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2237	Protein Solvent Shell Structure Provides Rapid Analysis of Hydration Dynamics.		
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- 2235 Fine-Tuning of the AMBER RNA Force Field with a New Term Adjusting Interactions of Terminal Nucleotides.
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- 2225 CPPE: An Open-Source C++ and Python Library for Polarizable Embedding.
- 2224 Self-Parametrizing System-Focused Atomistic Models.
- 2223 Improving Temperature Generator in Parallel Tempering Simulation in the NPT Condition.
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- 2221 Discovery of a Potent and Selective Coactivator Associated Arginine Methyltransferase 1 (CARM1) Inhibitor by Virtual Screening.
- 2220 .
- 2219 Identification of Dihydrofuro[3,4d]pyrimidine Derivatives as Novel HIV1 Non-Nucleoside Reverse Transcriptase Inhibitors with Promising Antiviral Activities and Desirable Physicochemical Properties.
- 2218 Comprehensive Characterization of Lipid-Guided G Protein-Coupled Receptor Dimerization.

2217 Dewetting of S1-Pocket via Water Channel upon Thrombin Substrate Association Reaction.

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2215 Unusual Influence of Fluorinated Anions on the Stretching Vibrations of Liquid Water.

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2213 Phase Diagram of a Stratum Corneum Lipid Mixture.

2212 Excited State Electronic Interconversion and Structural Transformation of Engineered Red-Emitting Green Fluorescent Protein Mutant.

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2206 Accurate Force Field Parameters and pH Resolved Surface Models for Hydroxyapatite to Understand Structure, Mechanics, Hydration and Biological Interfaces.

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2204 Multiscale Modeling of the HKUST-1/Poly(vinyl alcohol) Interface: From an Atomistic to a Coarse Graining Approach.

2203 Rattling Transport of Lithium Ion in the Cavities of Model Solid Electrolyte Interphase.

2202 Barrier-Free Charge Separation Enabled by Electronic Polarization in High-Efficiency Non-fullerene Organic Solar Cells.

2201 Quantifying Lateral Inhomogeneity of Cholesterol-Containing Membranes.

2200 Amide Rotation Hindrance Predicts Proteolytic Resistance of Cystine-Knot Peptides.

- 2199 Free Energies of Redox Half-Reactions from First-Principles Calculations.
- 2198 Solvent Polarity Governs Ion Interactions and Transport in a Solvated Room-Temperature Ionic Liquid.
- 2197 Kinetics-Controlled Amphiphile Self-Assembly Processes.
- 2196 Revealing the Solvation Structure and Dynamics of Carbonate Electrolytes in Lithium-Ion Batteries by Two-Dimensional Infrared Spectrum Modeling.
- 2195 Calcium Sensing by Recoverin: Effect of Protein Conformation on Ion Affinity.
- 2194 Merging In-Solution X-ray and Neutron Scattering Data Allows Fine Structural Analysis of MembraneProtein Detergent Complexes.
- 2193 Does Local Structure Bias How a Crystal Nucleus Evolves?.
- 2192 Evolution of All-Atom Protein Force Fields to Improve Local and Global Properties.
- 2191 Tracking Polariton Relaxation with Multiscale Molecular Dynamics Simulations.
- 2190 Helical Inclusions in Phospholipid Membranes: Lipid Adaptation and Chiral Order.
- 2189 Phospholipid Scramblases Remodel the Shape of Asymmetric Membranes.
- 2188 Small-Angle Xray Scattering Curves of Detergent Micelles: Effects of Asymmetry, Shape Fluctuations, Disorder, and Atomic Details.
- 2187 Surfactant Binding to PolymerWater Interfaces in Atomistic Simulations.
- 2186 Water-Mediated Interactions between Hydrophilic and Hydrophobic Surfaces.
- 2185 How Anionic Vesicles Steer the Oligomerization of Enzymatically Oxidized p-Aminodiphenylamine (PADPA) toward a Polyaniline Emeraldine Salt (PANI-ES)-Type Product.
- 2184 Melting Point and SolidLiquid Coexistence Properties of 1 Isotactic Polypropylene as Functions of Its Molar Mass: A Molecular Dynamics Study.
- 2183 Shuttlecock-Shaped Molecular Rectifier: Asymmetric Electron Transport Coupled with Controlled Molecular Motion.
- 2182 DNA Binding and Recognition of a CC Mismatch in a DNA Duplex by Water-Soluble Peptidocalix[4]arenes: Synthesis and Applications.

2181 Molecular Architectonics of Cyclic Dipeptide Amphiphiles and Their Application in Drug Delivery.

2180 Enhanced Polymer Crystallinity in Mixed-Matrix Membranes Induced by MetalOrganic Framework Nanosheets for Efficient CO₂ Capture.

2179 Tunable Ferroelectricity in RuddlesdenPopper Halide Perovskites.

2178 Effect of Trapped Solvent on the Interface between PSbPMMA Thin Films and P(SrMMA) Brush Layers.

2177 Organic Filling Mitigates Flaw-Sensitivity of Nanoscale Aragonite.

2176 Hollow Mesoporous MetalOrganic Frameworks with Enhanced Diffusion for Highly Efficient Catalysis.

2175 Versatile Peptide CTerminal Functionalization via a Computationally Engineered Peptide Amidase.

2174 Substrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivity.

2173 Thermal Stabilization of Enzymes with Molecular Brushes.

2172 Liquid-Phase Modeling in Heterogeneous Catalysis.

2171 Imidazole-Functionalized Pillar[5]arenes: Highly Reactive and Selective Supramolecular Artificial Enzymes.

2170 QM/MM Study of the Reaction Mechanism of the Dehydratase Domain from Mammalian Fatty Acid Synthase.

2169 In Silico Based Engineering Approach to Improve Transaminases for the Conversion of Bulky Substrates.

2168 Unpicking the Cause of Stereoselectivity in Actinorhodin Ketoreductase Variants with Atomistic Simulations.

2167 How To Break the Janus Effect of H₂O₂ in Biocatalysis? Understanding Inactivation Mechanisms To Generate more Robust Enzymes.

2166 Evidence for a Catalytic Strategy to Promote Nucleophile Activation in Metal-Dependent RNA-Cleaving Ribozymes and 817 DNAzyme.

2165 Translocation of an Intracellular Protein via Peptide-Directed Ligation.

2164 Biochemical Studies and Molecular Dynamic Simulations Reveal the Molecular Basis of Conformational Changes in DNA Methyltransferase 1.

2163 .

2162 Hexahydropyrrolo[2,3b]indole Compounds as Potential Therapeutics for Alzheimers Disease.

2161 V2+/V3+ Redox Kinetics on Glassy Carbon in Acidic Electrolytes for Vanadium Redox Flow Batteries.

2160 .

2159 .

2158 Threading of Unconcatenated Ring Polymers at High Concentrations: Double-Folded vs Time-Equilibrated Structures.

2157 Consequences of Depsipeptide Substitution on the ClpP Activation Activity of Antibacterial Acyldepsipeptides.

2156 Exploring Halogen Bonds in 5Hydroxytryptamine 2B ReceptorLigand Interactions.

2155 Cyanographene and Graphene Acid: Emerging Derivatives Enabling High-Yield and Selective Functionalization of Graphene.

2154 StructureStabilityFunction Mechanistic Links in the Anti-Measles Virus Action of Tocopherol-Derivatized Peptide Nanoparticles.

2153 Self-Assembly of Antimitotic Peptide at Membranes: Computational and Experimental Investigation.

2152 Design of a Helical-Stabilized, Cyclic, and Nontoxic Analogue of the Peptide Cm-p5 with Improved Antifungal Activity.

2151 Self-Sorted, Random, and Block Supramolecular Copolymers via Sequence Controlled, Multicomponent Self-Assembly.

2150 .

2149 Hydration Dynamics of a Peripheral Membrane Protein.

2148 Experimental and Computational Analysis of Protein Stabilization by Gly-todAla Substitution: A Convolution of Native State and Unfolded State Effects.

2147 Guanidinium can both Cause and Prevent the Hydrophobic Collapse of Biomacromolecules.

2146 Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations.

- 2145 Enzyme Architecture: Modeling the Operation of a Hydrophobic Clamp in Catalysis by Triosephosphate Isomerase.
- 2144 Origin of DNA-Induced Circular Dichroism in a Minor-Groove Binder.
- 2143 Exploiting ChromophoreProtein Interactions through Linker Engineering To Tune Photoinduced Dynamics in a Biomimetic Light-Harvesting Platform.
- 2142 Surface Dynamics and LigandCore Interactions of Quantum Sized Photoluminescent Gold Nanoclusters.
- 2141 .
- 2140 Stereodivergent Protein Engineering of a Lipase To Access All Possible Stereoisomers of Chiral Esters with Two Stereocenters.
- 2139 P450-BM3-Catalyzed Sulfoxidation versus Hydroxylation: A Common or Two Different Catalytically Active Species?.
- 2138 Toward Atomistic Resolution Structure of Phosphatidylcholine Headgroup and Glycerol Backbone at Different Ambient Conditions.
- 2137 Bound Na⁺ is a Negative Effector for Thrombin-Substrate Stereospecific Complex Formation.
- 2136 Na⁺ Binding Is Ineffective in Forming a Primary Substrate Pocket of Thrombin.
- 2135 Characterizing Conformational Dynamics of Proteins Using Evolutionary Couplings.
- 2134 Elucidating the Phosphate Binding Mode of Phosphate-Binding Protein: The Critical Effect of Buffer Solution.
- 2133 Catalytic Mechanism of Aryl-Ether Bond Cleavage in Lignin by LigF and LigG.
- 2132 Martini Coarse-Grained Model for ClayPolymer Nanocomposites.
- 2131 ATP Converts A42 Oligomer into Off-Pathway Species by Making Contact with Its Backbone Atoms Using Hydrophobic Adenosine.
- 2130 Contrasting Modes of Self-Assembly and Hydrogen-Bonding Heterogeneity in Chlorosomes of *Chlorobaculum tepidum*.
- 2129 In Situ Xray Spectroscopy of the Electrochemical Development of Iridium Nanoparticles in Confined Electrolyte.
- 2128 Unraveling the Fate of Host Excitons in HostGuest Phosphorescent Organic Light-Emitting Diodes.

- 2127 Theoretical Investigation on the Control of Macrocyclic Dihydroazulene/Azobenzene Photoswitches.
- 2126 Photoactive Yellow Protein Chromophore Photoisomerizes around a Single Bond if the Double Bond Is Locked.
- 2125 Physics behind Water Transport through Nanoporous Boron Nitride and Graphene.
- 2124 Benzene Probes in Molecular Dynamics Simulations Reveal Novel Binding Sites for Ligand Design.
- 2123 Unexpected Like-Charge Self-Assembly of a Biguanide-Based Antimicrobial Polyelectrolyte.
- 2122 Second-Harmonic Scattering as a Probe of Structural Correlations in Liquids.
- 2121 Anomalous Dynamics of Water Confined in ProteinProtein and ProteinDNA Interfaces.
- 2120 Ionization of Cellobiose in Aqueous Alkali and the Mechanism of Cellulose Dissolution.
- 2119 Coherent Light Harvesting through Strong Coupling to Confined Light.
- 2118 Rotational Cation Dynamics in Metal Halide Perovskites: Effect on Phonons and Material Properties.
- 2117 Self-Assembly of Nanocubic Molecular Capsules via Solvent-Guided Formation of Rectangular Blocks.
- 2116 Dodine as a Kosmo-Chaotropic Agent.
- 2115 Importance of the Force Field Choice in Capturing Functionally Relevant Dynamics in the von Willebrand Factor.
- 2114 The Contribution of Backbone Electrostatic Repulsion to DNA Mechanical Properties is Length-Scale-Dependent.
- 2113 Distinct and Nonadditive Effects of Urea and Guanidinium Chloride on Peptide Solvation.
- 2112 Nanoparticles Targeted against Cryptococcal Pneumonia by Interactions between Chitosan and Its Peptide Ligand.
- 2111 Toward an Understanding of the Microstructure and Interfacial Properties of PIMs/ZIF8 Mixed Matrix Membranes.
- 2110 Ion Gel Dynamic Templates for Large Modulation of Morphology and Charge Transport Properties of Solution-Coated Conjugated Polymer Thin Films.

2109 Molecular Mechanism of Inhibition of DNA Methylation by Zebularine.

2108 Enhancing the Steroid Sulfatase Activity of the Arylsulfatase from *Pseudomonas aeruginosa*.

2107 Redox Cofactor Rotates during Its Stepwise Decarboxylation: Molecular Mechanism of Conversion of Coproheme to Heme b.

2106 Complexities of the Reaction Mechanisms of CC Double Bond Reduction in Mammalian Fatty Acid Synthase Studied with Quantum Mechanics/Molecular Mechanics Calculations.

2105 Sequential Inactivation of Gliotoxin by the SMethyltransferase TmtA.

2104 Application of an Integrated GPCR SAR-Modeling Platform To Explain the Activation Selectivity of Human 5HT2C over 5HT2B.

2103 Insights into the Stereospecificity in Papain-Mediated Chemoenzymatic Polymerization from Quantum Mechanics/Molecular Mechanics Simulations.

2102 Transcriptional Bypass of DNAProtein and DNAPeptide Conjugates by T7 RNA Polymerase.

2101 Amyloid Properties of Asparagine and Glutamine in Prion-like Proteins.

2100 Identification of Inhibitors of CD36-Amyloid Beta Binding as Potential Agents for Alzheimers Disease.

2099 .

2098 Crystalline CyclophaneProtein Cage Frameworks.

2097 Superior Performance of the SQM/COSMO Scoring Functions in Native Pose Recognition of Diverse ProteinLigand Complexes in Cognate Docking.

2096 Combined Adsorption and Reaction in the Ternary Mixture N₂, N₂O₄, NO₂ on MIL-127 Examined by Computer Simulations.

2095 Molecular Signature for Receptor Engagement in the Metabolic Peptide Hormone Amylin.

2094 Self-Exfoliated Guanidinium-Based Ionic Covalent Organic Nanosheets (iCONs).

2093 .

2092 Switchable Chiral Selection of Aspartic Acids by Dynamic States of Brushite.

- 2091 Stress Propagation through Biological Lipid Bilayers in Silico.
- 2090 Differences in the Active Site of Water Oxidation among Photosynthetic Organisms.
- 2089 Nonadditive Ion Effects Drive Both Collapse and Swelling of Thermoresponsive Polymers in Water.
- 2088 Photocontrolling Protein/Peptide Interactions: From Minimal Perturbation to Complete Unbinding.
- 2087 Chirality Evolution from Sub-1 Nanometer Nanowires to the Macroscopic Helical Structure.
- 2086 Molecular Dynamics Simulations Reveal the Conformational Flexibility of Lipid II and Its Loose Association with the Defensin Plectasin in the *Staphylococcus aureus* Membrane.
- 2085 Molecular Simulations Reveal an Unresolved Conformation of the Type IA Protein Kinase A Regulatory Subunit and Suggest Its Role in the cAMP Regulatory Mechanism.
- 2084 Chemical Editing of Macrocyclic Natural Products and Kinetic Profiling Reveal Slow, Tight-Binding Histone Deacetylase Inhibitors with Picomolar Affinities.
- 2083 Intermolecular Recognition of the Antimalarial Drug Chloroquine: A Quantum Theory of Atoms in Molecules Density Functional Theory Investigation of the Hydrated Dihydrogen Phosphate Salt from the 103 K X-ray Structure.
- 2082 ¹⁹⁵Pt NMR and Molecular Dynamics Simulation Study of the Solvation of [PtCl₆]²⁻ in Water/Methanol and Water/Dimethoxyethane Binary Mixtures.
- 2081 PACKMOL-Memgen: A Simple-To-Use, Generalized Workflow for Membrane-Protein/Lipid-Bilayer System Building.
- 2080 Insights to the Binding of a Selective Adenosine A₃ Receptor Antagonist Using Molecular Dynamic Simulations MM-PBSA and MM-GBSA Free Energy Calculations, and Mutagenesis.
- 2079 Self-Assembly of Phosphocholine Derivatives Using the ELBA Coarse-Grained Model: Micelles, Bicelles, and Reverse Micelles.
- 2078 ProtoCaller: Robust Automation of Binding Free Energy Calculations.
- 2077 Using Local States To Drive the Sampling of Global Conformations in Proteins.
- 2076 pK_a Values of Titrable Amino Acids at the Water/Membrane Interface.
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2071	Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions.		
2070	Polarizable QM/MM Approach with Fluctuating Charges and Fluctuating Dipoles: The QM/FQF Model.		
2069	Residue-Residue Mutual Work Analysis of Retinal-Opsin Interaction in Rhodopsin: Implications for Protein-Ligand Binding.		
2068	Constraining Endomorphin1 by β -Hybrid Dipeptide/Heterocycle Scaffolds: Identification of a Novel Opioid Receptor Selective Partial Agonist.		
2067	Suppression of Tumor Growth and Metastases by Targeted Intervention in Urokinase Activity with Cyclic Peptides.		
2066	On the Price of the Factor of Safety in the Materials for Lightning-rods. 1887 , 9, 122-124		
2065	Molecular dynamics computer simulation of the hydration of two simple organic solutes. 1984 , 53, 1517-1526	12	
2064	A comparison of the structure and dynamics of avian pancreatic polypeptide hormone in solution and in the crystal. 1985 , 13, 77-88		51
2063	Canonical dynamics: Equilibrium phase-space distributions. 1985 , 31, 1695-1697		14620
2062	The Nose-Hoover thermostat. <i>Journal of Chemical Physics</i> , 1985 , 83, 4069-4074	3.9	1365
2061	A molecular dynamics computer simulation study of the hydration of bis(methylsulphonyl)methane in water. 1985 , 56, 1393-1409		4
2060	The Structure of Polar Molecular Liquids. 1985 , 36, 321-346		75
2059	A molecular dynamics study of the C-terminal fragment of the L7/L12 ribosomal protein. Secondary structure motion in a 150 picosecond trajectory. 1985 , 183, 461-77		143
2058	Structural changes in retinol binding protein induced by retinol removal. A molecular dynamics study. 1986 , 139, 564-70		11
2057	Molecular Dynamics Simulation Study of Polypeptide Conformational Equilibria: A Progress Report. 1986 , 482, 51-59		18
2056	Simulations of proteins in water. 1986 , 482, 269-86		148

2055	A molecular dynamics computer simulation of an eight-base-pair DNA fragment in aqueous solution: comparison with experimental two-dimensional NMR data. 1986 , 482, 287-303		96
2054	Tryptophan Structure and Dynamics Using GROMOS. 1986 , 482, 304-306		
2053	An extension of the canonical ensemble molecular dynamics method. 1986 , 57, 187-191		197
2052	Molecular dynamics simulations of the holo and apo forms of retinol binding protein. Structural and dynamical changes induced by retinol removal. 1986 , 192, 593-603		51
2051	Free energy of hydrophobic hydration: A molecular dynamics study of noble gases in water. <i>Journal of Chemical Physics</i> , 1986 , 85, 6720-6727	3.9	227
2050	Theoretical calculation of relative binding affinity in host-guest systems. 1986 , 83, 833-5		162
2049	Computer Simulation and the Design of New Biological Molecules. 1986 , 27, 211-215		51
2048	Restrained Molecular Dynamics Procedure for Protein Tertiary Structure Determination from NMR Data: A Lac Repressor Headpiece Structure Based on Information on J-coupling and from Presence and Absence of NOE's. 1986 , 27, 181-188		60
2047	Markov chain algorithms for canonical ensemble simulation. 1986 , 42, 29-35		5
2046	A molecular dynamics computer simulation study of the temperature dependence of hydration of 1,4-dioxane and 1,3-dioxane. 1986 , 101, 27-44		13
2045	Conformational dynamics of tryptophan: a proposal for the origin of the non-exponential fluorescence decay. 1986 , 126, 365-372		76
2044	Flows Far From Equilibrium Via Molecular Dynamics. 1986 , 18, 243-264		109
2043	Numerical test of the Liouville equation. 1986 , 34, 4229-4237		10
2042	Simulations of vibrational relaxation in dense molecular fluids. I. Methods. <i>Journal of Chemical Physics</i> , 1986 , 84, 3138-3146	3.9	20
2041	Free energy calculations by computer simulation. 1987 , 236, 564-8		386
2040	Molecular dynamics of a cytochrome c-cytochrome b5 electron transfer complex. 1987 , 238, 794-7		166
2039	Microcomputer simulation of a two-dimensional Lennard-Jones fluid: effects of repulsive and attractive forces. 1987 , 8, 117-124		8
2038	Analysis of discrete and continuum dielectric models; application to the calculation of protonation energies in solution. 1987 , 61, 293-311		46

2037	Rotational dynamics of a solvated dipole: A molecular dynamics study of dielectric friction. <i>Journal of Chemical Physics</i> , 1987 , 86, 7079-7083	3.9	25
2036	Molecular mechanics and dynamics in protein design. 1987 , 154, 430-49		9
2035	Effect of the lattice model on the dynamics of dissociative chemisorption of H ₂ on a Si(111) surface. 1987 , 188, 402-420		21
2034	Sidechain rotational isomerization in proteins. Dynamic simulation with solvent surroundings. 1987 , 51, 637-41		26
2033	A computer simulation study of the melting and freezing properties of a system of Lennard-Jones particles. 1987 , 61, 597-615		25
2032	Isothermal/isobaric molecular dynamics simulation of diatomic liquids and their mixtures. 1987 , 113, 43-52		32
2031	Molecular dynamics simulations of cyclosporin A: the crystal structure and dynamic modelling of a structure in apolar solution based on NMR data. 1987 , 1, 219-41		54
2030	A molecular dynamics simulation of crystalline alpha-cyclodextrin hexahydrate. 1987 , 15, 197-210		121
2029	The simulated dynamics of the insulin monomer and their relationship to the molecule's structure. 1987 , 14, 449-59		38
2028	A molecular dynamics study of associations in solution. an NPT simulation of the urea dimer in water. 1987 , 140, 401-405		19
2027	Biophysical applications of molecular dynamics. 1987 , 44, 233-242		19
2026	A specific inhibitor design approach by means of molecular dynamics calculation for porcine pancreatic elastase. 1987 , 8, 645-650		
2025	Molecular dynamics simulation of the 1:1 enzyme-ligand complex between porcine pancreatic elastase and acetyl-alanine-proline-alanine. 1987 , 8, 801-809		1
2024	Computergestütztes Moleküldesign (CAMD) – ein Überblick. 1987 , 99, 413-428		18
2023	Calculation of the relative change in binding free energy of a protein-inhibitor complex. 1987 , 235, 574-6		289
2022	The combined use of NMR, distance geometry, and restrained molecular dynamics for the conformational study of a cyclic somatostatin analogue. 1988 , 27, 323-38		30
2021	Computer simulation of biological interactions and reactivity. 1988 , 1, 313-22		5
2020	Dynamic simulation as an essential tool in molecular modeling. 1988 , 2, 217-21		10

2019	The structure of a membrane-spanning polypeptide studied by molecular dynamics. 1988 , 30, 279-92		58
2018	Molecular factors stabilizing protein crystals. 1988 , 90, 273-282		33
2017	Hydrogen bonds in concreto and in computro. 1988 , 177, 467-475		17
2016	Conformational aspects of malic acid: A multidisciplinary approach. 1988 , 189, 65-80		8
2015	Free energy of ionic hydration: Analysis of a thermodynamic integration technique to evaluate free energy differences by molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1988 , 89, 5876-5886	3.9	414
2014	New insights into the structure of B2O3 glass. 1988 , 103, 201-209		46
2013	Molecular dynamics simulation of a smectic liquid crystal with atomic detail. <i>Journal of Chemical Physics</i> , 1988 , 89, 3718-3732	3.9	271
2012	Conformational differences between alpha-cyclodextrin in aqueous solution and in crystalline form. A molecular dynamics study. 1988 , 203, 241-50		96
2011	Protein-ligand dynamics. A 96 picosecond simulation of a myoglobin-xenon complex. 1988 , 199, 195-211		65
2010	Molecular dynamics simulation of despentapeptide insulin in a crystalline environment. 1988 , 200, 571-7		9
2009	A molecular dynamics study of the structure of a model Langmuir monolayer of amphiphile molecules. <i>Journal of Chemical Physics</i> , 1988 , 89, 5898-5908	3.9	93
2008	Nonlinear Burnett coefficients. 1988 , 38, 5249-5252		10
2007	A velocity reset method of simulating thermal motion and damping in gas-solid collisions. <i>Journal of Chemical Physics</i> , 1988 , 88, 5934-5942	3.9	61
2006	Nonlinear equation for a one-dimensional oscillator: Resonance zones and the transition to large-scale irregular dynamics. 1988 , 38, 3120-3123		9
2005	Structures and energetics of monovalent ion-water microclusters. II. Thermal phenomena. <i>Journal of Chemical Physics</i> , 1988 , 89, 7492-7501	3.9	45
2004	On the Approximation of Solvent Effects on the Conformation and Dynamics of Cyclosporin A by Stochastic Dynamics Simulation Techniques. 1988 , 1, 369-383		59
2003	Three-dimensional solution structure of plastocyanin from the green alga <i>Scenedesmus obliquus</i> . 1988 , 240, 314-7		91
2002	A Gaussian Wave Packet Method for Studying Dissociation of Diatomic Molecules on Solid Surfaces. 1988 , 206-209		

2001	Procylin gene expression and loss of the variant surface glycoprotein during differentiation of <i>Trypanosoma brucei</i> . 1989 , 108, 737-46		262
2000	Nonequilibrium molecular dynamics of liquid sulfur in Couette flow. <i>Journal of Chemical Physics</i> , 1989 , 91, 3662-3669	3.9	3
1999	Treatment of rotational isomers in free energy calculations. II. Molecular dynamics simulation study of 18-crown-6 in aqueous solution as an example of systems with large numbers of rotational isomeric states. <i>Journal of Chemical Physics</i> , 1989 , 91, 3631-3637	3.9	82
1998	A perturbation-trajectory method for the study of gas-surface collision dynamics. <i>Journal of Chemical Physics</i> , 1989 , 90, 3363-3372	3.9	5
1997	Treatment of rotational isomers in free energy evaluations. Analysis of the evaluation of free energy differences by molecular dynamics simulations of systems with rotational isomeric states. <i>Journal of Chemical Physics</i> , 1989 , 90, 3300-3304	3.9	63
1996	The lag between the Hamiltonian and the system configuration in free energy perturbation calculations. <i>Journal of Chemical Physics</i> , 1989 , 91, 7831-7839	3.9	110
1995	Anisotropic spread of surface dimer openings in the initial stages of the epitaxial growth of Si on Si{100}. 1989 , 63, 302-305		70
1994	Molecular Dynamics Simulations of some Small Organic Molecules. 1989 , 4, 193-207		5
1993	A molecular dynamics study of the nematic phase of 4-n-pentyl-4'-cyanobiphenyl. 1989 , 6, 357-371		103
1992	Canonical molecular dynamics simulation. 1989 , 68, 1341-1352		4
1991	A combined 2D-NMR and molecular dynamics analysis of the structure of the actinomycin D: d(ATGCAT) ₂ complex. 1989 , 6, 929-69		18
1990	Three-dimensional solution structure of a single zinc finger DNA-binding domain. 1989 , 245, 635-7		580
1989	Molecular dynamics simulation techniques for determination of molecular structures from nuclear magnetic resonance data. 1989 , 177, 204-18		80
1988	Conformational aspects of β -hydroxy carboxylic acids, the heralds of stereochemistry. 1989 , 200, 169-187		11
1987	Application of molecular dynamics in the crystallographic refinement of colicin A. 1989 , 45 (Pt 7), 471-7		5
1986	Crystallographic refinement by incorporation of molecular dynamics: thermostable serine protease thermolysin complexed with eglin c. 1989 , 45 (Pt 5), 488-99		39
1985	Conformational Analysis of Didemnins. A multidisciplinary approach by means of X-Ray, NMR, molecular-dynamics, and molecular-mechanics techniques. 1989 , 72, 530-555		40
1984	Peptidkonformationen, 50. Synthese und Konformationsanalyse von cyclischen Alanin-Analogen des Thymopointins durch NMR-Spektroskopie und Molecular-Dynamics-Rechnungen im Vakuum und in Lösung. 1989 , 1989, 269-294		7

1983	Conformation of Antamanide. 1989 , 1989, 913-928	25
1982	NMR-Spectroscopic Assignment of the Aib-Methyl Groups in α -Helical and β -Turn Environment with the Use of Selectively Deuterated Aib The Solution Conformations of Boc-Ala-Aib-Ala-OMe. 1989 , 1989, 1017-1027	8
1981	Potential of mean force by thermodynamic integration: Molecular-dynamics simulation of decomplexation. 1989 , 164, 370-376	55
1980	Time-dependent distance restraints in molecular dynamics simulations. 1989 , 157, 289-294	245
1979	Glass transition in SPC/E water and in a protein solution: A molecular dynamics simulation study. 1989 , 154, 151-154	27
1978	Molecular dynamics simulation of protein hydration: Studies on tuna ferrocycytochrome-c and bovine erythrocyte superoxide dismutase. 1989 , 41, 193-206	1
1977	Simulation of finite patches of xenon on graphite. 1989 , 129, 273-284	5
1976	Molecular-dynamics simulations of α -D-ribose and α -D-deoxyribose solutions. 1989 , 195, 133-146	21
1975	The effects of truncating long-range forces on protein dynamics. 1989 , 6, 32-45	224
1974	An NMR-based molecular dynamics simulation of the interaction of the lac repressor headpiece and its operator in aqueous solution. 1989 , 6, 104-27	60
1973	Dynamical structure of carboxypeptidase A. 1989 , 207, 201-16	29
1972	Molecular dynamics refinement of a thermitase-eglin-c complex at 1.98 Å resolution and comparison of two crystal forms that differ in calcium content. 1989 , 210, 347-67	97
1971	Protein Stability and Function. 1989 , 149-159	3
1970	On the attribution of binding energy in antigen-antibody complexes McPC 603, D1.3, and HyHEL-5. 1989 , 28, 4735-49	384
1969	Water-like melting behaviour of SiO ₂ investigated by the molecular dynamics simulation technique. 1989 , 60, 753-775	80
1968	Isothermal̄obaric molecular dynamics simulation of polymorphic phase transitions in alkali halides. <i>Journal of Chemical Physics</i> , 1989 , 91, 3148-3159	3.9 25
1967	Counterion N.M.R. in heterogeneous aqueous systems. 1989 , 67, 537-573	54
1966	Computer Simulation by Molecular Dynamics as a Tool for Modelling of Molecular Systems. 1989 , 3, 187-200	7

1965	Molecular Dynamics Modelling of Polymer Materials. 1989 , 3, 27-47	43
1964	Predicting the Rheology of Complex Fluids. 1989 , 2, 253-279	17
1963	Tertiary structure of two-electron reduced <i>Megasphaera elsdenii</i> flavodoxin and some implications, as determined by two-dimensional ¹ H-NMR and restrained molecular dynamics. 1990 , 194, 185-98	33
1962	Slow-cooling protocols for crystallographic refinement by simulated annealing. 1990 , 46 (Pt 7), 585-93	420
1961	Molecular-dynamics simulation of crystalline 18-crown-6: thermal shortening of covalent bonds. 1990 , 46, 222-229	76
1960	Can the structure of proteins be calculated?. 1990 , 78, 137-143	10
1959	Hydrogen-bond geometry around sugar molecules: comparison of crystal statistics with simulated aqueous solutions. 1990 , 237, 315-325	46
1958	Mass and step length optimization for the calculation of equilibrium properties by molecular dynamics simulation. 1990 , 166, 425-428	52
1957	Fundamental aspects of chemical kinetics in condensed phases. 1990 , 149, 63-80	8
1956	Dynamical correlations in a binary metastable fluid. 1990 , 149, 221-231	12
1955	Solvent effect on the conformation of the hydroxymethyl group established by molecular dynamics simulations of methyl- ¹³ C-D-glucoside in water. 1990 , 29, 1243-1248	75
1954	A molecular dynamics investigation of the elastomeric restoring force in elastin. 1990 , 29, 1613-31	71
1953	Molecular dynamics simulation of the solution structure of the C-terminal fragment of L7/L12 ribosomal protein. 1990 , 30, 205-209	17
1952	Restrained and unrestrained molecular dynamics simulations in the NVT ensemble of alamethicin. 1990 , 30, 1083-99	47
1951	Molekulardynamik-Computersimulationen; Methodik, Anwendungen und Perspektiven in der Chemie. 1990 , 102, 1020-1055	83
1950	Solution Structure of [Me-L-Leu ⁷]Didemnin B Determined by NMR Spectroscopy and Refined by MD Calculation. 1990 , 73, 25-47	23
1949	Variable step molecular dynamics: An exploratory technique for peptides with fixed geometry. 1990 , 11, 468-486	50
1948	ARGOS, a vectorized general molecular dynamics program. 1990 , 11, 943-951	62

1947	Conserving energy during molecular dynamics simulations of water, proteins, and proteins in water. 1990 , 11, 1169-1180		82
1946	Hybrid molecular dynamics. 1990 , 60, 311-318		25
1945	Molecular dynamics simulation of ferrous and ferric ions in water. 1990 , 144, 353-362		43
1944	Molecular dynamics study of the primitive model of 1B electrolyte solutions. 1990 , 142, 203-211		18
1943	Parallelization of a molecular dynamics non-bonded force algorithm for MIMD architecture. 1990 , 14, 219-224		17
1942	Potentials and correlation functions for the copper halide and silver iodide melts. II. Time correlation functions and ionic transport properties. 1990 , 2, 6643-6650		32
1941	Molecular dynamics simulations of active site mutants of triosephosphate isomerase. 1990 , 3, 677-90		10
1940	Modified Nosé-Hoover equation for a one-dimensional oscillator: Enforcement of the virial theorem. 1990 , 42, 7467-7470		22
1939	Accurate solution of a highly asymmetric electrolyte: Molecular dynamics simulation and integral equation. <i>Journal of Chemical Physics</i> , 1990 , 93, 1376-1385	3.9	56
1938	Nonequilibrium molecular dynamics via a nondiverging subtraction technique. 1990 , 42, 5912-5916		4
1937	Molecular dynamics of liquid SiO ₂ under high pressure. 1990 , 42, 2081-2089		89
1936	Thermal dissociation of diatomics in inert gases: A Nosé equation approach. <i>Journal of Chemical Physics</i> , 1990 , 93, 5616-5620	3.9	2
1935	Molecular Dynamics Simulations of Phenyl-4-(4-benzoyloxy-)benzoyloxy-benzoate in the Crystalline and Nematic Phase. 1990 , 185, 141-153		4
1934	Application of the thermodynamic cycle perturbation method to systems with nonadditive potentials. <i>Journal of Chemical Physics</i> , 1990 , 93, 2762-2768	3.9	7
1933	Using molecular dynamics simulations on crambin to evaluate the suitability of different continuum dielectric and hydrogen atom models for protein simulations. 1990 , 7, 1019-41		15
1932	Inclusion of thermal motion in crystallographic structures by restrained molecular dynamics. 1990 , 249, 1149-52		114
1931	Pair Potentials from ab initio Calculations for use in MD Simulations of Molten Alkali Carbonates. 1990 , 5, 83-98		16
1930	Molecular-dynamics simulation of molten alkali carbonates. 1990 , 71, 413-426		37

1929	Computation Confirms Contraction: A Molecular Dynamics Study of Liquid Methanol, Water and a Methanol-Water Mixture. 1990 , 5, 175-179	15
1928	Molecular Dynamics Simulations with Interaction Potentials Including Polarization Development of a Noniterative Method and Application to Water. 1990 , 5, 181-192	108
1927	Conformation-activity relationship of sweet molecules. Comparison of aspartame and naphthimidazolesulfonic acids. 1990 , 33, 514-20	33
1926	Molecular dynamics study of the structure and dynamics of a protein molecule in a crystalline ionic environment, <i>Streptomyces griseus</i> protease A. 1990 , 29, 8658-76	56
1925	Time-averaged nuclear Overhauser effect distance restraints applied to tendamistat. 1990 , 214, 223-35	265
1924	Refinement of the influenza virus hemagglutinin by simulated annealing. 1990 , 212, 737-61	188
1923	Calculation of the relative binding free energy of 2'GMP and 2'AMP to ribonuclease T1 using molecular dynamics/free energy perturbation approaches. 1990 , 212, 197-209	36
1922	Insights into the function of the zinc hydroxide-Thr199-Glu106 hydrogen bonding network in carbonic anhydrases. 1990 , 214, 799-802	88
1921	Structure of vancomycin and a vancomycin/D-Ala-D-Ala complex in solution. 1990 , 29, 2271-7	35
1920	Isobaric and Isothermal Molecular Dynamics Simulations of Diatomic Systems. 1990 , 4, 371-398	3
1919	Computer simulation of glass structures. 1990 , 123, 48-70	40
1918	Computational methods for determining protein structures from NMR data. 1990 , 40, 15-22	62
1917	Solution conformation of purine-pyrimidine DNA octamers using nuclear magnetic resonance, restrained molecular dynamics and NOE-based refinement. 1990 , 215, 411-28	48
1916	Cooperative ligand reorientations in cytochrome c3: a molecular dynamics simulation. 1991 , 1058, 83-4	1
1915	Crystallographic phasing and refinement of macromolecules. 1991 , 1, 1016-1022	24
1914	Systolic Loop Methods for Molecular Dynamics Simulation, Generalised for Macromolecules. 1991 , 7, 59-69	10
1913	Computer Simulation of Liquid Methanol I. Molecular Dynamics on a Supernode Transputer Array. 1991 , 7, 155-169	2
1912	High-resolution solution structure of reduced French bean plastocyanin and comparison with the crystal structure of poplar plastocyanin. 1991 , 221, 533-55	104

