzed Imipenem in the Active Sites of Metallo-粗actamases and in Water Solution.	1
253	Spatial and Temporal Resolution of the Oxygen-Independent Photoinduced DNA Interstrand Cross-Linking by a Nitroimidazole Derivative. 2022 , 62, 3239-3252	О
252	Accurate and Efficient Estimation of LennardIIones Interactions for Coarse-Grained Particles via a Potential Matching Method.	O
251	The Effects of RNA.DNA-DNA Triple Helices on Nucleosome Structures and Dynamics.	
250	Resolution exchange with tunneling for enhanced sampling of protein landscapes. 2022, 106,	O
249	General Framework for the Study of Dynamical Properties and Arrested States of Ionic Liquids.	
248	Scalable Pillar[5]arene-Integrated Poly(arylate-amide) Molecular Sieve Membranes to Separate Light Gases.	O
247	COVID-19 serum can be cross-reactive and neutralizing against Dengue virus (DV) as observed by DV neutralization test. 2022 ,	1
246	Insight into substrate-assisted catalytic mechanism and stereoselectivity of bifunctional nocardicin thioesterase.	
245	The two-domain elevator-type mechanism of zinc-transporting ZIP proteins. 2022, 8,	1
244	Purification, Biochemical Characterization, and DPP-IV and thmylase inhibitory activity of Berberine from Cardiospermum halicacabum.	O
243	Introducing a New Bond-Forming Activity in an Archaeal DNA Polymerase by Structure-Guided Enzyme Redesign. 2022 , 17, 1924-1936	О
242	Allosteric inhibitors of the main protease of SARS-CoV-2. 2022 , 205, 105381	6
241	Size and displacement combining detection on physics properties of carbon nanotubes using a proposed energy approach. 2022 , 344, 113729	
240	Wettability of graphite under 2D confinement. 2022 , 198, 132-141	O

239	Room-temperature serial synchrotron crystallography of Drosophila cryptochrome. 2022, 78,	Ο
238	Lubrication Behavior of n-hexadecane on ZnO Layer at the Nanoscale: A Molecular Dynamic Exploration. 2022 , 70,	O
237	Use of Solvent Mapping for Characterizing the Binding Site and for Predicting the Inhibition of the Human Ether-EGo-Go-Related K+ Channel.	Ο
236	Cooperative Reaction of Hydrogen-Networked Water Molecules at the SiCH2O2 Solution Interface: Microscopic Insights from Ab Initio Molecular Dynamics.	O
235	Multi-scale modeling of an atomic force microscope tip for the study of frictional properties and oscillation behavior. 095440622211132	
234	Targeting the Major Groove of the Palindromic d(GGCGCC)2 Sequence by Oligopeptide Derivatives of Anthraquinone Intercalators.	1
233	Computational Modeling of Molecular Mechanics for the Experimentally Inclined.	
232	Insight into the mechanism of DNA synthesis by human terminal deoxynucleotidyltransferase. 2022 , 5, e202201428	O
231	FebRNA: An automated fragment-ensemble-based model for building RNA 3D structures. 2022,	1
230	Design and Synthesis of Benzene Homologues Tethered with 1,2,4-Triazole and 1,3,4-Thiadiazole Motifs Revealing Dual MCF-7/HepG2 Cytotoxic Activity with Prominent Selectivity via Histone Demethylase LSD1 Inhibitory Effect. 2022 , 23, 8796	O
229	Efficient Crystal Structure Prediction for Structurally Related Molecules with Accurate and Transferable Tailor-Made Force Fields.	1
228	Extension of the CHARMM Classical Drude Polarizable Force Field to N- and O-Linked Glycopeptides and Glycoproteins.	1
227	Conformational Heterogeneity of RNA Stem-Loop Hairpins Bound to FUS RNA Recognition Motif with Disordered RGG Tail Revealed by Unbiased Molecular Dynamics Simulations.	
