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- 2199 Interfacial Concentration Effect Facilitates Heterogeneous Nucleation from Solution.
- 2198 Classical Magnetic Dipole Moments for the Simulation of Vibrational Circular Dichroism by ab Initio Molecular Dynamics.
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- 2196 Repair Rate of Clustered Abasic DNA Lesions by Human Endonuclease: Molecular Bases of Sequence Specificity.
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2179 Large-Scale Biomolecular Conformational Transitions Explored by a Combined Elastic Network Model and Enhanced Sampling Molecular Dynamics.

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- 2176 Quantitative Comparison of Atomistic Simulations with Experiment for a Cross-Linked Epoxy: A Specific Volume Cooling Rate Analysis.
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- 2171 Perfect and Controllable Nesting in Minimally Twisted Bilayer Graphene.
- 2170 Transforming Complexity to Simplicity: Protein-Like Nanotransformer for Improving Tumor Drug Delivery Programmatically.
- 2169 An Active Site Opening Mechanism in a (Pyridylamide)hafnium(IV) Ion Pair Catalyst: An Associative Mechanism.
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- 2047 .
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- 2041 Understanding Complex Mechanisms of Enzyme Reactivity: The Case of Limonene-1,2-Epoxyde Hydrolases.
- 2040 Enhancing the Steroid Sulfatase Activity of the Arylsulfatase from *Pseudomonas aeruginosa*.
- 2039 Equatorial Active Site Compaction and Electrostatic Reorganization in Catechol O-methyltransferase.
- 2038 Dissecting the Stereocontrolled Conversion of Short-Lived Sulfenic Acid by Lachrymatory Factor Synthase.
- 2037 Semirational Design of Fluoroacetate Dehalogenase RPA1163 for Kinetic Resolution of α -Fluorocarboxylic Acids on a Gram Scale.
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- 2035 Elucidating the Catalytic Reaction Mechanism of Orotate Phosphoribosyltransferase by Means of X-ray Crystallography and Computational Simulations.
- 2034 Single Site Discrimination of Cytosine, 5-Methylcytosine and 5-Hydroxymethylcytosine in Target DNA Using Anthracene-Tagged Fluorescent Probes.
- 2033 Sequential Inactivation of Gliotoxin by the S-Methyltransferase TmtA.

- 2032 Discovery and Structural Characterization of ATP-Site Ligands for the Wild-Type and V617F Mutant JAK2 Pseudokinase Domain.
- 2031 Insights into the Stereospecificity in Papain-Mediated Chemoenzymatic Polymerization from Quantum Mechanics/Molecular Mechanics Simulations.
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- 2029 Cis-Selective Metathesis to Enhance the Living Character of Ring-Opening Polymerization: An Approach to Sequenced Copolymers.
- 2028 Discovery of Novel Nonpeptidic PAR2 Ligands.
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- 2017 Effect of HBonding on Order Amplification in the Growth of a Supramolecular Polymer in Water.
- 2016 Inhibition of Huntingtin Exon1 Aggregation by the Molecular Tweezer CLR01.
- 2015 Computational Design of Experiment Unveils the Conformational Reaction Coordinate of GH125 Mannosidases.

- 2014 Organelle-Specific Triggered Release of Immunostimulatory Oligonucleotides from Intrinsically Coordinated DNAMetalOrganic Frameworks with Soluble Exoskeleton.
- 2013 The Use of Fluoroproline in MUC1 Antigen Enables Efficient Detection of Antibodies in Patients with Prostate Cancer.
- 2012 Fundamental Insights into Proton-Coupled Electron Transfer in Soybean Lipoxygenase from Quantum Mechanical/Molecular Mechanical Free Energy Simulations.
- 2011 The Role of the Active Site Flap in Streptavidin/Biotin Complex Formation.
- 2010 A Block Supramolecular Polymer and Its Kinetically Enhanced Stability.
- 2009 Molecular Recognition of Hydrophilic Molecules in Water by Combining the Hydrophobic Effect with Hydrogen Bonding.
- 2008 Asymmetric Synthesis of Griffipavixanthone Employing a Chiral Phosphoric Acid-Catalyzed Cycloaddition.
- 2007 Structure-Based Design of Potent Tumor-Associated Antigens: Modulation of Peptide Presentation by Single-Atom O/S or O/Se Substitutions at the Glycosidic Linkage.
- 2006 Anion Recognition in Water by Charge-Neutral Halogen and Chalcogen Bonding Foldamer Receptors.
- 2005 Doped but Stable: Spirobisacridine Hole Transporting Materials for Hysteresis-Free and Stable Perovskite Solar Cells.
- 2004 Molecular Basis for Spirocycle Formation in the Paraherquamide Biosynthetic Pathway.
- 2003 Counterion-Mediated Crossing of the Cyanine Limit in Crystals and Fluid Solution: Bond Length Alternation and Spectral Broadening Unveiled by Quantum Chemistry.
- 2002 .
- 2001 Efficient and Selective Electrochemically Driven Enzyme-Catalyzed Reduction of Carbon Dioxide to Formate using Formate Dehydrogenase and an Artificial Cofactor.
- 2000 Adenosine Monophosphate Binding Stabilizes the KTN Domain of the *Shewanella denitrificans* Kef Potassium Efflux System.
- 1999 Multiscale Simulations of Clavulanate Inhibition Identify the Reactive Complex in Class A Lactamases and Predict the Efficiency of Inhibition.
- 1998 Bound Compound Interfacial Water, and Phenyl Ring Rotation Dynamics of a Compound in the DNA Minor Groove.
- 1997 Modulation of the *Gloeobacter violaceus* Ion Channel by Fentanyl: A Molecular Dynamics Study.

- 1996 Anticancer Activity of Dendriplexes against Advanced Prostate Cancer from Protumoral Peptides and Cationic Carbosilane Dendrimers.
- 1995 Chlorinated Polyfluoroalkylether Sulfonates Exhibit Similar Binding Potency and Activity to Thyroid Hormone Transport Proteins and Nuclear Receptors as Perfluorooctanesulfonate.
- 1994 Use of a Compact Tripodal Tris(bipyridine) Ligand to Stabilize a Single-Metal-Centered Chirality: Stereoselective Coordination of Iron(II) and Ruthenium(II) on a Semirigid Hexapeptide Macrocycle.
- 1993 Enabling Mitochondrial Uptake of Lipophilic Dications Using Methylated Triphenylphosphonium Moieties.
- 1992 SQM/COSMO Scoring Function at the DFTB3-D3H4 Level: Unique Identification of Native ProteinLigand Poses.
- 1991 QM/MM Studies of Dph5 A Promiscuous Methyltransferase in the Eukaryotic Biosynthetic Pathway of Diphthamide.
- 1990 PyLAT: Python LAMMPS Analysis Tools.
- 1989 Exploring Gatekeeper Mutations in EGFR through Computer Simulations.
- 1988 Evaluation of In Silico Multifeature Libraries for Providing Evidence for the Presence of Small Molecules in Synthetic Blinded Samples.
- 1987 Overcoming the Heuristic Nature of kMeans Clustering: Identification and Characterization of Binding Modes from Simulations of Molecular Recognition Complexes.
- 1986 ProtoCaller: Robust Automation of Binding Free Energy Calculations.
- 1985 Permeability Coefficients of Lipophilic Compounds Estimated by Computer Simulations.
- 1984 Ensemble- and Rigidity Theory-Based Perturbation Approach To Analyze Dynamic Allostery.
- 1983 Relative Principal Components Analysis: Application to Analyzing Biomolecular Conformational Changes.
- 1982 Discovery of an Orally Selective Inhibitor of Signal Transducer and Activator of Transcription 3 Using Advanced Multiple Ligand Simultaneous Docking.
- 1981 Inhibitors to Overcome Secondary Mutations in the Stem Cell Factor Receptor KIT.
- 1980 Paradoxically Most Flexible Ligand Binds Most Entropy-Favored: Intriguing Impact of Ligand Flexibility and Solvation on DrugKinase Binding.
- 1979 Positive Modulators of the NMethylaspartate Receptor: StructureActivity Relationship Study of Steroidal 3Hemiesters.

- 1978 Succinimide-Based Conjugates Improve IsoDGR Cyclopeptide Affinity to v3 without Promoting Integrin Allosteric Activation.
- 1977 Suppression of Tumor Growth and Metastases by Targeted Intervention in Urokinase Activity with Cyclic Peptides.
- 1976 Targeting DNA Repair in Tumor Cells via Inhibition of ERCC1XPF.
- 1975 From Inhibition to Degradation: Targeting the Antiapoptotic Protein Myeloid Cell Leukemia 1 (MCL1).
- 1974 Molecular modeling of nucleic acid structure: setup and analysis. **2001**, Chapter 7, Unit 7.10 4
- 1973 Halogen bonds in biological molecules. **2004**, 101, 16789-94 1324
- 1972 The structure of chondroitin B lyase complexed with glycosaminoglycan oligosaccharides unravels a calcium-dependent catalytic machinery. **2004**, 279, 32882-96 76
- 1971 Investigation of the effects of copper ions on protein aggregation using a model system. **2004**, 61, 982-91 27
- 1970 Receptor rigidity and ligand mobility in trypsin-ligand complexes. **2005**, 58, 407-17 21
- 1969 Threshold dissociation and molecular modeling of transition metal complexes of flavonoids. **2005**, 16, 139-51 45
- 1968 Molecular docking and 3D-QSAR studies of Yersinia protein tyrosine phosphatase YopH inhibitors. **2005**, 13, 1101-9 28
- 1967 Connecting traditional QSAR and molecular simulations of papain hydrolysis--importance of charge transfer. **2005**, 13, 3093-105 5
- 1966 Structural basis for the GSK-3beta binding affinity and selectivity against CDK-2 of 1-(4-aminofurazan-3yl)-5-dialkylaminomethyl-1H-[1,2,3] triazole-4-carboxylic acid derivatives. **2005**, 15, 5129-35 36
- 1965 Stability of a new class of unnatural hydrogen-bonded molecular duplexes: A computational study. **2005**, 410, 264-268 5
- 1964 Validation and use of the MM-PBSA approach for drug discovery. **2005**, 48, 4040-8 357
- 1963 Studies on binding free energies and the binding mode by docking and MM-PBSA in gp41-ligand complex. **2005**, 31, 1051-1056 6
- 1962 The Amber biomolecular simulation programs. *Journal of Computational Chemistry*, **2005**, 26, 1668-88 3.5 6155
- 1961 Exploring polymorphism: the case of benzene. **2005**, 44, 3769-73 121

1960	Vorhersage polymorpher Strukturen: der Fall Benzol. 2005 , 117, 3835-3839	18
1959	Characterization of flavonoids by aluminum complexation and collisionally activated dissociation. 2005 , 40, 350-63	40
1958	Binding site of activators of the cystic fibrosis transmembrane conductance regulator in the nucleotide binding domains. 2005 , 62, 446-60	99
1957	Scoring binding affinity of multiple ligands using implicit solvent and a single molecular dynamics trajectory: application to influenza neuraminidase. 2005 , 24, 147-56	29
1956	Modelling the interaction of catecholamines with the alpha 1A adrenoceptor towards a ligand-induced receptor structure. 2005 , 19, 357-67	2
1955	Role of hydrogen bonds in the fast dynamics of binary glasses of trehalose and glycerol: a molecular dynamics simulation study. 2005 , 122, 114505	51
1954	Identification of a specific inhibitor of the dishevelled PDZ domain. 2005 , 44, 15495-503	172
1953	The merits of the frozen-density embedding scheme to model solvatochromic shifts. 2005 , 122, 094115	187
1952	Probing the beta2 adrenoceptor binding site with catechol reveals differences in binding and activation by agonists and partial agonists. 2005 , 280, 22165-71	216
1951	Ab initio quantum chemistry: methodology and applications. 2005 , 102, 6648-53	217
1950	Laser-initiated shuttling of a water molecule between H-bonding sites. 2005 , 307, 1443-6	90
1949	Identification of a 14mer RNA that recognizes and binds flavin mononucleotide with high affinity. 2005 , 33, 6992-9	25
1948	C-H...O hydrogen bonding in 4-phenyl-benzaldehyde: a comprehensive crystallographic, spectroscopic and computational study. 2005 , 7, 3027-34	18
1947	Bioinformatics in drug development and assessment. 2005 , 37, 279-310	33
1946	Structure and dynamics of the hydrogen-bond network around (R,R)-pterocarpan with biological activity in aqueous solution. 2005 , 109, 16918-25	10
1945	Coupling between lysozyme and glycerol dynamics: microscopic insights from molecular-dynamics simulations. 2005 , 122, 244910	36
1944	Experimental and theoretical study of the interaction of single-stranded DNA homopolymers and a monomethine cyanine dye: nature of specific binding. 2005 , 4, 798-802	19
1943	Structure of hydrated Na-Nafion polymer membranes. 2005 , 109, 24244-53	62