1911	Interaction of troponin I and troponin C. Use of the two-dimensional nuclear magnetic resonance transferred nuclear Overhauser effect to determine the structure of the inhibitory troponin I peptide when bound to skeletal troponin C. 1991 , 222, 405-21		71
1910	The sensitivity of physical and spectral properties of silica glass to variations of interatomic potentials under high pressure. 1991 , 65, 210-230		19
1909	Na ⁺ Na ⁺ and Cl ⁻ Cl ⁻ ion pairs in water: Mean force potentials by constrained molecular dynamics. <i>Journal of Chemical Physics</i> , 1991 , 95, 2823-2831	3.9	149
1908	Time-correlation analysis of simulated water motion in flexible and rigid gramicidin channels. 1991 , 60, 273-85		81
1907	Microscopic theory of the dielectric properties of proteins. 1991 , 59, 670-90		89
1906	Collective vibrations of an alpha-helix. A molecular dynamics study. 1991 , 59, 795-804		17
1905	Transport Properties Computed by Linear Response through Weak Coupling to a Bath. 1991 , 139-155		39
1904	Diffusion of penetrants in amorphous polymers: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1991 , 94, 3192-3199	3.9	127
1903	Are time-averaged restraints necessary for nuclear magnetic resonance refinement? A model study for DNA. 1991 , 220, 457-79		133
1902	Calculation of relative free energy via indirect pathways. <i>Journal of Chemical Physics</i> , 1991 , 94, 3808-3816	3.9	70
1901	Combined procedures of distance geometry and molecular dynamics for determining protein structure from nuclear magnetic resonance data. 1991 , 202, 268-300		13
1900	Aspects of the design of conformationally constrained peptides. 1991 , 202, 411-36		5
1899	Studies on DNA-cleaving agents: computer modeling analysis of the mechanism of activation and cleavage of dynemicin-oligonucleotide complexes. 1991 , 88, 8835-9		36
1898	Coherent Nucleation and Growth of Martensite in B2 NiAl Observed in Computer Simulations. 1991 , 246, 3		5
1897	Atomistic Simulation of the Nanoindentation of Diamond and Graphite Surfaces. 1991 , 239, 573		15
1896	Atomistic mechanisms of adhesion and compression of diamond surfaces. 1991 , 206, 213-219		44
1895	Molecular dynamics simulations of the nanometer-scale mechanical properties of compressed Buckminsterfullerene. 1991 , 206, 220-223		168
1894	The effects of solvent on the conformation and the collective motions of protein: Normal mode analysis and molecular dynamics simulations of melittin in water and in vacuum. 1991 , 158, 447-472		335

1893	Conformation and aggregation of M13 coat protein studied by molecular dynamics. 1991 , 41, 193-202	16
1892	Hydrogen bonds in concreto and in computro: the sequel. 1991 , 243, 61-87	8
1891	Conformational analysis of antitumor cyclic hexapeptides, RA series. 1991 , 47, 2757-2772	54
1890	Structure solution and molecular dynamics refinement of the yeast Cu,Zn enzyme superoxide dismutase. 1991 , 47 (Pt 6), 918-27	20
1889	STRUCTURE OF BACTERIORHODOPSIN and in situ ISOMERIZATION OF RETINAL: A MOLECULAR DYNAMICS STUDY*. 1991 , 54, 937-948	36
1888	Calculations of relative free energy surfaces in configuration space using an integration method. 1991 , 179, 475-478	20
1887	Host-guest preorganization and complementarity: A molecular mechanics and molecular dynamics study of cation complexes of a cyclic urea-anisole spherand. 1991 , 12, 994-1007	13
1886	Molecular dynamics simulations of small peptides: dependence on dielectric model and pH. 1991 , 31, 285-304	72
1885	Conformational energy minimization by simulated annealing using molecular dynamics: Some improvements to the monitoring procedure. 1991 , 31, 663-670	10
1884	A molecular dynamics study of thermodynamic and structural aspects of the hydration of cavities in proteins. 1991 , 31, 919-31	67
1883	A molecular dynamics simulation of polyalanine: an analysis of equilibrium motions and helix-coil transitions. 1991 , 31, 1115-34	127
1882	Unfolding of an alpha-helix in water. 1991 , 31, 1351-61	130
1881	Solution structure of phalloidin obtained by NMR spectroscopy in [D6]DMSO and molecular dynamics calculation in vacuo and in water. 1991 , 1991, 179-184	11
1880	Potential of mean force by constrained molecular dynamics: A sodium chloride ion-pair in water. 1991 , 155, 187-195	190
1879	Stabilization of β -helical secondary structure during high-temperature molecular-dynamics simulations of β -lactalbumin. 1991 , 158, 295-301	14
1878	Free energy evaluation from molecular dynamics simulations using force fields including electronics polarization. 1991 , 177, 433-440	35
1877	The refinement of NMR structures by molecular dynamics simulation. 1991 , 62, 289-296	15
1876	A loose-coupling, constant-pressure, molecular dynamics algorithm for use in the modelling of polymer materials. 1991 , 62, 360-369	74

1875	Determination of the structure of an extracellular peptide produced by the mushroom saprotroph <i>Pseudomonas reactans</i> . 1991 , 47, 3645-3654		68
1874	The crystal structure of the "open" and the "closed" conformation of the flexible loop of trypanosomal triosephosphate isomerase. 1991 , 10, 33-49		79
1873	The adaptability of the active site of trypanosomal triosephosphate isomerase as observed in the crystal structures of three different complexes. 1991 , 10, 50-69		71
1872	Proline in alpha-helix: stability and conformation studied by dynamics simulation. 1991 , 10, 219-28		128
1871	Exploration of disorder in protein structures by X-ray restrained molecular dynamics. 1991 , 10, 340-58		90
1870	A 175-psec molecular dynamics simulation of camphor-bound cytochrome P-450cam. 1991 , 11, 184-204		67
1869	DNA bending studied by MD and 2D NMR NOESY simulations: Role of the junction sequence between the A/T tracts. 1991 , 40, 213-229		1
1868	Isomerization and inherent structures in liquids. A molecular dynamics study of liquid cyclohexane. <i>Journal of Chemical Physics</i> , 1991 , 95, 5953-5965	3.9	12
1867	Computer simulation of a model 2D electrolyte: Multiple time-step molecular dynamics. <i>Journal of Chemical Physics</i> , 1991 , 95, 9165-9171	3.9	22
1866	Experimental and molecular-dynamics study of the Ar emission mechanism during low-energy Ar ⁺ bombardment of Cu. 1991 , 43, 13695-13698		15
1865	Temperature and pressure constraints near the freezing point. 1991 , 43, 3514-3517		2
1864	Shear melting of colloids: A nonequilibrium phase diagram. 1991 , 66, 3004-3007		78
1863	Multiconfiguration thermodynamic integration. <i>Journal of Chemical Physics</i> , 1991 , 95, 1175-1188	3.9	226
1862	Automated modeling of coiled coils: application to the GCN4 dimerization region. 1991 , 4, 649-59		85
1861	Investigation of a poly(oxyethylene) chain by a molecular dynamics simulation in an aqueous solution and by Langevin dynamics simulations. 1991 , 74, 715-733		26
1860	MODELING OF MONOLAYERS. 1991 , 305-338		3
1859	Molecular Dynamics simulations of borate glasses. 1991 , 119-121, 493-498		15
1858	Analysis of active site motions from a 175 picosecond molecular dynamics simulation of camphor-bound cytochrome P450cam. 1991 , 9, 187-203		25

1857	Modeling DNA structures: molecular mechanics and molecular dynamics. 1992 , 211, 449-67		11
1856	Computer simulation on the temperature dependence of cooled ions in a Penning trap. 1992 , 46, 560-568		5
1855	3 Nsec molecular dynamics simulation of the protein ubiquitin and comparison with X-ray crystal and solution NMR structures. 1992 , 9, 935-49		14
1854	Molecular-dynamics studies of the structure and properties of monolayers of perfluorinated amphiphiles. <i>Journal of Chemical Physics</i> , 1992 , 96, 4735-4742	3.9	58
1853	Development of nonadditive intermolecular potentials using molecular dynamics: Solvation of Li ⁺ and F ⁻ ions in polarizable water. <i>Journal of Chemical Physics</i> , 1992 , 96, 6970-6977	3.9	202
1852	A molecular dynamics study of the packing structures in monolayers of partially fluorinated amphiphiles. <i>Journal of Chemical Physics</i> , 1992 , 96, 1352-1366	3.9	74
1851	Temperature dependence of interactions of an ion pair in water: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1992 , 97, 1919-1921	3.9	41
1850	Molecular-dynamics simulations of atomic-scale friction of diamond surfaces. 1992 , 46, 9700-9708		221
1849	Free energy perturbation calculations on multiple mutation bases. <i>Journal of Chemical Physics</i> , 1992 , 97, 6730-6736	3.9	19
1848	On the stability of type I gas hydrates in the presence of methanol. <i>Journal of Chemical Physics</i> , 1992 , 96, 5377-5382	3.9	28
1847	Random and ordered defects on ion-bombarded Si(100)-(2 x 1) surfaces. 1992 , 69, 3076-3079		93
1846	Use of molecular dynamics methods in conformational analysis. Glycol. A model study. <i>Journal of Chemical Physics</i> , 1992 , 97, 3639-3646	3.9	34
1845	Efficient Monte Carlo methods for the computer simulation of biological molecules. 1992 , 45, 8894-8901		98
1844	.		3
1843	Novel molecular dynamics simulations at constant pressure. 1992 , 75, 669-688		24
1842	Computer Simulation of Liquid Methanol II. System Size Effects. 1992 , 8, 273-283		19
1841	.		3
1840	Modeling DNA structures. 1992 , 43, 87-108		5

1839	Combining Molecular Dynamics and Monte Carlo Simulations to Model Chemical Vapor Deposition: Application to Diamond. 1992 , 278, 255		10
1838	Molecular dynamics simulation of the transport of small molecules across a polymer membrane. <i>Journal of Chemical Physics</i> , 1992 , 96, 4699-4704	3.9	182
1837	Structure and dynamics of the dilauroylphosphatidylethanolamine lipid bilayer. 1992 , 31, 7656-64		99
1836	Molecular-dynamics simulation of the growth of diamondlike films by energetic carbon-atom beams. 1992 , 68, 620-623		174
1835	Molecular dynamics simulations of dimer opening on a diamond {001}(2x1) surface. 1992 , 255, 835-8		182
1834	Empirical models for the hydration of protons. <i>Journal of Chemical Physics</i> , 1992 , 96, 3131-3136	3.9	58
1833	Structure and dynamics of water and aqueous solutions: The role of flexibility. <i>Journal of Chemical Physics</i> , 1992 , 96, 8450-8459	3.9	76
1832	Molecular dynamics simulations of ordered alkane chains physisorbed on graphite. <i>Journal of Chemical Physics</i> , 1992 , 96, 6213-6221	3.9	200
1831	Surface melting of the (0001) face of TIP4P ice. 1992 , 275, 365-382		172
1830	A molecular dynamics study of B2O3 glass using different interaction potentials. 1992 , 146, 267-278		47
1829	A molecular dynamics simulation of liquid benzene adsorbed on graphite. 1992 , 262, 180-188		18
1828	Nanoscale investigation of indentation, adhesion and fracture of diamond (111) surfaces. 1992 , 271, 57-67		96
1827	Leapfrog Rotational Algorithms. 1992 , 8, 165-178		193
1826	Polarizability effects in a four-charge model for water. <i>Journal of Chemical Physics</i> , 1992 , 96, 3120-3130	3.9	77
1825	Simulation of the thermal denaturation of hen egg white lysozyme: trapping the molten globule state. 1992 , 31, 7745-8		141
1824	Stress relaxation in a polymer melt of freely-rotating chains. <i>Journal of Chemical Physics</i> , 1992 , 97, 8698-8704	3.9	20
1823	Liquid-vapor interfaces of alkane oligomers: structure and thermodynamics from molecular dynamics simulations of chemically realistic models. 1992 , 96, 5077-5086		183
1822	Molecular dynamics of discotics in the isotropic phase. <i>Journal of Chemical Physics</i> , 1992 , 96, 2306-2317	3.9	18

1821	Molecular dynamics simulation of gas transport in amorphous polypropylene. <i>Journal of Chemical Physics</i> , 1992 , 96, 3200-3205	3.9	88
1820	Investigation of the solution conformation of cytochrome c-551 from <i>Pseudomonas stutzeri</i> . 1992 , 31, 8603-12		29
1819	Three-dimensional solution structure of Ca(2+)-loaded porcine calbindin D9k determined by nuclear magnetic resonance spectroscopy. 1992 , 31, 1011-20		43
1818	Determination of the solution structure of a synthetic two-site calcium-binding homodimeric protein domain by NMR spectroscopy. 1992 , 31, 9572-80		34
1817	Molecular-dynamics simulations of interfaces between water and crystalline urea. <i>Journal of Chemical Physics</i> , 1992 , 96, 7010-7018	3.9	43
1816	Molecular dynamics simulations on HiPIP from <i>Chromatium vinosum</i> and comparison with NMR data. 1992 , 114, 10683-10689		29
1815	Molecular dynamics simulation of solvated protein at high pressure. 1992 , 31, 10083-93		132
1814	Crystal structure solution and refinement of the semisynthetic cobalt-substituted bovine erythrocyte superoxide dismutase at 2.0 Å resolution. 1992 , 226, 227-38		46
1813	Crystal structure of yeast Cu,Zn superoxide dismutase. Crystallographic refinement at 2.5 Å resolution. 1992 , 225, 791-809		110
1812	Solution structure of the fibrin binding finger domain of tissue-type plasminogen activator determined by 1H nuclear magnetic resonance. 1992 , 225, 821-33		47
1811	Modeling of the structure of bacteriorhodopsin. A molecular dynamics study. 1992 , 226, 837-50		46
1810	Human epidermal growth factor. High resolution solution structure and comparison with human transforming growth factor alpha. 1992 , 227, 271-82		123
1809	Taming cut-off induced artifacts in molecular dynamics studies of solvated polypeptides. The reaction field method. 1992 , 228, 909-23		82
1808	Conformational search by potential energy annealing: algorithm and application to cyclosporin A. 1992 , 6, 97-112		38
1807	Conformational transition of an alpha-helix studied by molecular dynamics. 1992 , 21, 63-70		6
1806	Molecular dynamics studies of a DNA-binding protein: 1. A comparison of the trp repressor and trp aporepressor aqueous simulations. 1992 , 1, 1173-84		20
1805	Molecular dynamics studies of a DNA-binding protein: 2. An evaluation of implicit and explicit solvent models for the molecular dynamics simulation of the <i>Escherichia coli</i> trp repressor. 1992 , 1, 1185-205		93
1804	Substrate mobility in a deeply buried active site: analysis of norcamphor bound to cytochrome P-450cam as determined by a 201-psec molecular dynamics simulation. 1992 , 13, 26-37		19

1803	MD simulation of subtilisin BPN' in a crystal environment. 1992 , 14, 451-64	15
1802	Phase behaviour of metastable water. 1992 , 360, 324-328	1465
1801	A 1H-NMR and MD study of intramolecular hydrogen bonds in methyl beta-cellobioside. 1992 , 230, 41-61	93
1800	Presto(protein engineering simulator): A vectorized molecular mechanics program for biopolymers. 1992 , 16, 243-248	161
1799	Computer simulation of aromatic polyesters including molecular dynamics. 1992 , 33, 398-404	13
1798	Rotamer interconversion and its influence on the fluorescence decay of tyrosine: a molecular dynamics study. 1992 , 45, 41-50	12
1797	Free energy calculations in molecular biophysics. 1992 , 76, 251-275	79
1796	On the correlation between like ion pairs in water. <i>Journal of Chemical Physics</i> , 1992 , 96, 4046-4047	3.9 64
1795	Electrostatic forces and the structural stability of a modelled bacteriophage T4 glutaredoxin fold: molecular dynamics simulations of polyglycine 87-mers. 1992 , 256, 295-314	11
1794	Interaction of troponin I and troponin C: use of the two-dimensional transferred nuclear Overhauser effect to determine the structure of a Gly-110 inhibitory troponin I peptide analog when bound to cardiac troponin C. 1992 , 1160, 35-54	23
1793	A note on low energy recoils in collisional mixing. 1992 , 66, 508-510	3
1792	The conformational behaviour of the cardiac glycoside digoxin as indicated by NMR spectroscopy and molecular dynamics calculations. 1992 , 230, 201-12	15
1791	Computational evidence for anomalous diffusion of small molecules in amorphous polymers. 1992 , 199, 237-243	131
1790	Dynamic properties of salmon calcitonin bound to sodium dodecyl sulfate micelles: a restrained molecular dynamics study from NMR data. 1992 , 2, 335-48	18
1789	Three-dimensional solution structure of apo-neocarzinostatin from <i>Streptomyces carzinostaticus</i> determined by NMR spectroscopy. 1992 , 203, 505-11	28
1788	On the interpretation of biochemical data by molecular dynamics computer simulation. 1992 , 204, 947-61	105
1787	Neuropeptide Y. Optimized solid-phase synthesis and conformational analysis in trifluoroethanol. 1992 , 206, 39-48	41
1786	The three-dimensional structure of guanine-specific ribonuclease F1 in solution determined by NMR spectroscopy and distance geometry. 1992 , 208, 41-51	5

1785	The structure of the mammalian antibacterial peptide cecropin P1 in solution, determined by proton-NMR. 1992 , 209, 163-9	80
1784	Determination of the three-dimensional solution structure of the histidine-containing phosphocarrier protein HPr from Escherichia coli using multidimensional NMR spectroscopy. 1992 , 210, 881-91	24
1783	Anti-insulin antibody structure and conformation. II. Molecular dynamics with explicit solvent. 1992 , 32, 23-32	23
1782	Molecular dynamics study of the conformational behavior of a representative elastin building block: Boc-Gly-Val-Gly-Gly-Leu-OMe. 1992 , 32, 161-72	43
1781	Combined use of homo- and heteronuclear coupling constants as restraints in molecular dynamics simulations. 1992 , 32, 1277-82	33
1780	An MD simulation on the applicability of the diffusion equation for molecules adsorbed in a zeolite. 1992 , 198, 283-287	53
1779	Holonomic constraint contributions to free energy differences from thermodynamic integration molecular dynamics simulations. 1992 , 196, 297-302	51
1778	Fluoride-fluoride association in water from molecular dynamics simulations. 1992 , 200, 21-25	59
1777	Free energy perturbation calculations involving potential function changes. 1992 , 13, 362-370	29
1776	Precision of free energies calculated by molecular dynamics simulations of peptides in solution. 1992 , 13, 429-442	52
1775	THE weighted histogram analysis method for free-energy calculations on biomolecules. I. The method. 1992 , 13, 1011-1021	4722
1774	Peptide Conformation from Coupling Constants: Scalar Couplings as Restraints in MD Simulations. 1992 , 75, 2583-2592	19
1773	Molecular dynamics simulations of alumina surface stabilization by deposited silicon ions. 1993 , 211, 575-579	12
1772	The viscosity of SPC and SPC/E water at 277 and 300 K. 1993 , 215, 315-318	141
1771	Force oscillations and liquid structure in simulations of an atomic force microscope tip in a liquid. 1993 , 211, 328-332	21
1770	Solvation of ammonium ion. A molecular dynamics simulation with nonadditive potentials. 1993 , 213, 541-546	13
1769	Structure elucidation from rotation spectra: a penalty function approach. 1993 , 203, 88-92	2
1768	YASP: A molecular simulation package. 1993 , 78, 77-94	163

1767	Parallel molecular dynamics on a multi signalprocessor system. 1993 , 75, 65-86	3
1766	Synthesis, conformation, and activity of HCO-Met-delta Z Leu-Phe-OMe, an active analogue of chemotactic N-formyltripeptides. 1993 , 33, 437-51	31
1765	Molecular dynamics study of iduronate ring conformation. 1993 , 33, 575-588	67
1764	Molecular dynamics simulation of the stability of a 22-residue alpha-helix in water and 30% trifluoroethanol. 1993 , 33, 1159-66	94
1763	Molecular dynamics analysis of a ribonuclease C-peptide analogue. 1993 , 33, 1567-80	22
1762	Synthesis and Solvent Effects on the Conformation of Hymenistatin 1. 1993 , 76, 1649-1666	21
1761	Observations concerning the treatment of long-range interactions in molecular dynamics simulations. 1993 , 14, 278-284	87
1760	Conformational and energetic effects of truncating nonbonded interactions in an aqueous protein dynamics simulation. 1993 , 14, 295-311	90
1759	Conformational analysis and molecular dynamics simulation of cellobiose and larger celooligomers. 1993 , 14, 831-847	52
1758	Molecular dynamics simulation of cellobiose in water. 1993 , 14, 848-857	56
1757	AMBER force-field parameters for guanosine triphosphate and its imido and methylene analogs. 1993 , 14, 995-1005	8
1756	Comparison of two force fields by molecular dynamics simulations of glucose crystals: Effect of using ewald sums. 1993 , 14, 1281-1289	34
1755	Computation of the mean residence time of water in the hydration shells of biomolecules. 1993 , 14, 1396-1406	130
1754	Conformations of triglycyl-lysylvasopressin: 1H NMR spectroscopic and molecular dynamics study. 1993 , 31, 481-488	4
1753	On the diffusion mechanism of methane in a cation-free zeolite of type ZK4. 1993 , 174, 229-236	41
1752	Helix propensity of Ala and Val: a free energy perturbation study. 1993 , 47, 113-21	1
1751	Effect of atomic-scale surface roughness on friction: A molecular dynamics study of diamond surfaces. 1993 , 168, 127-133	88
1750	An approximate but efficient method to calculate free energy trends by computer simulation: application to dihydrofolate reductase-inhibitor complexes. 1993 , 7, 305-23	38

1749	Thermodynamic integration calculations of binding free energy difference for Gly-169 mutation in subtilisin BPN'. 1993 , 15, 5-9		19
1748	Characterization of proline-containing alpha-helix (helix F model of bacteriorhodopsin) by molecular dynamics studies. 1993 , 15, 26-41		34
1747	Absolute and relative binding free energy calculations of the interaction of biotin and its analogs with streptavidin using molecular dynamics/free energy perturbation approaches. 1993 , 16, 226-45		198
1746	A molecular dynamics study of solvent behavior around a protein. 1993 , 16, 268-77		47
1745	Molecular dynamics study of structure and stability of a model coiled coil. 1993 , 16, 384-92		21
1744	Essential dynamics of proteins. 1993 , 17, 412-25		2518
1743	Investigations of the thermostability of rubredoxin models using molecular dynamics simulations. 1993 , 2, 650-65		14
1742	Molecular dynamics in refinement against fiber diffraction data. 1993 , 49, 504-13		32
1741	Conformation dynamics in peptides: quantum chemical calculations and molecular dynamics simulations on N-acetylalanyl-N'-methylamide. 1993 , 285, 211-219		30
1740	Gas sorption and transport in polyisobutylene: Equilibrium and nonequilibrium molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1993 , 98, 9895-9904	3.9	99
1739	Melting of Yukawa systems: A test of phenomenological melting criteria. <i>Journal of Chemical Physics</i> , 1993 , 98, 2319-2324	3.9	120
1738	Simulations of aqueous solutions: the role of flexibility and the treatment of long-range forces. 1993 , 88, 79-87		13
1737	Lipid Membrane Structure and Dynamics Studied by All-Atom Molecular Dynamics Simulations of Hydrated Phospholipid Bilayers. 1993 , 10, 335-362		90
1736	Solution structure of lariat RNA by 500 MHz NMR spectroscopy and molecular dynamics studies in water. 1993 , 27, 229-59		20
1735	Dynamical properties of bovine pancreatic trypsin inhibitor from a molecular dynamics simulation at 5000 atm. 1993 , 323, 215-7		40
1734	Molecular dynamics study of the transport properties of perovskite melts under high temperature and pressure conditions. 1993 , 114, 373-384		27
1733	Conformational analysis of arachidonic and related fatty acids using molecular dynamics simulations. 1993 , 1178, 87-96		49
1732	Molecular dynamics investigation of the MBE growth of Si on Si{110}. 1993 , 284, 91-102		12

1731	Surface and bulk properties of metals modelled with Sutton-Chen potentials. 1993 , 281, 191-206		130
1730	Parallel Computing and Molecular Dynamics Simulations. 1993 , 473-495		5
1729	Transferability of ion models. 1993 , 97, 6524-6529		29
1728	Shell model simulations by adiabatic dynamics. 1993 , 5, 1031-1038		173
1727	Phase diagram for amorphous solid water. 1993 , 48, 4605-4610		163
1726	Optical activity of hemoproteins in the Soret region. Circular dichroism of the heme undecapeptide of cytochrome c in aqueous solution. 1993 , 32, 6674-9		121
1725	Computer simulation of a phospholipid monolayer-water system: The influence of long range forces on water structure and dynamics. <i>Journal of Chemical Physics</i> , 1993 , 98, 9798-9807	3.9	97
1724	Intermediate ordering in a liquid supported monolayer: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1993 , 99, 7020-7029	3.9	16
1723	Molecular dynamics simulation study of the adsorption of chain alkanes from solution onto graphite. <i>Journal of Chemical Physics</i> , 1993 , 99, 5528-5534	3.9	53
1722	Computer Simulation of Molecular Motions in Liquids: Infrared Spectra of Water and Heavy Water. 1993 , 11, 321-336		29
1721	Solution structure by 2D 1H-NMR of a chimeric peptide recognized by galanin and neuropeptide Y receptors. 1993 , 32, 7787-98		17
1720	Spinodal of liquid water. 1993 , 48, 3799-3817		188
1719	A molecular dynamics study of the bis-intercalation complexes of echinomycin with d(ACGT) ₂ and d(TCGA) ₂ : rationale for sequence-specific Hoogsteen base pairing. 1993 , 36, 1548-61		29
1718	Solvent-dependent conformation and hydrogen-bonding capacity of cyclosporin A: evidence from partition coefficients and molecular dynamics simulations. 1993 , 36, 3757-64		169
1717	Molecular dynamics simulation of winter flounder antifreeze protein variants in solution: correlation between side chain spacing and ice lattice. 1993 , 6, 19-27		33
1716	Molecular dynamics study of the lauryl alcohol-laurate model bilayer. 1993 , 64, 1344-53		6
1715	Liquid benzene confined between graphite surfaces. A constant pressure molecular dynamics study. <i>Journal of Chemical Physics</i> , 1993 , 99, 5405-5417	3.9	29
1714	Leapfrog Rotational Algorithms for Linear Molecules. 1993 , 11, 79-89		30

1713	Dynamic surface boundary conditions. 1993 , 79, 623-644		30
1712	Constant pressure molecular dynamics: Instantaneous external stress tensor in systems with periodic boundary conditions. 1993 , 65, 11-17		
1711	Stick and Slip Behaviour of Confined Oligomer Melts under Shear. A Molecular-Dynamics Study. 1993 , 24, 99-104		48
1710	Comment on molecular dynamics simulations of monolayers of fluorinated amphiphiles. <i>Journal of Chemical Physics</i> , 1993 , 98, 3469-3474	3.9	44
1709	Molecular dynamics simulations of aqueous ionic clusters using polarizable water. <i>Journal of Chemical Physics</i> , 1993 , 99, 6950-6956	3.9	163
1708	Solvent effect on translational diffusivity and orientational mobility of polymers in solution: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1993 , 99, 2235-2246	3.9	9
1707	Structure of H+(H ₂ O) _n clusters near the magic number n=21. <i>Journal of Chemical Physics</i> , 1993 , 99, 2978-2984	3.9	43
1706	Chemical sputtering of Si related to roughness formation of a Cl-passivated Si surface. 1993 , 74, 1303-1309		114
1705	The limiting behavior of water hydrating a phospholipid monolayer: A computer simulation study. <i>Journal of Chemical Physics</i> , 1993 , 99, 5547-5559	3.9	118
1704	Mobility of stretched water. <i>Journal of Chemical Physics</i> , 1993 , 98, 9859-9862	3.9	24
1703	Photoelectron spectra of the hydrated iodine anion from molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1993 , 99, 2972-2977	3.9	188
1702	Si-adatom dynamics and mechanisms of the epitaxial growth on a single-height-stepped Si{001} surface. 1993 , 47, 4464-4474		44
1701	Effect of pressure on molecular photodissociation in matrices: Molecular dynamics simulations of Cl ₂ in Xe. <i>Journal of Chemical Physics</i> , 1993 , 98, 331-335	3.9	21
1700	Calculations of the relative free energies of aqueous solvation of several fluorocarbons: A test of the bond potential of mean force correction. <i>Journal of Chemical Physics</i> , 1993 , 99, 9103-9110	3.9	25
1699	Molecular dynamics with combined quantum and empirical potentials: C ₂ H ₂ adsorption on Si(100). <i>Journal of Chemical Physics</i> , 1993 , 99, 1356-1372	3.9	89
1698	Stress-induced failure and melting of ideal solids. <i>Journal of Chemical Physics</i> , 1993 , 98, 9808-9818	3.9	21
1697	Sensitivity analysis of water thermodynamics. <i>Journal of Chemical Physics</i> , 1993 , 98, 8892-8899	3.9	43
1696	Molecular-dynamics simulation of stress relaxation on a triangular lattice. 1993 , 47, 7659-7667		39

1695	Crystallographic Refinement and Structure-Factor Time-Averaging by Molecular Dynamics in the Absence of a Physical Force Field. 1993 , 10, 377-395	14
1694	Atomistic Simulations of Friction at Sliding Diamond Interfaces. 1993 , 18, 50-53	44
1693	Computational challenges for macromolecular structure determination by X-ray crystallography and solution NMR-spectroscopy. 1993 , 26, 49-125	143
1692	Molecular dynamics study of the base pair opening process in the self-complementary octanucleotide d(CTGATCAG). 1993 , 11, 43-56	16
1691	Molecular dynamics of water transport through membranes: Water from solvent to solute. 1993 , 65, 2513-2520	44
1690	Multiple Time Steps: Limits on the Speedup of Molecular Dynamics Simulations of Aqueous Systems. 1993 , 11, 67-77	19
1689	Structure as a function of relaxation in glassy polymers. 1993 , 65, 99-107	
1688	Computer simulation of stress relaxation. 1993 , 65, 109-121	1
1687	Stress/strain analysis of polymeric materials by molecular dynamics simulations. 1993 , 65, 123-132	2
1686	Atomic-detail simulation studies of tilted smectics. 1994 , 6, A261-A268	18
1685	Molecular Dynamics Simulation of Equine Infectious Anemia Virus Tat Protein in Water and in 40% Trifluoroethanol. 1994 , 12, 19-36	10
1684	Molecular Dynamics Simulations With First Order Coupling to a Bath of Constant Chemical Potential. 1994 , 14, 21-34	9
1683	On The Berendsen Thermostat. 1994 , 13, 177-187	91
1682	Investigation of domain motions in bacteriophage T4 lysozyme. 1994 , 12, 457-74	18
1681	Molecular Dynamics Simulations of Chiral Nematic Liquid Crystals. 1994 , 63, 1025-1030	18
1680	Molecular modeling of the enthalpies of adsorption of hydrocarbons on smectite clay. 1994 , 98, 279-284	32
1679	Supercomputing Studies of Biomembranes. 1994 , 8, 6-23	8
1678	Influence of a mutation in the transmembrane domain of the p185c-erbB2 oncogene-encoded protein studied by molecular dynamics simulations. 1994 , 11, 983-1002	15

1677	Molecular dynamics simulations of phospholipid bilayers. 1994 , 11, 927-56		56
1676	Molecular dynamics simulation of protein denaturation: solvation of the hydrophobic cores and secondary structure of barnase. 1994 , 91, 1746-50		156
1675	Molecular dynamics simulations of a r(GA12G).d(CT12C) hybrid duplex. 1994 , 11, 1161-74		13
1674	Computer simulation studies of a model system for liquid crystals consisting of semiflexible molecules. <i>Journal of Chemical Physics</i> , 1994 , 101, 3157-3171	3.9	31
1673	Low frequency depolarized Raman spectra in water: Results from normal mode analysis. <i>Journal of Chemical Physics</i> , 1994 , 100, 5361-5366	3.9	31
1672	Molecular dynamics simulation of crystalline poly(ethylene oxide). <i>Journal of Chemical Physics</i> , 1994 , 101, 10064-10073	3.9	97
1671	Ab initio studies of hydrocarbon adsorption on stepped diamond surfaces. 1994 , 50, 15369-15380		23
1670	Confined thin films of a linear and branched octane. A comparison of the structure and solvation forces using molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1994 , 100, 3276-3285	3.9	89
1669	Comparative molecular dynamics simulation study of the benzene-graphite and the benzene-1,12-dodecanediol-graphite interface. <i>Journal of Chemical Physics</i> , 1994 , 100, 3930-3939	3.9	14
1668	Effect of shear on the desorption of oligomers in nanoscopically confined films. <i>Journal of Chemical Physics</i> , 1994 , 101, 1721-1724	3.9	32
1667	Consistent dielectric properties of the simple point charge and extended simple point charge water models at 277 and 300 K. <i>Journal of Chemical Physics</i> , 1994 , 100, 3169-3174	3.9	186
1666	Change of bond length in free-energy simulations: Algorithmic improvements, but when is it necessary?. <i>Journal of Chemical Physics</i> , 1994 , 100, 9129-9139	3.9	29
1665	Treatment of rotational isomeric states. III. The use of biasing potentials. <i>Journal of Chemical Physics</i> , 1994 , 101, 5032-5039	3.9	35
1664	Symplectic integrators for large scale molecular dynamics simulations: A comparison of several explicit methods. <i>Journal of Chemical Physics</i> , 1994 , 101, 4062-4072	3.9	127
1663	Molecular dynamics study of nucleation and melting of n-alkanes. <i>Journal of Chemical Physics</i> , 1994 , 101, 9033-9041	3.9	82
1662	Local chain dynamics of bulk amorphous polybutadienes: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1994 , 101, 6242-6254	3.9	55
1661	Growth of hexagonal string phases in sheared colloid simulation. <i>Journal of Chemical Physics</i> , 1994 , 101, 6096-6100	3.9	8
1660	Can the density maximum of water be found by computer simulation?. <i>Journal of Chemical Physics</i> , 1994 , 100, 6692-6699	3.9	57

1659	Anisotropic stress in a confined chain. Excluded volume effects. <i>Journal of Chemical Physics</i> , 1994 , 100, 682-686	3.9	5
1658	Predictions of free energy differences from a single simulation of the initial state. <i>Journal of Chemical Physics</i> , 1994 , 100, 577-585	3.9	63
1657	Structure and thermodynamics of the liquid-vapor interface of fluorocarbons and semifluorinated alkane diblocks: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1994 , 101, 4156-4165	3.9	54
1656	Effects of atomic-force-microscope tip characteristics on measurement of solvation-force oscillations. 1994 , 49, 2058-2066		32
1655	Time and internal energy dependent fluorescence spectra of naphthol-water clusters. <i>Journal of Chemical Physics</i> , 1994 , 101, 7327-7336	3.9	27
1654	Potential of mean force for the methane-methane pair in water. <i>Journal of Chemical Physics</i> , 1994 , 100, 9032-9034	3.9	65
1653	Molecular dynamics free energy calculation in four dimensions. <i>Journal of Chemical Physics</i> , 1994 , 101, 1417-1422	3.9	37
1652	A deterministic global optimization approach for molecular structure determination. <i>Journal of Chemical Physics</i> , 1994 , 100, 1247-1261	3.9	85
1651	Simulation of the formation and detection of one-dimensional ordered ion beams. 1994 , 50, 4073-4086		9
1650	Far-infrared spectra of HCl in dense Ar and time-dependent anisotropic potential autocorrelation functions. A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1994 , 100, 252-261	3.9	8
1649	Distance Dependence of Water Structure around Model Solutes. 1994 , 98, 5559-5564		52
1648	Existence of a density maximum in extended simple point charge water. <i>Journal of Chemical Physics</i> , 1994 , 101, 9837-9840	3.9	135
1647	Dynamical simulation of a quantum harmonic oscillator in a noble-gas bath by density-matrix evolution. 1994 , 50, 198-204		15
1646	The computation of a potential of mean force: Choice of the biasing potential in the umbrella sampling technique. <i>Journal of Chemical Physics</i> , 1994 , 100, 1492-1497	3.9	66
1645	Computer-simulation study of the interface between graphite and hydrocarbon mixtures: Preferential adsorption and dynamics. 1994 , 49, 910-913		13
1644	Determination of structure and conformation in solution of syringotoxin, a lipodepsipeptide from <i>Pseudomonas syringae</i> pv. <i>syringae</i> by 2D NMR and molecular dynamics. 1994 , 5, 43-50		18
1643	Perfect-structure regions in amorphous argon. 1994 , 35, 47-56		5
1642	High-performance liquid chromatography of amino acids, peptides and proteins: CXXV. Molecular dynamics simulation of n-butyl chains chemically bonded to silica-based reversed-phase high-performance liquid chromatography sorbents. 1994 , 660, 75-84		22

1641	Molecular dynamics simulations of the conformational behaviour of the synthetic dipeptide PIDOTIMOD, a new immunostimulating agent. 1994 , 317, 197-214	3
1640	Time- and ensemble-averaged direct NOE restraints. 1994 , 4, 143-9	53
1639	Molecular dynamics simulation of a phospholipid membrane. 1994 , 22, 423-36	248
1638	Coupling constants again: experimental restraints in structure refinement. 1994 , 8, 29-40	21
1637	Nucleotide-binding properties of adenylate kinase from Escherichia coli: a molecular dynamics study in aqueous and vacuum environments. 1994 , 8, 367-88	17
1636	Active-site mobility inhibits reductive dehalogenation of 1,1,1-trichloroethane by cytochrome P450cam. 1994 , 8, 389-404	10
1635	Solution conformation of hexameric & heptameric lariat-RNAs and their self-cleavage reactions which give products mimicking those from some catalytic RNAs (ribozymes). 1994 , 50, 1777-1810	17
1634	Harmonic and anharmonic aspects in the dynamics of BPTI: a normal mode analysis and principal component analysis. 1994 , 3, 936-43	102
1633	An evaluation of implicit and explicit solvent model systems for the molecular dynamics simulation of bacteriophage T4 lysozyme. 1994 , 18, 19-33	44
1632	Crystallization and structural analysis of bullfrog red cell L-subunit ferritins. 1994 , 18, 107-18	47
1631	The enzymatic mechanism of carboxypeptidase: a molecular dynamics study. 1994 , 18, 186-97	19
1630	Molecular dynamics studies on mutants of Cu,Zn superoxide dismutase: the functional role of charged residues in the electrostatic loop VII. 1994 , 18, 216-30	20
1629	Molecular dynamics simulation of the docking of substrates to proteins. 1994 , 19, 174-82	86
1628	Torsion angle dynamics: reduced variable conformational sampling enhances crystallographic structure refinement. 1994 , 19, 277-90	345
1627	Intrinsic pKas of ionizable residues in proteins: an explicit solvent calculation for lysozyme. 1994 , 20, 85-97	84
1626	Homology modeling of the Abl-SH3 domain. 1994 , 20, 203-15	17
1625	Computer assisted simulations and molecular graphics methods in molecular design. 1. Theory and applications to enzyme active-site directed drug design. 1994 , 3, 377-414	24
1624	The effect of stereochemistry upon carbohydrate hydration. A molecular dynamics simulation of α -D-galactopyranose and β -D-talopyranose. 1994 , 265, 215-225	66