226	Depolarizing Effects in Hydrogen Bond Energy in 310-Helices Revealed by Quantum Chemical Analysis. 2022 , 23, 9032	0
225	Sigma enlarging bridge correction of three dimensional Ornstein Zernike theory for solvation free energy of polyatomic solutes immersed in Lennard-Jones monatomic solvent. 2022 , 12, 085206	0
224	G-Quadruplex Recognition by DARPIns through Epitope/Paratope Analogy**.	
223	Exploring the Energy Landscape of Riboswitches Using Collective Variables Based on Tertiary Contacts. 2022 , 167788	1
222	Effect of Mass on the Dynamic Characteristics of Single- and Double-Layered Graphene-Based Nano Resonators. 2022 , 15, 5551	2

221	Mutagenic Activation of Glutathione Peroxidase-4: Approaches toward Rational Design of Allosteric Drugs.	0
220	New Benzimidazoles Targeting Breast Cancer: Synthesis, Pin1 Inhibition, 2D NMR Binding, and Computational Studies. 2022 , 27, 5245	
219	Molecular Simulations Matching Denaturation Experiments for N6-Methyladenosine. 2022, 8, 1218-1228	1
218	Carbon Nanodots from an In Silico Perspective. 2022 , 122, 13709-13799	2
217	Structural insight and characterization of human Twinkle helicase in mitochondrial disease. 2022 , 119,	0
216	Charging Effects in Inlet Capillaries.	
215	Novel Phenothiazine/Donepezil-like Hybrids Endowed with Antioxidant Activity for a Multi-Target Approach to the Therapy of Alzheimer Disease. 2022 , 11, 1631	0
214	Insight into the C-terminal SH3 domain mediated binding of Drosophila Drk to Sos and Dos. 2022 , 625, 87-93	
213	Exploring enzyme inhibition profiles of novel halogenated chalcone derivatives on some metabolic enzymes: Synthesis, characterization and molecular modeling studies. 2022 , 100, 107748	2
212	Solvation properties of silver ions in ionic liquids using attenuated total reflectance ultraviolet spectroscopy. 2022 , 364, 119998	
211	Insights into the mechanism of electrostatic field promoting ozone mass transfer in water: A molecular dynamics perspective. 2022 , 848, 157710	О
210	A systematic review of the molecular simulation of hybrid membranes for performance enhancements and contaminant removals. 2022 , 307, 135844	O
209	An Application of DipoleDipole Interaction Model in Stacking Dimers Including Protonated Arginine Residue. 2022 , 96, 1995-2001	О
208	Estimation of the Viscosity of an Antibody Solution from the Diffusion Interaction Parameter. 2022 , 45, 1300-1305	1
207	Molecular insight into C60-grafted graphene oxide as a novel reverse osmosis membrane with low energy consumption for seawater desalination. 2022 , 542, 116062	О
206	Local order of liquid propionic acid as studied by original neutron scattering, DFT calculations and molecular dynamics simulations. 2023 , 1272, 134096	O
205	Planning, executing and assessing the validity of SANS contrast variation experiments. 2022,	О
204	Lead Optimization in Drug Discovery. 2022 , 481-500	О

203	Structure and diffusive dynamics of aspartate Edecarboxylase (ADC) liganded with d-serine in aqueous solution. 2022 , 24, 20336-20347	1
202	Advanced spectral analysis of complex molecular system. 2022 , 25-54	Ο
201	Computational modeling and characterization of secondary bonding in compounds of late p-block elements. 2022 ,	О
200	MOFUN: a Python package for molecular find and replace.	О
199	Self-assembly in systems based on l-cysteinelilver-nitrate aqueous solution: multiscale computer simulation.	0
198	Modeling Metal Ions in Enzyme Catalysis. 2022 ,	O
197	End-to-end differentiable construction of molecular mechanics force fields.	1
196	Molecular designs of enhanced oil recovery chemicals. 2023 , 281-319	Ο
195	Sensitivity Analysis of ReaxFF Potential: The Case of Si/O System. 2022 , 126, 7027-7036	1
194	Contribution of Molecular Dynamics in pNMR for the Structural Determination of AnV and AnVI Complexes in Solution.	Ο
193	Molecular Dynamics Simulations of Protein RNA Complexes by Using an Advanced Electrostatic Model. 2022 , 126, 7343-7353	2