1942	Crystal structure of Methanobacterium thermoautotrophicum phosphoribosyl-AMP cyclohydrolase Hisl. 2005 , 44, 10071-80	23
1941	Ultrasonic velocities, densities, viscosities, electrical conductivities, Raman spectra, and molecular dynamics simulations of aqueous solutions of Mg(OAc) ₂ and Mg(NO ₃) ₂ : Hofmeister effects and ion pair formation. 2005 , 109, 24108-20	56
1940	Computational studies of the farnesyltransferase ternary complex part I: substrate binding. 2005 , 44, 16513-23	27
1939	Interior and interfacial aqueous solvation of benzene dicarboxylate dianions and their methylated analogues: A combined molecular dynamics and photoelectron spectroscopy study. 2005 , 109, 5042-9	20
1938	Modeling the similarity and divergence of dopamine D ₂ -like receptors and identification of validated ligand-receptor complexes. 2005 , 48, 694-709	41
1937	An explicit quantum chemical method for modeling large solvation shells applied to aminocoumarin C151. 2005 , 109, 7805-14	120
1936	Potential energy functions for atomic-level simulations of water and organic and biomolecular systems. 2005 , 102, 6665-70	770
1935	Mutagenic properties of 5-halogenuracils: correlated quantum chemical ab initio study. 2005 , 44, 1701-7	30
1934	Variational electrostatic projection (VEP) methods for efficient modeling of the macromolecular electrostatic and solvation environment in activated dynamics simulations. 2005 , 109, 536-56	25
1933	An all atom energy based computational protocol for predicting binding affinities of protein-ligand complexes. 2005 , 579, 6659-66	61
1932	Ligand-induced conformational change in the alpha7 nicotinic receptor ligand binding domain. 2005 , 88, 2564-76	62
1931	Protein/ligand binding free energies calculated with quantum mechanics/molecular mechanics. 2005 , 109, 10474-83	92
1930	Molecular Modeling. 2005 ,	
1929	Direct calculation of the binding free energies of FKBP ligands. 2005 , 123, 084108	165
1928	Can octupolar molecules be poled by an external electric field?. 2005 , 109, 16730-5	19
1927	Development and validation of empirical force field parameters for netropsin. 2005 , 45, 1546-52	27
1926	Simulation of Actuation by Polymeric Polyelectrolyte Helicenes. 2006 , 2, 1112-8	11
1925	High-throughput calculation of protein-ligand binding affinities: modification and adaptation of the MM-PBSA protocol to enterprise grid computing. 2006 , 46, 999-1005	79

1924	Trisubstituted acridines as G-quadruplex telomere targeting agents. Effects of extensions of the 3,6- and 9-side chains on quadruplex binding, telomerase activity, and cell proliferation. 2006 , 49, 582-99	174
1923	Adsorption of polycyclic aromatic hydrocarbons at the air-water interface: molecular dynamics simulations and experimental atmospheric observations. 2006 , 8, 4461-7	62
1922	Molecular dynamics simulations applied to electric field induced second harmonic generation in dipolar chromophore solutions. 2006 , 110, 8971-7	17
1921	Anthramycin-DNA binding explored by molecular simulations. 2006 , 110, 24687-95	23
1920	Conformational analysis of 2-substituted cyclobutane-alpha-amino acid derivatives. A synergistic experimental and computational study. 2006 , 71, 1869-78	19
1919	Specific interaction of citrate with bis(fluorophoric) bibrachial lariat aza-crown in comparison with the other components of the Krebs cycle. 2006 , 3824-6	29
1918	Thermochromatism and structural evolution of metastable polydiacetylenic crystals. 2006 , 110, 7221-5	65
1917	Molecular dynamics: survey of methods for simulating the activity of proteins. 2006 , 106, 1589-615	818
1916	A multistep approach to structure-based drug design: studying ligand binding at the human neutrophil elastase. 2006 , 49, 1837-44	73
1915	Parallelized-over-parts computation of absolute binding free energy with docking and molecular dynamics. 2006 , 125, 084901	81
1914	Atomic Charge Parameters for the Finite Difference Poisson-Boltzmann Method Using Electronegativity Neutralization. 2006 , 2, 1152-67	15
1913	Phenol red interacts with the protofibril-like oligomers of an amyloidogenic hexapeptide NFGAIL through both hydrophobic and aromatic contacts. 2006 , 91, 3664-72	55
1912	Absolute binding free energy calculations using molecular dynamics simulations with restraining potentials. 2006 , 91, 2798-814	284
1911	Subtype selectivity and flexibility of ionotropic glutamate receptors upon antagonist ligand binding. 2006 , 4, 1058-70	20
1910	Protein-ligand binding affinity predictions by implicit solvent simulations: a tool for lead optimization?. 2006 , 49, 7427-39	85
1909	Molecular dynamics studies of the size, shape, and internal structure of 0% and 90% acetylated fifth-generation polyamidoamine dendrimers in water and methanol. 2006 , 110, 4014-9	79
1908	Aqueous ionic and complementary zwitterionic soluble surfactants: molecular dynamics simulations and sum frequency generation spectroscopy of the surfaces. 2006 , 22, 2498-505	7
1907	Recognition of dicarboxylate anions by a ditopic hexaazamacrocycle containing bis-p-xylyl spacers. 2006 , 30, 247	30

1906	Discovery of a novel family of SARS-CoV protease inhibitors by virtual screening and 3D-QSAR studies. 2006 , 49, 3485-95	55
1905	Flexible 5-guanidino-4-nitroimidazole DNA lesions: structures and thermodynamics. 2006 , 45, 6644-55	12
1904	OH-stretching red shifts in bulky hydrogen-bonded alcohols: jet spectroscopy and modeling. 2006 , 110, 9839-48	52
1903	Controlling the shape and flexibility of arylamides: a combined ab initio, ab initio molecular dynamics, and classical molecular dynamics study. 2006 , 110, 3517-26	34
1902	Exploring the role of the active site cysteine in human muscle creatine kinase. 2006 , 45, 11464-72	17
1901	Computational study of antagonist/alpha1A adrenoceptor complexes--observations of conformational variations on the formation of ligand/receptor complexes. 2006 , 49, 501-10	15
1900	Investigation of the influence of spacer arm on the structural evolution of affinity ligands supported on agarose. 2006 , 110, 23564-77	29
1899	Molecular dynamics calculations of wild type vs. mutant protein C: relationship between binding affinity to endothelial cell protein C receptor and hereditary disease. 2006 , 24, 203-7	2
1898	HIV-1 protease flaps spontaneously open and reclose in molecular dynamics simulations. 2006 , 103, 915-20	298
1897	Chemical reactivity as a tool to study carcinogenicity: reaction between chloroethylene oxide and guanine. 2006 , 71, 4078-84	33
1896	Computational simulations of HIV-1 proteases--multi-drug resistance due to nonactive site mutation L90M. 2006 , 128, 7887-95	83
1895	Molecular dynamics simulations of hexahydro-1,3,5-trinitro-1,3,5-s-triazine (RDX) using a combined Sorescu-Rice-Thompson AMBER force field. 2006 , 110, 26185-8	30
1894	On the accuracy of force fields for predicting the physical properties of dimethylnitramine. 2006 , 110, 16082-8	6
1893	Effect of solvation on pinched cone-pinched cone interconversion of tetraethoxycalix[4]arene and tetraethoxythiacalix[4]arene. 2006 , 110, 861-7	10
1892	Linking ligand-induced alterations in androgen receptor structure to differential gene expression: a first step in the rational design of selective androgen receptor modulators. 2006 , 20, 1201-17	59
1891	Molecular dynamics investigation of bent-core molecules on a water surface. 2006 , 22, 9082-5	10
1890	Expect the unexpected or caveat for drug designers: multiple structure determinations using aldose reductase crystals treated under varying soaking and co-crystallisation conditions. 2006 , 363, 174-87	92
1889	RNA Three-Dimensional Structures, Computer Modeling of. 2006 ,	

1888	Determination of rotary diffusivity of poly(n-propyl isocyanate) by molecular dynamics. 2006 , 125, 244901	1
1887	The planar conformation of a strained proline ring: a QM/MM study. 2006 , 64, 700-10	13
1886	A computational analysis of the binding affinities of FKBP12 inhibitors using the MM-PB/SA method. 2006 , 64, 1058-68	66
1885	Molecular dynamics study of conformational changes in human serum albumin by binding of fatty acids. 2006 , 64, 730-9	59
1884	alpha-Conotoxin GI benzoylphenylalanine derivatives. (1)H-NMR structures and photoaffinity labeling of the Torpedo californica nicotinic acetylcholine receptor. 2006 , 273, 1373-88	13
1883	Coupling ligand structure to specific conformational switches in the beta2-adrenoceptor. 2006 , 2, 417-22	280
1882	Structure of the two most C-terminal RNA recognition motifs of PTB using segmental isotope labeling. 2006 , 25, 150-62	72
1881	Binding affinity prediction of non-peptide inhibitors of HIV-1 protease using COMBINE model introduced from peptide inhibitors. 2006 , 16, 6334-7	8
1880	Polarization effects and charge transfer in the KcsA potassium channel. 2006 , 124, 292-301	78
1879	Energy dispersive X-ray diffraction and molecular dynamics meet: The structure of liquid pyrrole. 2006 , 417, 200-205	32
1878	Furan and thiophene in liquid phase: An X-ray and molecular dynamics study. 2006 , 422, 256-261	14
1877	An evaluation of automated in silico ligand docking of amino acid ligands to Family C G-protein coupled receptors. 2006 , 14, 2032-9	16
1876	Modelling the interaction of several bisphosphonates with hydroxyapatite using the generalised AMBER force field. 2006 , 825, 134-142	28
1875	Theoretical framework for octopus rhodopsin crystallization. 2006 , 240, 260-9	2
1874	New dioxadiaz-, trioxadiaz- and hexaaza-macrocycles containing dibenzofuran units. 2006 , 62, 8550-8558	16
1873	Investigating interactions between HIV-1 gp41 and inhibitors by molecular dynamics simulation and MMBBSA/GBSA calculations. 2006 , 766, 77-82	20
1872	Effect of the structure of functionalized phosphoryl carriers on the membrane transport of proton-donor substrates. 2006 , 76, 1537-1544	7
1871	A novel, highly selective inhibitor of pestivirus replication that targets the viral RNA-dependent RNA polymerase. 2006 , 80, 149-60	72

1870	On the use of orientational restraints and symmetry corrections in alchemical free energy calculations. 2006 , 125, 084902		213
1869	AMBER force-field parameters for phosphorylated amino acids in different protonation states: phosphoserine, phosphothreonine, phosphotyrosine, and phosphohistidine. 2006 , 12, 281-9		256
1868	Possible dynamic anchor points in a benzoxazinone derivative-human oxytocin receptor system--a molecular docking and dynamics calculation. 2007 , 13, 1-10		5
1867	Extending the horizon: towards the efficient modeling of large biomolecular complexes in atomic detail. 2006 , 116, 194-205		47
1866	Development of novel brush-type chiral stationary phases based on terpenoid selectors: HPLC evaluation and theoretical investigation of enantioselective binding interactions. 2006 , 17, 3248-3264		18
1865	Synthesis and conformational preferences of unnatural tetrapeptides containing l-valine units. 2006 , 17, 3273-3281		7
1864	Automatic atom type and bond type perception in molecular mechanical calculations. 2006 , 25, 247-60		3191
1863	Stereoselectivity of 8-OH-DPAT toward the serotonin 5-HT1A receptor: biochemical and molecular modeling study. 2006 , 72, 498-511		16
1862	In quest of an empirical potential for protein structure prediction. 2006 , 16, 166-71		118
1861	Ab initio calculations of intramolecular parameters for a class of arylamide polymers. <i>Journal of Computational Chemistry</i> , 2006 , 27, 693-700	3-5	11
1860	Minimum sequence requirements for selective RNA-ligand binding: a molecular mechanics algorithm using molecular dynamics and free-energy techniques. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1631-40	3-5	6
1859	Coupled atomic charge selectivity for optimal ligand-charge distributions at protein binding sites. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1899-907	3-5	7
1858	Can MM-PBSA calculations predict the specificities of protein kinase inhibitors?. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1990-2007	3-5	49
1857	Aroyl-pyrrolyl hydroxyamides: influence of pyrrole C4-phenylacetyl substitution on histone deacetylase inhibition. 2006 , 1, 225-37		20
1856	Synthesis and biological evaluation of bicyclic nucleosides as inhibitors of M. tuberculosis thymidylate kinase. 2006 , 1, 1081-90		28
1855	Insight into the inhibition of human choline kinase: homology modeling and molecular dynamics simulations. 2006 , 1, 1216-28		14
1854	Molecular dynamics simulations of human tRNA Lys,3 UUU: the role of modified bases in mRNA recognition. 2006 , 34, 5361-8		33
1853	Recent Advances in Free Energy Calculations with a Combination of Molecular Mechanics and Continuum Models. 2006 , 2, 287-306		230

1852	Hierarchical Approach to Flow Calculations for Polymeric Liquid Crystals. 2006 , 22, 359-402	1
1851	Molecular dynamics simulations of melting of perfect crystalline hexahydro-1,3,5-trinitro-1,3,5-s-triazine. 2006 , 125, 084505	27
1850	Vibrational properties of inclusion complexes: the case of indomethacin-cyclodextrin. 2006 , 125, 44511	16
1849	PROXIMO--a new docking algorithm to model protein complexes using data from radical probe mass spectrometry (RP-MS). 2006 , 22, 1702-9	27
1848	Determination of binding site residues responsible for the subunit selectivity of novel marine-derived compounds on kainate receptors. 2006 , 69, 1849-60	28
1847	Coupling between lysozyme and trehalose dynamics: microscopic insights from molecular-dynamics simulations. 2006 , 124, 034901	31
1846	Crystal structure of TDP-fucosamine acetyltransferase (WecD) from Escherichia coli, an enzyme required for enterobacterial common antigen synthesis. 2006 , 188, 5606-17	25
1845	Structure of acyl carrier protein bound to FabI, the FASII enoyl reductase from Escherichia coli. 2006 , 281, 39285-39293	87
1844	Epac1 and cAMP-dependent protein kinase holoenzyme have similar cAMP affinity, but their cAMP domains have distinct structural features and cyclic nucleotide recognition. 2006 , 281, 21500-21511	113
1843	Energy analysis of chemistry for correct insertion by DNA polymerase beta. 2006 , 103, 13294-9	85
1842	Grid Assisted Ensemble Molecular Dynamics Simulations of HIV-1 Proteases Reveal Novel Conformations of the Inhibitor Saquinavir. 2006 , 150-161	2
1841	Critical role for polar residues in coupling leukotriene B4 binding to signal transduction in BLT1. 2007 , 282, 10005-10017	23
1840	Molecular dynamics simulations of local field factors. 2007 , 127, 014501	4
1839	Preference of small molecules for local minimum conformations when binding to proteins. 2007 , 2, e820	24
1838	ParDOCK: an all atom energy based Monte Carlo docking protocol for protein-ligand complexes. 2007 , 14, 632-46	103
1837	From drug target to leads--sketching a physicochemical pathway for lead molecule design in silico. 2007 , 13, 3454-70	52
1836	Consistent free energy landscapes and thermodynamic properties of small proteins based on a single all-atom force field employing an implicit solvation. 2007 , 127, 145104	26
1835	STD NMR spectroscopy and molecular modeling investigation of the binding of N-acetylneuraminic acid derivatives to rhesus rotavirus VP8* core. 2007 , 17, 68-81	55