1623	Theoretical analyses of O ₂ /H ₂ O systems under normal and supercritical conditions. 1994 , 222, 25-32	28
1622	Initial stages of electrophilic substitution studied with quantum molecular dynamics. 1994 , 223, 1-6	3
1621	High-pressure molecular dynamics of a nucleic acid fragment. 1994 , 224, 219-224	16
1620	Molecular dynamics study on the stability of ions around human lysozyme in the crystal condition. 1994 , 225, 196-201	1
1619	Free energies for association of Cs ⁺ to 18-crown-6 in water. A molecular dynamics study including counter ions. 1994 , 227, 211-214	40
1618	Computer simulation study of methane in silicalite. 1994 , 229, 250-256	31
1617	Interionic potentials of mean force for SrCl ₂ in polarizable water. 1994 , 230, 209-214	26
1616	PARALLACS: a benchmark for parallel molecular dynamics. 1994 , 84, 102-114	8
1615	Implementation of a data parallel, logical domain decomposition method for interparticle interactions in molecular dynamics of structured molecular fluids. 1994 , 15, 44-53	4
1614	Free energy perturbation calculations on parallel computers: Demonstrations of scalable linear speedup. 1994 , 15, 351-373	12
1613	Shape analysis of hydrogen-bonded networks in solvation clusters. 1994 , 15, 633-643	8
1612	New spherical-cutoff methods for long-range forces in macromolecular simulation. 1994 , 15, 667-683	865
1611	Thermodynamic integration calculations on the relative free energies of complex ions in aqueous solution: Application to ligands of dihydrofolate reductase. 1994 , 15, 704-718	11
1610	Combined molecular mechanical and quantum mechanical potential study of a nucleophilic addition reaction in solution. 1994 , 15, 1311-1318	29
1609	Algorithms for clustering molecular dynamics configurations. 1994 , 15, 1331-1340	78
1608	Conformational transitions of a dipeptide in water: Effects of imposed pathways using umbrella sampling techniques. 1994 , 34, 347-355	18
1607	Solution conformation of a pectic acid fragment by ¹ H-NMR and molecular dynamics. 1994 , 34, 457-62	14
1606	Coupling constants as restraints in ensemble distance driven dynamics. 1994 , 34, 559-563	48

1605	Molecular dynamics simulation of a leucine zipper motif predicted for the integrase of human immunodeficiency virus type 1. 1994 , 34, 1027-36	4
1604	Molecular modeling of the conformational and sodium ion binding properties of the oligosaccharide component of ganglioside GM1. 1994 , 34, 1311-26	12
1603	Kinked structures of isolated nicotinic receptor M2 helices: a molecular dynamics study. 1994 , 34, 1647-57	16
1602	Improving protein extraction yield in reversed micellar systems through surface charge engineering. 1994 , 44, 773-80	12
1601	Bestimmung der relativen Konfiguration durch Distanzgeometrie-Rechnungen mit Proton-Proton-Abständen aus NOESY-Spektren. 1994 , 106, 822-824	12
1600	Is there a second critical point in liquid water?. 1994 , 205, 122-139	88
1599	On the hydrogen bonding effects in liquid methanol: a molecular dynamics simulation study. 1994 , 62, 1-16	35
1598	Molecular dynamics calculation of the infrared spectra in liquid H ₂ O-D ₂ O mixtures. 1994 , 62, 17-31	57
1597	Comparative molecular field analysis of CCK-B antagonists. 1994 , 29, 487-494	6
1596	A molecular dynamics study of branched alpha-cyclodextrin. 1994 , 12, 297-301, 294	4
1595	Molecular dynamics of copper plastocyanin: simulations of structure and dynamics as a function of hydration. 1994 , 183, 155-166	22
1594	Evaluation of the hydrophilic behaviour of a β -casein peptide by molecular dynamics simulation. 1994 , 189, 511-521	1
1593	Calculation of the circular dichroism spectrum of cyclo-(L-tyr-L-tyr) based on a molecular dynamics simulation. 1994 , 49, 141-52	32
1592	Characterization of biomolecular structure and dynamics by NMR cross relaxation. 1994 , 26, 27-58	70
1591	Theory of diamondlike amorphous carbon. 1994 , 49, 16415-16422	173
1590	Improvements to the molecular dynamics simulated annealing procedures: conformational search of the elastin tetrapeptide Boc-Gly-Leu-Gly-Gly-NMe. 1994 , 308, 141-157	9
1589	The Virial of Angle Dependent Potentials in Molecular Dynamics Simulations. 1994 , 13, 367-374	5
1588	Molecular dynamics study of the binding of phenylalanine stereoisomers to thermolysin. 1994 , 50, 237-48	7

1587	High-resolution solution structures of oxidized and reduced Escherichia coli thioredoxin. 1994 , 2, 853-68		267
1586	Cross-validation tests of time-averaged molecular dynamics refinements for determination of protein structures by X-ray crystallography. 1994 , 50, 24-36		21
1585	The three-dimensional structure in solution of the paramagnetic high-potential iron-sulfur protein I from Ectothiorhodospira halophila through nuclear magnetic resonance. 1994 , 225, 715-25		87
1584	An extended x-ray absorption fine structure study of aqueous solutions by employing molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1994 , 100, 985-994	3.9	122
1583	Computer simulations of cesium-water clusters: Do ion-water clusters form gas-phase clathrates?. <i>Journal of Chemical Physics</i> , 1994 , 101, 7873-7881	3.9	54
1582	Simulation of viscoelasticity in polymer melts: effect of torsional potential. 1994 , 2, 755-766		12
1581	Computer Simulation of the Crystal Growth and Dissolution of Natural Gas Hydrates. 1994 , 715, 177-186		179
1580	The distal residue-CO interaction in carbonmonoxy myoglobins: a molecular dynamics study of two distal histidine tautomers. 1994 , 67, 2236-50		51
1579	A comparison of DMPC- and DLPE-based lipid bilayers. 1994 , 66, 1076-87		159
1578	Modeling of the three-dimensional structure of polypeptides in solution using potential-scaled/hot-solute molecular dynamics. 1994 , 66, 1815-22		4
1577	Molecular modeling of polymers: Molecular dynamics simulation of the rotator phase of C ₂₁ H ₄₄ . 1994 , 72, 661-664		12
1576	A critical evaluation of novel algorithms for the off-lattice Monte Carlo simulation of condensed polymer phases. 1994 , 283-318		50
1575	Molecular dynamics simulation of molten silica at high pressure. <i>Journal of Chemical Physics</i> , 1994 , 101, 7823-7827	3.9	10
1574	Computer simulations of NaCl association in polarizable water. <i>Journal of Chemical Physics</i> , 1994 , 100, 3757-3766	3.9	915
1573	Molecular structure of the cyanobacterial tumor-promoting microcystins. 1994 , 349, 319-23		42
1572	Investigation of shape variations in the antibody binding site by molecular dynamics computer simulation. 1994 , 236, 1186-95		15
1571	Protein three-dimensional structure determination and sequence-specific assignment of ¹³ C and ¹⁵ N-separated NOE data. A novel real-space ab initio approach. 1994 , 243, 696-718		54
1570	Observation of a volume minimum in computer simulations of supercooled, amorphous silica. 1994 , 167, 211-228		13

1569	Simulation studies of silicates and phosphates. 1994 , 177, 103-124		34
1568	Atomistic calculations on low-temperature layer-by-layer growth. 1994 , 307-309, 526-530		3
1567	Molecular dynamics simulations of ion impact on a supported rhodium cluster. 1994 , 306, 215-226		10
1566	Molecular dynamics simulation of the rare amino acid LL-dityrosine and a dityrosine-containing peptide: comparison with time-resolved fluorescence. 1994 , 1201, 345-52		4
1565	A molecular dynamics simulation study of chloroform. 1994 , 83, 381-403		143
1564	Molecular dynamics study of the mixing and demixing of a binary Lennard-Jones fluid. 1994 , 82, 1049-1062		9
1563	Separation-shifted scaling, a new scaling method for Lennard-Jones interactions in thermodynamic integration. <i>Journal of Chemical Physics</i> , 1994 , 100, 9025-9031	3.9	413
1562	Molecular-dynamics simulations of stress relaxation in metals and polymers. 1994 , 49, 6494-6500		47
1561	Pressure Calculation in Molecular Dynamics Simulations of Molecular Crystals. 1994 , 13, 221-230		5
1560	Dynamics of small molecules in bulk polymers. 1994 , 207-247		180
1559	Molecular dynamics simulation of MHC-peptide complexes as a tool for predicting potential T cell epitopes. 1994 , 33, 11476-85		88
1558	A reassessment of the structure of chymotrypsin inhibitor 2 (CI-2) using time-averaged NMR restraints. 1994 , 33, 14503-11		31
1557	Constant temperature molecular dynamics simulations by means of a stochastic collision model. I. Noninteracting particles. <i>Journal of Chemical Physics</i> , 1994 , 100, 566-576	3.9	57
1556	Open "back door" in a molecular dynamics simulation of acetylcholinesterase. 1994 , 263, 1276-8		258
1555	Molecular dynamics free energy simulations: Influence of the truncation of long-range nonbonded electrostatic interactions on free energy calculations of polar molecules. <i>Journal of Chemical Physics</i> , 1994 , 101, 7953-7962	3.9	44
1554	Molecular Dynamics Simulation of Hydrogenated Amorphous Silicon with Tersoff Potential. 1994 , 336, 177		13
1553	Computational chemistry and molecular modeling of electron-transfer proteins. 1994 , 243, 559-607		3
1552	Acetylcholine Recognition by an Aromatic Host: the Role of an All-Hydrogen Topology in Simulations of the Cation-Interaction. 1994 , 34, 159-163		6

1551	Thermodynamic parameters for the helix-coil transition of oligopeptides: molecular dynamics simulation with the peptide growth method. 1995 , 92, 10924-8	20
1550	An MD Study on the Correlation between Transport Diffusion and Self-Diffusion in Zeolites. 1995 , 189, 211-220	28
1549	Molecular-Dynamics Simulations of Hydrogenated Amorphous Silicon thin-Film Growth. 1995 , 408, 445	30
1548	On the Response of Dynamic Cracks to Increasing Overload. 1995 , 409, 297	3
1547	The structural origins of the unusual specificities observed in the isolation of chymopapain M and actinidin by covalent chromatography and the lack of inhibition of chymopapain M by cystatin. 1995 , 306 (Pt 1), 39-46	17
1546	Structural studies of DNA three-way junctions. 1995 , 261, 183-207	6
1545	Chapter 12 Simulated annealing applied to crystallographic structure refinement. 1995 , 259-280	1
1544	Chapter 14 Simulated annealing in the calculation of NMR structures. 1995 , 15, 303-328	1
1543	An extension of the GROMOS force field for carbohydrates, resulting in improvement of the crystal structure determination of β -D-galactose. 1995 , 51, 209-220	38
1542	Molecular dynamics and structure-based drug design for predicting non-natural nonapeptide binding to a class I MHC protein. 1995 , 51, 541-9	3
1541	Refined Solution Structure of the Tyr41->His Mutant of the M13 Gene V Protein. 1995 , 232, 506-514	16
1540	Studies of the bound conformations of methyl alpha-lactoside and methyl beta-allolactoside to ricin B chain using transferred NOE experiments in the laboratory and rotating frames, assisted by molecular mechanics and dynamics calculations. 1995 , 233, 618-30	50
1539	Solution conformation of the Pseudomonas syringae pv. syringae phytotoxic lipodepsipeptide syringopeptin 25-A. Two-dimensional NMR, distance geometry and molecular dynamics. 1995 , 234, 747-58	29
1538	Solution structure of the oxidized 2[4Fe-4S] ferredoxin from Clostridium pasteurianum. 1995 , 232, 192-205	73
1537	Molecular modeling of saccharides, 7. The conformation of sucrose in water: A molecular dynamics approach. 1995 , 1995, 1925-1937	70
1536	The Solution Structure of Oxidized HiPIP I from Ectothiorhodospira halophila; Can NMR Spectroscopy Be Used to Probe Rearrangements Associated with Electron Transfer Processes?. 1995 , 1, 598-607	27
1535	The use of the AMBER force field in conformational analysis of carbohydrate molecules: determination of the solution conformation of methyl alpha-lactoside by NMR spectroscopy, assisted by molecular mechanics and dynamics calculations. 1995 , 35, 55-73	95
1534	Dominant solvation effects from the primary shell of hydration: Approximation for molecular dynamics simulations. 1995 , 35, 171-178	64

1533	Fluctuations in molecular size, entanglement complexity, and anisometry along molecular dynamics trajectories of short β -helices. 1995 , 35, 393-409	18
1532	Structure of two microcystins: Refinement with nuclear overhauser effects and ensemble calculations. 1995 , 36, 811-828	10
1531	Constant temperature simulations of helix folding. 1995 , 173, 389-400	2
1530	Crystalline cellulose I β and I α studied by molecular dynamics simulation. 1995 , 273, 207-223	93
1529	Determination by NMR spectroscopy of the structure and conformational features of the enterobacterial common antigen isolated from Escherichia coli. 1995 , 273, 157-70	13
1528	Solution structure of the trisaccharide and hexasaccharide fragments of the O-antigen of the lipopolysaccharide of Rhizobium tropici CIAT899. 1995 , 279, 339-52	4
1527	Force field parametrization by weak coupling. Re-engineering SPC water. 1995 , 232, 429-436	143
1526	Umbrella sampling along linear combinations of generalized coordinates. Theory and application to a glycine dipeptide. 1995 , 237, 308-316	9
1525	Negative volumetric thermal expansion for proposed hinged phases. 1995 , 240, 180-184	11
1524	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
1523	GROMACS: A message-passing parallel molecular dynamics implementation. 1995 , 91, 43-56	6589
1522	Extended Lagrangian formalism applied to temperature control and electronic polarization effects in molecular dynamics simulations. 1995 , 91, 253-262	17
1521	Computer simulation of protein motion. 1995 , 91, 305-319	48
1520	Parameterization and evaluation of a flexible water model. 1995 , 16, 501-511	112
1519	Evaluating polarizable potentials on distributed memory parallel computers: Program development and applications. 1995 , 16, 1141-1152	10
1518	A molecular dynamics study of the inhibition of chicken dihydrofolate reductase by a phenyl triazine. 1995 , 16, 1378-1393	7
1517	Isothermal-isobaric molecular dynamics simulations with Monte Carlo volume sampling. 1995 , 91, 283-289	76
1516	Structure and dynamics of liquid formamide. 1995 , 190, 61-82	56

1515	Molecular dynamics study of water adopting a potential function with explicit atomic dipole moments and anisotropic polarizabilities. 1995 , 191, 195-202	61
1514	Molecular dynamics of amphotericin B I. Single molecule in vacuum and water. 1995 , 54, 49-60	15
1513	Chiral building blocks from streptomyces-2.1 stereoselective transformation of streptenol a into 3-methyl-lactones. 1995 , 51, 8247-8258	2
1512	Simulation of a fluid phase lipid bilayer membrane: Incorporation of the surface tension into system boundary conditions. 1995 , 5, 45-53	
1511	Biomolecules at phase boundaries. 1995 , 5, 235-243	
1510	Molecular dynamics study of a monomeric heme undecapeptide of cytochromec. 1995 , 2, 9-22	3
1509	Structure determination of a tetradecapeptide mimicking the RXVRG consensus sequence recognized by a <i>Xenopus laevis</i> skin endoprotease: an approach based on simulated annealing and ¹ H NMR. 1995 , 9, 160-70	2
1508	Conformation of the circular dumbbell d: structure determination and molecular dynamics. 1995 , 6, 403-22	21
1507	Parametrisation of time-averaged distance restraints in MD simulations. 1995 , 6, 313-20	45
1506	Structure refinement with molecular dynamics and a Boltzmann-weighted ensemble. 1995 , 6, 163-70	58
1505	Structure and atomic fluctuation patterns of potato carboxypeptidase a inhibitor protein. 1995 , 24, 1-11	7
1504	Dynamic modelling of a helical peptide in solution using NMR data: multiple conformations and multi-spin effects. 1995 , 6, 33-40	27
1503	Computational approaches to study protein unfolding: hen egg white lysozyme as a case study. 1995 , 21, 196-213	89
1502	Dramatic differences in the motions of the mouth of open and closed cytochrome P450BM-3 by molecular dynamics simulations. 1995 , 21, 237-43	56
1501	Automatic identification of discrete substates in proteins: singular value decomposition analysis of time-averaged crystallographic refinements. 1995 , 22, 311-21	66
1500	Structure and internal dynamics of the bovine pancreatic trypsin inhibitor in aqueous solution from long-time molecular dynamics simulations. 1995 , 23, 49-62	40
1499	Parametric sensitivity analysis of avian pancreatic polypeptide (APP). 1995 , 23, 218-32	15
1498	Modeling conformational changes in cyclosporin A. 1995 , 4, 2191-202	25

1497	Computational searching and mutagenesis suggest a structure for the pentameric transmembrane domain of phospholamban. 1995 , 2, 154-62	186
1496	Conformational variability in the refined structure of the chaperonin GroEL at 2.8 A resolution. 1995 , 2, 1083-94	207
1495	Three-dimensional structure of the single-stranded DNA-binding protein encoded by gene V of the filamentous bacteriophage M13 and a model of its complex with single-stranded DNA. 1995 , 17, 57-72	4
1494	Molecular mechanics and dynamics studies on two structurally related amide-modified DNA backbones for antisense technology. 1995 , 3, 321-35	15
1493	Conformational change due to esterification of hydroxy groups in erythromycin A and its major metabolite: analysis of these derivatives with different biological properties using NMR and molecular dynamics (MD) data. 1995 , 3, 587-604	10
1492	Theoretical analysis of the far-infrared spectra of HCl in liquid Ar along the Ar liquid-vapour coexistence line. 1995 , 63, 251-264	4
1491	Hydrogen bond analysis by MD simulation of copper plastocyanin at different hydration levels. 1995 , 201, 463-472	32
1490	Molecular dynamics simulations of yttria-stabilized zirconia. 1995 , 247, 386-390	75
1489	High field NMR techniques, molecular modelling and molecular dynamics simulations in the study of the inclusion complex of the cognition activator (-)-1-(4-methoxybenzoyl)-5-oxo-2-pyrrolidinepropanoic acid (CI-933) with β -cyclodextrin. 1995 , 350, 71-82	23
1488	¹ H, ¹³ C and ¹⁵ N NMR study of the solution structure of meta-bridged bis(benzo-15-crown-5 ether)s. 1995 , 356, 15-24	6
1487	Investigation of the atomic-scale friction and energy dissipation in diamond using molecular dynamics. 1995 , 260, 205-211	95
1486	Modelling molecular stability in gamma B crystallin. 1995 , 19, 65-74	9
1485	Structural and electronic properties of nitrogen doped fourfold amorphous carbon. 1995 , 93, 617-621	15
1484	C60 film growth and the interaction of fullerenes with bare and H terminated Si surfaces, studied by molecular dynamics. 1995 , 106, 74-79	12
1483	Ion bombardment of polyethylene. 1995 , 102, 223-227	45
1482	A molecular dynamics study of glutathione reductase. 1995 , 335, 243-254	2
1481	Conformational studies of a trisaccharide epitope in solution by using NMR spectroscopy and molecular mechanics and dynamics calculations with the MM3* program. 1995 , 713-721	4
1480	Constant pressure molecular dynamics simulation: The Langevin piston method. <i>Journal of Chemical Physics</i> , 1995 , 103, 4613-4621	3.9 3093

1479	MD simulations in Pseudo-Particle Fluids: Applications to active-site Protein Complexes. 1995 , 14, 229-241		2
1478	. 1995 ,		4
1477	Molecular dynamics simulations of liquids and glasses in the system NaAlSiO ₄ -SiO ₂ ; methodology and melt structures. 1995 , 80, 417-431		33
1476	Velocity reassignment echoes in proteins. <i>Journal of Chemical Physics</i> , 1995 , 103, 3124-3139	3.9	10
1475	Liquid densities and structural properties of molecular models of water. <i>Journal of Chemical Physics</i> , 1995 , 102, 6559-6565	3.9	39
1474	Analysis of friction kernels for n-butane isomerization in water by the generalized Langevin equation. <i>Journal of Chemical Physics</i> , 1995 , 102, 4976-4980	3.9	7
1473	Time dependent Monte Carlo simulations of H reactions on the diamond {001}(2 \times 1) surface under chemical vapor deposition conditions. <i>Journal of Chemical Physics</i> , 1995 , 102, 9401-9411	3.9	39
1472	Fracture simulations using large-scale molecular dynamics. 1995 , 51, 11275-11288		171
1471	Neutron-scattering and ab initio molecular-dynamics study of vibrations in glassy GeSe ₂ . 1995 , 52, 9133-9136		46
1470	Electric-field-gradient calculations on cadmium in cadmium-helium vacancy clusters in tungsten. 1995 , 52, 3909-3916		3
1469	Temperature quench echoes in proteins. <i>Journal of Chemical Physics</i> , 1995 , 103, 3112-3123	3.9	18
1468	Interaction of an amphiphilic peptide with a phospholipid bilayer surface by molecular dynamics simulation study. 1995 , 12, 937-56		42
1467	Thermostatted molecular dynamics: How to avoid the Toda demon hidden in Nosé-Hoover dynamics. 1995 , 52, 2338-2347		121
1466	Molecular-dynamics simulations of SiH ₃ radical deposition on hydrogen-terminated silicon (100) surfaces. 1995 , 52, 8283-8287		54
1465	Interactions of iron implants in transition metals. 1995 , 52, 8414-8422		22
1464	Small free energy barrier and postdesorption collisions: The keys towards the understanding of reactive ion etching of silicon. 1995 , 74, 1879-1882		19
1463	Effect of the treatment of long-range forces on the dynamics of ions in aqueous solutions. <i>Journal of Chemical Physics</i> , 1995 , 102, 450-456	3.9	139
1462	The polarization contribution to the free energy of hydration. <i>Journal of Chemical Physics</i> , 1995 , 102, 6145-6152	3.9	40

1461	Determination of force field parameters for molecular simulation by molecular simulation: An application of the weak-coupling method. <i>Journal of Chemical Physics</i> , 1995 , 102, 6199-6207	3.9	39
1460	Gibbs-ensemble molecular dynamics: Liquid-gas equilibrium in a Lennard-Jones system. 1995 , 51, 5116-5119		19
1459	A general pressure tensor calculation for molecular dynamics simulations. 1995 , 84, 577-595		82
1458	A molecular dynamics simulation study with a combined quantum mechanical and molecular mechanical potential energy function: Solvation effects on the conformational equilibrium of dimethoxyethane. <i>Journal of Chemical Physics</i> , 1995 , 102, 1722-1730	3.9	70
1457	The dipole moment of 18-crown-6: Molecular dynamics study of the structure and dynamics of the macrocycle in vacuo and in cyclohexane. <i>Journal of Chemical Physics</i> , 1995 , 103, 4637-4652	3.9	11
1456	New strategies to incorporate the solvent polarization in self-consistent reaction field and free-energy perturbation simulations. <i>Journal of Chemical Physics</i> , 1995 , 103, 10183-10191	3.9	46
1455	Free energy of cavity formation in solvent: Computational, methodological, and physical aspects. <i>Journal of Chemical Physics</i> , 1995 , 102, 3787-3793	3.9	54
1454	Kr incorporation in sputtered amorphous Si layers. 1995 , 77, 3467-3478		5
1453	Chemical and physical sputtering of fluorinated silicon. 1995 , 77, 1263-1274		92
1452	Molecular dynamics simulations of the glass former ortho-terphenyl. <i>Journal of Chemical Physics</i> , 1995 , 103, 8566-8576	3.9	39
1451	Phase equilibria in extended simple point charge ice-water systems. <i>Journal of Chemical Physics</i> , 1995 , 103, 9744-9755	3.9	104
1450	Molecular dynamics of linear and branched alkanes. <i>Journal of Chemical Physics</i> , 1995 , 103, 7156-7165	3.9	149
1449	Structure of human parathyroid hormone 1-37 in solution. 1995 , 270, 15194-202		56
1448	Path Dependence of Free Energy Components in Thermodynamic Integration. 1995 , 14, 417-423		3
1447	Atomic-Detail Simulation Studies of Smectic Liquid Crystals. 1995 , 14, 343-360		14
1446	Reaction Field Effects on the Simulated Properties of Liquid Water. 1995 , 15, 233-245		21
1445	Adsorption-desorption kinetics in nanoscopically confined oligomer films under shear. 1995 , 85, 1017-1032		32
1444	Perturbation-Relaxation Molecular Dynamics Simulations as a Tool to Explore Conformational Space. Reversible Response of the L3 Loop in Porin Towards Charge Screening Effects. 1995 , 15, 35-46		3

1443	Pressure and Temperature Dependence Study of the Denaturation of Ribonuclease A Solutions. 1995 , 15, 265-272	2
1442	Molecular dynamics simulations indicate that F87W,T185F-cytochrome P450cam may reductively dehalogenate 1,1,1-trichloroethane. 1995 , 13, 413-22	3
1441	Al K-edge XANES spectra of aluminosilicate minerals. 1995 , 80, 432-440	83
1440	Comment on Mean force potential for the calcium-chloride ion pair in water[J. Chem. Phys. 99, 4229 (1993)]. <i>Journal of Chemical Physics</i> , 1995 , 102, 3483-3484	3.9 84
1439	Structural basis for the extreme thermostability of D-glyceraldehyde-3-phosphate dehydrogenase from <i>Thermotoga maritima</i> : analysis based on homology modelling. 1995 , 8, 779-89	25
1438	Counterion Distribution around DNA Studied by Molecular Dynamics and Quantum Mechanical Simulations. 1995 , 99, 11591-11599	28
1437	L3 loop-mediated mechanisms of pore closing in porin: a molecular dynamics perturbation approach. 1995 , 8, 5-12	30
1436	Conformational modeling of elastin tetrapeptide Boc-Gly-Leu-Gly-Gly-NMe by molecular dynamics simulations with improvements to the thermalization procedure. 1995 , 12, 1173-202	20
1435	Molecular dynamics simulation of anesthetic-phospholipid bilayer interactions. 1995 , 12, 725-54	33
1434	Computer Simulation of Hydrophobic Hydration Forces on Stacked Plates at Short Range. 1995 , 99, 2893-2899	256
1433	Molecular dynamics simulations of liquid crystal molecules adsorbed on graphite. 1995 , 18, 45-49	29
1432	An Examination of a Hartree-Fock/Molecular Mechanical Coupled Potential. 1995 , 99, 17344-17348	47
1431	NMR and restrained molecular dynamics study of the three-dimensional solution structure of toxin FS2, a specific blocker of the L-type calcium channel, isolated from black mamba venom. 1995 , 34, 5923-37	60
1430	Exploring the role of the solvent in the denaturation of a protein: a molecular dynamics study of the DNA binding domain of the 434 repressor. 1995 , 34, 15057-67	19
1429	Molecular-dynamics simulations of direct reactive ion etching of silicon by fluorine and chlorine. 1995 , 78, 6604-6615	111
1428	Application of the free energy perturbation method to human carbonic anhydrase II inhibitors. 1995 , 38, 2061-9	16
1427	The three-dimensional solution structure of the reduced high-potential iron-sulfur protein from <i>Chromatium vinosum</i> through NMR. 1995 , 34, 206-19	72
1426	Aldose reductase as a target for drug design: molecular modeling calculations on the binding of acyclic sugar substrates to the enzyme. 1995 , 34, 8299-308	46

1425	Three-dimensional structure of cyclohexapeptides containing a phosphinic bond in aqueous solution: a template for zinc metalloprotease inhibitors. A NMR and restrained molecular dynamics study. 1995 , 38, 553-64	7
1424	Computational Chemistry on Workstation Clusters: Parallel Programming for Molecular Dynamics and Neural Networks. 1995 , 14, 209-233	1
1423	Molecular dynamics simulation of the solution structures of Ha-ras-p21 GDP and GTP complexes: flexibility, possible hinges, and levers of the conformational transition. 1995 , 34, 12038-47	41
1422	Methodological advances in molecular dynamics simulations of biological systems. 1995 , 5, 211-5	38
1421	The use of CVFF and CFF91 force fields in conformational analysis of carbohydrate molecules. Comparison with AMBER molecular mechanics and dynamics calculations for methyl alpha-lactoside. 1995 , 17, 137-48	75
1420	Molecular-dynamics simulation of the growth of diamond-like films. 1995 , 331-333, 975-977	15
1419	A smooth particle mesh Ewald method. <i>Journal of Chemical Physics</i> , 1995 , 103, 8577-8593	3.9 14532
1418	Osmotic permeability in a molecular dynamics simulation of water transport through a single-occupancy pore. 1995 , 1240, 159-66	3
1417	Structural Analysis of Carbyne Network Polymers. 1995 , 304-315	1
1416	Calculation of protein structures with ambiguous distance restraints. Automated assignment of ambiguous NOE crosspeaks and disulphide connectivities. 1995 , 245, 645-60	324
1415	Structure and dynamics of ferrocycytochrome c553 from <i>Desulfovibrio vulgaris</i> studied by NMR spectroscopy and restrained molecular dynamics. 1995 , 245, 661-81	64
1414	Internal mobility of the basic pancreatic trypsin inhibitor in solution: a comparison of NMR spin relaxation measurements and molecular dynamics simulations. 1995 , 246, 356-65	70
1413	Determination of the differential effects of hydrogen bonding and water release on the binding of FK506 to native and Tyr82-->Phe82 FKBP-12 proteins using free energy simulations. 1995 , 248, 696-717	40
1412	NMR cross-relaxation investigated by molecular dynamics simulation: a case study of ubiquitin in solution. 1995 , 249, 604-24	23
1411	Structure, dynamics and energetics of initiation sites in protein folding: I. Analysis of a 1 ns molecular dynamics trajectory of an early folding unit in water: the helix I/loop I-fragment of barnase. 1995 , 250, 239-57	10
1410	Fluctuation and cross-correlation analysis of protein motions observed in nanosecond molecular dynamics simulations. 1995 , 252, 492-503	332
1409	Acid and thermal denaturation of barnase investigated by molecular dynamics simulations. 1995 , 252, 672-708	160
1408	Molecular dynamics simulations of CaCO ₃ melts to mantle pressures and temperatures: implications for carbonatite magmas. 1995 , 131, 225-238	80

1407	Thermodynamics of water mediating protein-ligand interactions in cytochrome P450cam: a molecular dynamics study. 1995 , 69, 810-24		88
1406	Incorporation of surface tension into molecular dynamics simulation of an interface: a fluid phase lipid bilayer membrane. 1995 , 69, 1230-45		348
1405	Behavior of cholesterol and its effect on head group and chain conformations in lipid bilayers: a molecular dynamics study. 1995 , 68, 164-70		106
1404	Refinement of the solution structure of a branched DNA three-way junction. 1995 , 68, 266-74		25
1403	Molecular dynamics study of the 13-cis form (bR548) of bacteriorhodopsin and its photocycle. 1995 , 68, 1270-82		39
1402	Investigation of free volume percolation under the liquid-glass phase transition. <i>Journal of Chemical Physics</i> , 1995 , 102, 4981-4986	3.9	26
1401	A generalized reaction field method for molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1995 , 102, 5451-5459	3.9	1146
1400	Molecular dynamics simulations of liquid, interface, and ionic solvation of polarizable carbon tetrachloride. <i>Journal of Chemical Physics</i> , 1995 , 103, 7502-7513	3.9	74
1399	The Use of Molecular Dynamics Simulations for Modelling Nucleic Acids. 103-131		2
1398	Molecular dynamics simulation of vapor deposited amorphous ice. <i>Journal of Chemical Physics</i> , 1995 , 103, 4678-4692	3.9	32
1397	Three-dimensional solution structure of the cyanide adduct of a Met80Ala variant of <i>Saccharomyces cerevisiae</i> iso-1-cytochrome c. Identification of ligand-residue interactions in the distal heme cavity. 1995 , 34, 11385-98		61
1396	Structure and Properties of Neat Liquids Using Nonadditive Molecular Dynamics: Water, Methanol, and N-Methylacetamide. 1995 , 99, 6208-6219		440
1395	A computer simulation study of the chain configurations in poly(ethylene oxide)-homolog melts. <i>Journal of Chemical Physics</i> , 1995 , 102, 9725-9735	3.9	77
1394	Molecular Recognition of K ⁺ and Na ⁺ by Valinomycin in Methanol. 1995 , 117, 779-791		45
1393	Computer simulation of liquid/liquid interfaces. I. Theory and application to octane/water. <i>Journal of Chemical Physics</i> , 1995 , 103, 10252-10266	3.9	293
1392	Towards phase transferable potential functions: Methodology and application to nitrogen. <i>Journal of Chemical Physics</i> , 1995 , 103, 2272-2285	3.9	29
1391	Parameterizing polarizable intermolecular potentials for water with the ice 1h phase. 1995 , 85, 81-90		32
1390	The effect of environment on the stability of an integral membrane helix: molecular dynamics simulations of surfactant protein C in chloroform, methanol and water. 1995 , 247, 808-22		34

1389	A model for transmembrane helix with a cis-proline in the middle. 1995 , 374, 21-4	2
1388	Global fold determination from a small number of distance restraints. 1995 , 251, 308-26	117
1387	Potential Transformation Methods for Large-Scale Global Optimization. 1995 , 5, 871-891	5
1386	Molecular dynamics modeling of time-resolved fluorescence shifts in liquid solution. <i>Journal of Chemical Physics</i> , 1995 , 102, 9059-9068	3.9 31
1385	Interaction of small peptides with lipid bilayers. 1995 , 69, 1299-308	39
1384	Supercooled water and the kinetic glass transition. 1996 , 54, 6331-6343	295
1383	Molecular Dynamics Potential of Mean Force Calculations: A Study of the TolueneAmmonium Cation Interactions. 1996 , 118, 2998-3005	85
1382	Computer Simulations of the Solvent Dependence of Apolar Association Strength: Gibbs Free Energy Calculations on a CyclophaneByrene Complex in Water and Chloroform. 1996 , 118, 6044-6051	47
1381	Empirical potentials for C[sbnd]Si[sbnd]H systems with application to C60 interactions with Si crystal surfaces. 1996 , 74, 1439-1466	50
1380	Medium-range structure of amorphous silicon studied by the VoronoiDelaunay method. 1996 , 88, 1337-1348	14
1379	Local Structure and Dynamics in Solvent-Swollen Polymers. 1996 , 29, 4782-4791	123
1378	The consistency of large concerted motions in proteins in molecular dynamics simulations. 1996 , 71, 1707-13	84
1377	Solvation, water permeation, and ionic selectivity of a putative model for the pore region of the voltage-gated sodium channel. 1996 , 71, 2276-88	22
1376	Molecular modeling of the RNA binding N-terminal part of cowpea chlorotic mottle virus coat protein in solution with phosphate ions. 1996 , 71, 2920-32	18
1375	Free Energy Perturbation Calculations Within Quantum Mechanical Methodologies. 1996 , 142-153	1
1374	Molecular dynamics simulations of adipocyte lipid-binding protein: effect of electrostatics and acyl chain unsaturation. 1996 , 35, 1506-15	27
1373	Calculating Electrostatic Interactions Using the ParticleParticle ParticleMesh Method with Nonperiodic Long-Range Interactions. 1996 , 100, 2581-2587	133
1372	Atomistic Modeling of Amorphous Polymer Bulk Based on an ab Initio Optimized Force Field. 1996 , 29, 4051-4059	4

- 1371 Stabilization of a Cis Amide Bond in a Host-Guest Complex. **1996**, 118, 10220-10227 61
- 1370 pH-dependent structural changes in the active site of p-hydroxybenzoate hydroxylase point to the importance of proton and water movements during catalysis. **1996**, 35, 567-78 46
- 1369 Solvation and Dynamics of Chymotrypsin in Hexane. **1996**, 118, 6490-6498 33
- 1368 3D structure of ramoplanin: a potent inhibitor of bacterial cell wall synthesis. **1996**, 35, 12570-5 62
- 1367 Benzene Dimer: A Good Model for π -Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. **1996**, 118, 11217-11224 265
- 1366 Second Coordination Shell Water Exchange Rate and Mechanism: Experiments and Modeling on Hexaaquachromium(III). **1996**, 118, 12777-12787 75
- 1365 Molecular dynamics simulations of a fully hydrated dipalmitoylphosphatidylcholine bilayer with different macroscopic boundary conditions and parameters. *Journal of Chemical Physics*, **1996**, 105, 4871-4880 438
- 1364 Theoretical study of inhibition of adenosine deaminase by (8R)-coformycin and (8R)-deoxycoformycin. **1996**, 39, 277-84 35
- 1363 Experimental Evidence of Conformational Differences between C-Glycosides and O-Glycosides in Solution and in the Protein-Bound State: The C-Lactose/O-Lactose Case. **1996**, 118, 10862-10871 77
- 1362 Inhomogeneities in Sheared Ultrathin Lubricating Films. **1996**, 12, 4587-4593 80
- 1361 3D Structure of the Complex of MDL 63,246 with the Cell Wall Model Peptide Ac2-Lys-d-Ala-d-Ala. **1996**, 118, 5874-5880 5
- 1360 Hidden peculiarities in the potential energy time series of a tripeptide highlighted by a recurrence plot analysis: A molecular dynamics simulation. **1996**, 53, 6336-6340 40
- 1359 Surface growth modes analysed with modern microscopic and computing techniques. **1996**, 17, 311-321 11
- 1358 Constant-Pressure Molecular Dynamics Techniques Applied to Complex Molecular Systems and Solvated Proteins. **1996**, 100, 4314-4322 28
- 1357 Molecular dynamics simulations of the bis-intercalated complexes of ditercalinium and Flexi-Di with the hexanucleotide d(GCGCGC)₂: theoretical analysis of the interaction and rationale for the sequence binding specificity. **1996**, 39, 4810-24 19
- 1356 Intrinsic Shape Stability of Equilibrium Motions in Poly(l-alanine). **1996**, 29, 7594-7601 14
- 1355 Improved binding of cytochrome P450cam substrate analogues designed to fill extra space in the substrate binding pocket. **1996**, 35, 1485-99 53
- 1354 Molecular dynamics simulations of liquid crystal molecules on a polyimide monolayer. **1996**, 21, 347-359 23