192	Molecular simulations of thermodynamic properties of trigeminal tri-cationic ionic liquids: number of rings and anion type effects.	O
191	Force fields optimized against experimental data for large compound families using CombiFF: Validation considering non-target properties and polyfunctional compounds. 2022 , 108312	1
190	Influence of Carbon Nanotube Defects on the Elastic Modulus of Nanocomposite: Multiscale Simulation.	Ο
189	Effect of a Graphene Vacancy on the Kinetics of Heterogeneous Electron Transfer. 2022, 56, 333-338	0
188	Topological and Quantum Stability of Low-Dimensional Crystalline Lattices with Multiple Nonequivalent Sublattices.	2
187	Impact of non-proteinogenic amino acid norvaline and proteinogenic valine misincorporation on a secondary structure of a model peptide.	О
186	Interdomain Dynamics via Paramagnetic NMR on the Highly Flexible Complex Calmodulin/Munc13-1. 2022 , 144, 17041-17053	1

185	Indirect Measurement Methods for Quality and Process Control in Nanomanufacturing. 2022, 5, 209-229	0
184	It is in the flanks: Conformational flexibility of transcription factor binding sites. 2022,	O
183	Structure and Diffusive Properties of Water in Polymer Hydrogels.	1
182	Monoacylglycerol lipase from marine Geobacillus Sp showing lysophospholipase activity and its application in efficient soybean oil degumming. 2022 , 134506	O
181	Structural, Dynamical, and Entropic Differences between SARS-CoV and SARS-CoV-2 s2m Elements Using Molecular Dynamics Simulations.	О
180	A Novel Unspecific Peroxygenase from Galatian marginata for Biocatalytic Oxyfunctionalization Reactions. 2022 , 531, 112707	O
179	Comparison of the United- and All-Atom Representations of (Halo)alkanes Based on Two Condensed-Phase Force Fields Optimized against the Same Experimental Data Set.	2
178	pyDockDNA: A new web server for energy-based protein-DNA docking and scoring. 9,	O
177	Base-specific RNA force field improving the dynamics conformation of nucleotide. 2022 , 222, 680-690	1
176	Tuning a coiled-coil hydrogel via computational design of supramolecular fiber assembly.	O
175	Recent advances in solvation modeling applications: Chemical properties, reaction mechanisms and catalysis. 2022 ,	0
174	Prediction of Saturation Densities and Critical Properties of n-Decane, n-Pentadecane, and n-Eicosane Using Molecular Dynamics with Different Force-Fields.	O
173	RNA Captures More Cations than DNA: Insights from Molecular Dynamics Simulations. 2022 , 126, 8646-8654	1
172	Free energy perturbation calculations of tetrahydroquinolines complexed to the first bromodomain of BRD4.	O
171	Highly stretchable and self-healable polymer gels from physical entanglements of ultrahightholecular weight polymers. 2022 , 8,	1
170	Computational Studies on Selected Macrolides Active against Escherichia coli Combined with the NMR Study of Tylosin A in Deuterated Chloroform. 2022 , 27, 7280	O
169	Precise Steric Features Control Aminoacyl-tRNA Accommodation on the Ribosome. 2022 , 126, 8447-8459	0
168	Quantum-based machine learning and AI models to generate force field parameters for drug-like small molecules. 9,	O

167	Supramolecular Assembly and Small-Molecule Binding by Protein-Engineered Coiled-Coil Fibers.	O
166	Adsorption of oleic acid on magnetite facets. 2022 , 5,	O
165	Computational Study on the Conformational Preferences of Neutral, Protonated and Deprotonated Glycine Dimers. 2022 , 2, 252-266	О
164	The emergence of protein dynamics simulations: how computational statistical mechanics met biochemistry. 2022 , 47,	O
163	Molecular Simulation of Statherin Adsorption on Hydroxyapatite (001) Surface. 2201289	O
162	In Silico Simulations and Functional Cell Studies Evidence Similar Potency and Distinct Binding of Pacific and Caribbean Ciguatoxins.	O
161	Computer Aided Development of Nucleic Acid Applications in Nanotechnologies. 2204408	1