1834	Atomistic simulations of hydrated nafion and temperature effects on hydronium ion mobility. 2007 , 111, 7234-44	189
1833	Prediction of the Binding Mode between the Small Peptide Inhibitor EBR28 with Integrase through Molecular Modeling Methods. 2007 ,	
1832	R.E.DD.B.: a database for RESP and ESP atomic charges, and force field libraries. 2008 , 36, D360-7	76
1831	Solvent reaction field potential inside an uncharged globular protein: a bridge between implicit and explicit solvent models?. 2007 , 127, 155101	33
1830	Identification and characterization of a new tubulin-binding tetrasubstituted brominated pyrrole. 2007 , 72, 132-40	31
1829	Characterization of a pseudomonad 2-nitrobenzoate nitroreductase and its catabolic pathway-associated 2-hydroxylaminobenzoate mutase and a chemoreceptor involved in 2-nitrobenzoate chemotaxis. 2007 , 189, 3502-14	56
1828	In search of CS ₂ (H ₂ O)(n=1-4) clusters. 2007 , 126, 154320	20
1827	Comparative studies of anthraquinone- and anthracene-tetraamines as blockers of N-methyl-D-aspartate receptors. 2007 , 320, 47-55	24
1826	Crystal structure of StaL, a glycopeptide antibiotic sulfotransferase from <i>Streptomyces toyocaensis</i> . 2007 , 282, 13073-86	16
1825	Microscopic Insights into the Dynamics of Protein/Solvent Mixtures. 89-125	
1824	Molecular dynamics simulations and their application to four-stranded DNA. 2007 , 43, 278-90	91
1823	Molecular dynamics study of ethanolamine as a pure liquid and in aqueous solution. 2007 , 111, 3695-703	71
1822	Models for binding cooperativities of inhibitors with transthyretin. 2007 , 466, 85-97	13
1821	FTIR studies of the redox partner interaction in cytochrome P450: the Pdx-P450cam couple. 2007 , 1770, 420-31	15
1820	Analogue inhibitors by modifying oseltamivir based on the crystal neuraminidase structure for treating drug-resistant H5N1 virus. 2007 , 362, 525-31	60
1819	A 40.7 kDa Rpp30/Rpp1 homologue is a protein subunit of <i>Dictyostelium discoideum</i> RNase P holoenzyme. 2007 , 89, 301-10	6
1818	Discovering potassium channel blockers from synthetic compound database by using structure-based virtual screening in conjunction with electrophysiological assay. 2007 , 50, 83-93	26
1817	Computational characterization of structural role of the non-active site mutation M36I of human immunodeficiency virus type 1 protease. 2007 , 370, 598-607	48

1816	Predicting absolute ligand binding free energies to a simple model site. 2007 , 371, 1118-34	234
1815	Dual binding modes of Congo red to amyloid protofibril surface observed in molecular dynamics simulations. 2007 , 129, 1225-32	141
1814	Comparison of charge models for fixed-charge force fields: small-molecule hydration free energies in explicit solvent. 2007 , 111, 2242-54	232
1813	Efficient estimators for quantum instanton evaluation of the kinetic isotope effects: application to the intramolecular hydrogen transfer in pentadiene. 2007 , 127, 114309	56
1812	Simulated interactions between angiotensin-converting enzyme and substrate gonadotropin-releasing hormone: novel insights into domain selectivity. 2007 , 46, 8753-65	22
1811	Ligand-Based Approaches: Core Molecular Modeling. 2007 , 87-118	7
1810	Conformation and dynamics of arylthiol self-assembled monolayers on Au(111). 2007 , 23, 12208-16	15
1809	Conformational analysis of L-prolines in water. 2007 , 111, 14034-42	48
1808	Improving Docking Accuracy through Molecular Mechanics Generalized Born Optimization and Scoring. 2007 , 3, 1106-19	43
1807	General Transition-State Force Field for Cytochrome P450 Hydroxylation. 2007 , 3, 1765-73	49
1806	Evaluation of the binding ability of a novel dioxatetraazamacrocyclic receptor that contains two phenanthroline units: selective uptake of carboxylate anions. 2007 , 72, 4023-34	24
1805	Structure and absolute stereochemistry of syphonoside, a unique macrocyclic glycoterpenoid from marine organisms. 2007 , 72, 5625-30	30
1804	Parametrization and Validation of Intramolecular Force Fields Derived from DFT Calculations. 2007 , 3, 1803-17	75
1803	Structures of the di2dIII1 complex of proton-translocating transhydrogenase with bound, inactive analogues of NADH and NADPH reveal active site geometries. 2007 , 46, 3304-18	12
1802	Ion pairing as a possible clue for discriminating between sodium and potassium in biological and other complex environments. 2007 , 111, 14077-9	72
1801	A Distributed Computing Method for Crystal Structure Prediction of Flexible Molecules: An Application to N-(2-Dimethyl-4,5-dinitrophenyl) Acetamide. 2007 , 3, 201-9	15
1800	Entropy-driven population distributions in a prototypical molecule with two flexible side chains: O-(2-acetamidoethyl)-N-acetyltyramine. 2007 , 127, 234315	39
1799	A bibracchial lariat aza-crown ether as an abiotic catalyst of malonic acid enolization. 2007 , 31, 2065	

1798	Structure and Raman spectrum of clavulanic acid in aqueous solution. 2007 , 111, 2621-30	10
1797	Molecular dynamics simulations of polycarbonate doped with Lemke chromophores. 2007 , 111, 10645-50	9
1796	Structure of rhodamine 6G-DNA complexes from molecular dynamics simulations. 2007 , 8, 3429-38	7
1795	Solvated interaction energy (SIE) for scoring protein-ligand binding affinities. 1. Exploring the parameter space. 2007 , 47, 122-33	276
1794	Understanding the substrate selectivity and the product regioselectivity of Orf2-catalyzed aromatic prenylations. 2007 , 46, 1303-11	21
1793	Comment on "On the accuracy of force fields for predicting the physical properties of dimethylnitramine". 2007 , 111, 1900-2	13
1792	Insights into a mutation-assisted lateral drug escape mechanism from the HIV-1 protease active site. 2007 , 46, 14865-77	23
1791	Conformation-specific recognition of carcinogen-DNA adduct in escherichia coli nucleotide excision repair. 2007 , 20, 6-10	19
1790	Structure and energetics of diphenylalanine self-assembling on Cu(110). 2007 , 111, 12740-8	32
1789	Electric field poled polymeric nonlinear optical systems: molecular dynamics simulations of poly(methyl methacrylate) doped with disperse red chromophores. 2007 , 111, 3591-8	24
1788	Rapid estimation of relative protein-ligand binding affinities using a high-throughput version of MM-PBSA. 2007 , 47, 1493-503	53
1787	Propensity of Formate, Acetate, Benzoate, and Phenolate for the Aqueous Solution/Vapor Interface: Surface Tension Measurements and Molecular Dynamics Simulations. 2007 , 111, 8242-8247	48
1786	Computational Approaches in Molecular Recognition, Self-assembly, Electron Transport, and Surface Chemistry. 2007 , 19, 229-241	9
1785	A swift all-atom energy-based computational protocol to predict DNA-ligand binding affinity and ΔT_m . 2007 , 50, 2240-4	36
1784	Spectroscopic and theoretical insights into sequence effects of aminofluorene-induced conformational heterogeneity and nucleotide excision repair. 2007 , 46, 11263-78	32
1783	Mechanism of drug resistance due to N88S in CRF01_AE HIV-1 protease, analyzed by molecular dynamics simulations. 2007 , 50, 1768-77	43
1782	Computational studies of the farnesyltransferase ternary complex part II: the conformational activation of farnesyldiphosphate. 2007 , 46, 12375-81	25
1781	A linear scaling study of solvent-solute interaction energy of drug molecules in aqua solution. 2007 , 111, 10320-8	12

1780	Chromophore channeling in the G-protein coupled receptor rhodopsin. 2007 , 129, 6970-1	61
1779	Lesion specificity in the base excision repair enzyme hNeil1: modeling and dynamics studies. 2007 , 46, 5305-14	25
1778	Fretting about FRET: correlation between kappa and R. 2007 , 92, 4168-78	87
1777	The protonation state of the Glu-71/Asp-80 residues in the KcsA potassium channel: a first-principles QM/MM molecular dynamics study. 2007 , 93, 2315-24	32
1776	Molecular dynamics and free energy studies on the wild-type and double mutant HIV-1 protease complexed with amprenavir and two amprenavir-related inhibitors: mechanism for binding and drug resistance. 2007 , 50, 1177-88	216
1775	Fine-tuning ligand-receptor design for selective molecular recognition of dicarboxylic acids. 2007 , 46, 10632-8	18
1774	Solid-State Effects on NMR Chemical Shifts. 2007 , 115-178	46
1773	Multi-mannosides based on a carbohydrate scaffold: synthesis, force field development, molecular dynamics studies, and binding affinities for lectin Con A. 2007 , 72, 9032-45	70
1772	Computational Parameters. 2007 , 59-65	2
1771	Classification of water molecules in protein binding sites. 2007 , 129, 2577-87	225
1770	Protein-Ligand Complexes: Computation of the Relative Free Energy of Different Scaffolds and Binding Modes. 2007 , 3, 1645-55	40
1769	AMBER Force Field Parameters for the Naturally Occurring Modified Nucleosides in RNA. 2007 , 3, 1464-75	128
1768	Anions of Alkali Halide Salts at Surfaces of Formamide Solutions: Concentration Depth Profiles and Surface Topography. 2007 , 111, 4379-4387	28
1767	. 2007 ,	1
1766	Minimum sequence requirements for the binding of paromomycin to the rRNA decoding site A. 2007 , 86, 95-111	3
1765	Hybrid molecular dynamics-quantum mechanics simulations of solute spectral properties in the condensed phase: evaluation of simulation parameters. <i>Journal of Computational Chemistry</i> , 2007 , 28, 1572-1581	3.5 31
1764	Performance of the general amber force field in modeling aqueous POPC membrane bilayers. <i>Journal of Computational Chemistry</i> , 2007 , 28, 2051-8	3.5 109
1763	Synthesis, biological evaluation, and molecular modeling investigation of chiral phenoxyacetic acid analogues with PPARalpha and PPARgamma agonist activity. 2007 , 2, 641-54	26

1762	Homology modeling of NR2B modulatory domain of NMDA receptor and analysis of ifenprodil binding. 2007 , 2, 1498-510	35
1761	Segregation of inorganic ions at surfaces of polar nonaqueous liquids. 2007 , 8, 1457-63	23
1760	Design and synthesis of potential sheet nucleators via Suzuki coupling reaction. 2007 , 63, 12779-12785	15
1759	Stereoselective synthesis and conformational analysis of pseudo-heptapeptides: Part 5. 2007 , 18, 1448-1456	4
1758	The pheophorbide-a DAB dendrimer P4 in solution: MD-simulations based studies of exciton states. 2007 , 444, 118-124	22
1757	New antitumoral acetogenin 'Guanacone type' derivatives: isolation and bioactivity. Molecular dynamics simulation of diacetyl-guanacone. 2007 , 15, 4369-81	18
1756	Validation of an automated procedure for the prediction of relative free energies of binding on a set of aldose reductase inhibitors. 2007 , 15, 7865-77	87
1755	Calculation of absolute free energy of binding for theophylline and its analogs to RNA aptamer using nonequilibrium work values. 2007 , 337, 135-143	18
1754	Interaction of Estonian kukersite with organic solvents: A volumetric swelling and molecular simulation study. 2007 , 86, 17-21	29
1753	Analyzing the performance of conformational search programs on compound databases. 2007 , 25, 700-10	15
1752	Average and extreme multi-atom Van der Waals interactions: strong coupling of multi-atom Van der Waals interactions with covalent bonding. 2007 , 1, 21	8
1751	Parameterization of AZT, a widely used nucleoside inhibitor of HIV-1 reverse transcriptase. 2007 , 107, 292-298	6
1750	Computational protocol for predicting the binding affinities of zinc containing metalloprotein-ligand complexes. 2007 , 67, 1167-78	36
1749	Fast and reliable analysis of molecular motion using proximity relations and dimensionality reduction. 2007 , 67, 897-907	36
1748	Computational approach to site-directed ligand discovery. 2007 , 68, 551-60	2
1747	Protonation state and substrate binding to B2 metallo-beta-lactamase CphA from <i>Aeromonas hydrophila</i> . 2007 , 69, 595-605	31
1746	Substrate polarization in enzyme catalysis: QM/MM analysis of the effect of oxaloacetate polarization on acetyl-CoA enolization in citrate synthase. 2007 , 69, 521-35	29
1745	Binding pathways of ligands to HIV-1 protease: coarse-grained and atomistic simulations. 2007 , 69, 5-13	59