1353	Molecular dynamics simulation of a chloride ion in water under the influence of an external electric field. <i>Journal of Chemical Physics</i> , 1996 , 105, 650-657	3.9	61
1352	Molecular dynamics study of Na ⁺ and Cl ⁻ in methanol. <i>Journal of Chemical Physics</i> , 1996 , 105, 8826-8834	3.9	28
1351	Evaluation of dispersion relations of crystals from molecular-dynamics. 1996 , 6, 339-342		1
1350	An efficient mean solvation force model for use in molecular dynamics simulations of proteins in aqueous solution. 1996 , 256, 939-48		114
1349	Characterization of the electrostatic perturbation of a catalytic site (Cys)-S ⁻ /(His)-Im+H ion-pair in one type of serine proteinase architecture by kinetic and computational studies on chemically mutated subtilisin variants. 1996 , 257, 1088-111		31
1348	A combined quantum/classical molecular dynamics study of the catalytic mechanism of HIV protease. 1996 , 261, 454-69		93
1347	NMR solution structure of Cu(I) rusticyanin from <i>Thiobacillus ferrooxidans</i> : structural basis for the extreme acid stability and redox potential. 1996 , 263, 752-67		85
1346	Ectothiorhodospira halophila ferrocyclochrome c551: solution structure and comparison with bacterial cytochromes c. 1996 , 264, 567-84		8
1345	Chaos in Biomolecular Dynamics. 1996 , 100, 8101-8105		24
1344	Computation of Gibbs Free Energies of Hydration for Simple Aromatic Molecules: A Comparative Study Using Monte Carlo and Molecular Dynamics Computer Simulation Techniques. 1996 , 100, 4256-4260		16
1343	Integral equation theory for Lennard-Jones fluids: The bridge function and applications to pure fluids and mixtures. <i>Journal of Chemical Physics</i> , 1996 , 104, 6742-6754	3.9	117
1342	QM/MMpol: A Consistent Model for Solute/Solvent Polarization. Application to the Aqueous Solvation and Spectroscopy of Formaldehyde, Acetaldehyde, and Acetone. 1996 , 100, 14492-14507		227
1341	Molecular Dynamics Simulations of the Liquid/Vapor Interface of SPC/E Water. 1996 , 100, 11720-11725		243
1340	Molecular Dynamics Simulation of Benzene on Graphite: 1. Phase Behavior of an Adsorbed Monolayer. 1996 , 12, 2495-2500		19
1339	Molecular dynamics simulation of Li-Mg and Li-Na alloys. 1996 , 205-207, 907-910		9
1338	Hydration and DNA recognition by homeodomains. 1996 , 85, 1057-65		104
1337	Rational approach to improving reductive catalysis by cytochrome P450cam. 1996 , 78, 714-22		10
1336	A large scale molecular dynamics study of chain configurations in the n=100 alkane melt. <i>Journal of Chemical Physics</i> , 1996 , 104, 2078-2082	3.9	35

1335	Molecular dynamics simulation evidence of anomalous diffusion of protein hydration water. 1996 , 53, R3040-R3043		76
1334	Unusual Maxima in HPLC Retention of an Homologous Series Consisting of Longer Alkyl Chain Substitutions. 1996 , 68, 2379-2385		
1333	Synthesis and Evaluation of Thioether-Based Tris-Melamines as Components of Self-Assembled Aggregates Based on the CA.M Lattice. 1996 , 61, 1779-1786		21
1332	Slow dynamics of water molecules in supercooled states. 1996 , 76, 2730-2733		259
1331	Two-Dimensional Patterns of Magnetic Particles at Air/Water or Glass/Water Interfaces Induced by an External Magnetic Field: Theory and Simulation of the Formation Process. 1996 , 100, 3157-3162		15
1330	Molecular dynamics simulation of liquid water along the coexistence curve: Hydrogen bonds and vibrational spectra. <i>Journal of Chemical Physics</i> , 1996 , 105, 639-649	3.9	229
1329	A Molecular Dynamics and Quantum Mechanics Analysis of the Effect of DMSO on Enzyme Structure and Dynamics: Subtilisin. 1996 , 118, 4175-4180		91
1328	On the Structure and Dynamic Properties of Aqueous Solutions: Molecular Dynamics Simulation of Cl ⁻ and Cl ₂ ⁻ in Water. 1996 , 17, 83-94		15
1327	How does the Electrostatic Force Cut-Off Generate Non-uniform Temperature Distributions in Proteins?. 1996 , 16, 167-177		28
1326	Orientalional order in a liquid crystalline mixture studied by molecular dynamics simulation and NMR. <i>Journal of Chemical Physics</i> , 1996 , 104, 9620-9628	3.9	31
1325	SMD: visual steering of molecular dynamics for protein design. 1996 , 3, 38-45		64
1324	Self-assembly of domain wall of molecular twist defects in polyethylene crystal. 1996 , 106, 31-39		3
1323	How long does DNA keep the memory of its conformation? A time-dependent canonical correlation analysis of molecular dynamics simulation. 1996 , 38, 389-400		11
1322	A First Model of Amorphous GaN from ab Initio Molecular Dynamics. 1996 , 449, 947		1
1321	Atomic-Scale Simulations of Structural Properties of Ceramics. 1996 , 453, 209		
1320	Molecular dynamics simulations of liquids and glasses in the system NaAlSiO ₄ -SiO ₂ ; physical properties and transport mechanisms. 1996 , 81, 284-302		13
1319	Molecular Dynamics Studies of the Frictional Properties of Hydrocarbon Materials□ 1996 , 12, 4552-4556		38
1318	Molecular Dynamics Simulation of a Micellar System: 2,3,6,7,10,11-Hexakis(1,4,7-trioxaoctyl)triphenylene in Water. 1996 , 100, 12162-12171		22

1317	Molecular Dynamics Simulations of Reactions of Hyperthermal Fluorine Atoms with Fluorosilyl Adsorbates on the Si{100}-(2 × 1) Surface. 1996 , 100, 9471-9479	14
1316	A process model for sputter deposition of thin films using molecular dynamics. 1996 , 22, 117-IN3	2
1315	Conformational analysis of retinoids and restriction of their dynamics by retinoid-binding proteins. 1996 , 319 (Pt 2), 543-50	9
1314	Demonstration that 1-trans-epoxysuccinyl-L-leucylamido-(4-guanidino) butane (E-64) is one of the most effective low Mr inhibitors of trypsin-catalysed hydrolysis. Characterization by kinetic analysis and by energy minimization and molecular dynamics simulation of the E-64-beta-trypsin complex. 1996 , 316 (Pt 3), 777-86	53
1313	Permeation Process of Small Molecules across Lipid Membranes Studied by Molecular Dynamics Simulations. 1996 , 100, 16729-16738	358
1312	Computer simulations of crystal structures and elastic properties of cellulose. 1996 , 100, 1350-1354	31
1311	Threonine mutations in proline helix II of bacteriorhodopsin: a molecular dynamics study. 1996 , 361, 269-281	2
1310	Methodological procedures of Molecular Dynamics Simulated Annealing for the chain folding of the flexible tetrapeptide Boc-Gly-Leu-Gly-Gly-NMe with analysis of the evolution mechanism. 1996 , 363, 43-66	3
1309	Two step simulation of low energy ion beam mixing at different temperatures. 1996 , 117, 81-89	9
1308	The solution structure of cytochrome c 6 from the green alga <i>Monoraphidium braunii</i> . 1996 , 1, 330-340	21
1307	Gibbs-Ensemble Molecular Dynamics: A New Method for Simulations Involving Particle Exchange. 1996 , 2, 319-326	9
1306	Extensive and non-extensive thermodynamics. A molecular dynamic test. 1996 , 217, 47-51	38
1305	Mechanism of action of antifreeze polypeptide HPLC6 in solution: analysis of solvent behaviour by molecular dynamics. 1996 , 204, 251-261	15
1304	Molecular dynamics simulations of the bulk phases of 4-cyano-4'-n-pentyloxybiphenyl. 1996 , 208, 57-71	22
1303	Molecular dynamics of amphotericin B. II. Dimer in water. 1996 , 57, 205-17	44
1302	Chlorinated ethanes in aqueous solution: parameterization based on thermodynamics of hydration. 1996 , 259, 142-145	1
1301	Solution structure of the DNA-binding domain of the tomato heat-stress transcription factor HSF24. 1996 , 236, 911-21	49
1300	Secondary structural elements as a basis for antibody recognition in the immunodominant region of human immunodeficiency viruses 1 and 2. 1996 , 237, 188-204	18

1299	Conformational study of [Met5]enkephalin-Arg-Phe in the presence of phosphatidylserine vesicles. 1996 , 240, 540-9	20
1298	An NMR-derived model for the solution structure of oxidized <i>Thermotoga maritima</i> 1[Fe4-S4] ferredoxin. 1996 , 237, 726-35	20
1297	Molecular-dynamics simulation of domain movements in aspartate aminotransferase. 1996 , 240, 751-5	8
1296	Molecular dynamics investigations of the effects of debris molecules on the friction and wear of diamond. 1996 , 290-291, 211-215	28
1295	Pyranosyl-RNA (β -RNA) NMR and Molecular-Dynamics Study of the Duplex Formed by Self-pairing of Ribopyranosyl-(C-G-A-A-T-T-C-G). 1996 , 79, 2316-2345	36
1294	Molecular dynamics simulation of a rhinovirus capsid under rotational symmetry boundary conditions. 1996 , 17, 191-203	15
1293	Determination of the stereochemistry of natural products from nuclear magnetic resonance data by constrained molecular dynamics. 1996 , 17, 409-417	17
1292	Parametrization of GROMOS force field for oligosaccharides and assessment of efficiency of molecular dynamics simulations. 1996 , 17, 1068-1084	66
1291	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
1290	Hydrophilicity of cavities in proteins. 1996 , 24, 433-8	306
1289	Molecular dynamics simulations of N-terminal peptides from a nucleotide binding protein. 1996 , 24, 450-66	16
1288	On the sensitivity of MD trajectories to changes in water-protein interaction parameters: the potato carboxypeptidase inhibitor in water as a test case for the GROMOS force field. 1996 , 25, 89-103	33
1287	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
1286	Molecular mechanisms of pressure induced conformational changes in BPTI. 1996 , 25, 446-455	6
1285	Structural stability of disulfide mutants of basic pancreatic trypsin inhibitor: a molecular dynamics study. 1996 , 26, 66-71	6
1284	Exploring the interaction between D-xylose isomerase and D-xylose by free energy calculation. 1996 , 26, 157-66	2
1283	Dynamics of <i>Fusarium solani</i> cutinase investigated through structural comparison among different crystal forms of its variants. 1996 , 26, 442-58	51
1282	A technique to study molecular recognition in drug design: preliminary application of free energy derivatives to inhibition of a malarial cysteine protease. 1996 , 9, 103-12	4

1281	Molecular dynamics of subtilisin Carlsberg in aqueous and nonaqueous solutions. 1996 , 38, 791-9	11
1280	Molecular dynamics study of a new rigidified 18-crown-6 derivative using a QM / MM method. 1996 , 60, 1133-1141	5
1279	On the relative merits of flexible versus rigid models for use in computer simulations of molecular liquids. 1996 , 250, 19-24	76
1278	Analysis of interfacial water structure and dynamics in β -maltose solution by molecular dynamics simulation. 1996 , 251, 268-274	20
1277	Solvent dynamics in swollen polymers. 1996 , 252, 419-424	28
1276	Molecular dynamics simulations of maltose in water. 1996 , 281, 11-34	53
1275	Investigation of the β -cyclodextrin-myo-inositol phosphate inclusion complex by NMR spectroscopy and molecular modeling. 1996 , 287, 21-35	13
1274	Molecular Dynamics with a Quantum-Chemical Potential: Solvent Effects on an SN2 Reaction at Nitrogen. 1996 , 2, 191-195	22
1273	Diastereoselective recognition of enantiomers of phenyl glucosides by a cyclobis(paraquat-p-phenylene) receptor: A computational study. 1996 , 37, 287-290	13
1272	On the origin of the band at 960 cm^{-1} in the vibrational spectra of Ti-substituted zeolites. 1996 , 7, 133-138	49
1271	Molecular dynamics simulation of HCl in liquid Ar. 1996 , 70, 199-213	5
1270	Effective potentials for liquid simulation of the alternative refrigerants HFC-32: CH_2F_2 and HFC-23: CHF_3 . 1996 , 118, 61-76	25
1269	1,1,1-Trichloroethane-bound cytochrome P450cam dynamics. Does active site water make a difference?. 1996 , 204, 223-231	2
1268	Discrete time-reversible propagation scheme for mixed quantum-classical dynamics. 1996 , 208, 45-56	16
1267	Molecular dynamics simulations of cis-trans isomerization for a proline-containing tripeptide in solution. 1996 , 211, 227-234	3
1266	Correlations between the sugar-backbone conformation and the third strand orientation in triple helices. 1996 , 377, 57-74	2
1265	Transfer of CH_4 across the $\text{H}_2\text{O}/\text{CCl}_4$ liquid-liquid interface with polarizable potential models. 1996 , 263, 39-45	12
1264	Dielectric response of solvent surrounding an ion pair: Ewald potential versus spherical truncation. 1996 , 263, 521-529	27

1263	The dynamics of surfaces of metallic and monolayer systems: an embedded-atom molecular dynamics study. 1996 , 217-218, 112-115	2
1262	DL_POLY_2.0: a general-purpose parallel molecular dynamics simulation package. 1996 , 14, 136-41	1827
1261	Molecular dynamics simulations of silicon-fluorine etching. 1996 , 14, 260-71, 278	11
1260	Stress relaxation: Experiment, theory, and computer simulation. 1996 , 31, 432-445	7
1259	Nanorheology of strongly confined oligomeric lubricants. 1996 , 3, 319-328	1
1258	Molecular modelling simulation of gas transport in amorphous polyimide and poly(amide imide) membrane materials. 1996 , 37, 4773-4785	105
1257	Molecular dynamics simulations of peptides from BPTI: a closer look at amide-aromatic interactions. 1996 , 8, 229-38	79
1256	Molecular dynamics simulation using weak-coupling NOE distance restraining. 1996 , 8, 285-91	10
1255	Synthesis and conformational analysis by 1H NMR and restrained molecular dynamics simulations of the cyclic decapeptide [Ser-Tyr-Ser-Met-Glu-His-Phe-Arg-Trp-Gly]. 1996 , 10, 213-32	3
1254	Computer simulation and infrared investigation on a novolac formaldehyde phenolic resin. 1996 , 31, 3435-3440	14
1253	Solution structure of an SRYD-containing sequence (250-57) of the fibronectin-like Leishmania gp63 protein by restrained molecular dynamics. 1996 , 3, 317-326	3
1252	The new program OPAL for molecular dynamics simulations and energy refinements of biological macromolecules. 1996 , 8, 136-46	174
1251	Investigations of peptide hydration using NMR and molecular dynamics simulations: A study of effects of water on the conformation and dynamics of antamanide. 1996 , 8, 453-76	9
1250	Simulations of CRP:(cAMP) ₂ in noncrystalline environments show a subunit transition from the open to the closed conformation. 1996 , 5, 62-71	46
1249	Phosphorylation-induced torsion-angle strain in the active center of HPr, detected by NMR and restrained molecular dynamics refinement. 1996 , 5, 442-6	6
1248	Mobile unnatural amino acid side chains in the core of staphylococcal nuclease. 1996 , 5, 1026-31	30
1247	Bending of the calmodulin central helix: a theoretical study. 1996 , 5, 2044-53	66
1246	Solution structure of a mini IGF-1. 1996 , 5, 2193-202	30

1245	The Dielectric Properties of Simulated Water Droplets. 1996 , 17, 67-74		9
1244	Monte Carlo vs Molecular Dynamics for Conformational Sampling. 1996 , 100, 14508-14513		119
1243	Molecular Dynamics Studies of the Properties of Water around Simple Organic Solutes. 1996 , 100, 11460-11470	45	
1242	Dynamics of Long n-Alkanes in Silicalite: A Hierarchical Simulation Approach. 1996 , 100, 7155-7173		129
1241	Application of the Nosé-Hoover Chain Algorithm to the Study of Protein Dynamics. 1996 , 100, 1927-1937		111
1240	The NMR structure of 31mer RNA domain of Escherichia coli RNase P RNA using its non-uniformly deuterium labelled counterpart [the 'NMR-window' concept]. 1996 , 24, 2022-35		39
1239	Toward an exhaustive sampling of the configurational spaces of the two forms of the peptide hormone guanylin. 1996 , 13, 741-51		57
1238	Crystallographic Methods and Protocols. 1996 ,		
1237	Relationship between thermal stability and 3-D structure in a homology model of 3-isopropylmalate dehydrogenase from Escherichia coli. 1996 , 9, 663-70		11
1236	Free energy perturbation studies on binding of A-74704 and its diester analog to HIV-1 protease. 1996 , 9, 767-71		13
1235	Solvation Free Energies of the Nucleic Acid Bases. 1996 , 100, 8587-8594		69
1234	Molecular-dynamics study of thermodynamical properties of liquid copper. 1996 , 54, 15742-15746		49
1233	Constant pressure molecular dynamics simulations of the dodecamers: d(GCGCGCGCGCGC) ₂ and r(GCGCGCGCGCGC) ₂ . <i>Journal of Chemical Physics</i> , 1996 , 104, 6052-6057	3-9	41
1232	Free energy calculations of small molecules in dense amorphous polymers. Effect of the initial guess configuration in molecular dynamics studies. <i>Journal of Chemical Physics</i> , 1996 , 105, 8849-8857	3-9	74
1231	Molecular dynamics studies of Langmuir monolayers of F(CF ₂) ₂₀ F. <i>Journal of Chemical Physics</i> , 1996 , 104, 2114-2123	3-9	12
1230	Multielectron excitations at the L edges of barium in aqueous solution. 1996 , 54, 12129-12138		44
1229	Local structure and mobility of ions in polymer electrolytes: A molecular dynamics simulation study of the amorphous PEOxNaI system. <i>Journal of Chemical Physics</i> , 1996 , 104, 3797-3809	3-9	71
1228	Nosé-Andersen dynamics of partially rigid molecules: Coupling all degrees of freedom to heat and pressure baths. 1996 , 54, 6825-6837		13

1227	The influence of temperature on pairwise hydrophobic interactions of methane-like particles: A molecular dynamics study of free energy. <i>Journal of Chemical Physics</i> , 1996 , 104, 286-295	3.9	86
1226	The local energy approximation and the predictability of chain configurations in polymer melts. <i>Journal of Chemical Physics</i> , 1996 , 105, 2076-2088	3.9	29
1225	An extended x-ray absorption fine structure study by employing molecular dynamics simulations: Bromide ion in methanolic solution. <i>Journal of Chemical Physics</i> , 1996 , 104, 1779-1790	3.9	45
1224	Vibrational energy relaxation of HOD in liquid D2O. <i>Journal of Chemical Physics</i> , 1996 , 104, 2356-2368	3.9	233
1223	An All-Atom Force Field for Liquid Ethanol/Water Mixtures. 1996 , 18, 133-143		31
1222	Molecular dynamics studies of Langmuir monolayers of F(CF ₂) ₁₁ COOH. <i>Journal of Chemical Physics</i> , 1996 , 104, 2101-2113	3.9	21
1221	Molecular dynamics of linear and branched alkanes: Simulations and nuclear magnetic resonance results. <i>Journal of Chemical Physics</i> , 1996 , 105, 5208-5215	3.9	35
1220	Molecular dynamics simulation of a charged biological membrane. <i>Journal of Chemical Physics</i> , 1996 , 104, 2713-2720	3.9	105
1219	On the effects of truncating the electrostatic interactions: Free energies of ion hydration. <i>Journal of Chemical Physics</i> , 1996 , 104, 9578-9585	3.9	49
1218	Static and dynamic structural analysis of a saturated solution of ZnBr ₂ in water: Anomalous x-ray diffraction and molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1996 , 104, 7239-7248	3.9	4
1217	Molecular dynamics simulations of sliding friction of Langmuir/Blodgett monolayers. <i>Journal of Chemical Physics</i> , 1996 , 105, 6060-6067	3.9	51
1216	Molecular dynamics simulation study of adsorption of polymer chains with variable degree of rigidity. I. Static properties. <i>Journal of Chemical Physics</i> , 1996 , 104, 4806-4813	3.9	67
1215	A Molecular Dynamics Simulation Study of Liquid Carbon Tetrachloride. 1996 , 18, 1-11		25
1214	An efficient method for sampling the essential subspace of proteins. 1996 , 13, 615-25		234
1213	Effects of polymer surface structures on liquid crystal alignment studied with molecular dynamics simulations. 1996 , 21, 817-827		10
1212	Gibbs-Ensemble Molecular Dynamics: Liquid-Gas Equilibria for Lennard-Jones Spheres and n-Hexane. 1996 , 17, 95-112		16
1211	Direct Evaluation of Vapour-Liquid Equilibria of Mixtures by Molecular Dynamics Using Gibbs-Duhem Integration. 1996 , 18, 75-99		4
1210	Detailed description of an alpha helix->pi bulge transition detected by molecular dynamics simulations of the p185c-erbB2 V659G transmembrane domain. 1996 , 13, 753-69		23

1209	Molecular dynamics simulations of fluorinated ethanes. 1996 , 87, 167-187	12
1208	Molecular Dynamics of Microperoxidases in Aqueous and Nonaqueous Solutions. 1996 , 100, 19241-19250	22
1207	Molecular Dynamics Simulation of Water between Two Charged Layers of Dipalmitoylphosphatidylserine. 1996 , 100, 8621-8627	41
1206	Molecular Dynamics Study of Silica/Alumina Interfaces. 1996 , 100, 2201-2205	56
1205	Investigating the Anomalous Solvation Free Energies of Amines with a Polarizable Potential. 1996 , 100, 2367-2371	52
1204	Comparison of Continuum and Explicit Models of Solvation: Potentials of Mean Force for Alanine Dipeptide. 1996 , 100, 1439-1441	79
1203	Critical Study of Fluoride/Water Interactions. 1996 , 100, 3989-3995	96
1202	Prediction of pKa Shifts without Truncation of Electrostatic Interactions: An Explicit Solvent Calculation for Succinic Acid. 1996 , 100, 6389-6392	34
1201	Application of Free Energy Perturbation Calculations to the Mennis Ball/Dimer: Why Is CF ₄ Not Encapsulated by This Host?. 1996 , 100, 10779-10783	15
1200	16. Parallel Molecular Dynamics on a Torus Network. 1996 , 177-186	
1199	Recent developments for crystallographic refinement of macromolecules. 1996 , 56, 245-66	10
1198	Flexibility of serine protease in nonaqueous solvent. 1997 , 8, 693-702	
1197	Calculating protein structures from NMR data. 1997 , 60, 157-94	15
1196	Self-lubrication in scanning-force-microscope image formation on ionic surfaces. 1997 , 56, 12482-12489	44
1195	Structural changes during stress relaxation in simple liquids. <i>Journal of Chemical Physics</i> , 1997 , 107, 7214-7226	3.9
1194	Suppression of potential electron emission for impact of slow multicharged fullerenes on clean gold. 1997 , 56, 3007-3010	21
1193	Equation of state of supercooled water simulated using the extended simple point charge intermolecular potential. <i>Journal of Chemical Physics</i> , 1997 , 107, 7443-7450	3.9
1192	Can Amorphous GaN Serve as a Useful Electronic Material?. 1997 , 79, 677-680	94

1191	Soft-Landing Ion Deposition of Isolated Radioactive Probe Atoms on Surfaces: A Novel Method. 1997 , 78, 4075-4078		14
1190	Molecular dynamics simulation studies of the density profiles of water between (9-3) Lennard-Jones walls. <i>Journal of Chemical Physics</i> , 1997 , 106, 388-391	3.9	44
1189	Comparison of shear flow of hexadecane in a confined geometry and in bulk. <i>Journal of Chemical Physics</i> , 1997 , 106, 7303-7314	3.9	126
1188	Analysis of the optical spectra of aromaticAlkane clusters. <i>Journal of Chemical Physics</i> , 1997 , 107, 8338-8348	3.9	10
1187	Low-frequency dynamics of Lennard-Jones glasses. 1997 , 55, 12113-12120		9
1186	The Molecular Structure of Sodium Octanoate Micelles Studied by Molecular Dynamics Computer Experiments. 1997 , 101, 1485-1492		23
1185	Many-body components in the integrated far-infrared absorption coefficient of diatomic molecules in spherical solvents. <i>Journal of Chemical Physics</i> , 1997 , 107, 4844-4851	3.9	4
1184	Molecular Dynamics Simulations Find That 3[Phosphoramidate Modified DNA Duplexes Undergo a B to A Transition and Normal DNA Duplexes an A to B Transition. 1997 , 119, 6722-6730		73
1183	Theoretical study of a five-coordinated silica polymorph. 1997 , 56, 5797-5806		56
1182	Deposition of Cu atoms on a Pb single crystal surface. 1997 , 142, 51-62		3
1181	The reactive flux method applied to complex isomerization reactions: Using the unstable normal mode as a reaction coordinate. <i>Journal of Chemical Physics</i> , 1997 , 106, 5494-5508	3.9	17
1180	Far-infrared absorption spectra of water, ammonia, and chloroform calculated from instantaneous normal mode theory. <i>Journal of Chemical Physics</i> , 1997 , 106, 4389-4400	3.9	75
1179	Quantum energy gap law of outer-sphere electron transfer reactions: A molecular dynamics study on aqueous solution. <i>Journal of Chemical Physics</i> , 1997 , 106, 116-126	3.9	41
1178	Ionic and electronic processes at ionic surfaces induced by atomic-force-microscope tips. 1997 , 56, 15332-15344		9
1177	Electric field-gradient contributions to the chemical shifts of liquid water. <i>Journal of Chemical Physics</i> , 1997 , 106, 8332-8338	3.9	25
1176	Simulations of hydrocarbon adsorption and subsequent water penetration on an aluminum oxide surface. <i>Journal of Chemical Physics</i> , 1997 , 106, 7331-7342	3.9	35
1175	The frequency-dependent conductivity of a saturated solution of ZnBr ₂ in water: A molecular dynamics simulation. <i>Journal of Chemical Physics</i> , 1997 , 107, 3135-3143	3.9	15
1174	Dynamic relaxation of the elastic properties of hard carbon films. 1997 , 81, 7248-7254		27

1173	Solvation dynamics and electronic structure development of coumarin 120 in methanol: A theoretical modeling study. <i>Journal of Chemical Physics</i> , 1997 , 107, 4585-4596	3.9	46
1172	Protein dynamics determined by backbone conformation and atom packing. 1997 , 10, 373-80		22
1171	Modelling protein unfolding: hen egg-white lysozyme. 1997 , 10, 895-903		49
1170	Protein NMR Techniques. 1997 ,		2
1169	Chemistry of Polymerization Products of p-Benzoquinone. 13C NMR and Molecular Dynamics Study. 1997 , 29, 670-677		11
1168	Modelling pathways of alpha-chymotrypsin activation and deactivation. 1997 , 10, 1163-74		27
1167	Solution structure of porcine delta sleep-inducing peptide immunoreactive peptide A homolog of the shortsighted gene product. 1997 , 272, 30918-27		11
1166	Molecular switch in signal transduction: reaction paths of the conformational changes in ras p21. 1997 , 94, 11905-10		143
1165	Conformational Correlations in DNA. Molecular Dynamics Studies. 1997 , 19, 247-266		2
1164	Determination of The Solution Conformation of A Non-Uniformly Deuterium Labelled (Uppsala Nmr-Window) 21Mer Rna Hairpin by Nmr Spectroscopy And Computational Methods.. 1997 , 16, 743-750		1
1163	NMR Structure Determination of a 28-Nucleotide Signal Recognition Particle RNA with Complete Relaxation Matrix Methods Using Corrected Nuclear Overhauser Effect Intensities. 1997 , 122-149		2
1162	Crystallographic refinement by simulated annealing: methods and applications. 1997 , 277, 243-69		86
1161	Molecular Dynamics Simulation of Composition Dependence of Cohesive Energy, Lattice Constants and Elastic Constants in Nickel-Based Superalloys. 1997 , 38, 761-770		5
1160	Local Dynamics of Poly(ethylene oxide) in Solution. 1. Localization of Chain Motion. 1997 , 30, 5704-5713		13
1159	Azino-Fused Benzimidazolium Salts as DNA Intercalating Agents. 2.. 1997 , 62, 5476-5483		52
1158	Conformation Control of Peptides by Metal Ions. Coordination Conformation Correlation Observed in a Model for Cys-X-Y-Cys/M(2+) in Proteins. 1997 , 36, 4849-4859		14
1157	Conformational properties of the TATA-box binding sequence of DNA. 1997 , 14, 757-65		40
1156	Viscosity calculations of n-alkanes by equilibrium molecular dynamics. <i>Journal of Chemical Physics</i> , 1997 , 106, 9327-9336	3.9	185

1155	Thermodynamic Decomposition of Hydration Free Energies by Computer Simulation: Application to Amines, Oxides, and Sulfides. 1997 , 101, 10527-10534	53
1154	Effect of Polarizability on the Potential of Mean Force of Two Cations. The Guanidinium-Guanidinium Ion Pair in Water. 1997 , 101, 10910-10917	70
1153	Hydrogen Bonding of Water to Phosphatidylcholine in the Membrane As Studied by a Molecular Dynamics Simulation: Location, Geometry, and Lipid-Lipid Bridging via Hydrogen-Bonded Water. 1997 , 101, 3677-3691	205
1152	Incorporating Hydration Force Determined by Boundary Element Method into Stochastic Dynamics. 1997 , 101, 230-235	17
1151	Selectin-ligand interactions revealed by molecular dynamics simulation in solution. 1997 , 40, 362-9	37
1150	Molecular dynamics simulation of reactive ion etching of Si by energetic Cl ions. 1997 , 82, 3552-3559	72
1149	Determination of Equation-of-State Parameters by Molecular Simulations and Application to the Prediction of Surface Properties for Polyethylene. 1997 , 30, 1800-1805	11
1148	Solution structure of the cellulose-binding domain of the endoglucanase Z secreted by <i>Erwinia chrysanthemi</i> . 1997 , 36, 16074-86	92
1147	Chemical Shifts in Liquid Water Calculated by Molecular Dynamics Simulations and Shielding Polarizabilities. 1997 , 101, 4105-4110	52
1146	Point defect movement and annealing in collision cascades. 1997 , 56, 2421-2431	131
1145	Ligand Binding in the Catalytic Antibody 17E8. A Free Energy Perturbation Calculation Study. 1997 , 119, 11571-11577	35
1144	Atomistically Modeling the Chemical Potential of Small Molecules in Dense Polymer Microstructures. 1. Method. 1997 , 30, 6107-6113	42
1143	Structure Optimization Combining Soft-Core Interaction Functions, the Diffusion Equation Method, and Molecular Dynamics. 1997 , 101, 5926-5930	34
1142	Understanding the Mechanism for the Mass Accommodation of Ethanol by a Water Droplet. 1997 , 101, 5473-5476	40
1141	Simulation of a Protein Crystal at Constant Pressure. 1997 , 101, 2105-2108	13
1140	Constructing protein models for ligand-receptor binding thermodynamic simulations: an application to a set of peptidomimetic renin inhibitors. 1997 , 37, 779-91	34
1139	Effects of Molecular Structure on Frictional Properties of Langmuir-Blodgett Monolayers. 1997 , 13, 1718-1722	23
1138	Dielectric Constant and Structure of Liquid 18-Crown-6 Calculated from Molecular Dynamics Simulations. 1997 , 101, 1024-1034	10

1137	Investigation of the proton release channel of bacteriorhodopsin in different intermediates of the photo cycle. A molecular dynamics study. 1997 , 36, 2875-83	7
1136	Molecular Dynamics Simulation of the Interfacial Behavior of a Heptane/Water System in the Presence of Nonylphenol Triethoxylated Surfactants. 1. Surface Energy, Surface Entropy, and Interaction Energies as a Function of Temperature and Surfactant Concentration. 1997 , 13, 1644-1652	21
1135	Friction between Diamond Surfaces in the Presence of Small Third-Body Molecules. 1997 , 101, 1364-1373	64
1134	Molecular Dynamics and FEP Monte Carlo Studies of Calix[4]arene-Derived Complexes of Eu ³⁺ : The Role of the Counterions Investigated. 1997 , 101, 2755-2765	11
1133	DLC growth by ion beam assisted deposition: a molecular simulation. 1997 , 6, 1638-1642	8
1132	Atomistic simulation of the stretching of nanoscale metal wires. 1997 , 92, 705-714	76
1131	Computer simulation and boron nitride. 1997 , 141, 85-97	73
1130	Transmembrane helix structure, dynamics, and interactions: multi-nanosecond molecular dynamics simulations. 1997 , 73, 3-20	110
1129	The essential dynamics of Cu, Zn superoxide dismutase: suggestion of intersubunit communication. 1997 , 73, 1007-18	45
1128	A 5-nanosecond molecular dynamics trajectory for B-DNA: analysis of structure, motions, and solvation. 1997 , 73, 2313-36	280
1127	Observation of an A-DNA to B-DNA transition in a nonhelical nucleic acid hairpin molecule using molecular dynamics. 1997 , 73, 2702-10	17
1126	Ice-binding mechanism of winter flounder antifreeze proteins. 1997 , 73, 2851-73	87
1125	Molecular dynamics simulations of Leu-enkephalin in water and DMSO. 1997 , 72, 2032-41	99
1124	How hormone receptor-DNA binding affects nucleosomal DNA: the role of symmetry. 1997 , 72, 2056-67	21
1123	Role of water on unfolding kinetics of helical peptides studied by molecular dynamics simulations. 1997 , 72, 2445-56	39
1122	Solvated ion dynamics in the water-formamide mixtures using molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1997 , 107, 6908-6916	3.9 14
1121	Molecular dynamics modelling of amorphous polymers. 1997 , 33-83	3
1120	A simple nonequilibrium molecular dynamics method for calculating the thermal conductivity. <i>Journal of Chemical Physics</i> , 1997 , 106, 6082-6085	3.9 1033

1119	Crystal Growth of the Lennard-Jones (100) Surface by Means of Equilibrium and Nonequilibrium Molecular Dynamics. 1997 , 79, 5074-5077	64
1118	Dynamic Molecular Shape Analysis of Configurational Transitions Associated with Melting and Premelting of n-Alkane Chains. 1997 , 101, 4097-4104	6
1117	Derivation of Class II Force Fields. 4. van der Waals Parameters of Alkali Metal Cations and Halide Anions. 1997 , 101, 7243-7252	155
1116	Liquid-Liquid Phase Transition: Evidence from Simulations. 1997 , 78, 2409-2412	244
1115	[21] Stereoselectivity of lipase from <i>Rhizopus oryzae</i> toward triacylglycerols and analogs: Computer-aided modeling and experimental validation. 1997 , 353-376	11
1114	Calculation of Chloroform/Water Partition Coefficients for the N-Methylated Nucleic Acid Bases. 1997 , 101, 10971-10975	37
1113	Towards mechanosynthesis of diamondoid structures: I. Quantum-chemical molecular dynamics simulations of sila-adamantane synthesis on hydrogenated Si(111) surface with the STM. 1997 , 8, 132-144	5
1112	Molecular Dynamics Methods. 1997 , 83-115	1
1111	Energetics of nucleophile activation in a protein tyrosine phosphatase. 1997 , 265, 118-27	73
1110	Dynamical studies of peptide motifs in the <i>Plasmodium falciparum</i> circumsporozoite surface protein by restrained and unrestrained MD simulations. 1997 , 267, 1012-25	34
1109	Characterization of long-range structure in the denatured state of staphylococcal nuclease. II. Distance restraints from paramagnetic relaxation and calculation of an ensemble of structures. 1997 , 268, 170-84	270
1108	Automated NOESY interpretation with ambiguous distance restraints: the refined NMR solution structure of the pleckstrin homology domain from beta-spectrin. 1997 , 269, 408-22	395
1107	Structure of ribgrass mosaic virus at 2.9 Å resolution: evolution and taxonomy of tobamoviruses. 1997 , 269, 769-79	50
1106	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
1105	The effect of point mutations on the free energy of transmembrane alpha-helix dimerization. 1997 , 272, 266-75	223
1104	Torsion angle dynamics for NMR structure calculation with the new program DYANA. 1997 , 273, 283-98	2561
1103	Molecular dynamics study of water clusters, liquid, and liquid-vapor interface of water with many-body potentials. <i>Journal of Chemical Physics</i> , 1997 , 106, 8149-8159	3.9 578
1102	Atomic stress isobaric scaling for systems subjected to holonomic constraints. <i>Journal of Chemical Physics</i> , 1997 , 106, 195-199	3.9 31