160	Comparative Analysis of RNA Secondary Structure Accuracy on Predicted RNA 3D Models.	O
159	Getting Deeper into the Molecular Events of Heme Binding Mechanisms: A Comparative Multi-level Computational Study of HasAsm and HasAyp Hemophores. 2022 , 61, 17068-17079	0
158	Translocation pause of remdesivir-containing primer/template RNA duplex within SARS-CoV-2日 RNA polymerase complexes. 9,	O
157	Heterocyclic agrochemical hosted by cyclodextrin and hybrid cyclodextrin-silica materials: characterization, release behavior, and mobility in soil. 2022 , 130470	0
156	Structure-Based Discovery of a Novel Class of Small-Molecule Pure Antagonists of Integrin ₩₿.	O
155	Molecular Electronic Study of Spiro-[cyclopenta[1,2-b:5,4-b?]dithiophene-4,9?-fluorene] Derivatives: Route to Decent Hole-Transporting Materials. 2022 , 126, 18238-18250	0
154	Molecular dynamics simulation of the interaction of food proteins with small molecules. 2022 , 134824	1
153	Rational design of a novel multi-epitope peptide-based vaccine against Onchocerca volvulus using transmembrane proteins. 3,	O
152	Computational approaches for nanocluster science. 2023 , 313-343	O
151	Isolation and Computational Characterization of Glutathione Peroxidase Gene from an Aquatic Fern - <i>Salvinia molesta </i> . 51, 58-62	О
150	3D Modeling of Non-coding RNA Interactions. 2022 , 281-317	Ο

149	Controlling mechanical properties of ultrahigh molecular weight ion gels by chemical structure of ionic liquids and monomers.	1
148	Atomwise force fields for molten alkali chlorides (LiCl and KCl) and their mixtures: efficient parameterization via genetic algorithms. 2023 , 573, 154107	O
147	MOLECULAR AND MULTISCALE MODELING: REVIEW ON THE THEORIES AND APPLICATIONS IN CHEMICAL ENGINEERING. 2009 , 3, 205-223	4
146	Some Interfacial Properties of Water and CO2/H2S at Quasireservoir Conditions: A Molecular Dynamics Study. 2022 , 1-13	O
145	Retinal chromophore charge delocalization and confinement explain the extreme photophysics of Neorhodopsin. 2022 , 13,	3
144	Dynamic Docking of Small Molecules Targeting RNA CUG Repeats Causing Myotonic Dystrophy Type 1 (DM1). 2022 ,	О
143	Molecular Dynamics Simulation for Investigating AntigenAntibody Interaction. 2023, 101-107	0
142	The Importance of Charge Transfer and Solvent Screening in the Interactions of Backbones and Functional Groups in Amino Acid Residues and Nucleotides. 2022 , 23, 13514	2
141	Lubeluzole Repositioning as Chemosensitizing Agent on Multidrug-Resistant Human Ovarian A2780/DX3 Cancer Cells. 2022 , 27, 7870	O
140	MOLECULAR MODELLING OF CONFORMATIONAL FLEXIBITY OF HYLAMBATIN MOLECULE. 2022 , 7, 194-198	O
139	Enabling Donor:Acceptor Bicontinuous Networks via Short Contacts in Double-Cable Polymers with Pendant Rylene Diimides.	0
138	GPU-Accelerated All-Atom Particle-Mesh Ewald Continuous Constant pH Molecular Dynamics in Amber.	1
137	Stability and Metastability of Liquid Water in a Machine-Learned Coarse-Grained Model with Short-Range Interactions.	1
136	Computational drug discovery under RNA times. 1-21	O
135	Binding of the peptide deformylase on the ribosome surface modulates the exit tunnel interior. 2022 ,	O
134	CADD, Al and ML in Drug Discovery: A Comprehensive Review. 2022 , 106324	2
133	Conformational Heterogeneity of RNA Stem-Loop Hairpins Bound to FUS-RNA Recognition Motif with Disordered RGG Tail Revealed by Unbiased Molecular Dynamics Simulations. 2022 , 126, 9207-9221	0
132	What drives chorismate mutase to top performance? Insights from a combinedin silicoandin vitrostudy.	О

131	May the Force (Field) Be with You: On the Importance of Conformational Searches in the Prediction of NMR Chemical Shifts. 2022 , 20, 699	1
130	Adapting UFF4MOF for Heterometallic Rare-Earth Metal©rganic Frameworks.	O
129	Molecular dynamics investigation on the co-gasification of various components of sewage sludge in supercritical water. 2023 , 334, 126729	O
128	Valence Bond Methods for Molecules in Solution. 2022,	O