1744	Insight into the metabolism rate of quinone analogues from molecular dynamics simulation and 3D-QSMR methods. 2007 , 70, 290-301	4
1743	Prospects for octopus rhodopsin utilization in optical and quantum computation. 2007 , 4, 189-196	3
1742	Coumarin-based inhibitors of human NAD(P)H:quinone oxidoreductase-1. Identification, structure-activity, off-target effects and in vitro human pancreatic cancer toxicity. 2007 , 50, 6316-25	56
1741	Light driven molecular switches: exploring and tuning their photophysical and photochemical properties. 2007 , 117, 1041-1059	17
1740	A tunable QM/MM approach to chemical reactivity, structure and physico-chemical properties prediction. 2007 , 118, 219-240	73
1739	Charge-charge and cation- π interactions in ligand binding to G protein-coupled receptors. 2007 , 118, 579-588	7
1738	Investigating the mechanisms of 17beta-estradiol imprinting by computational prediction and spectroscopic analysis. 2007 , 389, 423-31	57
1737	Insights into amprenavir resistance in E35D HIV-1 protease mutation from molecular dynamics and binding free-energy calculations. 2007 , 13, 297-304	32
1736	Vibrational analysis of a solvated green fluorescent protein chromophore. 2007 , 13, 775-83	5
1735	Study on the drug resistance and the binding mode of HIV-1 integrase with LCA inhibitor. 2007 , 50, 665-674	5
1734	Simulation of mechanical properties of oriented glassy polystyrene. 2007 , 48, 7211-7220	10
1733	Stereoselective synthesis and conformational analysis of unnatural tetrapeptides. Part 2. 2007 , 18, 2695-2711	8
1732	Modelling the restoration of wild-type dynamic behaviour in DeltaF508-CFTR NBD1 by 8-cyclopentyl-1,3-dipropylxanthine. 2007 , 26, 691-9	5
1731	A molecular mechanism of P-loop pliability of Rho-kinase investigated by molecular dynamic simulation. 2008 , 22, 789-97	6
1730	Comparative structural dynamics of Tyrosyl-tRNA synthetase complexed with different substrates explored by molecular dynamics. 2008 , 38, 25-35	12
1729	Characterization of a complete cycle of acetylcholinesterase catalysis by ab initio QM/MM modeling. 2008 , 14, 409-16	64
1728	Automated conformational energy fitting for force-field development. 2008 , 14, 667-79	90
1727	On the electrostatic component of protein-protein binding free energy. 2008 , 1, 2	40

1726	Binding of ciguatera toxins to the voltage-gated Kv1.5 potassium channel in the open state. Docking of gambierol and molecular dynamics simulations of a homology model. 2008 , 21, 997-1001	12
1725	QSAR Study of Cyclic Urea Type HIV-1 PR Inhibitors Using Ab Initio MO Calculation of Their Complex Structures with HIV-1 PR. 2008 , 27, 694-703	27
1724	Computational optimization of AG18051 inhibitor for amyloid- β -binding alcohol dehydrogenase enzyme. 2008 , 108, 1982-1991	2
1723	Functionalization and molecular dynamics study of carboxy-terminated poly(1-vinylpyrrolidin-2-one): A potential soluble carrier of biomolecules. 2008 , 46, 1683-1698	6
1722	Molecular modeling of the second extracellular loop of G-protein coupled receptors and its implication on structure-based virtual screening. 2008 , 71, 599-620	89
1721	Evaluating the potency of HIV-1 protease drugs to combat resistance. 2008 , 71, 1163-74	103
1720	Protein-protein docking by simulating the process of association subject to biochemical constraints. 2008 , 71, 1955-69	24
1719	Comparative molecular dynamics simulations of histone deacetylase-like protein: binding modes and free energy analysis to hydroxamic acid inhibitors. 2008 , 73, 134-49	40
1718	Molecular simulations enlighten the binding mode of quercetin to lipoxygenase-3. 2008 , 73, 290-8	4
1717	Protein-protein recognition as a first step towards the inhibition of XIAP and Survivin anti-apoptotic proteins. 2008 , 21, 190-204	20
1716	The Energetics of Large Deformations of a Single Polyimide Molecular Chain: DFT and MO Calculations. 2008 , 17, 488-495	1
1715	Direct epoxidation in <i>Candida antarctica</i> lipase B studied by experiment and theory. 2008 , 9, 2443-51	73
1714	Supramolecular domains in mixed peptide self-assembled monolayers on gold nanoparticles. 2008 , 9, 2127-34	37
1713	Cooperative AND ion-pair recognition by heteroditopic calix[4]diquinone receptors. 2008 , 14, 2248-63	95
1712	Non-natural amino acids as modulating agents of the conformational space of model glycopeptides. 2008 , 14, 7042-58	24
1711	Glutathione transferase: new model for glutathione activation. 2008 , 14, 9591-8	51
1710	Thiobarbiturates as sirtuin inhibitors: virtual screening, free-energy calculations, and biological testing. 2008 , 3, 1965-76	56
1709	Deciphering the selectivity of <i>Bombyx mori</i> pheromone binding protein for bombykol over bombykal: a theoretical approach. 2008 , 9, 2785-93	3

1708	Structure and dynamics of phospholipid bilayers using recently developed general all-atom force fields. <i>Journal of Computational Chemistry</i> , 2008 , 29, 24-37	3.5	76
1707	The implementation of a fast and accurate QM/MM potential method in Amber. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1019-31	3.5	289
1706	Q-Dock: Low-resolution flexible ligand docking with pocket-specific threading restraints. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1574-88	3.5	36
1705	Basis set dependence of solute-solvent interaction energy of benzene in water: a HF/DFT study. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1725-32	3.5	7
1704	Role of structural water molecule in HIV protease-inhibitor complexes: a QM/MM study. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1840-9	3.5	27
1703	A poke in the eye: inhibiting HIV-1 protease through its flap-recognition pocket. 2008 , 89, 643-52		34
1702	Hierarchical Assembly of Organic/Inorganic Building Molecules with π Interactions. 2008 , 18, 1526-1535		29
1701	Structure-Based Insight into the Asymmetric Bioreduction of the C=C Double Bond of α,β -Unsaturated Nitroalkenes by Pentaerythritol Tetranitrate Reductase. 2008 , 350, 2789-2803		78
1700	Computational alanine scanning and free energy decomposition for E. coli type I signal peptidase with lipopeptide inhibitor complex. 2008 , 26, 813-23		27
1699	Binding modes of CCR5-targeting HIV entry inhibitors: partial and full antagonists. 2008 , 26, 1287-95		21
1698	Development and initial testing of an empirical forcefield for simulation of poly(alkylthiophenes). 2008 , 27, 34-44		12
1697	Binding of the tautomeric forms of isoniazid-NAD adducts to the active site of the Mycobacterium tuberculosis enoyl-ACP reductase (InhA): a theoretical approach. 2008 , 27, 536-45		14
1696	Flexible computational docking studies of new aminoglycosides targeting RNA 16S bacterial ribosome site. 2008 , 43, 1648-56		25
1695	Evaluation of Amber force field parameters for copper(II) with pyridylmethyl-amine and benzimidazolymethyl-amine ligands: A quantum chemical study. 2008 , 455, 354-360		27
1694	Modelling organic molecular crystals by hybrid quantum mechanical/molecular mechanical embedding. 2008 , 457, 154-158		14
1693	Solvent effects on the nitrogen NMR shielding and nuclear quadrupole coupling constants in 1-methyltriazoles. 2008 , 460, 129-136		15
1692	Propensities of oxalic, citric, succinic, and maleic acids for the aqueous solution/vapour interface: Surface tension measurements and molecular dynamics simulations. 2008 , 462, 217-221		27
1691	5'-Carbamoyl derivatives of 2'-C-methyl-purine nucleosides as selective A1 adenosine receptor agonists: affinity, efficacy, and selectivity for A1 receptor from different species. 2008 , 16, 336-53		22

1690	Activity of Mannich bases of 7-hydroxycoumarin against Flaviviridae. 2008 , 16, 2591-605	46
1689	Bornyl (3,4,5-trihydroxy)-cinnamate--an optimized human neutrophil elastase inhibitor designed by free energy calculations. 2008 , 16, 2385-90	58
1688	The discovery of small molecule chemical probes of Bcl-X(L) and Mcl-1. 2008 , 16, 7443-9	37
1687	Molecular dynamics simulations of the amyloid-beta binding alcohol dehydrogenase (ABAD) enzyme. 2008 , 16, 9511-8	10
1686	Synthesis, biological evaluation, and molecular modeling investigation of chiral 2-(4-chloro-phenoxy)-3-phenyl-propanoic acid derivatives with PPARalpha and PPARgamma agonist activity. 2008 , 16, 9498-510	18
1685	Discovery of dihydroquinoxalinone acetamides containing bicyclic amines as potent Bradykinin B1 receptor antagonists. 2008 , 18, 4477-81	23
1684	Structure-guided design of substituted aza-benzimidazoles as potent hypoxia inducible factor-1alpha prolyl hydroxylase-2 inhibitors. 2008 , 18, 5023-6	26
1683	Study on the molecular mechanism of inhibiting HIV-1 integrase by EBR28 peptide via molecular modeling approach. 2008 , 132, 69-80	20
1682	Mixed quantum classical simulations of electronic excitation energy transfer: The pheophorbide-a DAB dendrimer in solution. 2008 , 351, 117-128	23
1681	Binding studies of a protonated dioxatetraazamacrocycle with carboxylate substrates. 2008 , 64, 5392-5403	18
1680	Molecular dynamics simulation study on the interaction of KRN 7000 and three analogues with human CD1d. 2008 , 64, 9480-9489	27
1679	Interaction mode and selectivity of the 2PU inhibitor with the CDK4 and CDK2 cyclin-dependant kinases: A molecular dynamics study. 2008 , 849, 62-75	14
1678	Improving the performance of the coupled reference interaction site model-hyper-netted chain (RISM-HNC)/simulation method for free energy of solvation. 2008 , 112, 2340-8	6
1677	Docking ligands into flexible and solvated macromolecules. 2. Development and application of fitted 1.5 to the virtual screening of potential HCV polymerase inhibitors. 2008 , 48, 902-9	55
1676	Computation of binding free energy with molecular dynamics and grand canonical Monte Carlo simulations. 2008 , 128, 115103	103
1675	Comparison of protein force fields for molecular dynamics simulations. 2008 , 443, 63-88	132
1674	Hit identification and binding mode predictions by rigorous free energy simulations. 2008 , 51, 6654-64	56
1673	Revealing interaction mode between HIV-1 reverse transcriptase and diaryltriazine analog inhibitor. 2008 , 72, 350-9	6

1672	Endogenous tetrahydroisoquinolines associated with Parkinson's disease mimic the feedback inhibition of tyrosine hydroxylase by catecholamines. 2008 , 275, 2109-21	8
1671	Binding of berberine to human telomeric quadruplex - spectroscopic, calorimetric and molecular modeling studies. 2008 , 275, 3971-83	91
1670	Domain versatility in plant AB-toxins: evidence for a local, pH-dependent rearrangement in the 2gamma lectin site of the mistletoe lectin by applying ligand derivatives and modelling. 2008 , 582, 2309-12	24
1669	Equilibrium Molecular Dynamics Simulations. 2009 , 255-290	9
1668	Molecular dynamics of host-guest complexes of small gas molecules with calix[4]arenes. 2008 , 112, 6829-39	13
1667	Heterogeneous dynamics of ionic liquids from molecular dynamics simulations. 2008 , 129, 194501	122
1666	5-N-methylated quindoline derivatives as telomeric g-quadruplex stabilizing ligands: effects of 5-N positive charge on quadruplex binding affinity and cell proliferation. 2008 , 51, 6381-92	110
1665	Water inside a hydrophobic cavitand molecule. 2008 , 112, 10272-9	61
1664	Coarse-grained molecular modeling of non-ionic surfactant self-assembly. 2008 , 4, 2454	196
1663	Molecular motions in amorphous ibuprofen as studied by broadband dielectric spectroscopy. 2008 , 112, 11087-99	138
1662	Theoretical calculations of the catalytic triad in short-chain alcohol dehydrogenases/reductases. 2008 , 94, 1412-27	19
1661	Identification of high affinity fatty acid binding sites on human serum albumin by MM-PBSA method. 2008 , 94, 95-103	58
1660	Solid-state NMR and MD simulations of the antiviral drug amantadine solubilized in DMPC bilayers. 2008 , 94, 1295-302	44
1659	Sliding of alkylating anticancer drugs along the minor groove of DNA: new insights on sequence selectivity. 2008 , 94, 550-61	25
1658	Atomistic simulations of the HIV-1 protease folding inhibition. 2008 , 95, 550-62	9
1657	All-atom computer simulations of amyloid fibrils disaggregation. 2008 , 95, 5037-47	29
1656	Predicting small-molecule solvation free energies: an informal blind test for computational chemistry. 2008 , 51, 769-79	228
1655	Performance of SM8 on a test to predict small-molecule solvation free energies. 2008 , 112, 8651-5	52