1101	Atomistically Modeling the Chemical Potential of Small Molecules in Dense Polymer Microstructures. 2. Water Sorption by Polyamides. 1997 , 30, 6114-6119	48
1100	Molecular Simulation of Peptide Interactions with an RP-HPLC Sorbent. 1997 , 101, 10962-10970	38
1099	Atomistic simulations of fluid structure and solvation forces in atomic force microscopy. 1997 , 380, 224-244	28
1098	Molecular surface structure of ice(0001): dynamical low-energy electron diffraction, total-energy calculations and molecular dynamics simulations. 1997 , 381, 190-210	148
1097	Mechanical stability of compact modules of barnase. 1997 , 405, 47-54	6
1096	Effect of lithium and sodium ions on a charged membrane of dipalmitoylphosphatidylserine: a study by molecular dynamics simulation. 1997 , 1330, 145-56	27
1095	Inactive conformation of an insulin despite its wild-type sequence. 1997 , 6, 580-7	12
1094	Cross-validated maximum likelihood enhances crystallographic simulated annealing refinement. 1997 , 94, 5018-23	561
1093	A modular molecular dynamics / quantum dynamics program for non-adiabatic proton transfers in solution. 1997 , 107, 61-91	39
1092	Molecular dynamics simulations of Na ⁺ and Cl ⁻ ions solvation in aqueous mixtures of formamide. 1997 , 222, 43-57	16
1091	Mechanism of alpha-cyclodextrin-induced hemolysis. 1. The two-step extraction of phosphatidylinositol from the membrane. 1997 , 86, 935-43	60
1090	Molecular Dynamics Simulation of the Excited-State Dynamics of Bacteriorhodopsin. 1997 , 66, 735-740	10
1089	A computer perspective of membranes: molecular dynamics studies of lipid bilayer systems. 1997 , 1331, 235-70	622
1088	Computer-aided modelling of stereoselective triglyceride hydrolysis catalyzed by <i>Rhizopus oryzae</i> lipase. 1997 , 3, 73-82	24
1087	New applications of simulated annealing in X-ray crystallography and solution NMR. 1997 , 5, 325-36	183
1086	Dynamics of a type VI reverse turn in a linear peptide in aqueous solution. 1997 , 2, 35-46	51
1085	Role of a nonnative interaction in the folding of the protein G B1 domain as inferred from the conformational analysis of the alpha-helix fragment. 1997 , 2, 123-33	31
1084	Constitution and solution conformation of the antibiotic mersacidin determined by NMR and molecular dynamics. 1997 , 244, 501-12	39

1083	A molecular dynamics study in explicit water of the reduced and oxidized forms of yeast iso-1-cytochrome c--solvation and dynamic properties of the two oxidation states. 1997 , 249, 716-23	21
1082	Molecular dynamics study of conformational equilibria in aqueous d-glucose and d-galactose. 1997 , 395-396, 289-295	14
1081	The use of the MM3* and ESFF force fields in conformational analysis of carbohydrate molecules in solution: The methyl β -lactoside case. 1997 , 395-396, 245-270	20
1080	Cluster bombardment of solids: A molecular dynamics study. 1997 , 122, 311-317	56
1079	Quantitative Molecular Dynamics Simulation of High Pressure Adsorption Isotherms of Methane on Graphite. 1997 , 101, 79-83	3
1078	Development of a Hybrid Quantum Chemical and Molecular Mechanics Method with Application to Solvent Effects on the Electronic Spectra of Uracil and Uracil Derivatives. 1997 , 101, 2478-2488	51
1077	¹ H and ¹⁵ N NMR assignment and solution structure of the SH3 domain of spectrin: comparison of unrefined and refined structure sets with the crystal structure. 1997 , 9, 347-57	50
1076	The dynamic NMR structure of the T psi C-loop: implications for the specificity of tRNA methylation. 1997 , 9, 229-44	21
1075	Floating stereospecific assignment revisited: application to an 18 kDa protein and comparison with J-coupling data. 1997 , 9, 245-58	100
1074	TR-NOE and MD studies of Leishmania gp63 SRYD-containing sequences bound to anti-SRYD monoclonal antibody. 1997 , 4, 323-330	
1073	Conformation of the C-terminal pentapeptide of the message sequence of tachykinins as determined by consensus dynamic. 1997 , 22, 315-324	3
1072	Molecular Dynamics Simulations on the Complexes of Glucoamylase II (471) from <i>Aspergillus awamori</i> var. X100 with 1-Deoxynojirimycin and Lentiginosine. 1997 , 3, 249-260	17
1071	Simulation of Surface Excess Concentrations for a Binary Hydrocarbon Mixture on Graphite. 1997 , 3, 315-320	15
1070	Computer simulation of polymers. 1997 , 7, 35-46	12
1069	Polysiloxanes: ab initio force field and structural, conformational and thermophysical properties. 1997 , 53, 1301-1323	265
1068	Quantum chemistry based force fields for soft matter. 1997 , 53, 1325-1346	14
1067	Flickering noise in the potential energy fluctuations of proteins as investigated by MD simulation. 1997 , 236, 596-601	24
1066	Effective potentials for liquid simulation of the alternative refrigerants HFC-134a (CF ₃ CH ₂ F) and HFC-125 (CF ₃ CHF ₂). 1997 , 127, 83-102	10

1065	Critical point and coexistence curve for a flexible, simple point-charge water model. 1997 , 10, 119-125	8
1064	Multi-basin dynamics of a protein in a crystal environment. 1997 , 107, 225-239	76
1063	Water residence times around copper plastocyanin: a molecular dynamics simulation approach. 1997 , 214, 261-276	55
1062	Theoretical study of the solvatochromism of a merocyanine dye. 1997 , 223, 183-194	11
1061	Ion-water and water-water interactions in a gramicidinlike channel: effects due to group polarizability and backbone flexibility. 1997 , 65, 123-41	29
1060	Molecular dynamics simulation of a dye molecule in the interior of a bilayer: 1,6-diphenyl-1,3,5-hexatriene in dipalmitoylphosphatidylcholine. 1997 , 69, 1-8	22
1059	Long-term molecular dynamics simulation of copper plastocyanin in water. 1997 , 69, 185-98	30
1058	Theoretical and molecular dynamics studies of dense plasma microfield nonuniformity. 1997 , 58, 677-686	9
1057	Solvation of poly(vinyl alcohol) in water, ethanol and an equimolar water-ethanol mixture: structure and dynamics studied by molecular dynamics simulation. 1997 , 38, 2259-2268	80
1056	Molecular modelling of amorphous membrane polymers. 1997 , 38, 6145-6155	57
1055	NMR spectroscopic study of solution structure and complexational behaviour of bis-benzo crown ethers. 1997 , 404, 273-290	22
1054	Hydrogen bonding in liquid alcohols: a computer simulation study. 1997 , 416, 243-248	188
1053	Complexation Properties of Preorganized Receptor Molecules for Large, Neutral Guests. 1997 , 1997, 1577-1586	22
1052	Studying the Stability of a Helical α -Heptapeptide by Molecular Dynamics Simulations. 1997 , 3, 1410-1417	109
1051	MOLECULAR DYNAMICS STUDY OF THE COMPLEXATION OF LUMINESCENT CATIONS BY ENCAPSULATING LIGANDS WITH BIPYRIDINE UNITS. 1997 , 10, 292-304	11
1050	A molecular mechanics force field for NAD ⁺ NADH, and the pyrophosphate groups of nucleotides. 1997 , 18, 221-239	139
1049	Free energies of hydration from thermodynamic integration: Comparison of molecular mechanics force fields and evaluation of calculation accuracy. 1997 , 18, 449-462	32
1048	Free energy calculation methods: A theoretical and empirical comparison of numerical errors and a new method qualitative estimates of free energy changes. 1997 , 18, 902-919	94

1047	Finite element interpolation for combined classical/quantum mechanical molecular dynamics simulations. 1997 , 18, 1484-1495	18
1046	Coupled semiempirical molecular orbital and molecular mechanics model (QM/MM) for organic molecules in aqueous solution. 1997 , 18, 1496-1512	62
1045	Fast and accurate molecular dynamics simulation of a protein using a special-purpose computer. 1997 , 18, 1546-1563	64
1044	FAMUSAMM: An algorithm for rapid evaluation of electrostatic interactions in molecular dynamics simulations. 1997 , 18, 1729-1749	61
1043	Unification of box shapes in molecular simulations. 1997 , 18, 1930-1942	29
1042	Protein structure prediction force fields: parametrization with quasi-newtonian dynamics. 1997 , 27, 367-84	24
1041	Simulation of protein conformational freedom as a function of pH: constant-pH molecular dynamics using implicit titration. 1997 , 27, 523-544	142
1040	Calculation of pathways for the conformational transition between the GTP- and GDP-bound states of the Ha-ras-p21 protein: Calculations with explicit solvent simulations and comparison with calculations in vacuum. 1997 , 28, 434-451	52
1039	Correlation of the enzyme activities of Bacillus stearothermophilus lactate dehydrogenase on three substrates with the results of molecular dynamics/energy minimization conformational searching. 1997 , 29, 228-239	4
1038	Quantum chemical study of the molecular dynamics of hydrated Li ⁺ And Be ²⁺ cations. 1997 , 65, 803-816	16
1037	Characterization of lipid membrane dynamics by simulation: I. Torsion angle motions of the linear chains. 1997 , 41, 37-50	5
1036	Protein hinge bending as seen in molecular dynamics simulations of native and M61 mutant T4 lysozymes. 1997 , 41, 533-44	20
1035	Effects of substrate binding on the dynamics of RNase A: Molecular dynamics simulations of UpA bound and native RNase A. 1997 , 42, 505-520	16
1034	Torsion-angle molecular dynamics as a new efficient tool for NMR structure calculation. 1997 , 124, 154-64	284
1033	Generalized linear response approximation in discrete methods. 1997 , 265, 473-480	20
1032	Comparison of the interface between water and four surfaces of native crystalline cellulose by molecular dynamics simulations. 1998 , 306, 205-220	98
1031	Computer simulation of the cyclodextrin β phenylalanine complex. 1998 , 310, 253-259	16
1030	Molecular structure of the fullerene C ₇₀ at 825°C:: quantum-chemical molecular dynamics simulations. 1998 , 288, 183-187	3

1029	Molecular dynamics study of the tautomeric equilibrium in the Mannich base. 1998 , 289, 457-462	17
1028	Molecular dynamics simulation of water between hydrophobic surfaces. Implication for the long-range hydrophobic force. 1998 , 289, 567-571	24
1027	Ab initio molecular dynamics simulations on the hydrolysis of methyl chloride with explicit consideration of three water molecules. 1998 , 292, 474-480	38
1026	Local structural heterogeneities in liquid water under pressure. 1998 , 294, 9-12	79
1025	Simulation studies for liquid phenol: properties evaluated and tested over a range of temperatures. 1998 , 294, 135-142	68
1024	All-atom empirical potential for molecular modeling and dynamics studies of proteins. 1998 , 102, 3586-616	11429
1023	Structural and theoretical studies suggest domain movement produces an active conformation of thymidine phosphorylase. 1998 , 281, 285-99	64
1022	Solution structure of cytochrome c6 from the thermophilic cyanobacterium <i>Synechococcus elongatus</i> . 1998 , 17, 27-36	41
1021	Molecular Computer Simulations of the Swelling Properties and Interlayer Structure of Cesium Montmorillonite. 1998 , 14, 5959-5967	176
1020	Molecular simulation: Understanding polymer gels at the molecular level. 1998 , 102, 1679-1682	7
1019	A molecular dynamics study of carbon dioxide in water: diffusion, structure and thermodynamics. 1998 , 94, 963-972	55
1018	Demixing of Binary Water-Chloroform Mixtures Containing Ionophoric Solutes and Ion Recognition at a Liquid-Liquid Interface: A Molecular Dynamics Study. 1998 , 102, 10772-10788	72
1017	Structural homology of the central conserved region of the attachment protein G of respiratory syncytial virus with the fourth subdomain of 55-kDa tumor necrosis factor receptor. 1998 , 243, 293-302	47
1016	Structural transition in small gas-like clusters. 1998 , 86, 101-106	1
1015	Ambiguous NOEs and automated NOE assignment. 1998 , 32, 107-139	185
1014	The barrier for heme-protein separation estimated by non-equilibrium molecular dynamics simulations. 1998 , 291, 501-508	3
1013	A new simulated annealing method combined with a polarizable continuum model based on the boundary element method. 1998 , 291, 137-142	7
1012	A classical molecular dynamics study of the vibrational dynamics of the H/C(111)-(1 \times 1) system. 1998 , 230, 57-66	2

1011	Constant temperature simulations using the Langevin equation with velocity Verlet integration. 1998 , 236, 243-252	139
1010	MD simulation of atomic displacements in pure metals and metallic bilayers during low energy ion bombardment at 0 K. 1998 , 143, 455-472	13
1009	Molecular dynamics study of hyaluronic acid in water. 1998 , 422, 109-121	37
1008	Non-bonded organo-mineral interactions and sorption of organic compounds on soil surfaces: a model approach. 1998 , 422, 259-270	24
1007	Molecular dynamics simulation with atomic partial charges update of erythrol in water. 1998 , 431, 7-15	5
1006	Simulated annealing and molecular dynamics of an elastin-related tetrapeptide in aqueous solution. 1998 , 431, 205-218	10
1005	NMR-restrained molecular modeling of cobalt corrinoids: cyanocobalamin (vitamin B12) and methylcobalt corrinoids. 1998 , 453, 209-224	27
1004	Solution conformation of the <i>Pseudomonas syringae</i> MSU 16H phytotoxic lipodepsipeptide Pseudomycin A determined by computer simulations using distance geometry and molecular dynamics from NMR data. 1998 , 257, 449-56	9
1003	β - and β -Peptides with Proteinaceous Side Chains: Synthesis and solution structures of constitutional isomers, a novel helical secondary structure and the influence of solvation and hydrophobic interactions on folding. 1998 , 81, 932-982	287
1002	Solution structure of regioselectively addressable functionalized templates: an NMR and restrained molecular dynamics investigation. 1996 , 39, 297-308	55
1001	Theoretical studies of the intercalation of 9-hydroxyellipticine in DNA. 1998 , 39, 309-326	11
1000	Relationship between conformation and geometry as evidenced by molecular dynamics simulation of C β , β -dialkylated glycines. 1998 , 46, 239-244	17
999	Small structural ensembles for a 17-nucleotide mimic of the tRNA T ψ C-loop via fitting dipolar relaxation rates with the quadratic programming algorithm. 1998 , 46, 329-42	14
998	Structural similarities and differences between H1- and H2-family DNA minihairpin loops: NMR studies of octameric minihairpins. 1998 , 46, 375-393	19
997	Modeling large-scale dynamics of proteins. 1998 , 46, 493-501	14
996	Molecular dynamics simulation of organic glass formers: I. ortho-terphenyl and 1,3,5-tri- β -naphthyl benzene. 1998 , 19, 86-93	8
995	Parametrization of aliphatic CH n united atoms of GROMOS96 force field. 1998 , 19, 535-547	335
994	The flying ice cube: Velocity rescaling in molecular dynamics leads to violation of energy equipartition. 1998 , 19, 726-740	314

993	Free energy calculations in globular proteins: Methods to reduce errors. 1998 , 19, 1229-1240	6
992	Multiple time step algorithms for molecular dynamics simulations of proteins: How good are they?. 1998 , 19, 1534-1552	31
991	Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function. 1998 , 19, 1639-1662	7548
990	Structure prediction of a complex between the chromosomal protein HMG-D and DNA. 1998 , 30, 113-35	25
989	Mapping the active site of factor Xa by selective inhibitors: an NMR and MD study. 1998 , 30, 264-74	10
988	Improved protein free energy calculation by more accurate treatment of nonbonded energy: Application to chymotrypsin inhibitor 2, V57A. 1998 , 30, 388-400	37
987	Domain motions in bacteriophage T4 lysozyme: a comparison between molecular dynamics and crystallographic data. 1998 , 31, 116-27	141
986	Conformation of the Ras-binding domain of Raf studied by molecular dynamics and free energy simulations. 1998 , 31, 186-200	9
985	Essential spaces defined by NMR structure ensembles and molecular dynamics simulation show significant overlap. 1998 , 31, 370-382	58
984	Functional conformational changes of endo-1,4-xylanase II from <i>Trichoderma reesei</i> : A molecular dynamics study. 1998 , 31, 434-444	44
983	Reaction path and free energy calculations of the transition between alternate conformations of HIV-1 protease. 1998 , 32, 7-16	61
982	Molecular dynamics study of femtosecond events in photoactive yellow protein after photoexcitation of the chromophore. 1998 , 32, 268-75	19
981	Hydration energy landscape of the active site cavity in cytochrome P450cam. 1998 , 32, 381-396	47
980	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
979	Identification of functional and unfolding motions of cutinase as obtained from molecular dynamics computer simulations. 1998 , 33, 253-264	35
978	Molecular dynamics simulations of epidermal growth factor and transforming growth factor- β structures in water. 1998 , 33, 396-407	5
977	A bovine dander allergen, comparative modeling, and similarities and differences in folding with related proteins. 1998 , 17, 657-62	6
976	Investigating the dielectric effects of channel pore water on the electrostatic barriers of the permeation ion by the finite difference Poisson-Boltzmann method. 1998 , 27, 105-12	19

975	Molecular dynamics investigations of hammerhead ribozyme RNA. 1998 , 27, 153-65	60
974	A molecular dynamics study of intermolecular structure, thermodynamics and miscibility in hydrocarbon polymers. 1998 , 22, S19-S26	2
973	On the dynamics of electrochemical ion-transfer reactions. 1998 , 450, 303-311	11
972	Adsorption of water molecules in slit pores. 1998 , 450, 281-287	41
971	Computer simulation of the structure of the electrochemical double layer. 1998 , 450, 327-334	47
970	Atomistic modeling of finite-temperature properties of crystalline β -SiC: II. Thermal conductivity and effects of point defects. 1998 , 255, 139-152	216
969	Polyethylene (PEHD)/polypropylene (iPP) blends: mechanical properties, structure and morphology. 1998 , 39, 5283-5291	23
968	Substrate specificity of prostate-specific antigen (PSA). 1998 , 5, 475-88	81
967	The COMPASS force field: parameterization and validation for phosphazenes. 1998 , 8, 229-246	940
966	Q: a molecular dynamics program for free energy calculations and empirical valence bond simulations in biomolecular systems. 1998 , 16, 213-25, 261	258
965	Molecular mechanisms of resistance: free energy calculations of mutation effects on inhibitor binding to HIV-1 protease. 1998 , 7, 1750-6	21
964	Molecular simulation of gas permeability: poly(2,6-dimethyl-1,4-phenylene oxide). 1998 , 149, 115-126	58
963	Thermomechanical properties of the WCA Lennard-Jones model system in its fluid and solid states. 1998 , 250, 58-82	43
962	Enhancing the relaxivity of paramagnetic coordination complexes through the optimization of the molecular electrostatic potential. 1998 , 16, 811-28	5
961	Electron emission from a clean gold surface bombarded by slow multiply charged fullerenes. 1998 , 174, 317-328	20
960	Molecular dynamics simulation of POPC at low hydration near the liquid crystal phase transition. 1998 , 80, 415-9	11
959	Solution conformation of methylated macrolide antibiotics roxithromycin and erythromycin using NMR and molecular modelling. Ribosome-bound conformation determined by TRNOE and formation of cytochrome P450-metabolite complex. 1998 , 22, 103-27	26
958	Application of molecular dynamics calculations in the prediction of dynamical molecular properties. 1998 , 29, 1043-1050	21

957	The effects of conformational constraints on aspartic acid racemization. 1998 , 29, 1227-1232		43
956	Simulation of liquid benzene between two graphite surfaces: a molecular dynamics study. 1998 , 93, 767-776		17
955	Modelling the interaction of silane and disilane with Si{100}(211) using classical many-body potentials. 1998 , 11, 65-73		
954	Calculation of thermal properties of diamond from simulated phonon spectra. 1998 , 12, 9-25		25
953	Molecular dynamics investigations of silver diffusion in glass. 1998 , 232-234, 245-251		7
952	Empirical potential study of the chemisorption of C ₂ H ₂ and CH ₃ on the SiC(001) surface. 1998 , 396, 24-39		26
951	Water molecules in DNA recognition II: a molecular dynamics view of the structure and hydration of the trp operator. 1998 , 282, 859-73		75
950	Accurate simulation of highly asymmetric electrolytes with charge asymmetry 20:1 and 20:2. <i>Journal of Chemical Physics</i> , 1998 , 109, 3530-3541	3.9	55
949	Hydration and Dynamics of a Tetramethylammonium Ion in Water: A Computer Simulation Study. 1998 , 102, 7448-7454		48
948	Molecular dynamics studies of a-C:H film growth by energetic hydrocarbon molecule impact. 1998 , 7, 858-863		10
947	Dynamics of n-alkanes: Comparison to Rouse model. <i>Journal of Chemical Physics</i> , 1998 , 109, 798-805	3.9	111
946	The Application of the Reaction-Field Method to the Calculation of Dielectric Constants. 1998 , 20, 159-178		13
945	Molecular Dynamics Simulation of the Nematic Melt of a p-Hydroxybenzoic Acid/2-Hydroxy-6-naphthoic Acid Liquid Crystalline Copolyester. 1998 , 31, 7682-7690		10
944	The intrinsic curvature of a 51 bp K-DNA fragment of <i>Leishmania tarentolae</i> : a molecular model. 1998 , 15, 905-30		
943	The solution conformations of amino acids from molecular dynamics simulations of Gly-X-Gly peptides: comparison with NMR parameters. 1998 , 76, 164-170		15
942	Tertiary contacts in alpha-lactalbumin at pH 7 and pH 2: a molecular dynamics study. 1998 , 16, 355-65		3
941	Transformation of Diamond (sp ³) to Graphite (sp ²) Bonds by Ion-Impact. 1998 , 09, 61-69		58
940	Molecular dynamics simulations of low-energy (25000 eV) argon ion interactions with silicon surfaces: Sputter yields and product formation pathways. 1998 , 83, 4055-4063		67

939	Proteins in Vacuo. Denaturing of Disulfide-Intact and Disulfide-Broken Lysozyme Probed by Molecular Dynamics Simulations. 1998 , 102, 2277-2283	31
938	Continuum Corrections to the Polarization and Thermodynamic Properties of Ewald Sum Simulations for Ions and Ion Pairs at Infinite Dilution. 1998 , 102, 5673-5682	60
937	Structural and enzymatic studies of a new analogue of coenzyme B12 with an alpha-adenosyl upper axial ligand. 1998 , 37, 9704-15	38
936	Host-Guest Interactions Influence Stability of the Rebek Tennis Ball-Dimer Complex. 1998 , 63, 8027-8030	7
935	Application of the RESP Methodology in the Parametrization of Organic Solvents. 1998 , 102, 8070-8079	421
934	Interatomic potential for germanium dioxide empirically fitted to an ab initio energy surface. 1998 , 58, 14791-14803	64
933	Molecular Dynamics Study of the Structure and Dynamics of Water in Cylindrical Pores. 1998 , 102, 1241-1249	45
932	Generalized Langevin dynamics simulation: numerical integration and application of the generalized Langevin equation with an exponential model for the friction kernel. 1998 , 93, 901-912	4
931	Molecular Dynamics Study on Microheterogeneity and Preferential Solvation in Methanol/Chloroform Mixtures. 1998 , 102, 2027-2031	35
930	Molecular Modeling and Solid-State NMR of Short-Chain Molecules in Dianin's Compound and Zeolite 5A. 1998 , 120, 8113-8123	12
929	Solution structure of the oxidized Fe7S8 ferredoxin from the thermophilic bacterium <i>Bacillus schlegelii</i> by 1H NMR spectroscopy. 1998 , 37, 9812-26	45
928	Diffusion of a Mixture of Methane and Xenon in Silicalite: A Molecular Dynamics Study and Pulsed Field Gradient Nuclear Magnetic Resonance Experiments. 1998 , 102, 6375-6381	87
927	Use of Multiple Molecular Dynamics Trajectories To Study Biomolecules in Solution: The YTGP Peptide. 1998 , 102, 6260-6272	26
926	Brownian and essential dynamics studies of the HIV-1 integrase catalytic domain. 1998 , 16, 733-45	16
925	Proteins in Vacuo. Denaturation of Highly-Charged Lysozyme Studied by Molecular Dynamics Simulations. 1998 , 102, 9344-9352	38
924	Ordered Dendritic Nanorods with a Poly(p-phenylene) Backbone. 1998 , 120, 7691-7695	109
923	Estimation of the Surface Tension of Polar Fluids Long-Range Contributions. 1998 , 14, 396-406	9
922	Binding domain of human parathyroid hormone receptor: from conformation to function. 1998 , 37, 12737-43	67

921	Chain Length Effects on Frictional Behavior of Confined Ultrathin Films of Linear Alkanes under Shear. 1998 , 102, 3669-3675	39
920	Quantum chemical analysis of the enolization of ribulose bisphosphate: the first hurdle in the fixation of CO ₂ by Rubisco. 1998 , 37, 15414-22	33
919	Anaesthetic Mechanism on a Model Biological Membrane: A Molecular Dynamics Simulation Study. 1998 , 102, 625-631	30
918	Comparison of Selectively Polarizable Force Fields for Ion-Water-Peptide Interactions: Ion Translocation in a Gramicidin-like Channel. 1998 , 102, 9127-9138	15
917	Liquid Structure, Thermodynamics, and Mixing Behavior of Saturated Hydrocarbon Polymers. 1. Cohesive Energy Density and Internal Pressure. 1998 , 31, 6991-6997	58
916	SWARM-MD: Searching Conformational Space by Cooperative Molecular Dynamics. 1998 , 102, 5937-5943	58
915	Molecular Dynamics Simulation of Amorphous Poly(ethylene terephthalate). 1998 , 31, 1556-1564	51
914	Carbohydrate-Carbohydrate Interactions in Water with Glycophanes as Model Systems. 1998 , 63, 9212-9222	38
913	B-DNA's BI-> BII Conformer Substate Dynamics Is Coupled with Water Migration. 1998 , 102, 8934-8940	57
912	Molecular Dynamics Study of Viscoelastic Properties of Confined Oligomer Melts. 1998 , 31, 4605-4613	5
911	Self-Guided Molecular Dynamics Simulation for Efficient Conformational Search. 1998 , 102, 7238-7250	96
910	Solution structure of the glycosylated second type 2 module of fibronectin. 1998 , 276, 177-87	50
909	Are there non-trivial dynamic cross-correlations in proteins?. 1998 , 279, 911-20	45
908	Molecular dynamics simulations of peptide fragments from hen lysozyme: insight into non-native protein conformations. 1998 , 280, 703-19	12
907	Molecular dynamics simulations of an oligonucleotide duplex with adenine tracts phased by a full helix turn. 1998 , 281, 675-87	118
906	A structural homologue of colipase in black mamba venom revealed by NMR floating disulphide bridge analysis. 1998 , 283, 205-19	62
905	Essential dynamics from NMR clusters: dynamic properties of the Myb DNA-binding domain and a hinge-bending enhancing variant. 1998 , 14, 318-28	26
904	Simulation of self-associating polymer systems. I. Shear-induced structural changes. <i>Journal of Chemical Physics</i> , 1998 , 109, 9602-9613	3-9 42

903	Lipid properties and the orientation of aromatic residues in OmpF, influenza M2, and alamethicin systems: molecular dynamics simulations. 1998 , 37, 17554-61	151
902	Computational Study of a Terphenyl-Based Eu ³⁺ -Complex: Effect of Small Amounts of Water. 1998 , 102, 3060-3066	8
901	COMPASS: An ab Initio Force-Field Optimized for Condensed-Phase Applications Overview with Details on Alkane and Benzene Compounds. 1998 , 102, 7338-7364	3990
900	Adhesion forces of lipids in a phospholipid membrane studied by molecular dynamics simulations. 1998 , 74, 931-43	181
899	Simulating energy flow in biomolecules: application to tuna cytochrome c. 1998 , 75, 60-9	16
898	Sequence-dependent dynamics of TATA-Box binding sites. 1998 , 75, 372-81	54
897	NMR structure refinement and dynamics of the K ⁺ -[d(G3T4G3)] ₂ quadruplex via particle mesh Ewald molecular dynamics simulations. 1998 , 75, 968-81	93
896	Molecular dynamics simulation of cytochrome c ₃ : studying the reduction processes using free energy calculations. 1998 , 74, 1708-21	30
895	A molecular dynamics study of the pores formed by Escherichia coli OmpF porin in a fully hydrated palmitoylcholine bilayer. 1998 , 74, 2786-801	318
894	Importance of explicit salt ions for protein stability in molecular dynamics simulation. 1998 , 74, 2906-11	87
893	Molecular Dynamics Simulations of Ground and Transition States for the SN ₂ Displacement of Cl ⁻ from 1,2-Dichloroethane at the Active Site of Xanthobacter autotrophicus Haloalkane Dehalogenase. 1998 , 120, 5611-5621	57
892	The biological implications of damage to DNA incorporating an 8-oxodeoxyguanine:cytosine basepair. 1998 , 16, 651-61	4
891	Conformational analysis and automated receptor docking of selective arylacetamide-based kappa-opioid agonists. 1998 , 41, 4777-89	53
890	Stress relaxation and misfit dislocation nucleation in the growth of misfitting films: A molecular dynamics simulation study. 1998 , 83, 217-227	105
889	Molecular dynamics simulations of Ar ⁺ and Cl ⁺ impacts onto silicon surfaces: Distributions of reflected energies and angles. 1998 , 16, 3502-3514	81
888	Using molecular dynamics to obtain Maxwell-Stefan diffusion coefficients in liquid systems. 1998 , 94, 495-503	14
887	Relative diffusion and memory effects in supercooled water. 1998 , 57, R4871-R4874	12
886	A systematic study of water models for molecular simulation: Derivation of water models optimized for use with a reaction field. <i>Journal of Chemical Physics</i> , 1998 , 108, 10220-10230	3-9 514

885	Pancreatic lipase-related protein type I: a specialized lipase or an inactive enzyme. 1998 , 11, 135-42		21
884	Simulations of Wearless Friction at a Sliding Interface between Ordered Organic Monolayers. 1998 , 37, 6535-6543		19
883	A Feasibility Study of 3-D Ordering of Ion Beams in a Storage Ring. 1998 , 57, 36-44		
882	Molecular dynamics simulation with an ab initio potential energy function and finite element interpolation: The photoisomerization of cis-stilbene in solution. <i>Journal of Chemical Physics</i> , 1998 , 108, 8773-8781	3.9	37
881	Stress relaxation in a diatomic liquid. <i>Journal of Chemical Physics</i> , 1998 , 108, 4984-4991	3.9	12
880	A nonequilibrium simulation method for calculating tracer diffusion coefficients of small solutes in n-alkane liquids and polymers. <i>Journal of Chemical Physics</i> , 1998 , 108, 9558-9565	3.9	19
879	Dynamics of linear and branched alkane melts: Molecular dynamics test of theory for long time dynamics. <i>Journal of Chemical Physics</i> , 1998 , 108, 9155-9167	3.9	25
878	Modeling of angiogenin - 3-NMP complex. 1998 , 16, 715-22		4
877	Equation of state and stress tensor in inhomogeneous compressible copolymer melts: Dynamic mean-field density functional approach. <i>Journal of Chemical Physics</i> , 1998 , 108, 2638-2650	3.9	20
876	Assessment of the validity of intermolecular potential models used in molecular dynamics simulations by extended x-ray absorption fine structure spectroscopy: A case study of Sr ²⁺ in methanol solution. <i>Journal of Chemical Physics</i> , 1998 , 108, 9487-9497	3.9	43
875	A novel dynamic free-volume theory for molecular diffusion in fluids and interphases. <i>Journal of Chemical Physics</i> , 1998 , 109, 7876-7884	3.9	8
874	Efficient sampling of solvent free energies in polymers. <i>Journal of Chemical Physics</i> , 1998 , 109, 7578-7583	3.9	33
873	Rationalization of the dielectric properties of common three-site water models in terms of their force field parameters. <i>Journal of Chemical Physics</i> , 1998 , 109, 4927-4937	3.9	125
872	Effect of surface on defect creation by self-ion bombardment of Si(001). 1998 , 58, 9907-9915		30
871	Ionic charging free energies: Spherical versus periodic boundary conditions. <i>Journal of Chemical Physics</i> , 1998 , 109, 10921-10935	3.9	114
870	Mechanisms of ion beam mixing in metals and semiconductors. 1998 , 83, 1238-1246		65
869	Time-correlation functions in molecular liquids studied by the mode-coupling theory based on the interaction-site model. 1998 , 58, 7296-7308		29
868	Static structure and dynamics of the liquid Li-Na and Li-Mg alloys. 1998 , 58, 4747-4757		24

867	Molecular dynamics simulations of organically modified layered silicates. <i>Journal of Chemical Physics</i> , 1998 , 108, 7410-7415	3.9	200
866	Solvation dynamics: The role of hydrogen bonding. <i>Journal of Chemical Physics</i> , 1998 , 108, 6347-6352	3.9	17
865	Calculation of solid-fluid phase equilibria for systems of chain molecules. <i>Journal of Chemical Physics</i> , 1998 , 109, 318-328	3.9	42
864	Achieving constant pressure in molecular-dynamics simulations with constraint methods. <i>Journal of Chemical Physics</i> , 1998 , 109, 10138-10141	3.9	7
863	Coordinates scaling and multiple time step algorithms for simulation of solvated proteins in the NPT ensemble. <i>Journal of Chemical Physics</i> , 1998 , 109, 5194-5202	3.9	88
862	Alternative schemes for the inclusion of a reaction-field correction into molecular dynamics simulations: Influence on the simulated energetic, structural, and dielectric properties of liquid water. <i>Journal of Chemical Physics</i> , 1998 , 108, 6117-6134	3.9	105
861	Vibrational phase and energy relaxation of CN ₂ in water. <i>Journal of Chemical Physics</i> , 1998 , 108, 142-153	3.9	171
860	Water dynamical anomalies evidenced by molecular-dynamics simulations at the solvent-protein interface. 1998 , 57, 3315-3325		153
859	Addressing the tertiary structure of human parathyroid hormone-(1-34). 1998 , 273, 10420-7		90
858	An Extension of the LCAO Method Isothermal Dynamics. 1998 , 09, 649-666		1
857	Ion pairing between lipase and colipase plays a critical role in catalysis. 1998 , 273, 33604-9		16
856	Concerted motions in the photoactive yellow protein. 1998 , 11, 873-9		21
855	Low-frequency vibrations in monomers, dimers and polymers of propylene glycol. 1998 , 77, 699-707		7
854	Folding funnels and frustration in off-lattice minimalist protein landscapes. 1998 , 95, 5921-8		300
853	Molecular modeling of closed circular DNA thermodynamic ensembles. 1998 , 39, 243-258		6
852	Defect production and evolution during and after ion implantation studied by a combination of time-ordered BCA and MD simulations.		
851	Ion channels: molecular modeling and simulation studies. 1998 , 293, 647-93		4
850	Interfacial Behavior of Ionophoric Systems: Molecular Dynamics Studies on 18-Crown-6 and Its Complexes at the Water-Chloroform Interface.. 1998 , 14, 43-56		42

849	Optimization methods for conformational sampling using a Boltzmann-weighted mean field approach. 1998 , 39, 103-114		14
848	Extensive molecular dynamics simulations of a hairpin-forming peptide. 1998 , 39, 591-614		12
847	A COMPUTATIONAL CHEMISTRY APPROACH TO STUDY THE INTERACTIONS OF HUMIC SUBSTANCES WITH MINERAL SURFACES. 1998 , 133-145		4
846	The stability of transmembrane helices: A molecular dynamics study on the isolated helices of bacteriorhodopsin. 1998 , 38, 401-422		3
845	Molecular dynamics simulations of unsaturated lipids in monolayers: an investigation of bond ordering. 1999 ,		2
844	Hierarchical coupled map lattices as cascade models for hydrodynamical turbulence. 1999 , 45, 552-557		16
843	Interpretation of Difference in Wearless Friction Observed between Ordered Organic Monolayers with CH ₃ and CF ₃ Terminal Groups. 1999 , 38, L675-L678		18
842	A mini-protein designed by removing a module from barnase: molecular modeling and NMR measurements of the conformation. 1999 , 12, 673-80		8
841	Molecular dynamics simulation of energetic atom depositions of Au/Au(100) film. 1999 , 8, 296-305		5
840	Modelling of the disulphide-swapped isomer of human insulin-like growth factor-1: implications for receptor binding. 1999 , 12, 297-303		22
839	A structural snapshot of base-pair opening in DNA. 1999 , 96, 11809-14		30
838	Parallel Particle Simulations of Thin-Film Deposition. 1999 , 13, 16-32		6
837	A structural snapshot of an intermediate on the streptavidin-biotin dissociation pathway. 1999 , 96, 8384-9		57
836	Molecular Dynamics Simulations: The Limits and Beyond. 1999 , 3-36		16
835	Comparisons between integral equation theory and molecular dynamics simulations for realistic models of polyethylene liquids. <i>Journal of Chemical Physics</i> , 1999 , 111, 9073-9081	3.9	25
834	Molecular dynamics simulation with reversible heat addition. 1999 , 59, R44-R47		2
833	Direct simulation of ion-beam-induced stressing and amorphization of silicon. 1999 , 60, 12610-12616		41
832	Characterization of water octamer, nanomer, decamer, and iodide-water interactions using molecular dynamics techniques. <i>Journal of Chemical Physics</i> , 1999 , 110, 1526-1532	3.9	45