127	Molecular dynamics simulation of adsorption and separation of xylene isomers by Cu-HKUST-1. 2022 , 12, 35290-35299	1
126	Neutron crystallography and quantum chemical analysis of bilin reductase PcyA mutants reveal substrate and catalytic residue protonation states. 2023 , 299, 102763	O
125	A photodecarboxylase from Micractinium conductrix active on medium and short-chain fatty acids. 2023 , 44, 160-170	0
124	One-step production of biodiesel by wet Escherichia coli cells expressing a non-specific and methanol-resistant lipase. 2023 , 125, 75-83	Ο
123	Photochemistry of Biological Systems: Excited-State Electronic Structure Calculations and Nonadiabatic Dynamics Simulations with QM/MM Methods. 2022 ,	О
122	Photocatalytic Hydrogen Production and Carbon Dioxide Reduction Catalyzed by an Artificial Cobalt Hemoprotein. 2022 , 23, 14640	O
121	Computer-Aided Drug Design: An Update. 2023 , 123-152	1
120	Reactive Molecular Dynamics Simulation of the Structural Damages of the B-DNA Induced by the Oxidation/Nitration of Guanine. 2022 , 126, 10347-10359	Ο
119	Water Network in the Binding Pocket of Fluorinated BPTIII rypsin Complexes-Insights from Simulation and Experiment. 2022 , 126, 9985-9999	0
118	Osmotic Contribution of Synthesized Betaine by Choline Dehydrogenase Using In Vivo and In Vitro Models of Post-traumatic Syringomyelia.	Ο
117	Harmonizing Interstrand Electrostatic Repulsion by Conformational Rigidity in Counterion-Deprived Z-DNA: A Molecular Dynamics Study. 2022 , 126, 9956-9963	О
116	Toward Reliable and Insightful Entropy Calculations on Flexible Molecules. 2022, 18, 7166-7178	O
115	Sarcin/Ricin Domain RNA Retains Its Structure Better Than A-RNA in Adaptively Biased Molecular Dynamics Simulations. 2022 , 126, 10018-10033	0
114	Highlight on H-Bond Interaction-Associated Multiple Ion Layer Formation of an Imidazolium-Based Ionic Liquid on a Potential-Bias Surface: Molecular Dynamics Simulations. 2022 , 126, 20644-20657	O

113	Thermodynamic Architecture and Conformational Plasticity of GPCRs.	O
112	Collaborative Assessment of Molecular Geometries and Energies from the Open Force Field. 2022 , 62, 6094-6104	0
111	A Molecular Dynamics Study on the Tribological Performance of Imidazolium B ased Ionic Liquids Mixed with Oil in Comparison to Pure Liquids. 2022 , 7, 384	О
110	Multiscale Modeling of Phosphate Contacts in RNA U-Turns Exposes Differences between Quantum-Chemical and AMBER Force Field Descriptions. 2022 , 62, 6182-6200	O
109	Molecular Insights into Bifunctional Ambruticin DH3 for Substrate Specificity and Catalytic Mechanism.	О
108	An Efficient Approach to Large-Scale Ab Initio Conformational Energy Profiles of Small Molecules. 2022 , 27, 8567	0
107	Identification and mechanistic basis of non-ACE2 blocking neutralizing antibodies from COVID-19 patients with deep RNA sequencing and molecular dynamics simulations. 9,	О
106	Simulation of high-concentration self-interactions for monoclonal antibodies from well-behaved to poorly-behaved systems.	O
105	Phenols, antioxidant and anticancer properties of Tagetes minuta, Euphorbia granulata and Galinsoga parviflora: in vitro and in silico evaluation.	О
104	Polarizable Molecular Block Model: Toward the Development of an Induced Dipole Force Field for DNA. 2022 , 126, 10646-10661	O
103	The development of nucleic acids force fields: From an unchallenged past to a competitive future. 2022 ,	О
102	DeePKS + ABACUS as a Bridge between Expensive Quantum Mechanical Models and Machine Learning Potentials. 2022 , 126, 9154-9164	O
101	13C ENDOR Spectroscopy-Guided MD Computations Reveals the Structure of the Enzyme-Substrate Complex of an Active, N-linked Glycosylated Lipoxygenase.	О
100	A Biologically Active Chromone from Bomarea setacea (alstroemeriaceae): Leishmanicidal, Antioxidant and Multilevel Computational Studies. 2022 , 7,	O
99	Direct or Indirect ESPT Mechanism in CFP psamFP488? A Theoretical-Computational Investigation. 2022 , 23, 15640	О