1654	Refinement of a low-resolution crystal structure to better understand erythromycin interactions on large ribosomal subunit. 2008 , 26, 131-46	2
1653	United-atom acyl chains for CHARMM phospholipids. 2008 , 112, 7008-15	70
1652	Persistence of camptothecin analog-topoisomerase I-DNA ternary complexes: a molecular dynamics study. 2008 , 130, 17928-37	20
1651	Engineering of Crystalline Materials Properties. 2008 ,	23
1650	In silico mutagenesis and docking studies of Pseudomonas aeruginosa PA-III lectin predicting binding modes and energies. 2008 , 48, 2234-42	15
1649	Comparison of docking methods for carbohydrate binding in calcium-dependent lectins and prediction of the carbohydrate binding mode to sea cucumber lectin CEL-III. 2008 , 34, 469-479	29
1648	Transition-State Docking of Flunitrazepam and Progesterone in Cytochrome P450. 2008 , 4, 673-81	24
1647	Prediction of partition coefficients by multiscale hybrid atomic-level/coarse-grain simulations. 2008 , 112, 657-60	77
1646	Rescoring docking hit lists for model cavity sites: predictions and experimental testing. 2008 , 377, 914-34	149
1645	The binding of thioflavin T and its neutral analog BTA-1 to protofibrils of the Alzheimer's disease Abeta(16-22) peptide probed by molecular dynamics simulations. 2008 , 384, 718-29	119
1644	pH-dependent interdomain tethers of CD1b regulate its antigen capture. 2008 , 28, 774-86	45
1643	Energetics of the human Tel-22 quadruplex-telomestatin interaction: a molecular dynamics study. 2008 , 112, 6828-36	54
1642	Activation mechanism of the human histamine H4 receptor--an explicit membrane molecular dynamics simulation study. 2008 , 48, 1199-210	34
1641	On the molecular mechanism of drug intercalation into DNA: a simulation study of the intercalation pathway, free energy, and DNA structural changes. 2008 , 130, 9747-55	151
1640	Force field parameters for S-nitrosocysteine and molecular dynamics simulations of S-nitrosated thioredoxin. 2008 , 377, 612-616	23
1639	Automated molecular simulation based binding affinity calculator for ligand-bound HIV-1 proteases. 2008 , 48, 1909-19	43
1638	Rapid and accurate prediction of binding free energies for saquinavir-bound HIV-1 proteases. 2008 , 130, 2639-48	130
1637	Protein-ligand docking accounting for receptor side chain and global flexibility in normal modes: evaluation on kinase inhibitor cross docking. 2008 , 51, 3499-506	78

1636	Acylguanidines as bioisosteres of guanidines: NG-acylated imidazolylpropylguanidines, a new class of histamine H2 receptor agonists. 2008 , 51, 7193-204	63
1635	Biomolecular simulations of membranes: physical properties from different force fields. 2008 , 128, 125103	227
1634	Modeling the catalysis of anti-cocaine catalytic antibody: competing reaction pathways and free energy barriers. 2008 , 130, 5140-9	84
1633	Treating entropy and conformational changes in implicit solvent simulations of small molecules. 2008 , 112, 938-46	97
1632	Molecular dynamics and principal components analysis of human telomeric quadruplex multimers. 2008 , 95, 296-311	169
1631	The multiscale coarse-graining method. I. A rigorous bridge between atomistic and coarse-grained models. 2008 , 128, 244114	550
1630	Ionization of imidazole in the gas phase, microhydrated environments, and in aqueous solution. 2008 , 112, 3499-505	77
1629	Structure-activity studies on splitomicin derivatives as sirtuin inhibitors and computational prediction of binding mode. 2008 , 51, 1203-13	147
1628	Hydronium and hydroxide at the interface between water and hydrophobic media. 2008 , 10, 4975-80	65
1627	Aqueous solutions of ionic liquids: study of the solution/vapor interface using molecular dynamics simulations. 2008 , 10, 5765-75	55
1626	An analytical potential energy function to model protonated peptide soft-landing experiments. The CH ₃ NH ₃ ⁺ /CH ₄ interactions. 2008 , 10, 4565-72	14
1625	Sulfate anion templation of a neutral pseudorotaxane assembly using an indolocarbazole threading component. 2008 , 3154-6	73
1624	Sulfate anion-templated assembly of a [2]catenane. 2008 , 4610-2	55
1623	Investigations into conformational transitions and solvation structure of a 7-piperidino-5,9-methanobenzo[8] annulene in water. 2008 , 10, 6135-43	6
1622	Sequence dependence in base flipping: experimental and computational studies. 2008 , 6, 485-92	8
1621	Structural origin of selectivity in class II-selective histone deacetylase inhibitors. 2008 , 51, 2898-906	107
1620	CHARMMing: a new, flexible web portal for CHARMM. 2008 , 48, 1920-9	105
1619	Charge asymmetries in hydration of polar solutes. 2008 , 112, 2405-14	84

1618	Molecular Modeling of Geometries, Charge Distributions, and Binding Energies of Small, Drug-Like Molecules Containing Nitrogen Heterocycles and Exocyclic Amino Groups in the Gas Phase and Aqueous Solution. 2008 , 4, 1718-1732	12
1617	Asymmetric synthesis of 2,3-dihydro-2-arylquinazolin-4-ones: methodology and application to a potent fluorescent tubulin inhibitor with anticancer activity. 2008 , 51, 4620-31	150
1616	Studies of the mechanism of selectivity of protein tyrosine phosphatase 1B (PTP1B) bidentate inhibitors using molecular dynamics simulations and free energy calculations. 2008 , 48, 2030-41	22
1615	Molecular dynamics simulation of the energetic room-temperature ionic liquid, 1-hydroxyethyl-4-amino-1,2,4-triazolium nitrate (HEATN). 2008 , 112, 3121-31	74
1614	Origins of Resistance Conferred by the R292K Neuraminidase Mutation via Molecular Dynamics and Free Energy Calculations. 2008 , 4, 1526-40	62
1613	Structural studies of heparan sulfate hexasaccharides: new insights into iduronate conformational behavior. 2008 , 130, 12435-44	24
1612	Molecular dynamics investigation of the effects of a water surface on the aggregation of bent-core molecules. 2008 , 24, 4456-60	7
1611	New endomorphin analogues containing alicyclic beta-amino acids: influence on bioactive conformation and pharmacological profile. 2008 , 51, 4270-9	41
1610	Aqueous Partial Molar Volumes from Simulation and Individual Group Contributions. 2008 , 47, 5169-5174	19
1609	Molecular dynamics simulations of functional group effects on solvation thermodynamics of model solutes in decane and tricapylin. 2008 , 5, 1023-36	19
1608	Solvent dependence on conformational transition, dipole moment, and molecular geometry of 1,2-dichloroethane: insight from Car-Parrinello molecular dynamics calculations. 2008 , 112, 14673-7	11
1607	An anchor-dependent molecular docking process for docking small flexible molecules into rigid protein receptors. 2008 , 48, 1638-55	6
1606	Ground- and Excited-State Pinched Cone Equilibria in Calix[4]arenes Bearing Two Perylene Bisimide Dyes. 2008 , 112, 14626-14638	72
1605	Conformational sampling of druglike molecules with MOE and catalyst: implications for pharmacophore modeling and virtual screening. 2008 , 48, 1773-91	94
1604	Analysis of the unfolding process of green fluorescent protein by molecular dynamics simulation. 2008 , 112, 8672-80	4
1603	Active site pressurization: a new tool for structure-guided drug design and other studies of protein flexibility. 2008 , 48, 1448-54	23
1602	Protein-ligand binding affinity by nonequilibrium free energy methods. 2008 , 112, 14985-92	10
1601	Insights into ligand selectivity in estrogen receptor isoforms: molecular dynamics simulations and binding free energy calculations. 2008 , 112, 2719-26	37

1600	Selective structure-based virtual screening for full and partial agonists of the beta2 adrenergic receptor. 2008 , 51, 4978-85	124
1599	Surface polarity of beta-HMX crystal and the related adhesive forces with Estane binder. 2008 , 24, 13477-82	8
1598	Docking to RNA via root-mean-square-deviation-driven energy minimization with flexible ligands and flexible targets. 2008 , 48, 1257-68	62
1597	Mechanism for the transport of ammonia within carbamoyl phosphate synthetase determined by molecular dynamics simulations. 2008 , 47, 2935-44	15
1596	Theoretical analysis of antisense duplexes: determinants of the RNase H susceptibility. 2008 , 130, 3486-96	27
1595	Molecular dynamics simulations of dendrimer-encapsulated alpha-Keggin ions in trichloromethane solution. 2008 , 112, 5153-62	19
1594	Hepatitis C virus NS5B polymerase: QM/MM calculations show the important role of the internal energy in ligand binding. 2008 , 112, 3168-76	13
1593	Calculating chemically accurate redox potentials for engineered flavoproteins from classical molecular dynamics free energy simulations. 2008 , 112, 13053-7	14
1592	Nitrate ion photochemistry at interfaces: a new mechanism for oxidation of alpha-pinene. 2008 , 10, 3063-71	24
1591	Protein polarization is critical to stabilizing AF-2 and helix-2' domains in ligand binding to PPAR-gamma. 2008 , 130, 17129-33	67
1590	Digging a hole: Scaled-particle theory and cavity solvation in organic solvents. 2008 , 129, 174505	15
1589	Fast tools for calculation of atomic charges well suited for drug design. 2008 , 19, 153-65	15
1588	Many-atom van der Waals interactions lead to direction-sensitive interactions of covalent bonds. 2008 , 6, 693-707	2
1587	Differential roles of phosphatidylserine, PtdIns(4,5)P2, and PtdIns(3,4,5)P3 in plasma membrane targeting of C2 domains. Molecular dynamics simulation, membrane binding, and cell translocation studies of the PKCalpha C2 domain. 2008 , 283, 26047-58	73
1586	Adaptively biased molecular dynamics for free energy calculations. 2008 , 128, 134101	138
1585	Soluble guanylyl cyclase activation by HMR-1766 (ataciguat) in cells exposed to oxidative stress. 2008 , 295, H1763-71	38
1584	Dissociation of minor groove binders from DNA: insights from metadynamics simulations. 2008 , 36, 5910-21	59
1583	Intramolecular cohesion of coils mediated by phenylalanine-glycine motifs in the natively unfolded domain of a nucleoporin. 2008 , 4, e1000145	43

1582	Incorrect nucleotide insertion at the active site of a G:A mismatch catalyzed by DNA polymerase beta. 2008 , 105, 5670-4	46
1581	Adaptive protein evolution grants organismal fitness by improving catalysis and flexibility. 2008 , 105, 20605-10	84
1580	A minimalist network model for coarse-grained normal mode analysis and its application to biomolecular x-ray crystallography. 2008 , 105, 15358-63	40
1579	Metabolism of phenylahistin enantiomers by cytochromes P450: a possible explanation for their different cytotoxicity. 2008 , 36, 2381-92	8
1578	Designing a ligand for pharmaceutical purposes. 2008 , 3, 579-90	4
1577	Linear absorbance of the pheophorbide-a butanediamine dendrimer P(4) in solution: computational studies using a mixed quantum classical methodology. 2008 , 128, 154905	23
1576	Molecular dynamics study of the dynamics near the glass transition in ionic liquids. 2008 , 24, 1321-7	21
1575	Comparative docking assessment of glucokinase interactions with its allosteric activators. 2008 , 2, 76-89	12
1574	Methods for Studying Nucleic Acid Structure. 2008 , 1-19	5
1573	Molecular Dynamics Computations for Proteins: A Case Study in Membrane Ion Permeation. 2009 ,	
1572	Molecular dynamics simulation of Axillaridine-A: a potent natural cholinesterase inhibitor. 2009 , 24, 1101-5	2
1571	Analytical energy gradient for reference interaction site model self-consistent field explicitly including spatial electron density distribution. 2009 , 131, 214504	35
1570	A mechanism for S-adenosyl methionine assisted formation of a riboswitch conformation: a small molecule with a strong arm. 2009 , 37, 6528-39	43
1569	Conformational toggle switches implicated in basal constitutive and agonist-induced activated states of 5-hydroxytryptamine-4 receptors. 2009 , 75, 982-90	49
1568	Nanosculpting reversed wavelength sensitivity into a photoswitchable iGluR. 2009 , 106, 6814-9	75
1567	QUANTUM CALCULATION OF PROTEIN SOLVATION AND PROTEIN-LIGAND BINDING FREE ENERGY FOR HIV-1 PROTEASE/WATER COMPLEX. 2009 , 08, 1265-1279	22
1566	Coarse grain molecular dynamics simulation for the prediction of tertiary conformation of lysozyme adsorbed on silica surface. 2009 , 35, 974-985	6
1565	Conformational analysis of hexapeptide mimicking reverse turn structures induced by a modified (S)-proline. A combined spectroscopic and molecular dynamics investigation. Part 4. 2009 , 107, 653-663	2

1564	Essential role of proximal histidine-asparagine interaction in mammalian peroxidases. 2009 , 284, 25929-37	62
1563	Structural and functional analysis of Campylobacter jejuni PseG: a udp-sugar hydrolase from the pseudaminic acid biosynthetic pathway. 2009 , 284, 20989-1000	15
1562	SMALL PURE CARBON MOLECULES WITH SMALL-WORLD NETWORKS USING DENSITY FUNCTIONAL THEORY SIMULATIONS. 2009 , 20, 1345-1356	2
1561	COMPUTER SIMULATIONS OF THE INTERACTION OF CIGUATOXIN 3C, BREVENAL AND ent-BREVENAL LADDER POLYETHERS WITH A HOMOLGY MODEL OF THE VOLTAGE-GATED Kv1.5 POTASSIUM CHANNEL. 2009 , 08, 957-971	5
1560	High-performance drug discovery: computational screening by combining docking and molecular dynamics simulations. 2009 , 5, e1000528	109
1559	Path integral evaluation of equilibrium isotope effects. 2009 , 131, 024111	33
1558	Molecular Dynamics as a Tool in Rational Drug Design: Current Status and Some Major Applications. 2009 , 5, 225-240	33
1557	Kinetic and thermodynamic characterization of dihydrotestosterone-induced conformational perturbations in androgen receptor ligand-binding domain. 2009 , 23, 1231-41	18
1556	A guide to template based structure prediction. 2009 , 10, 270-85	35
1555	Molecular Mechanics Force Fields and their Applications in Drug Design. 2009 , 8, 128-150	10
1554	Conformational sampling and energetics of drug-like molecules. 2009 , 16, 3381-413	56
1553	A computer simulation model for proton transport in liquid imidazole. 2009 , 113, 4507-17	49
1552	Dynamic allostery in the methionine repressor revealed by force distribution analysis. 2009 , 5, e1000574	48
1551	Coarse-grained molecular dynamics of ligands binding into protein: The case of HIV-1 protease inhibitors. 2009 , 130, 215102	24
1550	Hierarchical modeling of activation mechanisms in the ABL and EGFR kinase domains: thermodynamic and mechanistic catalysts of kinase activation by cancer mutations. 2009 , 5, e1000487	63
1549	Further analysis and comparative study of intermolecular interactions using dimers from the S22 database. 2009 , 131, 065102	75
1548	FINDSITE: a threading-based approach to ligand homology modeling. 2009 , 5, e1000405	64
1547	DOCK 6: combining techniques to model RNA-small molecule complexes. 2009 , 15, 1219-30	510