831	Molecular dynamics studies of semifluorinated hydrocarbon monolayers. <i>Journal of Chemical Physics</i> , 1999 , 111, 6556-6564	3.9	12
830	Unfolded in vacuo lysozyme folds into native, quasinate, and compact structures. 1999 , 59, 5981-6		23
829	Model of noncontact scanning force microscopy on ionic surfaces. 1999 , 59, 2436-2448		127
828	Tight-binding molecular-dynamics study of amorphous carbon deposits over silicon surfaces. 1999 , 60, 2762-2770		7
827	Simulation of an asymmetric electrolyte with charge asymmetry 60:1 using hard-sphere and soft-sphere models. <i>Journal of Chemical Physics</i> , 1999 , 111, 4300-4309	3.9	88
826	Molecular dissolution processes in lipid bilayers: A molecular dynamics simulation. <i>Journal of Chemical Physics</i> , 1999 , 110, 1807-1818	3.9	24
825	Reactive ion etching of Si by Cl and Cl ₂ ions: Molecular dynamics simulations with comparisons to experiment. 1999 , 17, 1510-1513		16
824	A molecular-dynamics simulation study of water on NaCl(100) using a polarizable water model. <i>Journal of Chemical Physics</i> , 1999 , 110, 12097-12107	3.9	65
823	Quasiharmonic versus exact surface free energies of Al: A systematic study employing a classical interatomic potential. 1999 , 60, 5055-5064		44
822	Folding of a 16-residue helical peptide using molecular dynamics simulation with Tsallis effective potential. <i>Journal of Chemical Physics</i> , 1999 , 111, 4359-4361	3.9	36
821	A new mechanism for penetrant diffusion in amorphous polymers: Molecular dynamics simulations of phenol diffusion in bisphenol-A-polycarbonate. <i>Journal of Chemical Physics</i> , 1999 , 111, 6061-6068	3.9	59
820	Structural transition in hot small clusters. <i>Journal of Chemical Physics</i> , 1999 , 110, 7770-7778	3.9	21
819	TIT for TAT: the properties of inosine and adenosine in TATA box DNA. 1999 , 16, 787-810		19
818	Dynamic heterogeneities of translational and rotational motion of a molecular glass former from computer simulations. <i>Journal of Chemical Physics</i> , 1999 , 110, 4514-4522	3.9	54
817	Recurrence quantification analysis as a tool for characterization of molecular dynamics simulations. 1999 , 59, 992-998		46
816	Dielectric constant of water at high electric fields: Molecular dynamics study. <i>Journal of Chemical Physics</i> , 1999 , 110, 7935-7942	3.9	164
815	Quantum-classical molecular dynamics simulation of femtosecond spectroscopy on I ₂ in inert gases: Mechanisms for the decay of pump-probe signals. <i>Journal of Chemical Physics</i> , 1999 , 111, 7807-7817	3.9	18
814	Molecular dynamics simulations in the grand canonical ensemble: Formulation of a bias potential for umbrella sampling. <i>Journal of Chemical Physics</i> , 1999 , 110, 8295-8302	3.9	31

813	Slow Dynamics of Water under Pressure. 1999 , 82, 3629-3632		103
812	Structure of supercooled and glassy water under pressure. 1999 , 60, 1084-7		68
811	Viscosity dependence and solvent effects in the photoisomerization of cis-stilbene: Insight from a molecular dynamics study with an ab initio potential-energy function. <i>Journal of Chemical Physics</i> , 1999 , 111, 8987-8999	3.9	13
810	Proteins in vacuo: a molecular dynamics study of the unfolding behavior of highly charged disulfide-bond-intact lysozyme subjected to a temperature pulse. 1999 , 60, 7277-84		19
809	Molecular Dynamics Simulation of Self-Diffusion and Maxwell-Stefan Diffusion Coefficients in Liquid Mixtures of Methanol and Water. 1999 , 23, 79-94		15
808	On the convergence of simulation of asymmetric electrolytes with charge asymmetry 60:1. <i>Journal of Chemical Physics</i> , 1999 , 110, 3493-3501	3.9	22
807	Molecular dynamics study of the solution of semiflexible telechelic polymer chains with strongly associating end-groups. <i>Journal of Chemical Physics</i> , 1999 , 110, 6039-6049	3.9	53
806	Secondary structures and intramolecular interactions in fragments of the B-loops of naturally occurring analogs of epidermal growth factor. 1999 , 17, 393-407		6
805	Unidirectional diffusion of methane in AlPO ₄ -5. <i>Journal of Chemical Physics</i> , 1999 , 110, 11511-11516	3.9	40
804	Inverse Kirkendall mixing in collision cascades. 1999 , 59, 20-23		73
803	Trapping dynamics of ethane on Si(100)-(2×1): Molecular beam experiments and molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1999 , 111, 7567-7575	3.9	17
802	Variations in chain compactness and topological complexity uncover folding processes in the relaxation dynamics of unfolded in vacuo lysozyme. <i>Journal of Chemical Physics</i> , 1999 , 111, 4774-4779	3.9	20
801	Analysis of the mechanical behavior of poly(trimethylene terephthalate) in an amorphous state under uniaxial extension/compression condition through atomistic modeling. <i>Journal of Chemical Physics</i> , 1999 , 110, 7524-7532	3.9	29
800	Molecular dynamics simulation of silicon surface smoothing by low-energy argon cluster impact. 1999 , 86, 6758-6762		6
799	An integral equation study of a simple point charge model of water. <i>Journal of Chemical Physics</i> , 1999 , 110, 1148-1153	3.9	61
798	The X-ray Structure of Epoxide Hydrolase from <i>Agrobacterium radiobacter</i> AD1. 1999 , 274, 14579-14586		140
797	Rotation-Vibration Coupling in Liquid Water Investigated by Molecular Dynamics Simulation. 1999 , 23, 55-62		0
796	New Free Energy Calculation Methods for Structure-Based Drug Design and Prediction of Protein Stability. 1999 , 37-52		1

795	MD-simulation study of the hydrophobic hydration of nonionic surfactants. 1999 , 156, 489-500	8
794	Concepts of Rehbinder's school and modern theories of spreading. 1999 , 160, 63-77	14
793	Polar interactions of chondroitinsulfate. 1999 , 13, 143-156	7
792	The temperature dependence of single-file separation mechanisms in one-dimensional nanoporous materials. 1999 , 74, 33-42	10
791	Molecular simulation of the glass transition of polyphosphazenes. 1999 , 9, 111-116	48
790	Cause and effect reversed in non-equilibrium molecular dynamics: an easy route to transport coefficients. 1999 , 9, 203-209	115
789	Molecular dynamics study of quartz into stishovite. 1999 , 270, 164-171	5
788	Critical temperature and nonextensivity in long-range interacting Lennard-Jones-like fluids. 1999 , 264, 270-275	17
787	Molecular dynamics simulations of real systems: application to chloro-fluoro-hydrocarbons and polymers. 1999 , 158-160, 49-58	10
786	A novel approach to thermophysical properties prediction for chloro-fluoro-hydrocarbons. 1999 , 166, 21-37	22
785	L-Alanyl-L-alanine in the zwitterionic state: structures determined in the presence of explicit water molecules and with continuum models using density functional theory. 1999 , 240, 63-77	83
784	A molecular model of p-terphenyl and its disorder-order transition. 1999 , 246, 323-334	29
783	Nonadiabatic processes in solution: molecular dynamics and surface hopping. 1999 , 246, 315-322	13
782	Towards molecular dynamics simulation of large proteins with a hydration shell at constant pressure. 1999 , 78, 157-82	52
781	Long-term molecular dynamics simulation of copper azurin: structure, dynamics and functionality. 1999 , 78, 247-57	32
780	Computer simulation of intramolecular mobility of dendrimers. 1999 , 82, 105-116	15
779	Water in porous glasses. A computer simulation study. 1999 , 80, 165-178	59
778	Simulation of a laser diagnostics to detect the string configuration of an ion beam in a storage ring. 1999 , 430, 10-23	

777	Determination of two- and three-body correlation functions in ionic solutions by means of MD and EXAFS investigations. 1999 , 6, 281-3	4
776	Monte Carlo studies on the deformation behaviour of glassy model systems. 1999 , 9, 99-109	5
775	Aqueous solution near charged Ag(111) surfaces: comparison between a computer simulation and experiment. 1999 , 301, 81-86	31
774	On the validity of Stokes' law at the molecular level. 1999 , 303, 583-586	43
773	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
772	Photocontrolled nanophase segregation in a liquid-crystal solvent. 1999 , 398, 54-57	106
771	The role of mat-forming diatoms in the formation of Mediterranean sapropels. 1999 , 398, 57-61	145
770	Erratum: Experimental verification of the quasi-unit-cell model of quasicrystal structure. 1999 , 399, 84-84	4
769	Erratum: Extreme Th1 bias of invariant V β 24J β Q T cells in type 1 diabetes. 1999 , 399, 84-84	2
768	Erratum: In vivo regulation of axon extension and pathfinding by growth-cone calcium transients. 1999 , 399, 84-84	1
767	Erratum: The role of mat-forming diatoms in the formation of Mediterranean sapropels. 1999 , 399, 84-84	2
766	Recurrence quantification analysis in molecular dynamics. 1999 , 879, 258-66	9
765	Conformational chaos of an elastin-related peptide in aqueous solution. 1999 , 879, 284-7	28
764	Simulations of the dynamics at an RNA-protein interface. 1999 , 6, 540-4	35
763	Stability of hairpin ribozyme tertiary structure is governed by the interdomain junction. 1999 , 6, 544-9	132
762	Molecular simulation of the electrochemical double layer. 1999 , 44, 1697-1705	101
761	Hydration of glucose in the rubbery and glassy states studied by molecular dynamics simulation. 1999 , 315, 63-69	36
760	Molecular dynamics of a tetrasaccharide subunit of chondroitin 4-sulfate in water. 1999 , 318, 1-9	14

759	Improved carbohydrate force field for gromos: ring and hydroxymethyl group conformations and exo-anomeric effect. 1999 , 322, 264-273	39
758	One transition state leading to two product states: ab initio molecular dynamics simulations of the reaction of formaldehyde radical anion and methyl chloride. 1999 , 300, 583-587	46
757	'ChairBoat' transitions and side groups affect the stiffness of polysaccharides. 1999 , 305, 202-208	46
756	Classical simulations on the pump-probe spectroscopy of I2 encapsulated in DDR porosil. 1999 , 311, 146-152	6
755	Analysis of single-molecule dynamics in liquid HF. 1999 , 315, 109-114	5
754	Molecular dynamics investigation of bond ordering of unsaturated lipids in monolayers. 1999 , 25, 245-62	5
753	Computer simulation of sliding hydroxylated alumina surfaces. 1999 , 7, 153-159	8
752	Fluoroalkoxyaluminate-based ionic liquids as electrolytes for sodium-ion batteries. 2023 , 369, 120919	o
751	The pursuit of new alternative ways to eradicate Helicobacter pylori continues: Detailed characterization of interactions in the adenylosuccinate synthetase active site. 2023 , 226, 37-50	o
750	Novel biosurfactants: Rationally designed surface-active peptides and in silico evaluation at the decane-water interface. 2023 , 125, 84-95	o
749	Molecular insight into nano-heterogeneity of localized high-concentration electrolyte: Correlation with lithium dynamics and solid-electrolyte interphase formation. 2023 , 557, 232545	o
748	Kinetic Temperature of Structures for Resilience, Instability, and Failure Analysis of Building Systems. 2023 , 149,	o
747	Plasma membrane lipid bilayer is druggable: Selective delivery of gemcitabine-squalene nano-medicine to cancer cells. 2023 , 1869, 166614	o
746	A synergistic effect of NH ₃ BH ₃ and H ₂ on their pressurization metallization: An Ab initio molecular dynamics study. 2023 , 218, 111972	o
745	Machine learning and molecular simulation ascertain antimicrobial peptide against Klebsiella pneumoniae from public database. 2023 , 102, 107800	o
744	Glycation restrains open-closed conformation of Insulin. 2023 , 102, 107803	o
743	Insights into pathways and solvent effects of fructose dehydration to 5-hydroxymethylfurfural in acetone/water solvent. 2023 , 267, 118352	o
742	Identification of possible binding modes of SARS-CoV-2 spike N-terminal domain for ganglioside GM1. 2023 , 812, 140260	o

- 741 Designing sequence-defined peptoids for fibrillar self-assembly and silicification. **2023**, 634, 450-459 ○
- 740 New insights into the effect of mutations on affibody-Fc interaction, a molecular dynamics simulation approach. **2023**, 215, 107925 ○
- 739 Microstructural evolution of bitumen during the glass transition: An application of digital oil. **2023**, 335, 127048 ○
- 738 Pore density effect on separations of water/ethanol and methanol/ethanol through graphene oxide membranes: A theoretical study. **2023**, 308, 122975 ○
- 737 Inhibitory mechanism of phenolic compounds in rapeseed oil on α -amylase and α -glucosidase: Spectroscopy, molecular docking, and molecular dynamic simulation. **2023**, 289, 122251 ○
- 736 Structural basis of Nrf2 activation by flavonolignans from silymarin. **2023**, 119, 108393 ○
- 735 Low-frequency spectra of reline and its mixtures with water: A comparative study based on femtosecond Raman-induced Kerr effect spectroscopy and molecular dynamics simulations. **2023**, 437, 114504 ○
- 734 Investigation on surface generation mechanism of single-crystal silicon in grinding: Surface crystal orientation effect. **2023**, 34, 105125 ○
- 733 The protein dynamics of bovine and caprine β -lactoglobulin differ as a function of pH. **2023**, 408, 135229 ○
- 732 Abnormal methylation in the NDUFA13 gene promoter of breast cancer cells breaks the cooperative DNA recognition by transcription factors. **2022**, 3, ○
- 731 The concentration-dependent effect of hydrocortisone on the structure of model lung surfactant monolayer by using an in silico approach. **2022**, 12, 33313-33328 ○
- 730 Drug and Anti-Viral Peptide Design to Inhibit the Monkeypox Virus by Restricting A36R Protein. **2022**, 16, 117793222211411 ○
- 729 Atomistic modeling of the properties of gold in the region of phase transitions of the first order. **2022**, 55, 53-66 ○
- 728 How Do Salt and Lipids Affect Conformational Dynamics of A β 42 Monomers in Water?. ○
- 727 Convenient Way to Create an MD Model of a Hot Crystal with an Open Surface. **2022**, ○
- 726 The role of surface activity on the amyloid fibrillation pathway of bovine serum albumin upon interaction with glyphosate. **2022**, ○
- 725 A Zn-dependent structural transition of SOD1 modulates its ability to undergo phase separation. ○
- 724 Revealing druggable cryptic pockets in the Nsp1 of SARS-CoV-2 and other β -coronaviruses by simulations and crystallography. 11, ○

- 723 Structural differences in 3C-like protease (Mpro) from SARS-CoV and SARS-CoV-2: molecular insights revealed by Molecular Dynamics Simulations. ○
- 722 Human Milk Oligosaccharide 2'-Fucosyllactose Inhibits Ligand Binding to C-Type Lectin DC-SIGN but Not to Langerin. **2022**, 23, 14745 ○
- 721 Upstream of N-Ras C-terminal cold shock domains mediate poly(A) specificity in a novel RNA recognition mode and bind poly(A) binding protein during translation regulation. ○
- 720 Distinct conformational and energetic features define the specific recognition of (di)aromatic peptide motifs by PEX14. **2022**, ○
- 719 Encapsulation dynamics of neuromuscular blocking drugs by sugammadex. **2022**, 1
- 718 Kinetic and thermodynamic allostery in the Ras protein family. ○
- 717 Sampling the Bulk Viscosity of Water with Molecular Dynamics Simulation in the Canonical Ensemble. **2022**, 126, 10172-10184 ○
- 716 In silico study on probing atomistic insights into structural stability and tensile properties of Fe-doped hydroxyapatite single crystals. **2022**, 12, ○
- 715 Insights into the Interactions of Peptides with Monolayer-Protected Metal Nanoclusters. ○
- 714 Structural Anomaly in Glasses: Molecular Dynamics Study of Organic Radical in Dibutylphthalate at Different Temperatures. **2022**, 23, 14859 ○
- 713 Automated Path Searching Reveals the Mechanism of Hydrolysis Enhancement by T4 Lysozyme Mutants. **2022**, 23, 14628 ○
- 712 Spiro heterocycles bearing piperidine moiety as potential scaffold for antileishmanial activity: synthesis, biological evaluation, and in silico studies. **2023**, 38, 330-342 ○
- 711 Mutational Insight into Allosteric Regulation of Kir Channel Activity. **2022**, 7, 43621-43634 ○
- 710 Molecular Mechanism of Drug Transport and Release through Zeolitic imidazole framework nanospheres for Versatile Drug Delivery Applications. **2022**, 120822 ○
- 709 Thermal tuning of protein hydration in a hyperthermophilic enzyme. 9, ○
- 708 Hierarchical Coarse-Grained Strategy for Macromolecular Self-Assembly: Application to Hepatitis B Virus-Like Particles. **2022**, 23, 14699 ○
- 707 Computational Study of Helicase from SARS-CoV-2 in RNA-Free and Engaged Form. **2022**, 23, 14721 ○
- 706 Why Does Synergistic Activation of WASP, but Not N-WASP, by Cdc42 and PIP2 Require Cdc42 Prenylation?. 1

- 705 Structural and electronic properties of the Te-Si(111) surface from first principles. **2022**, 106, ○
- 704 Atomic mechanisms of self-diffusion in amorphous silicon. **2022**, 12, 115325 ○
- 703 Molecular Factors of Ice Growth Inhibition for Hyperactive and Globular Antifreeze Proteins: Insights from Molecular Dynamics Simulation. **2022**, 38, 15132-15144 ○
- 702 Cancer regulator EGFR-ErbB4 heterodimer is stabilized through glycans at the dimeric interface. **2022**, 28, ○
- 701 Folding Dynamics of 3,4,3-LI(1,2-HOPO) in Its Free and Bound State with U4+ Implicated by MD Simulations. **2022**, 27, 8151 1
- 700 Biological Characterization of Natural Peptide Bcl-1003 from *Boana cordobae* (anura): Role in Alzheimer's Disease and Microbial Infections. **2023**, 29, ○
- 699 Adaptive insertion of a hydrophobic anchor into a poly(ethylene glycol) host for programmable surface functionalization. ○
- 698 Dynamics and Allosteric Information Pathways of Unphosphorylated c-Cbl. **2022**, 62, 6148-6159 ○
- 697 Uptake mechanism of iron-phytosiderophore from the soil based on the structure of yellow stripe transporter. **2022**, 13, ○
- 696 Strength of nano-twinned gradient nano-grained copper: Molecular dynamic simulation. **2022**, 1270, 012069 ○
- 695 Molecular and thermodynamic insights into interfacial interactions between collagen and cellulose investigated by molecular dynamics simulation and umbrella sampling. ○
- 694 A mini-TGA protein modulates gene expression through heterogeneous association with transcription factors. ○
- 693 Machine learning aided atomic structure identification of interfacial ionic hydrates from AFM images. ○
- 692 Evaluation of docking procedures reliability in affitins-partners interactions. 10, ○
- 691 Interactions of Apigenin and Safranal with the 5HT1A and 5HT2A Receptors and Behavioral Effects in Depression and Anxiety: A Molecular Docking, Lipid-Mediated Molecular Dynamics, and In Vivo Analysis. **2022**, 27, 8658 1
- 690 Stomatal CO₂/bicarbonate sensor consists of two interacting protein kinases, Raf-like HT1 and non-kinase-activity activity requiring MPK12/MPK4. **2022**, 8, ○
- 689 Exploration of natural product database for the identification of potent inhibitor against IDH2 mutational variants for glioma therapy. **2023**, 29, ○
- 688 Quantitative Predictions and Experimental Validation of Liquid-Vapor Interfacial Tension in Binary and Ternary Mixtures of Alkanes Using Molecular Dynamics Simulations. ○

- 687 Supramolecular Semiconductivity through Emerging Ionic Gates in Ion Nanoparticle Superlattices. ○
- 686 Weak Interactions between Poly(ether imide) and Carbon Dioxide: A Multiscale Investigation Combining Experiments, Theory, and Simulations. **2022**, 55, 10773-10787 1
- 685 How Aberrant N-Glycosylation Can Alter Protein Functionality and Ligand Binding: an Atomistic View. ○
- 684 Structure-based discovery and in vitro validation of inhibitors of Chloride Intracellular Channel 4 protein. **2022**, ○
- 683 Protein-Ligand Binding Free-Energy Calculations with ARROW-A Purely First-Principles Parameterized Polarizable Force Field. **2022**, 18, 7751-7763 ○
- 682 Dual aromatase-steroid sulfatase inhibitors (DASI's) for the treatment of breast cancer: a structure guided ligand based designing approach. 1-23 ○
- 681 (-)-Epigallocatechin-3-gallate Directly Binds Cyclophilin D: A Potential Mechanism for Mitochondrial Protection. **2022**, 27, 8661 ○
- 680 Thermal conductivity and conductance of protein in aqueous solution: Effects of geometrical shape. ○
- 679 Molecular Dynamics and Structural Studies of Zinc Chloroquine Complexes. ○
- 678 In vitro and computational studies of the β -lactamase inhibition and β -lactam potentiating properties of plant secondary metabolites. 1-21 ○
- 677 The H163A Mutation Unravels an Oxidized Conformation of the SARS-CoV-2 Main Protease and Opens a New Avenue for Anti-Viral Therapeutic Design. ○
- 676 Machine learning in accelerating microsphere formulation development. ○
- 675 Aggregation propensities of proteins with varying degrees of disorder. ○
- 674 Design of ionic liquids containing glucose and choline as drug carriers, finding the link between QM and MD studies. **2022**, 12, ○
- 673 Development of a novel circular mRNA vaccine of six protein combinations against *Staphylococcus aureus*. 1-21 ○
- 672 Molecular Modeling, Virtual Screening, and Molecular Dynamics for *Leishmania infantum* Methionyl-tRNA Synthetase. ○
- 671 Selective Distribution of BaTiO₃ and Graphene in PS/PVDF Blends: Molecular Dynamics Simulations. **2022**, 105247 ○
- 670 Reorganization of the outer layer of a model of the plasma membrane induced by a neuroprotective aminosterol. **2022**, 113115 1

669	Elucidating the Protonation State of the β -Secretase Catalytic Dyad.	0
668	Nirmatrelvir-resistant SARS-CoV-2 variants with high fitness in an infectious cell culture system. 2022 , 8,	3
667	Molecular Basis for Non-Covalent, Non-Competitive FAAH Inhibition. 2022 , 23, 15502	0
666	Effect of Water on the Mechanical Properties of Cyclic Peptide Polymers.	0
665	Mechanistic investigation of SARS-CoV-2 main protease to accelerate design of covalent inhibitors. 2022 , 12,	1
664	Molecular interactions underlying the phase separation of HP1 β : role of phosphorylation, ligand and nucleic acid binding.	1
663	Disparate Effect of Hybrid Peptidomimetics Containing Isomers of Aminobenzoic Acid on hIAPP Aggregation. 2022 , 126, 10427-10444	1
662	Myristoyl dual role in allosterically regulating and localizing Abl kinase.	0
661	Effect of the Thermal Fluctuations of the Photophysics of GC and CG DNA Steps: A Computational Dynamical Study. 2022 , 126, 10608-10621	1
660	From Molecule to Device: Prediction and Validation of the Optical Orientation of Iridium Phosphors in Organic Light-Emitting Diodes.	0
659	Modeling the Interaction of Human Lipoyxygenase LOX 15 with Free Arachidonic Acid. 2022 , 16, 929-933	0
658	Accelerated Enveloping Distribution Sampling (AEDS) Allows for Efficient Sampling of Orthogonal Degrees of Freedom.	0
657	Identifying antibiotics based on structural differences in the conserved allostery from mitochondrial heme-copper oxidases. 2022 , 13,	0
656	The human signal peptidase complex acts as a quality control enzyme for membrane proteins. 2022 , 378, 996-1000	1
655	A Crystalline Dimeric Steroidal Diboronate with Electronically Impeded Rotation.	0
654	Nanoscale mechanism on lime stabilization of expansive soil.	0
653	An In-Silico Evaluation of Anthraquinones as Potential Inhibitors of DNA Gyrase B of Mycobacterium tuberculosis. 2022 , 10, 2434	0
652	Unraveling the Structural Changes in the DNA-Binding Region of Tumor Protein p53 (TP53) upon Hotspot Mutation p53 Arg248 by Comparative Computational Approach. 2022 , 23, 15499	0

- 651 Particle size and temperature effects on thermal conductivity of aqueous Ag nanofluids: modelling and simulations using classical molecular dynamics. **2022**, 76, 0
- 650 Solvation Structure and Ion Solvent Hydrogen Bonding of Hydrated Fluoride, Chloride and Bromide. A Comparative QM/MM MD Simulation Study. **2022**, 2, 445-464 0
- 649 Internal Normal Mode Analysis applied to RNA flexibility and conformational changes. 0
- 648 Quinoxalinones as A Novel Inhibitor Scaffold for EGFR (L858R/T790M/C797S) Tyrosine Kinase: Molecular Docking, Biological Evaluations, and Computational Insights. **2022**, 27, 8901 0
- 647 Amentoflavone and methyl hesperidin, novel lead molecules targeting epitranscriptomic modulator in acute myeloid leukemia: in silico drug screening and molecular dynamics simulation approach. **2023**, 29, 0
- 646 Conformational Effects of Regioisomeric Substitution on the Catalytic Activity of Copper/Calix[8]arene CB Coupling. 0
- 645 Network Analysis of Molecular Dynamics Sectors in the p53 Protein. 0
- 644 Atomic-Level Thermodynamics Analysis of the Binding Free Energy of SARS-CoV -2 Neutralizing Antibodies. 0
- 643 Network analysis uncovers the communication structure of SARS-CoV-2 Spike protein identifying sites for immunogen design. **2022**, 105855 0
- 642 Structural Remodeling Mechanism of the Toxic Amyloid Fibrillary Mediated by Epigallocatechin-3-gallate. **2022**, 7, 48047-48058 0
- 641 Influence mechanism of different organic solvents on API solvation behaviors: Molecular dynamics simulations. **2022**, 113708 1
- 640 Bioactive compounds from Pandanus fascicularis as potential therapeutic candidate to tackle hepatitis a inhibition: Docking and molecular dynamics simulation study. 1-17 2
- 639 Emerging variants of SARS-CoV-2 NSP10 highlight strong functional conservation of its binding to two non-structural proteins, NSP14 and NSP16. 0
- 638 Is the Stalk of the SARS-CoV-2 Spike Protein Druggable?. **2022**, 14, 2789 0
- 637 Reversible H₂ Storage Capacity of Ni Functionalized Carbyne (C₁₀) Complex. 0
- 636 Proton Transfers to DNA in Native Electrospray Ionization Mass Spectrometry: A Quantum Mechanics/Molecular Mechanics Study. 12004-12010 0
- 635 HIF-1 signalling pathway was identified as a potential new pathway for Icariin treatment against Alzheimer disease based on preclinical evidence and bioinformatics. 13, 0
- 634 Benchmarking biomolecular force field-based Zn²⁺ for mono- and bimetallic ligand binding sites. 2

- 633 Cumulative Millisecond-Long Sampling for a Comprehensive Energetic Evaluation of Aqueous Ionic Liquid Effects on Amino Acid Interactions. ○
- 632 Pull-Out of Pristine and Functionalized Carbon Nanotubes from Cement: A Molecular Modelling Study. **2022**, 8, 80 ○
- 631 Locating dynamic contributions to allostery via determining rates of vibrational energy transfer . ○
- 630 Computational Exploration of Anti-cancer Potential of Flavonoids against Cyclin-Dependent Kinase 8: An In Silico Molecular Docking and Dynamic Approach. 1
- 629 Improvements and new functionalities of UNRES server for coarse-grained modeling of protein structure, dynamics, and interactions. 9, ○
- 628 Thermally Controlled Exciplex Fluorescence in a Dynamic Homo[2]catenane. ○
- 627 Simulation Reveals the Chameleonic Behavior of Macrocycles. ○
- 626 Phosphorylation of the Hsp90 co-chaperone Hop changes its conformational dynamics and biological function. **2022**, 167931 ○
- 625 Interfacial Role of Ionic Liquids in CO₂ Electrocatalytic Reduction: A Mechanistic Investigation. **2022**, 141076 ○
- 624 Application of Nano-SiO₂ Reinforced Urea-Formaldehyde Resin and Molecular Dynamics Simulation Study. **2022**, 15, 8716 ○
- 623 MoBioTools : A toolkit to setup quantum mechanics/molecular mechanics calculations. ○
- 622 An α -Transition in S6 shapes the conformational cycle of the bacterial sodium channel NavAb. **2023**, 155, ○
- 621 Does Supramolecular Gelation Require an External Trigger?. **2022**, 8, 813 ○
- 620 Screening of Novel Antimicrobial Diastereomers of Azithromycin β -thiosemicarbazone Conjugates: A Combined LC-SPE/Cryo NMR, MS/MS and Molecular Modeling Approach. **2022**, 11, 1738 ○
- 619 Non-micelle-like Amyloid Aggregate Stabilizes Amyloid β (1-42) Growth Nuclei Formation. ○
- 618 Purine 5 β -Ribonucleotide- l -Glutamate Hybrids As Potential Tools To Investigate The Mechanism Of Umami Taste Reception. **2022**, 7, ○
- 617 Molecular Dynamic Simulations and Experiments Study on the Mechanical Properties of HTPE Binders. **2022**, 14, 5491 ○
- 616 In Silico Profiling of Non-Synonymous SNPs of Fat Mass and Obesity- Associated Gene: Possible impacts on the treatment of Non-Alcoholic Fatty Liver Disease. ○

- 615 Enhancing the Coherent Phonon Transport in SiGe Nanowires with Dense Si/Ge Interfaces. **2022**, 12, 4373
- 614 Efficient hydrogen storage capacity of La₃B₁₈: A DFT study. **2022**,
- 613 Toehold clipping: A mechanism for remote control of DNA strand displacement.
- 612 Allosteric rescue of catalytically impaired ATP phosphoribosyltransferase variants links protein dynamics to active-site electrostatic preorganisation. **2022**, 13,
- 611 Destabilizers of the thymidylate synthase homodimer accelerate its proteasomal degradation and inhibit cancer growth. 11,
- 610 Study of Human Lipoygenase by the Method of Molecular and Quantum Mechanics. **2022**, 16, 1089-1093
- 609 Convergence in Determining Enzyme Functional Descriptors across Kemp Eliminate Variants.
- 608 Investigation of the Interaction between Aloe vera Anthraquinone Metabolites and c-Myc and C-Kit G-Quadruplex DNA Structures. **2022**, 23, 16018
- 607 Effects of Active-Center Reduction of Plant-Type Ferredoxin on Its Structure and Dynamics: Computational Analysis Using Molecular Dynamics Simulations. **2022**, 23, 15913
- 606 Potential inhibitors of FemC to combat Staphylococcus aureus: virtual screening, molecular docking, dynamics simulation, and MM-PBSA analysis. 1-12
- 605 Diclofenac and other Non-Steroidal Anti-Inflammatory Drugs (NSAIDs) are Competitive Antagonists of the human P2X₃ Receptor.
- 604 Computational evaluation of relevant species in inorganic sulfur biochemistry.
- 603 Csk β C Helix: A Computational Analysis of an Essential Region for Conformational Transitions. **2022**, 126, 10587-10596
- 602 Collagen-Derived Cryptides: Machine-Learning Prediction and Molecular Dynamic Interaction Against Klebsiella pneumoniae Biofilm Synthesis Precursor. **2022**, 51, 59-75
- 601 Effect of moisture content on the microscopic properties of amorphous cellulose: a molecular dynamics simulations. **2022**, 9, 125308
- 600 Inspection on the Mechanism of SARS-CoV-2 Inhibition by Penciclovir: A Molecular Dynamic Study. **2023**, 28, 191
- 599 Molecular characterization of glutor-GLUT interaction and prediction of glutor β drug-likeness: implications for its utility as an antineoplastic agent. 1-12
- 598 Cryo-EM structures of human ABCA7 provide insights into its phospholipid translocation mechanisms.

- 597 In silico study revealed the inhibitory activity of selected phytochemicals of *C. rotundus* against VacA implicated in gastric ulcer. 1-12 ○
- 596 Potential targets of severe acute respiratory syndrome coronavirus 2 of clinical drug fluvoxamine: Docking and molecular dynamics studies to elucidate viral action. ○
- 595 Inorganic Drugs as a Tool for Protein Structure Solving and Studies on Conformational Changes. ○
- 594 Interference of malvidin and its mono- and di-glucosides on the membrane [Combined in vitro and computational chemistry study. **2022**, 99, 105340 ○
- 593 Force-tuned avidity of spike variant-ACE2 interactions viewed on the single-molecule level. **2022**, 13, ○
- 592 Molecular mechanism underlying desensitization of the proton-activated chloride channel PAC. 11, 1 ○
- 591 Variability of Phenylalanine side chain conformations facilitates promiscuity of Fatty acid binding in Cockroach milk proteins. ○
- 590 Crosstalk between regulatory elements in the disordered TRPV4 N-terminus modulates lipid-dependent channel activity. ○
- 589 Assembly and Synthesis Mechanism of CdSe Quantum Dots in Recombinant *Escherichia coli* Expressing Metallothionein. ○
- 588 Synthesis of Benzothiazole Linked Triazole Conjugates and Their Evaluation Against Cholinesterase Enzymes. **2022**, 7, ○
- 587 Synergistic effect of conformational changes in phosphoglycerate kinase 1 product release. 1-11 ○
- 586 Unraveling the friction response from selective hydrogenation of textured amorphous carbon surface. **2022**, 156246 ○
- 585 Serine/threonine kinase of human Monkeypox virus: computational modeling and structural analysis. ○
- 584 Conformational switch and multiple supramolecular structures of a newly identified self-assembling protein-mimetic peptide from *Pseudomonas aeruginosa* YeaZ protein. 10, ○
- 583 Structural and molecular insight into the disintegration of BRPs released by massive wasp stings using serratiopeptidase. ○
- 582 Studies on the Interaction between Model Proteins and Fluorinated Ionic Liquids. **2023**, 15, 157 1
- 581 Odorant Receptor OR2C1 Is an Essential Modulator of Boar Sperm Capacitation by Binding with Heparin. **2023**, 24, 1664 ○
- 580 Comparative Study of Receptor-, Receptor State-, and Membrane-Dependent Cholesterol Binding Sites in A2A and A1 Adenosine Receptors Using Coarse-Grained Molecular Dynamics Simulations. ○

- 579 Discovery of TP0597850: A Selective, Chemically Stable, and Slow Tight-Binding Matrix Metalloproteinase-2 Inhibitor with a Phenylbenzamide-Pentapeptide Hybrid Scaffold. **2023**, 66, 822-836 ○
- 578 Modeling the molecular fingerprint of protein-lipid interactions of MLKL on complex bilayers. 10, ○
- 577 A role of salt bridges in mediating drug potency: A lesson from the N-myristoyltransferase inhibitors. 9, ○
- 576 Understanding water structure and hydrogen association on platinum-electrolyte interface. **2022**, 2, ○
- 575 Understanding the emergence of the boson peak in molecular glasses. **2023**, 14, ○
- 574 The specificity of pectate lyase VdPelB from *Verticillium dahliae* is highlighted by structural, dynamical and biochemical characterizations. **2023**, 123137 ○
- 573 Peptide-nucleic acid aptamer pair biosensor for disease biomarker detection in clinical samples. **2023**, 141499 ○
- 572 Development of a QM/MM(ABEEM) method combined with a polarizable force field to investigate the excision reaction mechanism of damaged thymine. ○
- 571 Rational design of potent ultrashort antimicrobial peptides with programmable assembly into nanostructured hydrogels. 10, ○
- 570 Molecular Insights into Substrate Binding of the Outer Membrane Enzyme OmpT. **2023**, 13, 214 ○
- 569 Reentrant 2D Nanostructured Liquid Crystals by Competition between Molecular Packing and Conformation: Potential Design for Multistep Switching of Ionic Conductivity. ○
- 568 How Does Multiple Substrate Binding Lead to Substrate Inhibition of CYP2D6 Metabolizing Dextromethorphan? A Theoretical Study. ○
- 567 Discovery of Novel Drug-like PHGDH Inhibitors to Disrupt Serine Biosynthesis for Cancer Therapy. **2023**, 66, 285-305 ○
- 566 Molecular mechanism of LIP05 derived from *Monascus purpureus* YJX-8 for synthesizing fatty acid ethyl esters under aqueous phase. 13, 1
- 565 Membrane-binding properties of NS1 proteins from Zika and Dengue viruses: Comparative simulations in explicit bilayers reveal significant differences. ○
- 564 Water Flow in Graphene Nanochannels driven by Imposed Thermal Gradients: The Role of Flexural Phonons. ○
- 563 The DNA Radical Code. Resolution of Identity in Dissociations of Trinucleotide Codon Cation Radicals in the Gas Phase. 1
- 562 Conformational Selection of a Tryptophan Side Chain Drives the Generalized Increase in Activity of PET Hydrolases through a Ser/Ile Double Mutation. ○

561	Specificity of Monoterpene Interactions with Insect Octopamine and Tyramine Receptors: Insights from in Silico Sequence and Structure Comparison.	0
560	Multi-ligand molecular docking, simulation, free energy calculations and wavelet analysis of the synergistic effects between natural compounds baicalein and cubebin for the inhibition of the main protease of SARS-CoV-2. 2023 , 121253	0
559	Pharmacophore-based virtual screening and in-silico study of natural products as potential DENV-2 RdRp inhibitors. 1-18	0
558	All-temperature zinc batteries with high-entropy aqueous electrolyte.	2
557	A structure-based virtual high-throughput screening, molecular docking, molecular dynamics and MM/PBSA study identified novel putative drug-like dual inhibitors of trypanosomal cruzain and rhodesain cysteine proteases.	0
556	A molecular insight into the dehydration of metal-organic framework and its impact on the CO ₂ capture.	0
555	Artificial extracellular matrix scaffolds of mobile molecules enhance maturation of human stem cell-derived neurons. 2023 ,	0
554	A novel fold for acyltransferase-3 (AT3) proteins provides a framework for transmembrane acyl-group transfer. 12,	0
553	Effects of a Semisynthetic Catechin on Phosphatidylglycerol Membranes: A Mixed Experimental and Simulation Study. 2023 , 28, 422	0
552	Preparation of Temperature-Sensitive SiO ₂ /PSBMA for Reducing the Viscosity of Heavy Oil.	0
551	Modulating membrane shape and mechanics of minimal cells by light: area increase, softening and interleaflet coupling of membrane models doped with azobenzene-lipid photoswitches.	0
550	4-Cyanotryptophan as a Sensitive Fluorescence Probe of Local Electric Field of Proteins.	0
549	Seleno-Analogs of Scaffolds Resembling Natural Products a Novel Warhead toward Dual Compounds. 2023 , 12, 139	1
548	Microfluidics-Based Force Spectroscopy Enables High-Throughput Force Experiments with Sub-Nanometer Resolution and Sub-Piconewton Sensitivity. 2206713	0
547	On the Propensity of Excess Hydroxide Ions at the Alcohol Monolayer/Water Interface.	0
546	Martini 3 Coarse-Grained Model for Second-Generation Unidirectional Molecular Motors and Switches.	0
545	Equivalence of charge imbalance and external electric fields during free energy calculations of membrane electroporation.	0
544	ACES: Optimized Alchemically Enhanced Sampling.	0