98	Toehold clipping: A mechanism for remote control of DNA strand displacement.	O
97	Improved docking of peptides and small molecules in iMOLSDOCK. 2023, 29,	1
96	Molecular Insights into Curvature Effects on the Capacitance of Electrical Double Layers in Tricationic Ionic Liquids with Carbon Nanotube Electrodes.	O

95	Protein structure determination in human cells by in-cell NMR and a reporter system to optimize protein delivery or transexpression. 2022 , 5,	1
94	Quantum chemical studies on hydrogen bonds in helical secondary structures. 2022 , 14, 1369-1378	Ο
93	The Same Natural Ligand Is Involved in Allorecognition of Multiple HLA-B27 Subtypes by a Single T Cell Clone: Role of Peptide and the MHC Molecule in Alloreactivity. 1998 , 161, 5481-5490	17
92	Glass-box molecular dynamics simulation for teaching the van der Waals interaction.	Ο
91	A dual organelle-targeting mechanosensitive probe. 2023 , 9,	1
90	Computational protein design repurposed to explore enzyme vitality and help predict antibiotic resistance. 9,	Ο
89	gmak: A Parameter-Space Mapping Strategy for Force-Field Calibration.	0
88	MEodos computacionales para estimar la afinidad de un complejo ligando-receptor. 2023 , 5, 27-46	O
87	Discovery of aromatic 2-(3-(methylcarbamoyl) guanidino)-N-aylacetamides as highly potent chitinase inhibitors. 2023 , 117172	0
86	Thermodynamic architecture and conformational plasticity of GPCRs. 2023, 14,	O
85	Molecular Dynamics-Assisted Interaction of Vanadium ComplexAMPK: From Force Field Development to Biological Application for Alzheimer Treatment.	O
84	Sequence and structural similarities of ACCase protein of Phalaris minor and wheat: An insight to explain herbicide selectivity. 13,	O
83	Design, synthesis, and biological activity studies on benzimidazole derivatives targeting myeloperoxidase. 2023 , 248, 115083	O
82	Multi spectroscopic and molecular simulation studies of propyl acridone binding to calf thymus DNA in the presence of electromagnetic force. 2023 , 13, 5-16	O
81	A Baseline Cellular Antiviral State Is Maintained by cGAS and Its Most Frequent Naturally Occurring Variant rs610913. 2022 , 209, 535-547	0
80	Redesigning methionyl-tRNA synthetase formethionine activity with adaptive landscape flattening and experiments.	O
79	Computer Simulation Techniques for Modelling Statics and Dynamics of Nanoscale Structures. 2014 , 230-299	О
78	Recognizing the power of machine learning and other computational methods to accelerate progress in small molecule targeting of RNA. rna.079497.122	0

77	Molecular Simulation Study of Montmorillonite in Contact with Ethanol.	0
76	What Drives Chorismate Mutase to Top Performance? Insights from a Combined In Silico and In Vitro Study. 2023 , 62, 782-796	O
75	Transferability of the Electrostatic Parameters of the Polarizable Gaussian Multipole Model.	O
74	In Silico Study of the Binding of Daunomycin and Phenylalanine Transfer RNA: Probe Molecular Recognition for Structure-Based Drug Design.	O
73	Revealing the Molecular Interactions between Human ACE2 and the Receptor Binding Domain of the SARS-CoV-2 Wild-Type, Alpha and Delta Variants. 2023 , 24, 2517	1
72	Molecular Dynamics and Raman Optical Activity Spectra Reveal Nucleotide Conformation Ratios in Solution.	O
71	Coenzyme Engineering of Glucose-6-phosphate Dehydrogenase on a Nicotinamide-Based Biomimic and Its Application as a Glucose Biosensor. 2023 , 13, 1983-1998	О
70	Click and Detect: Versatile Ampicillin Aptasensor Enabled by Click Chemistry on a GrapheneAlkyne Derivative. 2207216	1
69	Deconvoluting binding sites in amyloid nanofibrils using time-resolved spectroscopy. 2023 , 14, 1072-1081	О
68	MetaDOCK: A Combinatorial Molecular Docking Approach.	O
67	Computational assessment of hexadecane freezing by equilibrium atomistic molecular dynamics simulations. 2023 , 638, 743-757	1