1546	Differences in conformational dynamics of [Pt3(HPTAB)]6+-DNA adducts with various cross-linking modes. 2009 , 37, 5930-42		13
1545	Molecular determinants of non-competitive antagonist binding to the mouse GPRC6A receptor. 2009 , 46, 323-32		44
1544	Computer- and Structure-Based Lead Identification for Epigenetic Targets. 2009 , 57-85		
1543	Ferroelectric Response and Induced Biaxiality in the Nematic Phase of Bent-Core Mesogens. 2009 , 19, 2592-2600		178
1542	Modeling Polymer Dielectric/Pentacene Interfaces: On the Role of Electrostatic Energy Disorder on Charge Carrier Mobility. 2009 , 19, 3254-3261		72
1541	Design of protonated polyazamacrocycles based on phenanthroline motifs for selective uptake of aromatic carboxylate anions and herbicides. 2009 , 15, 3277-89		21
1540	Bifunctional catalysis by natural cinchona alkaloids: a mechanism explained. 2009 , 15, 7913-21		55
1539	Electron density shift in imidazolium derivatives upon complexation with cucurbit[6]uril. 2009 , 15, 6926-31		38
1538	Counterions control the self-assembly of structurally persistent micelles: theoretical prediction and experimental observation of stabilization by sodium ions. 2009 , 15, 8586-92		18
1537	N(G)-acylated aminothiazolylpropylguanidines as potent and selective histamine H(2) receptor agonists. 2009 , 4, 232-40		38
1536	Mechanistic insights into cyclooxygenase irreversible inactivation by aspirin. 2009 , 4, 939-45		30
1535	Design and discovery of plasmepsin II inhibitors using an automated workflow on large-scale grids. 2009 , 4, 1164-73		38
1534	Site-dependent excited-state dynamics of a fluorescent probe bound to avidin and streptavidin. 2009 , 10, 1517-32		16
1533	In silico prediction of drug solubility: 4. Will simple potentials suffice?. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1859-71	3.5	20
1532	Crystal structure prediction of flexible molecules using parallel genetic algorithms with a standard force field. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1973-85	3.5	28
1531	Insights into docking and scoring neuronal alpha4beta2 nicotinic receptor agonists using molecular dynamics simulations and QM/MM calculations. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2443-54	3.5	22
1530	Theoretical study of the prion protein based on the fragment molecular orbital method. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2594-601	3.5	112
1529	Roles of K151 and D180 in L-2-haloacid dehalogenase from <i>Pseudomonas</i> sp. YL: analysis by molecular dynamics and ab initio fragment molecular orbital calculations. <i>Journal of Computational Chemistry</i> , 2009 , 30, 2625-34	3.5	24

1528	The use of time-averaged 3JHH restrained molecular dynamics (tar-MD) simulations for the conformational analysis of five-membered ring systems: methodology and applications. <i>Journal of Computational Chemistry</i> , 2010 , 31, 561-72	3.5	10
1527	How to obtain statistically converged MM/GBSA results. <i>Journal of Computational Chemistry</i> , 2010 , 31, 837-46	3.5	129
1526	CHARMM general force field: A force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields. <i>Journal of Computational Chemistry</i> , 2010 , 31, 671-90	3.5	2953
1525	Fast and accurate predictions of binding free energies using MM-PBSA and MM-GBSA. <i>Journal of Computational Chemistry</i> , 2010 , 31, 797-810	3.5	377
1524	Blind docking method combining search of low-resolution binding sites with ligand pose refinement by molecular dynamics-based global optimization. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1080-92	3.5	12
1523	Basic ingredients of free energy calculations: a review. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1569-82	3.5	225
1522	Parameterization of the torsional potential for calix[4]arene-substituted poly(thiophene)s. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1741-51	3.5	5
1521	Investigation of Thermal Expansion of Polyimide/SiO ₂ Nanocomposites by Molecular Dynamics Simulations. 2009 , 19, NA-NA		34
1520	Alchemical free energy simulations for biological complexes: powerful but temperamental. 2010 , 23, 117-27		46
1519	Vibrational properties of ibuprofen β -cyclodextrin inclusion complexes investigated by Raman scattering and numerical simulation. 2009 , 40, 453-458		43
1518	Molecular dynamic simulations of the metallo-beta-lactamase from <i>Bacteroides fragilis</i> in the presence and absence of a tight-binding inhibitor. 2009 , 15, 133-45		21
1517	Mimicking direct protein-protein and solvent-mediated interactions in the CDP-methylerythritol kinase homodimer: a pharmacophore-directed virtual screening approach. 2009 , 15, 997-1007		16
1516	Parameterization of aromatic azido groups: application as photoaffinity probes in molecular dynamics studies. 2009 , 15, 1291-7		10
1515	Hofmeister series and specific interactions of charged headgroups with aqueous ions. 2009 , 146, 42-7		332
1514	A new method for in-silico drug screening and similarity search using molecular dynamics maximum volume overlap (MD-MVO) method. 2009 , 27, 628-36		9
1513	Molecular modeling of ligand-receptor interactions in GABA C receptor. 2009 , 27, 813-21		19
1512	An improved method to predict the entropy term with the MM/PBSA approach. 2009 , 23, 63-71		103
1511	Studies of chirality effect of 4-(phenylamino)-pyrrolo[2,1-f][1,2,4]triazine on p38alpha by molecular dynamics simulations and free energy calculations. 2009 , 23, 737-45		5

1510	Complexation of N-methyl-4-(p-methyl benzoyl)-pyridinium methyl cation and its neutral analogue by cucurbit[7]uril and β -cyclodextrin: a computational study. 2009 , 64, 357-365	11
1509	A three-point method for evaluations of AMBER force field parameters: an application to copper-based artificial nucleases. 2009 , 122, 167-178	15
1508	Glutathione transferase A1-1: catalytic role of water. 2009 , 124, 71-83	6
1507	Ligand unbinding pathways from the vitamin D receptor studied by molecular dynamics simulations. 2009 , 38, 185-98	50
1506	Movements of native C505 during channel gating in CNGA1 channels. 2009 , 38, 465-78	5
1505	Predicting drug resistance of the HIV-1 protease using molecular interaction energy components. 2009 , 74, 837-46	72
1504	Insights into lid movements of Burkholderia cepacia lipase inferred from molecular dynamics simulations. 2009 , 77, 509-23	76
1503	Synthesis and differentiation of alpha- and beta-glycoporphyrin stereoisomers by electrospray tandem mass spectrometry. 2009 , 23, 3478-83	8
1502	Computational studies of H5N1 influenza virus resistance to oseltamivir. 2009 , 18, 707-15	22
1501	Quantum chemical justification of the specificity of enzyme catalysis: Correlations between the rate of enzyme catalysis by acetylcholinesterase and substrate structure. 2009 , 426, 98-100	
1500	Binding estimation after refinement, a new automated procedure for the refinement and rescoring of docked ligands in virtual screening. 2009 , 73, 283-6	87
1499	QM/MM study of epitope peptides binding to HLA-A*0201: the roles of anchor residues and water. 2009 , 74, 611-8	14
1498	Gas-Phase Hydrogen/Deuterium Exchange of Dinucleotides and 5'-Monophosphate Dinucleotides in a Quadrupole Ion Trap. 2009 , 287, 87-95	3
1497	Cycloaddition reactions of cross-conjugated enaminones. 2009 , 65, 8478-8485	22
1496	Molecular dynamics of d(CGCGAATTCGCG) ₂ complexed with netropsin and its minor groove methylating analog, Me-lex, using explicit and implicit water models. 2009 , 894, 50-58	5
1495	DFT RX3LYP and RPBEPBE studies on the structural, electronic, and vibrational properties of some amino-alcohol ligands. 2009 , 915, 20-32	9
1494	Modelling beta-1,3-exoglucanase-saccharide interactions: structure of the enzyme-substrate complex and enzyme binding to the cell wall. 2009 , 27, 908-20	8
1493	Theoretical studies on the interaction of modified pyrimidines and purines with purine riboswitch. 2009 , 28, 37-45	11

1492	Molecular modeling of human cytochrome P450 2W1 and its interactions with substrates. 2009 , 28, 170-6	16
1491	Structure and function of the glycopeptide N-methyltransferase MtfA, a tool for the biosynthesis of modified glycopeptide antibiotics. 2009 , 16, 401-10	33
1490	Time and frequency resolved spontaneous emission from supramolecular pheophorbide-a complexes: A mixed quantum classical computation. 2009 , 362, 19-26	14
1489	Understanding ligand-protein interactions in affinity membrane chromatography for antibody purification. 2009 , 1216, 8687-96	31
1488	Single-molecule DNA conductance in water solutions: Role of DNA low-frequency dynamics. 2009 , 467, 369-374	12
1487	Theoretical and computational strategies for rational molecularly imprinted polymer design. 2009 , 25, 543-52	140
1486	Calculation of binding free energies for non-zinc chelating pyrimidine dicarboxamide inhibitors with MMP-13. 2009 , 19, 47-50	9
1485	A Theoretical Study of Polyoxometalates and Dendrzyme Model Compounds. 2009 , 129-142	1
1484	Computations of standard binding free energies with molecular dynamics simulations. 2009 , 113, 2234-46	415
1483	A molecular dynamics simulation study of crystalline 1,3,5-triamino-2,4,6-trinitrobenzene as a function of pressure and temperature. 2009 , 131, 224703	65
1482	Molecular insights into 14-membered macrolides using the MM-PBSA method. 2009 , 49, 1558-67	17
1481	Fluorine bonding--how does it work in protein-ligand interactions?. 2009 , 49, 2344-55	201
1480	Permeability of small molecules through a lipid bilayer: a multiscale simulation study. 2009 , 113, 12019-29	123
1479	Thyroid hormone interactions with DMPC bilayers. A molecular dynamics study. 2009 , 113, 13357-64	8
1478	Alternating pattern of stereochemistry in the nonactin macrocycle is required for antibacterial activity and efficient ion binding. 2009 , 131, 17155-65	28
1477	Conformational variability of benzamidinium-based inhibitors. 2009 , 131, 7742-54	28
1476	Conformationally constrained peptidomimetic inhibitors of signal transducer and activator of transcription. 3: Evaluation and molecular modeling. 2009 , 52, 2429-42	53
1475	Molecular dynamics simulations on binding models of Dervan-type polyamide + Cu(II) nuclease ligands to DNA. 2009 , 113, 839-48	16

1474	Reduced Catalytic Activity of P450 2A6 Mutants with Coumarin: A Computational Investigation. 2009 , 5, 1411-20	22
1473	Computational insights into the mechanism of ligand unbinding and selectivity of estrogen receptors. 2009 , 113, 10436-44	43
1472	Accommodation of an N-(deoxyguanosin-8-yl)-2-acetylaminofluorene adduct in the active site of human DNA polymerase β : Hoogsteen or Watson-Crick base pairing?. 2009 , 48, 7-18	20
1471	Identification of anxiolytic/nonsedative agents among indol-3-ylglyoxylamides acting as functionally selective agonists at the gamma-aminobutyric acid-A (GABAA) $\alpha 2$ benzodiazepine receptor. 2009 , 52, 3723-34	25
1470	Theoretical characterization of the dynamical behavior and transport properties of alpha,gamma-peptide nanotubes in solution. 2009 , 131, 15678-86	40
1469	Identification of specific small molecule ligands for stem loop 3 ribonucleic acid of the packaging signal Psi of human immunodeficiency virus-1. 2009 , 52, 5462-73	22
1468	Integrated Continuum Dielectric Approaches to treat Molecular Polarizability and the Condensed Phase: Refractive Index and Implicit Solvation. 2009 , 5, 1785-1802	18
1467	Surface residence and uptake of methyl chloride and methyl alcohol at the air/water interface studied by vibrational sum frequency spectroscopy and molecular dynamics. 2009 , 113, 2015-24	24
1466	Computational studies of load-dependent guest dynamics and free energies of inclusion for CO ₂ in low-density p-tert-butylcalix[4]arene at loadings up to 2:1. 2009 , 113, 3369-74	6
1465	Ion-specific interactions between halides and basic amino acids in water. 2009 , 113, 1969-75	46
1464	Exploring damage recognition models in prokaryotic nucleotide excision repair with a benzo[a]pyrene-derived lesion in UvrB. 2009 , 48, 8948-57	22
1463	Molecular dynamics of water-mediated interactions of a linear benzimidazole-biphenyl diamidine with the DNA minor groove. 2009 , 131, 7618-25	34
1462	Chemical Detail Force Fields for Mesogenic Molecules. 2009 , 5, 1865-76	18
1461	Structure-based CoMFA as a predictive model - CYP2C9 inhibitors as a test case. 2009 , 49, 853-64	24
1460	Controlled Isomerization of a Light-Driven Molecular Motor: A Theoretical Study. 2009 , 113, 3574-3580	21
1459	Quantifying Correlations Between Allosteric Sites in Thermodynamic Ensembles. 2009 , 5, 2486-2502	172
1458	Hybrid quantum/classical molecular dynamics simulations of the proton transfer reactions catalyzed by ketosteroid isomerase: analysis of hydrogen bonding, conformational motions, and electrostatics. 2009 , 48, 10608-19	32
1457	Computational structure activity relationship studies on the CD1d/glycolipid/TCR complex using AMBER and AUTODOCK. 2009 , 49, 410-23	12