- 543 Rational design of tryptophan hydroxylation 1 for improving 5-Hydroxytryptophan production. **2023**, 110198 ○
- 542 The pathogenic effect of SNPs on structure and function of human TLR4 using a computational approach. 1-14 ○
- 541 Determining interchromophore effects for energy transport in molecular networks using machine-learning algorithms. ○
- 540 Molecular Dynamic Simulations and Experiments Study on the Mechanical Properties of HTPE/PEG Interpenetrating Polymer Network (IPN) Binders. **2023**, 13, 268 ○
- 539 Mechanisms by Which Small Molecules of Diverse Chemotypes Arrest Sec14 Lipid Transfer Activity. **2023**, 102861 ○
- 538 DNA Recognition Site of Anticancer Tinidazole Copper(II) Complexes. 1
- 537 Revealing the biotoxicity of phosphorene oxide nanosheets based on the villin headpiece. ○
- 536 Synthesis, Biological Evaluation and Molecular Modeling Studies of Naphthoquinone Sulfonamides and Sulfonate Ester Derivatives as P2X7 Inhibitors. **2023**, 28, 590 ○
- 535 Dynamics Simulation of the Effect of Cosolvent on the Solubility and Tackifying Behavior of PDMS Tackifier in Supercritical CO2 Fracturing Fluid. **2023**, 130985 ○
- 534 Fructose-1,6-bisphosphatase 1 dephosphorylates IB β and suppresses colorectal tumorigenesis. ○
- 533 Interaction of Chondroitin and Hyaluronan Glycosaminoglycans with Surfaces of Carboxylated Carbon Nanotubes Studied Using Molecular Dynamics Simulations. **2023**, 28, 826 ○
- 532 In silico insights into procathepsin S maturation mediated by glycosaminoglycans. **2023**, 108406 ○
- 531 Molecular mechanism of binding between a therapeutic RNA aptamer and its protein target VEGF : A molecular dynamics study. ○
- 530 Conformational dynamics and putative substrate extrusion pathways of the N-glycosylated outer membrane factor CmeC from *Campylobacter jejuni*. **2023**, 19, e1010841 ○
- 529 Elucidation of Structure-Function Relationships of Hyaluronic Acid-Based Polymers via Combinatorial Approaches. ○
- 528 In Silico Mining of Natural Products Atlas (NPAtlas) Database for Identifying Effective Bcl-2 Inhibitors: Molecular Docking, Molecular Dynamics, and Pharmacokinetics Characteristics. **2023**, 28, 783 ○
- 527 Design of CO2 Thickeners and Role of Aromatic Rings in Enhanced Oil Recovery Using Molecular Dynamics. ○
- 526 Specific Binding of the B-Component of the Lantibiotic Lichenicidin to the Peptidoglycan Precursor Lipid II Predetermines Its Antimicrobial Activity. **2023**, 24, 1332 1

- 525 Does twist angle affect the properties of water confined inside twisted bilayer graphene?. **2023**, 158, 034501 ○
- 524 Ability of ionic liquids to inhibit the formation of methane hydrate: Insights from molecular dynamics simulations. **2023**, 204878 ○
- 523 Fluorescent protein lifetimes report increased local densities and phases of nuclear condensates during embryonic stem cell differentiation. ○
- 522 Molecular Dynamics Study on Thermal Conductance between Nanotip and Substrate under Vertical Forces and Horizontal Sliding. ○
- 521 Amphiphilic Co-Solvents Modulate the Structure of Membrane Domains. ○
- 520 Discovery of All-d-Peptide Inhibitors of SARS-CoV-2 3C-like Protease. ○
- 519 Discovery of Natural Bisbenzylisoquinoline Analogs from the Library of Thai Traditional Plants as SARS-CoV-2 3CLPro Inhibitors: In Silico Molecular Docking, Molecular Dynamics, and In Vitro Enzymatic Activity. 1
- 518 Multifunctional Electrolyte Additive Enables Highly Reversible Anodes and Enhanced Stable Cathodes for Aqueous Zinc-Ion Batteries. ○
- 517 Transthyretin binds soluble endoglin and increases its uptake by hepatocytes: A possible role for transthyretin in preeclampsia?. **2023**, 562, 111851 ○
- 516 Diffusivities of ketones and aldehydes in liquid ethanol by molecular dynamics simulations. **2023**, 371, 121068 1
- 515 Effect of microwave electric field on asphaltene aggregation in a heavy oil system: MD and DFT investigation. **2023**, 372, 121212 ○
- 514 Enhancing the fabrication yield of NV centers in diamond by pre-doping using molecular dynamics simulation. **2023**, 132, 109683 ○
- 513 Exploring the adsorption behavior of pyrazinamide on the surface of X₁₂Y₁₂ (X' = B, Al; Y' = N, P) nanocages: A in-silico study. **2023**, 372, 121211 ○
- 512 Theoretical superlubricity and its friction stability of amorphous carbon film induced by simple surface graphitization. **2023**, 615, 156318 ○
- 511 Effect of tryptophan mutation on the structure of LOV1 domain of phototropin1 protein of *Ostreococcus tauri*: A combined molecular dynamics simulation and biophysical approach. **2023**, 1867, 130304 ○
- 510 Interfacial tension of carbon dioxide - water under conditions of CO₂ geological storage and enhanced geothermal systems: A molecular dynamics study on the effect of temperature. **2023**, 337, 127219 ○
- 509 Electrophoretic coalescence behavior of oil droplets in oil-in-water emulsions containing SDS under DC electric field: A molecular dynamics study. **2023**, 338, 127258 ○
- 508 Combustion characteristics of three linear monohydric alcohols CH₃(CH₂)_n-1OH (n = 16, 18, 22): Combined ignition experiments and molecular dynamics simulations. **2023**, 338, 127264 ○

- 507 Experimental and ReaxFF molecular dynamic study of NO emission during municipal sludge/coal co-combustion. **2023**, 338, 127342 ○
- 506 Molecular interactions of resveratrol with A β 2 peptide and fibril during in-vitro A β 2 aggregation. **2023**, 7, 100060 ○
- 505 Exploring depolymerization mechanism and complex reaction networks of aromatic structures in chemical looping combustion via ReaxFF MD simulations. **2023**, 107, 101180 ○
- 504 Exploration of interaction between α -lactalbumin and β -lactoglobulin under dUHT treatment and storage: Experimental and molecular dynamics study. **2023**, 138, 108469 ○
- 503 Construction of LipidDrug Conjugates for Beclomethasone Dipropionate. ○
- 502 Role of Thylakoid Lipids in Protochlorophyllide Oxidoreductase Activation: Allosteric Mechanism Elucidated by a Computational Study. **2023**, 24, 307 ○
- 501 In silico identification of potential β -secretase inhibitor of marine-algal origin: an anticancer intervention. 1-10 ○
- 500 On the Permeation of Polychlorinated Dibenzodioxins and Dibenzofurans through Lipid Membranes: Classical MD and Hybrid QM/MM-EDA Analysis. **2023**, 13, 28 ○
- 499 Mechanism of β hairpin formation in AzoChignolin and Chignolin. ○
- 498 CLIP-Seq Analysis Enables the Design of Ribosomal RNA Bait Oligonucleotides That Protect Against C9ORF72ALS/FTD-Associated Poly-GR Pathophysiology. ○
- 497 Computational and structural insights into the pre- and post-hydrolysis states of multidrug resistance associated protein 1 in lipid bilayer membranes. ○
- 496 Additive-Driven Interfacial Engineering of Aluminum Metal Anode for Ultralong Cycling Life. **2023**, 15, ○
- 495 Effect of Local Stress on Accurate Modeling of Bacterial Outer Membranes Using All-Atom Molecular Dynamics. **2023**, 19, 363-372 ○
- 494 Accurate Metalimidazole Interactions. ○
- 493 Thermal-oxidative aging behavior of graphene and graphene oxide-filled nitrile butadiene rubber: A molecular simulation approach. ○
- 492 An Efficient, Short Stimulus PANC-1 Cancer Cell Ablation and Electrothermal Therapy Driven by Hydrophobic Interactions. **2023**, 15, 106 ○
- 491 Molecular dynamics simulation and nonlinear analysis of density fluctuations in Lennard-Jones fluid system near the critical point. **2022**, ○
- 490 Increasing the O₂ Resistance of the [FeFe]-Hydrogenase CbA5H through Enhanced Protein Flexibility. **2023**, 13, 856-865 ○

- 489 Structural Factors That Determine the Activity of the Xenobiotic Reductase B Enzyme from *Pseudomonas putida* on Nitroaromatic Compounds. **2023**, 24, 400 ○
- 488 Native and Irradiation-Induced Defects in Graphene: What Can We Learn from Atomistic Simulations?. **2011**, 334-376 ○
- 487 Comparative Analysis of the Interfaces between Monomers in the Dimers of Bacterial Histone-Like HU Proteins by the MM-GBSA Method. **2022**, 67, 897-904 ○
- 486 Comparison of force fields to study the zinc-finger containing protein NPL4, a target for Antabuse in cancer therapy. ○
- 485 Elucidating the Hydrotropic Mechanism of the Antagonistic Salt PPh4Cl. **2023**, 127, 996-1012 ○
- 484 Mechanical Properties of Polypropylene/Cellulose Biocomposites: Molecular Dynamics Simulations Combined with Constant Strain Method. **2023**, 28, 1115 ○
- 483 Calculation of the Transport and Relaxation Properties of the Ar⁴⁴HCl van der Waals Complex Using a New Potential Energy Surface: Comparison of the Classical and Full Quantum Mechanical Kinetic Theory Results with Molecular Dynamics Simulations. **2023**, 127, 1053-1067 ○
- 482 Conformational preferences of inosine and its methyl derivatives: Comparison of the AMBER derived force field parameters and reparameterization of the glycosidic torsion parameters. ○
- 481 Nucleoside-Based Cross-Linkers for Hydrogels with Tunable Properties. **2023**, 15, 7359-7370 ○
- 480 Computational investigation on the antioxidant activities and on the Mpro SARS-CoV-2 non-covalent inhibition of isorhamnetin. 11, ○
- 479 Insight into the Competitive and Synergistic Effects during Coal/NH₃ Cofiring via Reactive Molecular Dynamics Simulations. ○
- 478 Azobenzene-Based Amino Acids for the Photocontrol of Coiled-Coil Peptides. ○
- 477 The *Mythimna separata* general odorant binding protein 2 (MsepGOBP2) is involved in the larval detection of the sex pheromone (Z)-11-hexadecenal. ○
- 476 State-specific morphological deformations of the lipid bilayer explain mechanosensitive gating of MscS ion channels. 12, ○
- 475 Resistance to a tyrosine kinase inhibitor mediated by changes to the conformation space of the kinase. ○
- 474 In Silico Targeting of Fascin Protein for Cancer Therapy: Benchmarking, Virtual Screening and Molecular Dynamics Approaches. **2023**, 28, 1296 ○
- 473 Assessment of Enzyme Functionality at Metal/Organic Framework Interfaces Developed through Molecular Simulations. **2023**, 39, 1750-1763 ○
- 472 pH modulates the role of SP6 RNA polymerase in transcription process: an in silico study. 1-18 ○

471	Robust anti-inflammatory activity of genistein against neutrophil elastase: a microsecond molecular dynamics simulation study. 1-17	1
470	Molecular dynamics simulations depict structural motions of the whole human aryl hydrocarbon receptor influencing its binding of ligands and HSP90. 1-16	0
469	Capillary force exerted by water bridge on cellulose nanocrystals: Effect of an external electric field..	0
468	Structural Investigation of CDCA3-Cdh1 Protein-Protein Interactions using in-vitro Studies and Molecular Dynamics Simulation.	0
467	Polypropylene carbonate-based electrolytes as model for a different approach towards improved ion transport properties for novel electrolytes. 2023 , 25, 4810-4823	0
466	Phosphorylation of Tau R2 Repeat Destabilizes Its Binding to Microtubules: A Molecular Dynamics Simulation Study. 2023 , 14, 458-467	2
465	In silico profiling of nonsynonymous SNPs of fat mass and obesity-associated gene: possible impacts on the treatment of non-alcoholic fatty liver disease. 2023 , 22,	0
464	HuR modulation with tanshinone mimics impairs LPS response in murine macrophages.	0
463	Reconfigurable Peptide Analogs of Apolipoprotein A-I Reveal Tunable Features of Nanodisc Assembly.	0
462	Assessment of Different Parameters on the Accuracy of Computational Alanine Scanning of ProteinProtein Complexes with the Molecular Mechanics/Generalized Born Surface Area Method. 2023 , 127, 944-954	0
461	A Top-down and Bottom-up Combined Strategy for Parameterization of Coarse-grained Force Fields for Phospholipids.	
460	Partial Mimicry of the Microtubule Binding of Tau by Its Membrane Binding.	0
459	Physical properties of phospholipids at low temperatures through Slipid force field. 2023 , 2436, 012025	1
458	Upstream of N-Ras C-terminal cold shock domains mediate poly(A) specificity in a novel RNA recognition mode and bind poly(A) binding protein.	0
457	Analytical model of critical buckling transition for smectic liquid crystal based on the viscoelastic scaling of coarse-grained molecular dynamics. 2023 , 107,	0
456	Influence of salt and temperature on the self-assembly of cyclic peptides in water: a molecular dynamics study.	0
455	Interaction of Tryptophan- and Arginine-Rich Antimicrobial Peptide with E. coli Outer MembraneA Molecular Simulation Approach. 2023 , 24, 2005	1
454	Impact of an Ionic Liquid on Amino Acid Side Chains: A Perspective from Molecular Simulation Studies.	0

- 453 Solvation Structure and Dynamics of Aqueous Solutions of Au⁺ Ions: A Molecular Dynamics Simulation Study. ○
- 452 A physicochemical cause of betaine lipid evolutionary loss in seed plants?. ○
- 451 AMOEBA Polarizable Force Field for Molecular Dynamics Simulations of Glyme Solvents. ○
- 450 In silico investigation of cytochrome bc₁ molecular inhibition mechanism against *Trypanosoma cruzi*. **2023**, 17, e0010545 ○
- 449 Structure of a 28.5 kDa duplex-embedded G-quadruplex system resolved to 7.4 Å resolution with cryo-EM. ○
- 448 Roles of Tryptophan and Charged Residues on the Polymorphisms of Amyloids Formed by K-Peptides of Hen Egg White Lysozyme Investigated through Molecular Dynamics Simulations. **2023**, 24, 2626 ○
- 447 Antibiotic hyper-resistance in a class I aminoacyl-tRNA synthetase with altered active site signature motif. ○
- 446 The discovery of some promising putative binders of KRAS G12D receptor using computer-aided drug discovery approach. **2023**, 37, 101170 ○
- 445 Effect of the QM Size, Basis Set, and Polarization on QM/MM Interaction Energy Decomposition Analysis. 1
- 444 Molecular dynamics simulation of shock response of CL-20 co-crystals containing void defects. **2023**, , ○
- 443 The reconciliation between the experimental and calculated octanol-water partition coefficient of 1,2-dipalmitoyl-sn-glycero-3-phosphatidylcholine using atomistic molecular dynamics: an open question. 1-8 1
- 442 Understanding the Key Roles of pH Buffer in Accelerating Lignin Degradation by Lignin Peroxidase. ○
- 441 A molecular dynamics approach to investigate effect of pressure on asphaltene self-aggregation. **2023**, 121347 ○
- 440 Molecular Dynamics Simulations of Asphaltene Aggregation: Machine-Learning Identification of Representative Molecules, Molecular Polydispersity, and Inhibitor Performance. **2023**, 8, 4862-4877 ○
- 439 A Molecular Dynamics and Quantum Mechanical Investigation of Intermolecular Interaction and Electron-transfer Mechanism between Copper-containing Nitrite Reductase and Redox Partner Pseudoazurin. ○
- 438 Structure of human NaV1.6 channel reveals Na⁺selectivity and pore blockade by 4,9-anhydro-tetrodotoxin. ○
- 437 Monomer morphology selection rules for an accurate design of bulk heterojunction: An updated theoretical account. ○
- 436 Click and Detect: Versatile Ampicillin Aptasensor Enabled by Click Chemistry on a GrapheneAlkyne Derivative. 2207216 1

- 435 Sigmoid Accelerated Molecular Dynamics: An Efficient Enhanced Sampling Method for Biosystems. **2023**, 14, 1103-1112 ○
- 434 Druggable sites identification in Streptococcus mutans VicRK system evaluated by catechols. 1-16 ○
- 433 A comparative analysis of the influence of hydrofluoroethers as diluents on solvation structure and electrochemical performance in non-flammable electrolytes. ○
- 432 Porous Electrospun Films with Reversible Photoresponsive Microenvironmental Humidity Regulation: A Controllable Hydrogen-Bonding Synergistic Effect Exhibited by Acrylic Acid Segments. **2023**, 15, 6187-6201 ○
- 431 Structural Insights into Plasticity and Discovery of Flavonoid Allosteric Inhibitors of Flavivirus NS2B/NS3 Protease. **2023**, 3, 71-92 ○
- 430 Torque generation mechanism in Fo motor of ATP synthase elucidated by free-energy and Coulomb-energy landscapes along the c-ring rotation. **2023**, ○ 1
- 429 Structural characteristics, binding behaviors, and stability of ternary nanocomplexes of lecithin, polyvinylpyrrolidone, and curcumin. **2023**, 175, 114489 ○
- 428 Role of hinge motion and ATP dynamics in factors for inversion stimulation FIS protein deduced while targeting drug resistant Orientia tsutsugamushi. **2023**, 120, 108425 ○
- 427 Improved surface flashover voltage of epoxy following polythiourea-assisted coating with high gas adsorption ability. **2023**, 618, 156546 ○
- 426 Nature of the dative Nitrogen-Coinage metal bond in molecular Motors. Evaluation of NHC-M pyrazine bond (M=Cu, Ag, Au) from relativistic DFT. **2023**, 549, 121401 ○
- 425 Computational assessment of hexadecane freezing by equilibrium atomistic molecular dynamics simulations. **2023**, 638, 743-757 ○ 1
- 424 Modeling of the Interaction of Cytochrome c with Cardiolipin. **2022**, 67, 892-896 ○
- 423 Distinct effects of zwitterionic molecules on ionic solvation in (ethylene oxide)₁₀: a molecular dynamics simulation study. **2023**, 25, 8180-8189 ○
- 422 The substrate specificity in the O-demethylation of 4-alkylguaiaacols by cytochrome P450 AgcAP450. **2023**, 13, 2070-2079 ○
- 421 The Effect of Cholesterol in SOPC Lipid Bilayers at Low Temperatures. **2023**, 13, 275 ○
- 420 Influence of the Chemical Structure on the Mechanical Relaxation of Dendrimers. **2023**, 15, 833 ○
- 419 The SAH7 Homologue of the Allergen Ole e 1 Interacts with the Putative Stress Sensor SBP1 (Selenium-Binding Protein 1) in Arabidopsis thaliana. **2023**, 24, 3580 ○
- 418 Computational analysis of structural and functional evaluation of the deleterious missense variants in the human CTLA4 gene. 1-18 ○

- 417 Shedding light on the metal-phthalocyanine EXAFS spectra through classical and ab initio molecular dynamics. **2023**, 158, 064110 ○
- 416 Generic maximum-valence model for fluid polyamorphism. **2023**, 107, ○
- 415 Effect of Pressurized Hydrothermal Treatment on the Properties of Cellulose Amorphous Region Based on Molecular Dynamics Simulation. **2023**, 14, 314 ○
- 414 Molecular Dynamics Study on Mechanical Properties of Cellulose with Water Molecules Diffusion Behavior at Different Oxygen Concentrations. **2023**, 14, 371 ○
- 413 Stability and structural evolution of double-stranded DNA molecules under high pressures: A molecular dynamics study. 11, ○
- 412 Salinity Effect on the Interfacial Tension of CO₂-Brine: Estimation and Investigation by Molecular Dynamics Simulations. **2023**, ○
- 411 Metabolite-induced in vivo fabrication of substrate-free organic bioelectronics. **2023**, 379, 795-802 2
- 410 Evaluation of 6-OxP-CD, an Oxime-based cyclodextrin as a viable medical countermeasure against nerve agent poisoning: Experimental and molecular dynamic simulation studies on its inclusion complexes with cyclosarin, soman and VX. **2023**, 18, e0283181 ○
- 409 Physics-based generative model of curvature sensing peptides; distinguishing sensors from binders. **2023**, 9, ○
- 408 DNA methylation of the promoter region at the CREB1 binding site is a mechanism for the epigenetic regulation of brain-specific PKM β . **2023**, 1866, 194909 ○
- 407 Modeling the Infrared Spectroscopy of Oligonucleotides with ¹³C Isotope Labels. **2023**, 127, 2351-2361 ○
- 406 Stabilization of Interdomain Interactions in G protein β iSubunits Determines G β iSubtype Signaling Specificity. ○
- 405 Magnesium ions mediate ligand binding and conformational transition of the SAM/SAH riboswitch. ○
- 404 Storage and diffusion of CO₂ in covalent organic frameworks: A neural network-based molecular dynamics simulation approach. 11, ○
- 403 Insight to the Local Structure of Mixtures of Imidazolium-Based Ionic Liquids and Molecular Solvents from Molecular Dynamics Simulations and Voronoi Analysis. **2023**, 127, 2534-2545 ○
- 402 Multi-dimensional structural footprint identification for the design of potential scaffolds targeting METTL3 in cancer treatment from natural compounds. **2023**, 29, ○
- 401 Cage Dynamics-Mediated High Ionic Transport in Li-O₂ Batteries with a Hybrid Aprotic Electrolyte: LiTFSI, Sulfolane, and N,N-Dimethylacetamide. **2023**, 127, 2991-3000 ○
- 400 Migration mediated by the oxysterol receptor GPR183 depends on arrestin coupling but not receptor internalization. **2023**, 16, ○

- 399 Partial Destabilization of Amyloid- β Protofibril by Methionine Photo-Oxidation: A Molecular Dynamic Simulation Study. **2023**, 8, 10148-10159 ○
- 398 Why Does Synergistic Activation of WASP, but Not N-WASP, by Cdc42 and PIP2 Require Cdc42 Prenylation?. **2023**, 435, 168035 ○
- 397 Application of molecular dynamics simulation for exploring the roles of plant biomolecules in promoting environmental health. **2023**, 869, 161871 ○
- 396 Molecular dynamics simulation on CH₄ combustion in CO₂/O₂/N₂ atmosphere subjected to electric field. 1-7 ○
- 395 Genetically engineered PD-1 displaying nanovesicles for synergistic checkpoint blockades and chemo-metabolic therapy against non-small cell lung cancer. **2023**, 161, 184-200 ○
- 394 Effect of temperature and salt addition on the structural properties of Triton X-100. **2023**, 615, 128614 ○
- 393 Unique structure of ozoralizumab, a trivalent anti-TNF β NANOBODY β compound, offers the potential advantage of mitigating the risk of immune complex-induced inflammation. 14, ○
- 392 Thermal conductivity across transition metal dichalcogenide bilayers. **2023**, 26, 106447 ○
- 391 The Effect of Miscibility and Morphology of Porphyrin Donors and Non-Fullerene Acceptors on Exciton Dissociation Processes: A Quantum Chemical and Molecular Dynamics Study. ○
- 390 Embedding Beyond Electrostatics: The Extended Polarizable Density Embedding Model. **2023**, 127, 3248-3256 ○
- 389 Phosphatidylcholine in the tear film of the eye: Enhanced topical delivery of fluorometholone to the eye. **2023**, 150, 110506 ○
- 388 Contribution of proteins to ceramic membrane fouling at the early stage of membrane filtration. **2023**, 312, 123450 ○
- 387 Computer simulation study of ion-water and water-water hydrogen bonds in methanesulfonic acid solutions at room temperature. **2023**, 377, 121518 ○
- 386 Extraction of estrogenic pollutants in aqueous solution using poly(lactic acid). **2023**, 377, 121577 ○
- 385 Computational probing of Nigella sativa bioactive metabolites against chickungunya nsP2 cysteine protease. **2023**, 35, 102651 ○
- 384 Targeting hPKM2 in cancer: A bio isosteric approach for ligand design. **2023**, 158, 106852 ○
- 383 Room for improvement in the initial martini 3 parameterization of peptide interactions. **2023**, 819, 140436 ○
- 382 Highly thermally conductive polymer-based composites with 3D exfoliated BNNS/functionalized SiC networks prepared by rapid solidification and hot pressing. **2023**, 186, 105539 ○

- 381 Identification of alkaloid compounds as potent inhibitors of Mycobacterium tuberculosis NadD using computational strategies **2023**, 158, 106863 ○
- 380 The effect of alumina as an interfacial layer on the reactivity of Al/PTFE energetic composites. **2023**, 24, 3033-3047 ○
- 379 Click chemistry-initiated highly uniform semi-interpenetrating polymer electrolyte with dual salts for high-performance lithium metal batteries. **2023**, 565, 232884 ○
- 378 Exploring the basal/prismatic slip transfer at grain boundaries in magnesium: A molecular dynamic simulation. **2023**, 212, 111995 ○
- 377 Molecular insights on PS-PLA1 lipase activity of human ABHD16B. **2023**, 296, 106976 ○
- 376 A comparative study on inclusion complex formation between formononetin and β -cyclodextrin derivatives through multiscale classical and umbrella sampling simulations. **2023**, 310, 120729 ○
- 375 Directional movement of gold nanoparticles on the silicon substrate due to the Laplace pressure: A molecular dynamics simulation study. **2023**, 380, 121767 ○
- 374 Assessment of CO₂-Oil swelling behavior using molecular dynamics simulation: CO₂ utilization and storage implication. **2023**, 379, 121582 ○
- 373 Molecular dynamics simulation study of DNA conformation changes caused by the dinuclear platinum(II) complexes with the bisphosphonate group. **2023**, 243, 112179 ○
- 372 A modified bonded model approach for molecular dynamics simulations of New Delhi Metallo- β -lactamase. **2023**, 121, 108431 ○
- 371 GAP positions catalytic H-Ras residue Q61 for GTP hydrolysis in molecular dynamics simulations, complicating chemical rescue of Ras deactivation. **2023**, 104, 107835 ○
- 370 Experimental and computational approaches to characterize a novel amidase that initiates the biodegradation of the herbicide propanil in Borea sp. P5. **2023**, 451, 131155 ○
- 369 On the angular distributions of atoms sputtered by gas cluster ion beam. **2023**, 212, 112061 ○
- 368 Computational identification of drug-like marine natural products as potential RNA polymerase inhibitors against Nipah virus. **2023**, 104, 107850 ○
- 367 Structure-based virtual screening for potent inhibitors of GH-20 N -acetylglucosaminidase: Classical and machine learning scoring functions, and molecular dynamics simulations. **2023**, 104, 107856 ○
- 366 Insight into surfactant adsorption performance at asphaltene surface by in-situ DPI experiment and microscopic MD simulation. **2023**, 666, 131313 ○
- 365 Effects of modified single-wall carbon nanotubes on the mechanical properties of polyvinyl alcohol composites by molecular dynamics simulation. **2023**, 35, 105598 ○
- 364 Decoupling effects of C₃H₃/C₄H₅/*i*-C₄H₅/CN radicals on the formation and growth of aromatics: A ReaxFF molecular dynamics study. **2023**, 171, 106185 ○

- 363 Is imogolite a suitable adsorbent agent for the herbicides like diuron and atrazine?. **2023**, 380, 121732 ○
- 362 Interaction of neutral and protonated Tamoxifen with the DPPC lipid bilayer using molecular dynamics simulation. **2023**, 194, 109225 ○
- 361 Elucidating the effects of emulsification on the thermal performances of palm oil-based phase change materials by molecular dynamics simulations. **2023**, 64, 107071 ○
- 360 Introducing NMR strategies to define water molecules that drive metal binding in a transcriptional regulator. **2023**, 16-17, 100114 ○
- 359 Epigenetic CpG duplex marks probed by an evolved DNA reader via a well-tempered conformational plasticity. ○
- 358 Shifting the selectivity of pyrido[2,3-d]pyrimidin-7(8H)-one inhibitors towards the salt-inducible kinase (SIK) subfamily. **2023**, 115347 ○
- 357 Ionizable lipids penetrate phospholipid bilayers with high phase transition temperatures: perspectives from free energy calculations. **2023**, 253, 105294 ○
- 356 Accurate and efficient constrained molecular dynamics of polymers using Newton's method and special purpose code. **2023**, 288, 108742 ○
- 355 The molecular basis of the antidepressant action of the magic mushroom extract, psilocin. **2023**, 1871, 140914 ○
- 354 Composition effects on thermodynamic properties and interfacial structure in styrene-butadiene rubber: A combined experimental and simulation study. **2023**, 275, 118750 ○
- 353 Uncovering the mechanisms of cyclic peptide self-assembly in membranes with the chirality-aware MA(R/S)TINI forcefield. **2023**, 642, 84-99 ○
- 352 Effect of molecular dynamics water models on flux, diffusivity, and ion dynamics for polyamide membrane simulations. **2023**, 678, 121630 ○
- 351 Surface-induced demixing of self-assembled isomeric mixtures of citral. **2023**, 381, 121803 ○
- 350 Influence of High Concentration Vacancy-Type Defects on the Mobility of Edge Dislocation in β -Iron: An Atomistic Investigation. **2022**, ○
- 349 Pressure-driven flow behavior of small molecules through a carbon nanotube. **2023**, 374, 121276 ○
- 348 Structure restoration and aggregate inhibition of V30M mutant transthyretin protein by potential quinoline molecules. **2023**, 231, 123318 2
- 347 Nanoscale insights into the interfacial characteristics between calcium silicate hydrate and silica. **2023**, 616, 156478 ○
- 346 Computer-aided affinity enhancement of a cross-reactive antibody against dengue virus envelope domain III. ○

- 345 Polishing process of 4H-SiC under different pressures in a water environment. **2023**, 133, 109710 ○
- 344 Asymmetry and Ion Selectivity Properties of Bacterial Channel NaK Mutants Derived from Ionotropic Glutamate Receptors. **2023**, 435, 167970 ○
- 343 Deciphering the interactions of genistein with cyclodextrin derivatives through experimental and microsecond timescale umbrella sampling simulations. **2023**, 374, 121295 ○
- 342 Integration of terpesomes loaded Levocetazine dihydrochloride gel as a repurposed cure for Methicillin-Resistant Staphylococcus aureus (MRSA)-Induced skin infection; D-optimal optimization, ex-vivo, in-silico, and in-vivo studies. **2023**, 633, 122621 ○
- 341 Evaluating the active site-substrate interplay between x-ray crystal structure and molecular dynamics in chorismate mutase. **2023**, 158, 065101 ○
- 340 Distant sequence regions of JBP1 contribute to J-DNA binding. ○
- 339 Computational analysis of protein-ligand interaction by targeting a cell cycle restrainer. **2023**, 231, 107367 2
- 338 The Physical Foundations of 3D-Printing Technology. Molecular Dynamics Simulation. **2022**, 65, 1290-1298 ○
- 337 Simulation strategies for ReaxFF molecular dynamics in coal pyrolysis applications: A review. **2023**, 170, 105882 ○
- 336 A computational strategy for therapeutic development against superoxide dismutase (SOD1) amyloid formation: effect of polyphenols on the various events in the aggregation pathway. **2023**, 25, 6232-6246 ○
- 335 On the Behavior of the Ethylene Glycol Components of Polydisperse Polyethylene Glycol PEG200. **2023**, 127, 1178-1196 ○
- 334 A concurrent multiscale method based on smoothed molecular dynamics for large-scale parallel computation at finite temperature. **2023**, 406, 115898 ○
- 333 Integration of Ultrastructural and Computational Approaches Reveals the Protective Effect of Astaxanthin against BPA-Induced Nephrotoxicity. **2023**, 11, 421 ○
- 332 Investigation of the effects of N-Acetylglucosamine on the stability of the spike protein in SARS-CoV-2 by molecular dynamics simulations. **2023**, 1222, 114049 ○
- 331 Protein dynamics provide mechanistic insights about epistasis among common missense polymorphisms. **2023**, ○
- 330 Elucidating the Molecular Origins of the Transference Number in Battery Electrolytes Using Computer Simulations. **2023**, 3, 306-315 ○
- 329 The hydration of Li⁺ and Mg²⁺ in subnano carbon nanotubes using a multiscale theoretical approach. 11, ○
- 328 Bifunctional electrolyte regulation towards low-temperature and high-stability Zn-ion hybrid capacitor. **2023**, 79, 495-504 ○

- 327 Molecular surveillance of Kelch-13 gene in Plasmodium falciparum field isolates from Mayurbhanj District, Odisha, India, and in silico artemisinin-Kelch-13 protein interaction study. **2023**, 122, 717-727 ○
- 326 Structural Basis for Agonistic Activity and Selectivity toward Melatonin Receptors hMT1 and hMT2. **2023**, 24, 2863 1
- 325 How Can Static and Oscillating Electric Fields Serve in Decomposing Alzheimer's and Other Senile Plaques?. **2023**, 145, 3543-3553 ○
- 324 Multi-Hydration Induced Zwitterionic Hydrogel with Open Environment Stability for Chemical Sensing. 2200061 ○
- 323 On the interplay between lipids and asymmetric dynamics of an NBS degenerate ABC transporter. **2023**, 6, ○
- 322 Rohitukine content across the geographical distribution of Dysoxylum binectariferum Hook F. and its natural derivatives as potential sources of CDK inhibitors. **2023**, 9, e13469 ○
- 321 Coulombic Organization in Membrane-Embedded Rotary Motor of ATP Synthase. **2023**, 127, 1552-1562 1
- 320 Nano-structured Hydrotrope-Caged Cytochrome c with Boosted Stability in Harsh Environments: A Molecular Insight. ○
- 319 The effects of size and surface functionalization of polystyrene nanoplastics on stratum corneum model membranes: An experimental and computational study. **2023**, 638, 778-787 ○
- 318 Two-temperature activity induces liquid-crystal phases inaccessible in equilibrium. **2023**, 107, ○
- 317 Distal Mutations in the β -Clamp of DNA Polymerase III* Disrupt DNA Orientation and Affect Exonuclease Activity. **2023**, 145, 3478-3490 ○
- 316 High-throughput single-molecule quantification of individual base stacking energies in nucleic acids. **2023**, 14, ○
- 315 HPV and molecular mimicry in systemic lupus erythematosus and an impact of compiling B-cell epitopes and MHC-class II binding profiles with in silico evidence. 1-9 ○
- 314 Entropically-Driven Co-assembly of L-Histidine and L-Phenylalanine to Form Supramolecular Materials. **2023**, 17, 3506-3517 ○
- 313 Quantum-corrected thickness-dependent thermal conductivity in amorphous silicon predicted by machine learning molecular dynamics simulations. **2023**, 107, ○
- 312 Computational analysis of the effect of Gly100Ala mutation on the thermostability of SazCA. 1-9 ○
- 311 In-silico approaches towards development of model irreversible HIV-1 protease inhibitors. ○
- 310 Molecular dynamics study of SiO₂ nanohole etching by fluorocarbon ions. **2023**, 41, 023001 1

- 309 Dislocation mechanisms in strengthening and softening of nanotwinned materials. **2023**, 133, 055106 ○
- 308 Molecular dynamics simulation studies of 1,3-dimethyl imidazolium nitrate ionic liquid with water. **2023**, 158, 084505 ○
- 307 Targeting Troponin C with Small Molecules Containing Diphenyl Moieties: Calcium Sensitivity Effects on Striated Muscle and Structure Activity Relationship. ○
- 306 In silico drug discovery of SIRT2 inhibitors from natural source as anticancer agents. **2023**, 13, ○
- 305 Evaluation of free radical quenching, anti-inflammatory activity together with anticancer potential of *Lychnis coronaria* and characterization of novel molecules from its extract through high resolution-liquid chromatography mass spectrometry coupled to structural biochemistry approach. 1-15 ○
- 304 RNA G-quadruplex folding is a multi-pathway process with a variety of short-lived intermediates. ○
- 303 Machine learning based modeling of disordered elemental semiconductors: understanding the atomic structure of a-Si and a-C. **2023**, 38, 043001 ○
- 302 Enhanced adhesion friction behaviors of nature rubber composites by applications of carbon nanotube: Experiment and molecular insight. **2023**, 181, 108333 ○
- 301 In Silico Discovery of Small Molecule Modulators Targeting the Achilles' Heel of SARS-CoV-2 Spike Protein. ○
- 300 New molecular insights for 4H-1,2,4-triazole derivatives as inhibitors of tankyrase and Wnt-signaling antagonist: a molecular dynamics simulation study. 1-13 ○
- 299 Effect of single-vacancy- and vacancy-adsorbed-atom-defective CNTs on the mechanical and tribological properties of NBR composites: molecular dynamics simulations. **2023**, 30, ○
- 298 Lipidation Alters the Structure and Hydration of Myristoylated Intrinsically Disordered Proteins. **2023**, 24, 1244-1257 ○
- 297 Molecular Dynamic and Dissipative Particle Dynamic Simulation on the Miscibility of NR/CR Blends. **2023**, 15, 856 ○
- 296 Structural Insights into the Antiparallel G-Quadruplex in the Presence of K⁺ and Mg²⁺ Ions. **2023**, 127, 1499-1512 ○
- 295 Design of a multi-epitope vaccine against six *Nocardia* species based on reverse vaccinology combined with immunoinformatics. 14, ○
- 294 Lessons for Oral Bioavailability: How Conformationally Flexible Cyclic Peptides Enter and Cross Lipid Membranes. **2023**, 66, 2773-2788 ○
- 293 A study of polyethylene glycol terephthalate (PET) pyrolysis mechanisms using reactive molecular dynamic simulations. **2023**, 45, 1079-1090 ○
- 292 Caffeic Acid Has Antiviral Activity against Influenza Virus In Vitro. **2023**, 15, 494 ○