66	Characterising RNA Dynamics using NMR Residual Dipolar Couplings. 2012 , 184-215	O
65	In silico approaches for elastomers. 2023 , 349-397	0
64	Spherical PEG/SiO2 promising agents for Lamivudine antiviral drug delivery, a molecular dynamics simulation study. 2023 , 13,	O
63	Accelerated Quantum Mechanics/Molecular Mechanics Simulations via Neural Networks Incorporated with Mechanical Embedding Scheme. 2023 , 19, 1157-1169	0
62	EnCPdock: a web-interface for direct conjoint comparative analyses of complementarity and binding energetics in inter-protein associations.	O
61	Molecular dynamics simulation of the surface wettability of typical minerals in shale.	0
60	Impact of the Force Field on the Calculation of Density and Surface Tension of EpoxyResins. 2023 , 127, 2617-2628	O

59	Consequences of Overfitting the van der Waals Radii of Ions. 2023, 19, 2064-2074	О
58	Computer-Assisted Design of Peptide-Based Radiotracers. 2023 , 24, 6856	O
57	Molecular dynamics investigation on the vapor l lquid interface behavior of long-chain alkanes, alcohols, and their mixtures. 2023 , 375, 121283	0
56	The inorganic chemistry of the cobalt corrinoids han update. 2023 , 242, 112154	O
55	Bioinformatics approaches to discovering food-derived bioactive peptides: Reviews and perspectives. 2023 , 162, 117051	О
54	PDA-Pred: Predicting the binding affinity of protein-DNA complexes using machine learning techniques and structural features. 2023 , 213, 10-17	1
53	In silico evaluation of geroprotective phytochemicals as potential sirtuin 1 interactors. 2023, 161, 114425	O
52	Aqueous solutions of chiral ionic liquids based on (Ill menthol: An experimental and computational study of volumetric and transport properties. 2023 , 378, 121591	O
51	Multiscale analysis of nonlinear systems using a hierarchy of deep neural networks. 2023, 271-272, 112261	O
50	Classification of k-defect holes on a graphene sheet. 2023 , 225, 112181	O
49	Prominently improved CO2/N2 separation efficiency by ultrathin-ionic-liquid-covered MXene membrane. 2023 , 311, 123296	О
48	On the Behavior of the Ethylene Glycol Components of Polydisperse Polyethylene Glycol PEG200. 2023 , 127, 1178-1196	Ο
47	Simulating dynamic interaction between diazepam and ethanol targeting the GABAA receptor via in silico model. 2023 , 95, 136-143	О
46	Molecular and kinetic properties of copper nitrite reductase from Sinorhizobium meliloti 2011 upon substituting the interfacial histidine ligand coordinated to the type 2 copper active site for glycine. 2023 , 241, 112155	Ο
45	Quantum Dynamics and Bi Metal Force Field Parameterization Yielding Significant Antileishmanial Targets. 2023 , 63, 1371-1385	0
44	Recent advances of computational studies on bioethanol to light olefin reactions using zeolite and metal oxide catalysts. 2023 , 270, 118532	O
43	Alternative Strategy for Spectral Tuning of Flavin-Binding Fluorescent Proteins. 2023, 127, 1301-1311	Ο
42	Evidence That Less Can Be More for Transferable Force Fields. 2023 , 63, 1188-1195	Ο

41	A riboswitch separated from its ribosome-binding site still regulates translation. 2023 , 51, 2464-2484	1
40	The peptide bond rupture mechanism in the serine proteases: an in silico study based on sequential scale models. 2023 , 25, 8043-8049	Ο
39	RNA G-quadruplex folding is a multi-pathway process with a variety of short-lived intermediates.	O
38	Revealing Structural and Physical Properties of Polylactide: What Simulation Can Do beyond the Experimental Methods. 1-39	O
37	Impact of non-proteinogenic amino acid norvaline and proteinogenic valine misincorporation on a secondary structure of a model peptide.	O
36	Greedy Theory Using Improved Performance Prim Algorithm, Big Bang Speedup of the Bellman Flord Algorithm. 2023 , 493-500	O
35	Therapeutic phosphorodiamidate morpholino oligonucleotides: Physical properties, solution structures, and folding thermodynamics. 2023 , 31, 631-647	О