1456	Entropic cost of protein-ligand binding and its dependence on the entropy in solution. 2009 , 113, 5871-84	53
1455	Charge equilibration force fields for lipid environments: applications to fully hydrated DPPC bilayers and DMPC-embedded gramicidin A. 2009 , 113, 9183-96	40
1454	Cluster hydration model for binding energy calculations of protein-ligand complexes. 2009 , 113, 809-17	19
1453	E-novo: an automated workflow for efficient structure-based lead optimization. 2009 , 49, 1797-809	31
1452	Specificity of ion-protein interactions: complementary and competitive effects of tetrapropylammonium, guanidinium, sulfate, and chloride ions. 2009 , 113, 3227-34	60
1451	Hydrogen bonding in ortho-substituted arylamides: the influence of protic solvents. 2009 , 113, 7041-4	19
1450	Crystal structures of constitutive nitric oxide synthases in complex with de novo designed inhibitors. 2009 , 52, 2060-6	18
1449	Predictions of hydration free energies from all-atom molecular dynamics simulations. 2009 , 113, 4533-7	76
1448	A combined crystallographic and molecular dynamics study of cathepsin L retrobinding inhibitors. 2009 , 52, 6335-46	10
1447	Polarization effects in molecular mechanical force fields. 2009 , 21, 333102	192
1446	Binding ensemble profiling with photoaffinity labeling (BProFL) approach: mapping the binding poses of HDAC8 inhibitors. 2009 , 52, 7003-13	39
1445	1,2-dichloroethane in haloalkane dehalogenase protein and in water solvent: a case study of the confinement effect on structural and dynamical properties. 2009 , 113, 3257-63	8
1444	Synergistic regulation and ligand-induced conformational changes of tryptophan synthase. 2009 , 48, 9921-31	21
1443	Role of dynamic flexibility in computing solvatochromic properties of dye-solvent systems: o-betaine in water. 2009 , 113, 2572-7	27
1442	Exploring complex protein-ligand recognition mechanisms with coarse metadynamics. 2009 , 113, 4807-16	61
1441	Free energies and entropies of water molecules at the inhibitor-protein interface of DNA gyrase. 2009 , 131, 6608-13	36
1440	Ab Initio Raman Spectra of β -Lactamase Inhibitor Intermediates Bound to E166A SHV β -Lactamase. 2009 , 5, 2158-72	12
1439	Oriental dynamics of transient molecules measured by nonequilibrium two-dimensional infrared spectroscopy. 2009 , 113, 8907-16	29

1438	Theoretical studies on inclusion complexes of cyclodextrins. 2009 , 113, 9533-42	30
1437	Catalytic Mechanism of Diaminopimelate Epimerase: A QM/MM Investigation. 2009 , 5, 1915-30	11
1436	Improved Hydrogen Bonding at the NDDO-Type Semiempirical Quantum Mechanical/Molecular Mechanical Interface. 2009 , 5, 2206-11	18
1435	Intramolecular hydrogen bonding in ortho-substituted arylamide oligomers: a computational and experimental study of ortho-fluoro- and ortho-chloro-N-methylbenzamides. 2009 , 113, 12809-15	24
1434	Molecular dynamical approach to the conformational transition in peptide nanorings and nanotubes. 2009 , 113, 1473-84	9
1433	The energy gap as a universal reaction coordinate for the simulation of chemical reactions. 2009 , 113, 7867-73	34
1432	Modulation of catalytic function by differential plasticity of the active site: case study of Trypanosoma cruzi trans-sialidase and Trypanosoma rangeli sialidase. 2009 , 48, 3398-406	28
1431	The cluster of hydrophobic residues controls the entrance to the active site of choline oxidase. 2009 , 48, 9599-605	24
1430	Validation of all-atom phosphatidylcholine lipid force fields in the tensionless NPT ensemble. 2009 , 1788, 638-49	37
1429	Insight into estrogenicity of phytoestrogens using in silico simulation. 2009 , 379, 139-44	10
1428	A short guide for molecular dynamics simulations of RNA systems. 2009 , 47, 187-97	60
1427	Insights into the enzymatic mechanism of 6-phosphogluconolactonase from Trypanosoma brucei using structural data and molecular dynamics simulation. 2009 , 388, 1009-21	12
1426	Ligand entry and exit pathways in the beta2-adrenergic receptor. 2009 , 392, 1102-15	80
1425	Binding modes of thioflavin-T to the single-layer beta-sheet of the peptide self-assembly mimics. 2009 , 394, 627-33	104
1424	Halogen bonding--a novel interaction for rational drug design?. 2009 , 52, 2854-62	485
1423	Solution structure of a covalently bound pyrrolo[2,1-c][1,4]benzodiazepine-benzimidazole hybrid to a 10mer DNA duplex. 2009 , 48, 12223-32	13
1422	Influence of local sequence context on damaged base conformation in human DNA polymerase iota: molecular dynamics studies of nucleotide incorporation opposite a benzo[a]pyrene-derived adenine lesion. 2009 , 37, 7095-109	15
1421	Understanding the mechanism of drug resistance due to a codon deletion in protoporphyrinogen oxidase through computational modeling. 2009 , 113, 4865-75	43

1420	Selective recognition of tetrahedral dianions by a hexaaza cryptand receptor. 2009 , 7, 4661-73	58
1419	Synthesis and structure-activity relationships of cyanoguanidine-type and structurally related histamine H4 receptor agonists. 2009 , 52, 6297-313	57
1418	Binding regularities in complexes of transcription factors with operator DNA: homeodomain family. 2009 , 26, 687-700	9
1417	Computational modeling of structurally conserved cancer mutations in the RET and MET kinases: the impact on protein structure, dynamics, and stability. 2009 , 96, 858-74	39
1416	Analysis of the interaction of the nucleotide base with myosin and the effect on substrate efficacy. 2009 , 97, 1952-60	1
1415	Tetracycline-tet repressor binding specificity: insights from experiments and simulations. 2009 , 97, 2829-38	13
1414	The properties of water: insights from quantum simulations. 2009 , 113, 5702-19	187
1413	Benzothiopyranoindole-based antiproliferative agents: synthesis, cytotoxicity, nucleic acids interaction, and topoisomerases inhibition properties. 2009 , 52, 5429-41	27
1412	Molecular dynamics study of a polymeric reverse osmosis membrane. 2009 , 113, 10177-82	111
1411	Nanosecond to submillisecond dynamics in dye-labeled single-stranded DNA, as revealed by ensemble measurements and photon statistics at single-molecule level. 2009 , 113, 13917-25	27
1410	Anion recognition by a macrobicycle based on a tetraoxadiazia macrocycle and an isophthalamide head unit. 2009 , 74, 4819-27	35
1409	SINGLE-MOLECULE DNA CONDUCTANCE IN WATER SOLUTIONS: ROLE OF EXPLICIT WATER COUNTERION SHEATH AND CHEMICAL MODIFICATION OF NUCLEOBASES. 2009 , 04, 231-243	3
1408	Conformational study of the PCU cage mono-peptide: a key role of some force-field parameters. 2009 , 113, 5234-8	
1407	Paramagnetic perturbation of the ¹⁹ F NMR chemical shift in fluorinated cysteine by O ₂ : a theoretical study. 2009 , 113, 10916-22	4
1406	Prediction of spin-spin coupling constants in solution based on combined density functional theory/molecular mechanics. 2009 , 130, 134508	46
1405	Steered molecular dynamics simulations reveal the likelier dissociation pathway of imatinib from its targeting kinases c-Kit and Abl. 2009 , 4, e8470	37
1404	High-Level ab Initio Calculations To Improve Protein Backbone Dihedral Parameters. 2009 , 5, 1155-65	45
1403	Solvent dependence on bond length alternation and charge distribution in phenol blue: a Car-Parrinello molecular dynamics investigation. 2009 , 113, 4833-9	21

1402	Molecular simulation of electric double-layer capacitors based on carbon nanotube forests. 2009 , 131, 12373-6	109
1401	Quantum mechanics/molecular mechanics studies on the sulfoxidation of dimethyl sulfide by compound I and compound 0 of cytochrome P450: which is the better oxidant?. 2009 , 113, 11635-42	49
1400	Parallel Genetic Algorithms for Crystal Structure Prediction: Successes and Failures in Predicting Bicalutamide Polymorphs. 2009 , 120-129	
1399	Molecular dynamics simulations on the stability and assembly mechanisms of quadruple and double helical aromatic amide foldamers. 2009 , 113, 10934-41	5
1398	Copper-1,10-phenanthroline complexes binding to DNA: structural predictions from molecular simulations. 2009 , 113, 10881-90	69
1397	Conformational free energy surface of alpha-N-acetylneuraminic acid: an interplay between hydrogen bonding and solvation. 2009 , 113, 9589-94	29
1396	Importance of dispersion and electron correlation in ab initio protein folding. 2009 , 113, 5290-300	61
1395	Predictions of binding for dopamine D2 receptor antagonists by the SIE method. 2009 , 49, 2369-75	22
1394	Solution structure and thermodynamics of 2',5' RNA intercalation. 2009 , 131, 5831-8	17
1393	Molecular basis of inactive B-RAF(WT) and B-RAF(V600E) ligand inhibition, selectivity and conformational stability: an in silico study. 2009 , 6, 144-57	15
1392	Validating CHARMM parameters and exploring charge distribution rules in structure-based drug design. 2009 , 5, 1680-1691	10
1391	WISDOM-II: screening against multiple targets implicated in malaria using computational grid infrastructures. 2009 , 8, 88	22
1390	Synthesis of new serotonin 5-HT7 receptor ligands. Determinants of 5-HT7/5-HT1A receptor selectivity. 2009 , 52, 2384-92	44
1389	Association of a weakly acidic anti-inflammatory drug (ibuprofen) with a poly(amidoamine) dendrimer as studied by molecular dynamics simulations. 2009 , 113, 10984-93	71
1388	Dynamic behavior of avian influenza A virus neuraminidase subtype H5N1 in complex with oseltamivir, zanamivir, peramivir, and their phosphonate analogues. 2009 , 49, 2323-32	46
1387	The influence of protein dynamics on the success of computational enzyme design. 2009 , 131, 14111-5	52
1386	Toward understanding the conformational dynamics of RNA ligation. 2009 , 48, 709-19	11
1385	Characterizing loop dynamics and ligand recognition in human- and avian-type influenza neuraminidases via generalized born molecular dynamics and end-point free energy calculations. 2009 , 131, 4702-9	117

1384	In silico fragment screening by replica generation (FSRG) method for fragment-based drug design. 2009 , 49, 925-33	16
1383	Mixed Quantum Classical Simulations of Electronic Excitation Energy Transfer and Related Optical Spectra: Supramolecular Pheophorbide β Complexes in Solution. 2009 , 35-71	1
1382	A Multiscale Treatment of Angeli's Salt Decomposition. 2009 , 5, 37-46	11
1381	Molecular insights on the two fluorescence lifetimes displayed by warfarin from fluorescence anisotropy and molecular dynamics studies. 2009 , 113, 7945-9	16
1380	Molecular dynamics simulations of polyamidoamine dendrimers and their complexes with linear poly(ethylene oxide) at different pH conditions: static properties and hydrogen bonding. 2009 , 11, 10017-28	44
1379	Large-scale application of high-throughput molecular mechanics with Poisson-Boltzmann surface area for routine physics-based scoring of protein-ligand complexes. 2009 , 52, 3159-65	77
1378	Structure and dynamics of monomer-template complexation: an explanation for molecularly imprinted polymer recognition site heterogeneity. 2009 , 131, 13297-304	98
1377	UV-vis spectra of the anticancer camptothecin family drugs in aqueous solution: specific spectroscopic signatures unraveled by a combined computational and experimental study. 2009 , 113, 5369-75	35
1376	Massively parallel computation of absolute binding free energy with well-equilibrated states. 2009 , 79, 021914	70
1375	Binding free energy calculations of adenosine deaminase inhibitor and the effect of methyl substitution in inhibitors. 2009 , 49, 615-22	2
1374	Quantitative prediction of fold resistance for inhibitors of EGFR. 2009 , 48, 8435-48	61
1373	Computations of Absolute Solvation Free Energies of Small Molecules Using Explicit and Implicit Solvent Model. 2009 , 5, 919-30	125
1372	Interlocked host anion recognition by an indolocarbazole-containing [2]rotaxane. 2009 , 131, 4937-52	66
1371	Solvent dependence of conformational distribution, molecular geometry, and electronic structure in adenosine. 2009 , 113, 1012-21	13
1370	An explicit solvent quantum chemistry study on the water environment influence on the interactions of fluoride with phenol. 2009 , 33, 831	4
1369	X-ray reflectometry studies on the effect of water on the surface structure of [C4mpyr][NTf2] ionic liquid. 2009 , 11, 11507-14	38
1368	Hydration of diazoles in water solution: pyrazole. A theoretical and X-ray diffraction study. 2009 , 11, 9431-9	8
1367	Solvation shell structure of cyclooctylpyranone in water solvent and its comparative structure, dynamics and dipole moment in HIV protease. 2009 , 11, 6482-9	2