- 291 Small molecule inhibitors of 15-PGDH exploit a physiologic induced-fit closing system. **2023**, 14, ○
- 290 Structures of NF- κ B p52 homodimer-DNA complexes rationalize binding mechanisms and transcription activation. 12, ○
- 289 Molecular dynamics simulations reveal the effect of mutations in the RING domains of BRCA1-BARD1 complex and its relevance to the prognosis of breast cancer. 1-19 ○
- 288 Correlation between protein conformations and water structure and thermodynamics at high pressure: A molecular dynamics study of the Bovine Pancreatic Trypsin Inhibitor (BPTI) protein. **2023**, 158, 095102 ○
- 287 The combination of polyphenols and phospholipids as an efficient platform for delivery of natural products. **2023**, 13, ○
- 286 Impact of non-proteinogenic amino acid norvaline and proteinogenic valine misincorporation on a secondary structure of a model peptide. ○
- 285 Effect of Organic Ions on The Formation and Collapse of Nanometric Bubbles in Ionic Liquid/Water Solutions: A Molecular Dynamics Study. **2023**, 127, 1628-1644 ○
- 284 Hexamethylenetetramine additive with zincophilic head and hydrophobic tail for realizing ultra-stable Zn anode. **2023**, 460, 141902 ○
- 283 Evaluation of the affinity of asphaltene molecular models A1 and A2 by the water/oil interfaces based on a novel concept of solubility parameter profiles obtained from MD simulations. **2023**, 376, 121430 ○
- 282 Using High-Throughput Molecular Dynamics Simulation to Enhance the Computational Design of Kemp Elimination Enzymes. **2023**, 63, 1323-1337 ○
- 281 Phosphorylation at Ser289 Enhances the Oligomerization of Tau Repeat R2. **2023**, 63, 1351-1361 ○
- 280 Stability of the A β 2 Peptide in Mixed Solutions of Denaturants and Proline. **2023**, 127, 1572-1585 ○
- 279 Efficient production of salvianic acid A from L-dihydroxyphenylalanine through a tri-enzyme cascade. ○
- 278 Virtual Screening of Hepatitis B Virus Pre-Genomic RNA as a Novel Therapeutic Target. **2023**, 28, 1803 ○
- 277 Modelling of nanocrystalline insulators response to swift heavy ion irradiation. **2023**, 221, 112078 ○
- 276 Influence of gelation temperature on physicochemical properties of cellulose hydrogels prepared from ionic liquid/DMSO solution. **2023**, 376, 121465 ○
- 275 Site-Specific Phosphorylation of RTK KIT Kinase Insert Domain: Interactome Landscape Perspectives. **2023**, 1, 39-71 ○
- 274 How Do Cyclopropane Fatty Acids Protect the Cell Membrane of Escherichia coli in Cold Shock?. **2023**, 127, 1607-1617 ○

- 273 Study on host-guest interaction of aroma compounds/ β -cyclodextrin inclusion complexes. **2023**, 178, 114589 ○
- 272 Molecular dynamics simulations of the interactions between CO₂ and branched unreacted and reacted polyethylenimine films. **2023**, 111, 204928 ○
- 271 Silk Assembly against Hydrophobic Surfaces-Modeling and Imaging of Formation of Nanofibrils. **2023**, 6, 1011-1018 ○
- 270 Relaxation dynamics measure the aggregation propensity of amyloid- β and its mutants. **2023**, 158, 105101 ○
- 269 i-Motif folding intermediates with zero-nucleotide loops are trapped by 2'-fluoroarabincytidine via F⁻⁻⁻H and O⁻⁻⁻H hydrogen bonds. **2023**, 6, 1 ○
- 268 Co-occurring pathogenic variants in 6q27 associated with dementia spectrum disorders in a Peruvian family. 16, ○
- 267 Thermodynamics and transport properties of valine and cysteine peptides in water. **2023**, 376, 121472 ○
- 266 Inhibition of 3-Hydroxykynurenine Transaminase from *Aedes aegypti* and *Anopheles gambiae*: A Mosquito-Specific Target to Combat the Transmission of Arboviruses. **2023**, 3, 211-222 ○
- 265 NanoModeler CG: A Tool for Modeling and Engineering Functional Nanoparticles at a Coarse-Grained Resolution. **2023**, 19, 1582-1591 ○
- 264 Structural basis for membrane attack complex inhibition by CD59. **2023**, 14, ○
- 263 Toward Force Fields with Improved Base Stacking Descriptions. **2023**, 19, 1529-1536 ○
- 262 Discovery of potent inhibitors targeting Glutathione S-transferase of *Wuchereria bancrofti*: a step toward the development of effective anti-filariasis drugs. ○
- 261 Dynamic Heterogeneity of Solvent Motion and Ion Transport in Concentrated Electrolytes. **2023**, 127, 1803-1810 ○
- 260 Long-time scale simulations of virus-like particles from three human-norovirus strains. ○
- 259 Unraveling topoisomerase IA gate dynamics in presence of PPEF and its preclinical evaluation against multidrug-resistant pathogens. **2023**, 6, ○
- 258 Structural Characterization of Nanobodies during Germline Maturation. **2023**, 13, 380 ○
- 257 Interaction of Amphipathic Peptide from Influenza Virus M1 Protein with Mitochondrial Cytochrome Oxidase. **2023**, 24, 4119 1
- 256 Thermal transport across copper/water interfaces according to deep potential molecular dynamics. **2023**, 25, 6746-6756 ○

- 255 Influence of Mutations of Conserved Arginines on Neuropeptide Binding in the DPP III Active Site. **2023**, 28, 1976 ○
- 254 Utilizing Machine Learning to Greatly Expand the Range and Accuracy of Bottom-Up Coarse-Grained Models through Virtual Particles. 1
- 253 Phosphorylation-Competent Metastable State of Escherichia coli Toxin HipA. **2023**, 62, 989-999 ○
- 252 All-Atom Molecular Dynamics Simulations Indicated the Involvement of a Conserved Polar Signaling Channel in the Activation Mechanism of the Type I Cannabinoid Receptor. **2023**, 24, 4232 ○
- 251 The chemosensory protein 1 contributes to indoxacarb resistance in *Plutella xylostella* (L.). ○
- 250 Conformational landscapes of artificial peptides predicted by various force fields: are we ready to simulate amino acids?. **2023**, 25, 7466-7476 ○
- 249 Evaluation of polyanionic cyclodextrins as high affinity binding scaffolds for fentanyl. **2023**, 13, ○
- 248 Determination of elastic parameters of lipid membranes from simulation under varied external pressure. **2023**, 107, ○
- 247 Field-Induced Hydration Shell Reorganization Enables Electro-osmotic Flow in Nanochannels. **2023**, 130, ○
- 246 Understanding Drug Resistance of Wild-Type and L38HL Insertion Mutant of HIV-1 C Protease to Saquinavir. **2023**, 14, 533 ○
- 245 AI-Accelerated Design of Targeted Covalent Inhibitors for SARS-CoV-2. **2023**, 63, 1438-1453 1
- 244 Exploring Core Genes by Comparative Transcriptomics Analysis for Early Diagnosis, Prognosis, and Therapies of Colorectal Cancer. **2023**, 15, 1369 ○
- 243 Combined quantum mechanics and molecular dynamics study on the calcite scale inhibition mechanism of carboxymethyl dextran. **2023**, 553, 116503 ○
- 242 Experimental and Simulation Study for the Dissociation Behavior of Gas Hydrates-Part II: sII Mixed Gas Hydrates. **2023**, 37, 4497-4514 ○
- 241 FERM domains recruit ample PI(4,5)P2s to form extensive protein-membrane attachments. **2023**, 122, 1325-1333 ○
- 240 Probing the Mechanisms of Inhibitors Binding to Presenilin Homologue Using Molecular Dynamics Simulations. **2023**, 28, 2076 ○
- 239 Hierarchical Aggregation in a Complex Fluid-The Role of Isomeric Interconversion. **2023**, 127, 2052-2065 ○
- 238 Venetoclax analogs as promising anticancer therapeutics via targeting Bcl-2 protein: in-silico drug discovery study. 1-17 ○

- 237 In Vitro and In Silico Study on the Molecular Encapsulation of β -Tocopherol in a Large-Ring Cyclodextrin. **2023**, 24, 4425 ○
- 236 Isolation, characterization and in silico study of propenamide alkaloids from *Hymenocallis bicolor* poison against active β opioid receptor. 1-17 ○
- 235 Phenotypic Discovery of Thiocarbohydrazone with Anticancer Properties and Catalytic Inhibition of Human DNA Topoisomerase II β . **2023**, 16, 341 ○
- 234 Vapor-liquid phase transition behavior and thermophysical properties of R448A and R449A at temperatures from 233.15 K to 308.15 K. **2023**, 37, 1473-1483 ○
- 233 Structure of human NaV1.6 channel reveals Na⁺ selectivity and pore blockade by 4,9-anhydro-tetrodotoxin. **2023**, 14, ○
- 232 Experimental and Simulation Study for the Dissociation Behavior of Gas Hydrates [Part I: CH₄ Hydrates]. **2023**, 37, 4484-4496 1
- 231 Uncovering the Interaction Interface Between Harpin (Hpa1) and Rice Aquaporin (OsPIP1;3) Through Protein-Protein Docking: An In Silico Approach. ○
- 230 Repurposing of phyto-ligand molecules from the honey bee products for Alzheimer's disease as novel inhibitors of BACE-1: small molecule bioinformatics strategies as amyloid-based therapy. **2023**, 30, 51143-51169 ○
- 229 HilE represses the activity of HilD via a mechanism distinct from that of intestinal long-chain fatty acids. ○
- 228 Tween-80 on Water/Oil Interface: Structure and Interfacial Tension by Molecular Dynamics Simulations. **2023**, 39, 3255-3265 ○
- 227 Polyethylene glycol regulated carnallite decomposition-crystallization: Experimental and theoretical analysis. **2023**, 195, 108021 ○
- 226 The Mechanism of Action of SAAP-148 Antimicrobial Peptide as Studied with NMR and Molecular Dynamics Simulations. **2023**, 15, 761 ○
- 225 Chelation Behaviors of 3,4,3-LI(1,2-HOPO) with Lanthanides and Actinides Implicated by Molecular Dynamics Simulations. **2023**, 62, 4304-4313 ○
- 224 Inert-gas ion scattering at grazing incidence on smooth and rough Si and SiO₂ surfaces. **2023**, 41, 023003 ○
- 223 Effect of macrocyclization and tetramethylrhodamine labeling on chemokine binding peptides. ○
- 222 Million-atom molecular dynamics simulations reveal the interfacial interactions and assembly of plant PSII-LHCII supercomplex. **2023**, 13, 6699-6712 ○
- 221 2D MoS₂ and BN Nanosheets Damage Mitochondria through Membrane Penetration. **2023**, 17, 4716-4728 ○
- 220 The molecular mechanism of Y473 phosphorylation of UGDH relieves the inhibition effect of UDP-glucose on HuR. **2023**, 25, 8714-8724 ○

- 219 SorptionDeformationPercolation Model for Diffusion in Nanoporous Media. **2023**, 17, 4507-4514 ○
- 218 Simulated Tempering-Enhanced Umbrella Sampling Improves Convergence of Free Energy Calculations of Drug Membrane Permeation. **2023**, 19, 1898-1907 ○
- 217 Adsorption of Biomimetic Amphiphilic Heteropolymers onto Graphene and Its Derivatives. **2023**, 56, 1798-1809 ○
- 216 Fluorescent Probes cis- and trans-Parinaric Acids in Fluid and Gel Lipid Bilayers: A Molecular Dynamics Study. **2023**, 28, 2241 ○
- 215 Interfacial Shear Strength of Single-Walled Carbon Nanotubes-Cement Composites from Molecular Dynamics and Finite Element Studies. **2023**, 16, 1992 ○
- 214 In-silico natural product database mining for novel neuropilin-1 inhibitors: molecular docking, molecular dynamics and binding energy computations. **2023**, 17, ○
- 213 Alchemical Metadynamics: Adding Alchemical Variables to Metadynamics to Enhance Sampling in Free Energy Calculations. **2023**, 19, 1805-1817 ○
- 212 Novel Mixed Matrix Membranes Based on Poly(vinylidene fluoride): Development, Characterization, Modeling. **2023**, 15, 1222 ○
- 211 The coat protein of tobacco mosaic virus as an anti-tobacco mosaic virus: a molecular dynamics simulation. 1-6 ○
- 210 The interactions of monomeric acridines and unsymmetrical bisacridines (UAs) with DNA duplexes: an insight provided by NMR and MD studies. **2023**, 13, ○
- 209 The Intrinsic Radius as a Key Parameter in the Generalized Born Model to Adjust Protein-Protein Electrostatic Interaction. **2023**, 24, 4700 ○
- 208 On the Mechanism of Membrane Permeabilization by Tamoxifen and 4-Hydroxytamoxifen. **2023**, 13, 292 ○
- 207 Singlet fission as a polarized spin generator for dynamic nuclear polarization. **2023**, 14, ○
- 206 Phenothiazine-Based LSD1 Inhibitor Promotes T-Cell Killing Response of Gastric Cancer Cells. **2023**, 66, 3896-3916 ○
- 205 Different Dynamic Behavior of Methyl Groups in Crystalline Carbimazole as Revealed by a Multitechnique Experimental and Theoretical Approach. **2023**, 127, 5186-5196 ○
- 204 Effects of N₂ and CO₂ on the flammability of 2,3,3,3-tetrafluoropropene at elevated temperatures. **2023**, 83, 105024 ○
- 203 Molecular Dynamics Assessment of Mechanical Properties of the Thin Filaments in Cardiac Muscle. **2023**, 24, 4792 ○
- 202 Extension of the TraPPE Force Field for Battery Electrolyte Solvents. **2023**, 127, 2224-2236 ○

- 201 Probing Redox Properties of Extreme Concentrations Relevant for Nonaqueous Redox-Flow Batteries. **2023**, 6, 2819-2831 ○
- 200 Molecular Insights into Cyclodextrin-Adamantane-Modified Copolymer Host-Guest Interactions. **2023**, 39, 3619-3627 ○
- 199 Computational Procedure for Analysis of Crystallites in Polycrystalline Solids of Quasilinear Molecules. **2023**, 28, 2327 ○
- 198 Solvation free energy arithmetic for small organic molecules. **2023**, 44, 1263-1277 ○
- 197 Rational Computational Approaches in Drug Discovery: Potential Inhibitors for Allosteric Regulation of Mutant Isocitrate Dehydrogenase-1 Enzyme in Cancers. **2023**, 28, 2315 ○
- 196 Insights at the atomistic resolution of antibiotics using multiscale simulations. **2023**, 241-253 ○
- 195 Microscopic Understanding of the Conformational Stability of the Aggregated Nonamyloid β Components of β -Synuclein. **2023**, 63, 1542-1555 ○
- 194 Triterpene Derivatives as Potential Inhibitors of the RBD Spike Protein from SARS-CoV-2: An In Silico Approach. **2023**, 28, 2333 ○
- 193 Ligand-Ligand-Interaction-Dominated Self-Assembly of Gold Nanoparticles at the Oil/Water Interface: An Atomic-Scale Simulation. **2023**, 127, 2258-2266 ○
- 192 Conformational dynamics of C1r inhibitor proteins from Lyme disease and relapsing fever spirochetes ○
- 191 The thermodynamics of enhanced dope stability of cellulose solution in NaOH solution by urea. **2023**, 311, 120744 ○
- 190 SARS-CoV-2-related bat virus behavior in human-relevant models sheds light on the origin of COVID-19. **2023**, 24, 1 ○
- 189 In Silico Exploration of Microtubule Agent Griseofulvin and Its Derivatives Interactions with Different Human β -Tubulin Isoforms. **2023**, 28, 2384 ○
- 188 Expanding the molecular language of protein liquid-liquid phase separation. ○
- 187 Stereo-complementary epoxidation of 4-vinyl-2,3-dihydrobenzofuran using mutants of SeStyA with enhanced stability and enantioselectivity. **2023**, 540, 113055 ○
- 186 Thermal cloaking phenomenon in the convex structure silicon film. **2023**, 364, 115131 ○
- 185 In silico screening of inhibitors against human dihydrofolate reductase to identify potential anticancer compounds. 1-13 ○
- 184 Light-Induced Subnanometric Modulation of a Single-Molecule Electron Source. **2023**, 130, ○

- 183 Combining experiments and simulations to examine the temperature-dependent behaviour of a disordered protein. ○
- 182 IDP Force Fields Applied to Model PPII-Rich 33-mer Gliadin Peptides. **2023**, 127, 2407-2417 ○
- 181 Mechanism of Chiral-Selective Aminoacylation of an RNA Minihelix Explored by QM/MM Free-Energy Simulations. **2023**, 13, 722 ○
- 180 Binding of Anionic Polyacrylamide with Amidase and Laccase under 298, 303, and 308 K: Docking and Molecular Dynamics Simulation Studies Combined with Experiments. **2023**, 8, 10040-10050 ○
- 179 NiAl (0 0 1) terminated surface effect on the growth of the Al thin film. **2023**, 222, 112117 ○
- 178 Molecular interactions of CO₂ and CH₄ and their adsorption behaviour in kerogens with different grades of maturity. **2023**, 49, 536-550 ○
- 177 Unsupervised Data-Driven Reconstruction of Molecular Motifs in Simple to Complex Dynamic Micelles. **2023**, 127, 2595-2608 ○
- 176 How NaFTA salt affects the structural landscape and transport properties of Pyr₁,3FTA ionic liquid. **2023**, 158, 104502 ○
- 175 Computational insight into structural basis of human ELOVL1 inhibition. **2023**, 157, 106786 ○
- 174 Theoretical Study on the Gas-Phase and Aqueous Interface Reaction Mechanism of Criegee Intermediates with 2-Methylglyceric Acid and the Nucleation of Products. **2023**, 24, 5400 ○
- 173 HuR modulation counteracts lipopolysaccharide response in murine macrophages. **2023**, 16, ○
- 172 Frontiers, challenges, and solutions in modeling of swift heavy ion effects in materials. **2023**, 133, 100701 ○
- 171 Development of multi-epitope vaccines against the monkeypox virus based on envelope proteins using immunoinformatics approaches. 14, ○
- 170 Interfacial interactions of humic acids with polystyrene nano-plastics in aqueous/ionic environments: a molecular dynamics exploration. ○
- 169 Anesthetic-Binding Induced Motion of GABA_A Receptors Revealed by Coarse-Grained Molecular Dynamics Simulations. ○
- 168 Computational Analysis and Experimental Testing of the Molecular Mode of Action of Gatastatin and Its Derivatives. **2023**, 15, 1714 ○
- 167 Performance analysis of thermal cloak with porous silicon structure. **2023**, 143, 106730 ○
- 166 Metastable hybridized structure transformation in amorphous carbon films during friction study combining experiments and MD simulation. ○

- 165 Structural Optimization of an β -Hairpinin Blocking Potassium Channels KV1.3. **2023**, 59, 192-199 ○
- 164 The Impact of Antimicrobial Peptides on the *Acinetobacter baumannii* Inner Membrane Is Modulated by Lipid Polyunsaturation. **2023**, 9, 815-826 ○
- 163 Slow spectral diffusion of the NO stretching mode of $[\text{RuCl}_5(\text{NO})]_2$ in D₂O studied by 2D-IR spectroscopy and molecular dynamics simulations. **2023**, 158, 134510 ○
- 162 Relaxation time scales of interfacial water upon fluid to ripple to gel phase transitions of bilayers. **2023**, 158, 114503 ○
- 161 Stable LiF-Rich Electrode/Electrolyte Interface toward High-Voltage and High-Energy-Density Lithium Metal Solid Batteries. 2300494 ○
- 160 Cristae formation is a mechanical buckling event controlled by the inner membrane lipidome. ○
- 159 Influence of the Lennard-Jones Combination Rules on the Simulated Properties of Organic Liquids at Optimal Force-Field Parametrization. **2023**, 19, 2048-2063 ○
- 158 Molecular Basis of RNA-Driven ATP Hydrolysis in DEXH-Box Helicases. **2023**, 145, 6691-6701 ○
- 157 Aggregation of chlorophylls on plant thylakoid membranes using coarse-grained simulations. ○
- 156 Conformational Behavior of SARS-Cov-2 Spike Protein Variants: Evolutionary Jumps in Sequence Reverberate in Structural Dynamic Differences. **2023**, 19, 2120-2134 ○
- 155 Decoding the Dual Recognition Mechanism of Glucocorticoid Receptor for DNA and RNA: Sequence vs. Shape. ○
- 154 Diclofenac and other non-steroidal anti-inflammatory drugs (NSAIDs) are competitive antagonists of the human P2X₃ receptor. 14, ○
- 153 In Silico Prediction of Stratum Corneum Partition Coefficients via COSMOmic and Molecular Dynamics Simulations. **2023**, 127, 2719-2728 ○
- 152 The neglected autoxidation pathways for the formation of highly oxygenated organic molecules (HOMs) and the nucleation of the HOMs generated by limonene. **2023**, 304, 119727 ○
- 151 Intrinsic relationship between viscosity, viscosity index, and molecular structure of isoalkanes. **2023**, 29, ○
- 150 Molecular dynamics simulation of polymorphic transformation between β -CL-20 and β -CL-20 by short range order and orientational order parameter. **2023**, 610, 127179 ○
- 149 Insights into selectivity of some oxygen containing gases by the CHCl_3 anion from molecular simulation. **2023**, 49, 758-768 ○
- 148 Mechanical properties and structure of injection molded poly(hydroxybutyrate-co-hydroxyvalerate)/poly(butylene adipate-co-terephthalate) (PHBV / PBAT) blends. ○

- 147 Ultraviolet irradiation confers titanium oxide oleophilicity. **2023**, 58, 5258-5268 ○
- 146 Molecular basis of polyglutamine-modulated ELF3 phase change in Arabidopsis temperature response. ○
- 145 Effects of neutron irradiation on densities and elastic properties of aggregate-forming minerals in concrete. **2023**, ○
- 144 Sappanin-type homoisoflavonoids from *Scilla nervosa* inhibits acetylcholinesterase enzyme: a combined in silico and in vitro approach. 1-12 ○
- 143 Solution Structures of Europium Terpyridyl Complexes with Nitrate and Triflate Counterions in Acetonitrile. **2023**, 62, 5207-5218 ○
- 142 Immunoinformatics aided approach for predicting potent cytotoxic T cell epitopes of respiratory syncytial virus. 1-13 ○
- 141 Adsorption Studies at the Graphene Oxide/Liquid Interface: A Molecular Dynamics Study. **2023**, 127, 5920-5930 ○
- 140 SchNetPack 2.0: A neural network toolbox for atomistic machine learning. **2023**, 158, 144801 ○
- 139 Insights Into Targeting the SARS-CoV-2: Design, Synthesis, In Silico Studies and Antiviral Evaluation of New Dimethylxanthine Derivatives. ○
- 138 The Unusual Architecture of RNA-Dependent RNA Polymerase (RdRp) Catalytic Chamber Provides a Potential Strategy for Combination Therapy against COVID-19. **2023**, 28, 2806 1
- 137 Mitigation of membrane morphology defects explain stability and orientational specificity of CLC dimers. ○
- 136 Nucleolar Essential Protein 1 (Nep1): Elucidation of Enzymatic Catalysis Mechanism by Combined Molecular Dynamics Simulation and Quantum Chemical Calculations. ○
- 135 Structural basis of mitochondrial membrane bending by the $\text{F}_1\text{F}_0\text{F}_2$ supercomplex. **2023**, 615, 934-938 ○
- 134 Bacterial Lectin FimH and Its Aggregation Hot-Spots: An Alternative Strategy against Uropathogenic *Escherichia coli*. **2023**, 15, 1018 ○
- 133 Computational studies of potential antiviral compounds from some selected Nigerian medicinal plants against SARS-CoV-2 proteins. **2023**, 38, 101230 ○
- 132 Phase transition of three-dimensional finite-sized charged dust clusters in a plasma environment. **2023**, 107, ○
- 131 Characterization of the mechanism of bile salt hydrolase substrate specificity by experimental and computational analyses. **2023**, ○
- 130 Diphenyl Diselenide and SARS-CoV-2: in silico Exploration of the Mechanisms of Inhibition of Main Protease (Mpro) and Papain-like Protease (PLpro). **2023**, 63, 2226-2239 ○

- 129 Intermolecular And Dynamic Investigation of The Mechanism of Action of Reldesemtiv on Fast Skeletal Muscle Troponin Complex Toward the Treatment of Impaired Muscle Function. ○
- 128 FTD-tau S320F mutation stabilizes local structure and allosterically promotes amyloid motif-dependent aggregation. **2023**, 14, ○
- 127 Impact of Drug Repurposing on SARS-Cov-2 Main Protease. **2022**, 96, 3311-3330 ○
- 126 A Multi-Enzyme Cascade for Efficient Production of Pyrrolidone from L- Glutamate. ○
- 125 Research progress and prospect of silica-based polymer nanofluids in enhanced oil recovery. **2023**, 12, ○
- 124 Finite-Temperature Mechanical Properties of Organic Molecular Crystals from Classical Molecular Simulation. **2023**, 23, 2155-2168 ○
- 123 Misorientation and Temperature Dependence of Small Angle Twist Grain Boundaries in Silicon: Atomistic Simulation of Directional Growth. **2023**, 23, 2893-2904 ○
- 122 An Arg/Ala-rich helix in the N-terminal region of *M. tuberculosis* FtsQ is a potential membrane anchor of the Z-ring. **2023**, 6, ○
- 121 Two gates mediate NMDA receptor activity and are under subunit-specific regulation. **2023**, 14, ○
- 120 Structure of interpolymer complex between poly(acrylic acid) and poly(ethylene oxide) in aqueous salt solution: a molecular dynamics simulation study. **2023**, 49, 743-757 ○
- 119 An extended Tudor domain within Vreteno interconnects Gtsf1L and Ago3 for piRNA biogenesis in *Bombyx mori*. ○
- 118 Electric-field induced entropic effects in liquid water. ○
- 117 Conformational dynamics of A30G β -synuclein that causes familial Parkinson disease. 1-13 ○
- 116 Exploring and targeting potential druggable antimicrobial resistance targets ArgS, SecY and MurA in *Staphylococcus sciuri* with TCM inhibitors through subtractive genomics strategy. ○
- 115 Molecular modeling and simulations of some antiviral drugs, benzyloquinoline alkaloid, and coumarin molecules to investigate the effects on Mpro main viral protease inhibition. **2023**, 34, 101459 ○
- 114 Hydroperoxidation of Docosahexaenoic Acid by Human ALOX12 and pigALOX15-mini-LOX. **2023**, 24, 6064 ○
- 113 Optimizing the binding of OGT and a peptidic substrate towards pseudo-substrate inhibitors via molecular dynamic simulations. ○
- 112 Calculations of the binding free energies of the Comprehensive <i>in vitro</i> Proarrhythmia Assay (CiPA) reference drugs to cardiac ion channels. **2023**, 20, n/a ○

- 111 Decarboxylation and Protonation Enigma in the H85Q Mutant of Cytochrome P450leT. **2023**, 127, 2927-2933 ○
- 110 Shifting the selectivity of pyrido[2,3-d]pyrimidin-7(8H)-one inhibitors towards the salt-inducible kinase (SIK) subfamily. ○
- 109 Molecular mechanisms of inorganic-phosphate release from the core and barbed end of actin filaments. ○
- 108 Structural mechanism of Fab domain dissociation as a measure of interface stability. **2023**, 37, 201-215 ○
- 107 Internal Normal Mode Analysis Applied to RNA Flexibility and Conformational Changes. ○
- 106 Calcium carbonate from chicken eggshells as filler in composite Nafion membrane for direct ethanol fuel cell: a molecular dynamics study. ○
- 105 Exploring biogenic chalcones as DprE1 inhibitors for antitubercular activity via in silico approach. **2023**, 29, ○
- 104 Parametric crystalline characterization of Anatase/Rutile polymorphic ceramic. **2023**, 129, ○
- 103 Effects of pH and NaCl on the Spatial Structure and Conformation of Myofibrillar Proteins and the Emulsion Gel System Insights from Computational Molecular Dynamics on Myosin of Golden Pompano. **2023**, 9, 270 ○
- 102 Identification of new oxospiro chromane quinoline-carboxylate antimalarials that arrest parasite growth at ring stage. 1-22 ○
- 101 Discrimination between cyclic nucleotides in a cyclic nucleotide-gated ion channel. **2023**, 30, 512-520 ○
- 100 Synthetic Curcumin Analogues Present Antiflavivirus Activity In Vitro with Potential Multiflavivirus Activity from a Thiazolyldrazone Moiety. **2023**, 3, 364-378 ○
- 99 Soft Matter under Pressure: Pushing Particle Field Molecular Dynamics to the Isobaric Ensemble. **2023**, 63, 2207-2217 ○
- 98 A theoretical survey to find potential natural compound for inhibition of binding the RBD domain to ACE2 receptor based on plant antivirals. 1-26 ○
- 97 Structures and Dynamics of DNA Mini-Dumbbells Are Force Field Dependent. ○
- 96 Investigation of the Entry Pathway and Molecular Nature of β Receptor Ligands. **2023**, 24, 6367 ○
- 95 Mechanistic Insights on Permeation of Water over Iron Cations in Nanoporous Silicon Oxide Films for Selective H₂ and O₂ Evolution. **2023**, 15, 17814-17824 ○
- 94 Unraveling the molecular mechanism of novel leukemia mutations on NTRK2 (A203T & R458G) and NTRK3 (E176D & L449F) genes using molecular dynamics simulations approach. 12, 345 ○

- 93 Deep Boosted Molecular Dynamics (DBMD): Accelerating molecular simulations with Gaussian boost potentials generated using probabilistic Bayesian deep neural network. ○
- 92 Converging PMF calculations of antibiotic permeation across an outer membrane porin with sub-kilocalorie per mole accuracy. ○
- 91 High-entropy alloy nanopatterns by prescribed metallization of DNA origami templates. **2023**, 14, ○
- 90 Energetics and kinetics of membrane permeation of photoresists for bioprinting. ○
- 89 Identification of potential inhibitor against CTX-M-3 and CTX-M-15 proteins: an in silico and in vitro study. 1-17 ○
- 88 Effect of temperature on hepatitis a virus and exploration of binding mode mechanism of phytochemicals from *tinospora cordifolia*: an insight into molecular docking, MM/GBSA, and molecular dynamics simulation study. 1-17 ○
- 87 Theoretical design of a new hydrogen storage based on the decorated phosphorene nanosheet by alkali metals. **2023**, 178, 111354 ○
- 86 Formation of parallel and perpendicular ripples on solid amorphous surfaces by ion beam-driven atomic flow on and under the surface. **2023**, 7, ○
- 85 AmberMDrun: A Scripting Tool for Running Amber MD in an Easy Way. **2023**, 13, 635 ○
- 84 Autocatalytic effect boosts the production of medium-chain hydrocarbons by fatty acid photodecarboxylase. **2023**, 9, ○
- 83 Molecular insights into the stereospecificity of arginine in RNA tetraloop folding. ○
- 82 Exploring the Macroscopic Properties of Humic Substances Using Modeling and Molecular Simulations. **2023**, 13, 1044 ○
- 81 The targeted next-generation sequence revealed SMAD4, AKT1, and TP53 mutations from circulating cell-free DNA of breast cancer and its effect on protein structure: A computational approach. 1-14 ○
- 80 Identification of EGFR inhibitors as potential agents for cancer therapy: pharmacophore-based modeling, molecular docking, and molecular dynamics investigations. **2023**, 29, ○
- 79 Effect of Force Field Resolution on Membrane Mechanical Response and Mechanoporation Damage under Deformation Simulations. ○
- 78 1-Benzyl-5-bromo-3-hydrazonoindolin-2-ones as Novel Anticancer Agents: Synthesis, Biological Evaluation and Molecular Modeling Insights. **2023**, 28, 3203 ○
- 77 Charge-optimized many-body interaction potential for AlN revisited to explore plasma-surface interactions. **2023**, 13, ○
- 76 Designing a multi-epitope vaccine against chickenpox virus using in silico approach. ○

- 75 An Affordable Topography-Based Protocol for Assigning a Residue's Character on a Hydrophathy (PARCH) Scale.
- 74 The Role of C2 Domains in Two Different Phosphatases: PTEN and SHIP2. **2023**, 13, 408
- 73 Novel Strategy of Machine Learning for Predicting Henry's Law Constants of CO₂ in Ionic Liquids. **2023**, 11, 6090-6099
- 72 Identification of the precursor cluster in thermolysin crystallization solution by molecular dynamics methods. **2023**, 33, 225-227
- 71 Deep Eutectic Solvents for the Enzymatic Synthesis of Sugar Esters: A Generalizable Strategy?. **2023**, 11, 5926-5936
- 70 Carbon nanotube recognition by human Siglec-14 provokes inflammation.
- 69 Sodium is a negative allosteric regulator of the ghrelin receptor. **2023**, 42, 112320
- 68 Influence of hydrostatic pressure during gelation on physicochemical properties of cellulose hydrogels prepared from ionic liquid/DMSO solution. **2023**, 381, 121810
- 67 Novel hits for autosomal dominated polycystic kidney disease (ADPKD) targeting derived by in silico screening on ZINC-15 natural product database. 1-18
- 66 Rehydration Post-orientation: Investigating Field-Induced Structural Changes via Computational Rehydration.
- 65 Conformational cycle of human polyamine transporter ATP13A2. **2023**, 14,
- 64 Molecular origin of the two-step mechanism of gellan aggregation. **2023**, 9,
- 63 In silico investigation of the structural stability as the origin of the pathogenicity of β -synuclein protofibrils. 1-13
- 62 Ceramide-1-phosphate transfer protein enhances lipid transport by disrupting hydrophobic lipid-membrane contacts. **2023**, 19, e1010992
- 61 Ion Conduction Mechanisms in Potassium Channels Revealed by Permeation Cycles.
- 60 Computational and structural insights into the pre- and post-hydrolysis states of bovine multidrug resistance-associated protein 1.
- 59 Molecular Rotations, Multiscale Order, Hyperuniformity, and Signatures of Metastability during the Compression/Decompression Cycles of Amorphous Ices.
- 58 Does non-thermal plasma modify biopolymers in solution? A chemical and mechanistic study for alginate.

- 57 Magnetic Polaron States in Photoluminescent Carbon Dots Enable Hydrogen Peroxide Photoproduction. ○
- 56 Binding to the Conserved and Stably Folded Guide RNA Pseudoknot Induces Cas12a Conformational Changes During Ribonucleoprotein Assembly. **2023**, 104700 ○
- 55 Crystal morphology prediction of CL-20 and 1,4-DNI co-crystal at different temperatures. **2023**, 29, ○
- 54 Binding kinetics study of SARS-CoV-2 main protease and potential inhibitors via molecular dynamics simulations. ○
- 53 Molecular Dynamics Simulation on Tensile Behavior of Cellulose at Different Strain Rates. **2023**, 2023, 1-10 ○
- 52 Exploitation of Dimeric Cyclic Cysteine as Helix Inducer in Ultra-Short Peptides for Cu(II)-Catalysed Asymmetric Michael Addition on Chalcones. ○
- 51 Activation and substrate specificity of the human P4-ATPase ATP8B1. ○
- 50 Equivalence of Charge Imbalance and External Electric Fields during Free Energy Calculations of Membrane Electroporation. ○
- 49 Uncovering the Mechanism of the Proton-Coupled Fluoride Transport in the CLCF Antiporter. ○
- 48 Identification of a novel drug molecule for Neurodegenerative Disease from marine algae through In-silico analysis. ○
- 47 Unpolarized laser method for infrared spectrum calculation of amide I C O bonds in proteins using molecular dynamics simulation. **2023**, 159, 106902 ○
- 46 Coarse-Grained Modeling of Polystyrene-Modified CNTs and Their Interactions with Lipid Bilayers. **2023**, ○
- 45 The Interaction Mechanism of Intramuscular Gene Delivery Materials with Cell Membranes. **2023**, 14, 219 ○
- 44 Dielectric Saturation in Water from a Long-Range Machine Learning Model. ○
- 43 Reactive molecular dynamics simulations on interaction mechanisms of cold atmospheric plasmas and peptides. **2023**, 30, 043512 ○
- 42 Synthesis, antiviral activity, and computational study of β -xylofuranosyl nucleoside phosphonates. **2023**, 115379 ○
- 41 Computer-aided de novo design and optimization of novel potential inhibitors of HIV-1 Nef protein. **2023**, 104, 107871 ○
- 40 Structural Dynamics of the Precatalytic State of Human Cytochrome c upon T28C, G34C, and A50C Mutations: A Molecular Dynamics Simulation Perspective. ○

- 39 Profiling the disintegration of BRPs released by massive wasp stings using serratiopeptidase: An in-silico insight. **2023**, 159, 106951 ○
- 38 Influence of Ethanol Parametrization on Diffusion Coefficients Using OPLS-AA Force Field. **2023**, 24, 7316 ○
- 37 Intermediate-aided allosteric mechanism for β -glucosidase by Xanthene-11v as an inhibitor using residue interaction network analysis. **2023**, 108495 ○
- 36 Hofmeister Effects Influence Bulk Nanostructure in a Protic Ionic Liquid. **2023**, ○
- 35 Theoretical Analysis of the Role of Water in Ligand Binding to Cucurbit[n]uril of Different Sizes. ○
- 34 Structural and Dynamic Characterization of Ionic Liquid Electrolyte Solutions for Application in Li-Ion Batteries: A Molecular Dynamics Approach. **2023**, 9, 234 ○
- 33 Molecular Dynamics Study on the Aggregation Behavior of Triton X Micelles with Different PEO Chain Lengths in Aqueous Solution. **2023**, 28, 3557 ○
- 32 Atomic level mechanisms of graphene healing by methane-based plasma radicals. **2023**, 100506 ○
- 31 How to obtain high monolayer content in liquid phase exfoliation of graphene: A molecular dynamic simulation. **2023**, 121873 ○
- 30 The effect of grain boundary on irradiation resistance of CoCrCuFeNi high entropy alloy. **2023**, 225, 112185 ○
- 29 Biophysical and in-silico studies on the structure-function relationship of Brugia malayi protein disulfide isomerase. 1-11 ○
- 28 Molecular-level fabrication strategies for the POSS cross-linked polybenzoxazines. ○
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- 3 Catalytic Reaction Mechanism of Glyoxalase II: A Quantum Mechanics/Molecular Mechanics Study. ○
- 2 Dissociation Rate Calculation via Constant-Force Steered Molecular Dynamics Simulation. ○
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