34	Non-active Site Residue in Loop L4 Alters Substrate Capture and Product Release in d-Arginine Dehydrogenase. 2023 , 62, 1070-1081	O
33	The effects of RNA.DNA-DNA triple helices on nucleosome structures and dynamics. 2023, 122, 1229-1239	О
32	Toward Force Fields with Improved Base Stacking Descriptions. 2023 , 19, 1529-1536	O
31	A review on microfluidic-assisted nanoparticle synthesis, and their applications using multiscale simulation methods. 2023 , 18,	O
30	Direct Proton-Coupled Electron Transfer between Interfacial Tyrosines in Ribonucleotide Reductase. 2023 , 145, 4784-4790	O
29	A review on shale oil and gas characteristics and molecular dynamics simulation for the fluid behavior in shale pore. 2023 , 376, 121507	О
28	Free energy change in the complete transport of all water molecules through a carbon nanotube. 2023 , 25, 7032-7046	O
27	Molecular dynamics simulation of phosphatidylcholine membrane in low ionic strengths of sodium chloride. 1-11	О
26	Static Binding and Dynamic Transporting-Based Design of Specific Ring-Chain-Ring Acetylcholinesterase Inhibitor: From Galantamine to Natural Product.	O
25	GAFF-AIC: reoptimisation of the GAFF force field for realistic densities and viscosities in aromatic isocyanates. 2023 , 49, 576-588	О
24	ATP binding by an F1Fo ATP synthase $\bar{\mu}$ subunit is pH dependent, suggesting a diversity of $\bar{\mu}$ subunit functional regulation in bacteria. 10,	O

23	The Intrinsic Radius as a Key Parameter in the Generalized Born Model to Adjust Protein-Protein Electrostatic Interaction. 2023 , 24, 4700	О
22	Prediction and Control in DNA Nanotechnology.	O
21	CN bond formation by a polyketide synthase. 2023 , 14,	O
20	Electronic Excitation Response of DNA to High-Energy Proton Radiation in Water. 2023, 130,	О
19	Structural Analysis of Interactions between Epidermal Growth Factor Receptor (EGFR) Mutants and Their Inhibitors. 2023 , 3, 203-213	О
18	Human Pol®Natural Polymorphic Variants G118V and R149I Affects Substate Binding and Catalysis. 2023 , 24, 5892	O
17	Structural and dynamic properties of the YTH domain in complex with N\$lt;sup\$gt;6\$lt;/sup\$gt;-methyladenosine RNA studied by accelerated molecular dynamics simulations. 2023 , 11, 72	О
16	Machines on Genes through the Computational Microscope. 2023 , 19, 1945-1964	О
15	Investigation of Solid Formation Enthalpy and Molecular Mechanics Energies of Amino Acids via Force Field Approach. 2023 , 12, 10-16	О
14	Modeling of SARS-CoV-2 Virus Proteins: Implications on Its Proteome. 2023 , 265-299	О
13	Exploration of the binding of antifungal drugs to human P450 2C9 based on docking and molecular dynamics simulation.	О
12	Approach of Electronic Structure Calculations to Crystal. 2023 , 209-255	О
11	Design and Pharmacological Characterization of All Integrin Cyclopeptide Agonists: Computational Investigation of Ligand Determinants for Agonism versus Antagonism. 2023, 66, 5021-5040	О
10	Desensitization dynamics of the AMPA receptor. 2023 ,	О
9	Towards Computational Modeling of Ligand Binding to the ILPR G-Quadruplex. 2023, 28, 3447	О
8	Strategy for Ultrafast Cathode Reaction in Magnesium-Ion Batteries Using BF4 Anion Based Dual-Salt Electrolyte Systems: A Case Study of FePO4.	О
7	Theories and radial distribution function of MD and MC simulations. 2023, 271-290	О
6	A Peptide Potential Based on a Bond Dipole Representation of Electrostatics. 2023 , 11, 1291	О

5	Hydrated solvation suppression of zinc ions for highly reversible zinc anodes. 2023, 466, 143189	O
4	Atomistic Picture of Openingtosing Dynamics of DNA Holliday Junction Obtained by Molecular Simulations. 2023 , 63, 2794-2809	O
3	Modern Approaches to Protein Engineering to Create Enzymes with New Catalytic Properties. 2023 , 57, 204-213	O
2	Interlayered Interface of a Thin Film Composite Janus Membrane for Sieving Volatile Substances in Membrane Distillation. 2023 , 57, 7612-7623	O
1	Molecular Dynamics Simulations of Ionic Liquid Crystals. 2023 ,	О