1366	A novel biomimetic photochemical switch at work: design of a photomodulable peptide. 2009 , 8, 1639-49	12
1365	Diazo transfer-click reaction route to new, lipophilic teicoplanin and ristocetin aglycon derivatives with high antibacterial and anti-influenza virus activity: an aggregation and receptor binding study. 2009 , 52, 6053-61	34
1364	Protein-ligand binding free energy calculation by the Smooth Reaction Path Generation (SRPG) Method. 2009 , 49, 1944-51	22
1363	Stabilizing unusual conformations in small peptides and glucopeptides using a hydroxylated cyclobutane amino acid. 2009 , 7, 2885-93	12
1362	Isaindigotone derivatives: a new class of highly selective ligands for telomeric G-quadruplex DNA. 2009 , 52, 2825-35	75
1361	Small molecule hydration free energies in explicit solvent: An extensive test of fixed-charge atomistic simulations. 2009 , 5, 350-358	279
1360	Standard Free Energy of Binding from a One-Dimensional Potential of Mean Force. 2009 , 5, 909-18	144
1359	A combined theoretical and experimental study of the ammonia tunnel in carbamoyl phosphate synthetase. 2009 , 131, 10211-9	28
1358	Molecular Simulation of Cross-Linked Epoxy and EpoxyBOSS Nanocomposite. 2009 , 42, 4319-4327	147
1357	Molecular dynamics and quantum chemistry study on conformations and optical properties of hydrogen bonded dipolar merocyanine dyes. 2009 , 113, 10271-6	12
1356	Discovery of potent thermolysin inhibitors using structure based virtual screening and binding assays. 2009 , 52, 48-61	26
1355	ONIOM Study of the Mechanism of the Enzymatic Hydrolysis of Biodegradable Plastics. 2009 , 82, 338-346	4
1354	Serum albumin complexation of acetylsalicylic acid metabolites. 2009 , 10, 448-58	5
1353	Protein Flexibility in In Silico Screening. 2010 , 867-887	
1352	Impact of human leukocyte antigen-B*51-restricted cytotoxic T-lymphocyte pressure on mutation patterns of nonnucleoside reverse transcriptase inhibitor resistance. 2010 , 24, F15-22	9
1351	[In-silico approaches for fragment-based drug design]. 2010 , 130, 349-54	0
1350	Communication: Direct observation of a hydrophobic bond in loop closure of a capped (-OCH ₂ CH ₂ -) _n oligomer in water. 2010 , 133, 231102	8
1349	Computational study of the three-dimensional structure of N-acetyltransferase 2-acetyl coenzyme a complex. 2010 , 33, 1639-43	4

1348	Bioinformatic search for plant homologs of the protein kinase Bub1 β key component of the mitotic spindle assembly checkpoint. 2010 , 44, 376-388	4
1347	Symmetrical bisbenzimidazoles with benzenediyl spacer: the role of the shape of the ligand on the stabilization and structural alterations in telomeric G-quadruplex DNA and telomerase inhibition. 2010 , 21, 1148-59	51
1346	Simulating POPC and POPC/POPG Bilayers: Conserved Packing and Altered Surface Reactivity. 2010 , 6, 3267-73	71
1345	Cyclobutane amino acid analogues of furanomycin obtained by a formal [2 + 2] cycloaddition strategy promoted by methylaluminumoxane. 2010 , 75, 545-52	24
1344	Vinblastine perturbation of tubulin protofilament structure: a computational insight. 2010 , 12, 15530-6	9
1343	Inclusion of carboxyl function inside of cucurbiturils and its use in molecular switches. 2010 , 5, 2386-92	11
1342	Prediction of Absolute Solvation Free Energies using Molecular Dynamics Free Energy Perturbation and the OPLS Force Field. 2010 , 6, 1509-19	959
1341	Gatekeeper mutations mediate resistance to BRAF-targeted therapies. 2010 , 2, 35ra41	127
1340	Working mechanism for a redox switchable molecular machine based on cyclodextrin: a free energy profile approach. 2010 , 114, 6561-6	44
1339	Molecular dynamics simulations of structure and dynamics of organic molecular crystals. 2010 , 12, 14916-29	43
1338	Field-Induced Transport in Sulfonated Poly(styrene-co-divinylbenzene) Membranes. 2010 , 43, 10521-10527	11
1337	Quantum Chemistry Calculations Provide Support to the Mechanism of the Light-Induced Structural Changes in the Flavin-Binding Photoreceptor Proteins. 2010 , 6, 2293-302	36
1336	Molecular dynamics study of a heteroditopic-calix[4]diquinone-assisted transfer of KCl and dopamine through a water-chloroform liquid-liquid interface. 2010 , 114, 11173-80	10
1335	Update of the CHARMM all-atom additive force field for lipids: validation on six lipid types. 2010 , 114, 7830-43	2654
1334	Practical considerations for building GROMOS-compatible small-molecule topologies. 2010 , 50, 2221-35	154
1333	Rationalizing perhydrolase activity of aryl-esterase and subtilisin Carlsberg mutants by molecular dynamics simulations of the second tetrahedral intermediate state. 2010 , 125, 375-386	9
1332	Factors influencing the binding of a potassium cation to a polyethylene glycol type podand in liquid-liquid extraction β molecular dynamics study. 2010 , 127, 681-687	5
1331	Asymmetric synthesis of (S)-3-chloro-1-phenyl-1-propanol using <i>Saccharomyces cerevisiae</i> reductase with high enantioselectivity. 2010 , 87, 185-93	25

1330	GROW: A gradient-based optimization workflow for the automated development of molecular models. 2010 , 181, 499-513	39
1329	Assessment of numerical optimization algorithms for the development of molecular models. 2010 , 181, 887-905	25
1328	Theoretical study on the absorption maxima of real GFPs. 2010 , 484, 324-329	8
1327	Some insights into mechanism for binding and drug resistance of wild type and I50V V82A and I84V mutations in HIV-1 protease with GRL-98065 inhibitor from molecular dynamic simulations. 2010 , 45, 227-35	30
1326	Investigating the structural basis of arylamides to improve potency against M. tuberculosis strain through molecular dynamics simulations. 2010 , 45, 5585-93	41
1325	Recognition of selected monosaccharides by Pseudomonas aeruginosa Lectin II analyzed by molecular dynamics and free energy calculations. 2010 , 345, 1432-41	17
1324	Evaluation of the binding ability of a macrobicyclic receptor for anions by potentiometry and molecular dynamics simulations in solution. 2010 , 66, 8714-8721	7
1323	Pyridine-containing chiral macrocycles for the enantioselective recognition of amino acid derivatives and their molecular dynamics simulations. 2010 , 21, 990-996	9
1322	Insight into ligand selectivity in HCV NS5B polymerase: molecular dynamics simulations, free energy decomposition and docking. 2010 , 16, 49-59	18
1321	Hemolytic mechanism of dioscin proposed by molecular dynamics simulations. 2010 , 16, 107-18	41
1320	Homology modeling of Mycobacterium tuberculosis 2C-methyl-D-erythritol-4-phosphate cytidyltransferase, the third enzyme in the MEP pathway for isoprenoid biosynthesis. 2010 , 16, 1061-73	6
1319	An improved generalized AMBER force field (GAFF) for urea. 2010 , 16, 1427-40	54
1318	Effects of the V82A and I54V mutations on the dynamics and ligand binding properties of HIV-1 protease. 2010 , 16, 1577-83	11
1317	Investigating reaction pathways in rare events simulations of antibiotics diffusion through protein channels. 2010 , 16, 1701-8	12
1316	Three applications of path integrals: equilibrium and kinetic isotope effects, and the temperature dependence of the rate constant of the [1,5] sigmatropic hydrogen shift in (Z)-1,3-pentadiene. 2010 , 16, 1779-87	17
1315	Reactivity versus steric effects in fluorinated ketones as esterase inhibitors: a quantum mechanical and molecular dynamics study. 2010 , 16, 1753-64	8
1314	Effect of the Enhanced Cyan Fluorescent Protein framework on the UV/visible absorption spectra of some chromophores. 2010 , 2, 38-47	25
1313	Insight into herbicide resistance of W574L mutant Arabidopsis thaliana acetohydroxyacid synthase: molecular dynamics simulations and binding free energy calculations. 2010 , 53, 91-102	8

1312	Molecular dynamics simulations exploring drug resistance in HIV-1 proteases. 2010 , 55, 2677-2683	6
1311	A computational workflow for the design of irreversible inhibitors of protein kinases. 2010 , 24, 183-94	9
1310	Predictions of hydration free energies from continuum solvent with solute polarizable models: the SAMPL2 blind challenge. 2010 , 24, 361-72	8
1309	Prediction of tautomer ratios by embedded-cluster integral equation theory. 2010 , 24, 343-53	30
1308	Rapid prediction of solvation free energy. 3. Application to the SAMPL2 challenge. 2010 , 24, 373-83	15
1307	Tautomers and reference 3D-structures: the orphans of in silico drug design. 2010 , 24, 605-11	12
1306	Predicting hydration free energies using all-atom molecular dynamics simulations and multiple starting conformations. 2010 , 24, 307-16	85
1305	Prediction of protein-ligand binding affinity by free energy simulations: assumptions, pitfalls and expectations. 2010 , 24, 639-58	198
1304	A computational analysis of the binding model of MDM2 with inhibitors. 2010 , 24, 687-97	30
1303	Dependency of ligand free energy landscapes on charge parameters and solvent models. 2010 , 24, 699-712	6
1302	Modeling of the mechanism of hydrolysis of succinylcholine in the active site of native and modified (Asp70Gly) human butyrylcholinesterase. 2010 , 59, 55-60	5
1301	Interaction of manzamine A with glycogen synthase kinase 3 α molecular dynamics study. 2010 , 59, 1983-1993	8
1300	Oxidation of human cytochrome P450 1A2 substrates by <i>Bacillus megaterium</i> cytochrome P450 BM3. 2010 , 63, 179-187	20
1299	Inhibitory effect of quercetin on matrix metalloproteinase 9 activity molecular mechanism and structure-activity relationship of the flavonoid-enzyme interaction. 2010 , 644, 138-45	48
1298	Dual role of FMN in flavodoxin function: electron transfer cofactor and modulation of the protein-protein interaction surface. 2010 , 1797, 262-71	16
1297	Correlation between the substrate structure and the rate of acetylcholinesterase hydrolysis modeled with the combined quantum mechanical/molecular mechanical studies. 2010 , 187, 59-63	4
1296	Experimental and computational determination of tRNA dynamics. 2010 , 584, 376-86	56
1295	Molecular Dynamics Simulation of HIV-1 Integrase Dimer Complexed with Viral DNA. 2010 , 28, 33-40	7

1294	Discovery of potent vascular endothelial growth factor receptor-2 inhibitors. 2010 , 5, 118-29		8
1293	Interaction of the sigma(2) receptor ligand PB28 with the human nucleosome: computational and experimental probes of interaction with the H2A/H2B dimer. 2010 , 5, 268-73		28
1292	Novel monocyclam derivatives as HIV entry inhibitors: Design, synthesis, anti-HIV evaluation, and their interaction with the CXCR4 co-receptor. 2010 , 5, 1272-81		16
1291	Understanding the key factors that control the inhibition of type II dehydroquinase by (2R)-2-benzyl-3-dehydroquinic acids. 2010 , 5, 1726-33		20
1290	On the reliability of the AMBER force field and its empirical dispersion contribution for the description of noncovalent complexes. 2010 , 11, 2399-408		29
1289	A new force field for simulating phosphatidylcholine bilayers. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1117-25	3.5	261
1288	A toolkit to assist ONIOM calculations. <i>Journal of Computational Chemistry</i> , 2010 , 31, 2363-9	3.5	42
1287	Incorporation of deMon2k as a new parallel quantum mechanical code for the PUPIL system. <i>Journal of Computational Chemistry</i> , 2010 , 31, 2669-76	3.5	4
1286	Less is more when simulating unsulfated glycosaminoglycan 3D-structure: comparison of GLYCAM06/TIP3P, PM3-CARB1/TIP3P, and SCC-DFTB-D/TIP3P predictions with experiment. <i>Journal of Computational Chemistry</i> , 2010 , 31, 2932-47	3.5	24
1285	A Novel Water-Soluble Hexanuclear Bismuth Oxido Cluster Synthesis, Structure and Complexation with Polyacrylate. 2010 , 2010, 4763-4769		37
1284	Multimeric lactoside "click clusters" as tools to investigate the effect of linker length in specific interactions with peanut lectin, galectin-1, and -3. 2010 , 11, 1430-42		38
1283	Antimicrobial peptides and their superior fluorinated analogues: structure-activity relationships as revealed by NMR spectroscopy and MD calculations. 2010 , 11, 2424-32		6
1282	PAMAM dendrimers for siRNA delivery: computational and experimental insights. 2010 , 16, 7781-95		83
1281	Sodium effect on self-organization of amphiphilic carboxylates: formation of structured micelles and superlattices. 2010 , 16, 9544-54		18
1280	Synthesis and molecular modelling of double-functionalised nucleosides with aromatic moieties in the 5'-(S)-position and minor groove interactions in DNA zipper structures. 2010 , 16, 12904-19		19
1279	Rotaxanes capable of recognising chloride in aqueous media. 2010 , 16, 13082-94		55
1278	Insight into the stability of cross-beta amyloid fibril from molecular dynamics simulation. 2010 , 93, 578-86		15
1277	Characterization of a clinical polymer-drug conjugate using multiscale modeling. 2010 , 93, 936-51		19

1276	Calculation of the standard binding free energy of sparsomycin to the ribosomal peptidyl-transferase P-site using molecular dynamics simulations with restraining potentials. 2010 , 23, 128-41	13
1275	Comparison of the complexation between methylprednisolone and different cyclodextrins in solution by 1H-NMR and molecular modeling studies. 2010 , 99, 3863-73	20
1274	NAD(+) -dependent histone deacetylases (sirtuins) as novel therapeutic targets. 2010 , 30, 861-89	69
1273	'tieredScreen' - Layered Virtual Screening Tool for the Identification of Novel Estrogen Receptor Alpha Modulators. 2010 , 29, 421-30	6
1272	Rigorous Free Energy Calculations in Structure-Based Drug Design. 2010 , 29, 570-8	60
1271	Asymmetric synthesis of (S)-ethyl-4-chloro-3-hydroxy butanoate using a <i>Saccharomyces cerevisiae</i> reductase: enantioselectivity and enzyme-substrate docking studies. 2010 , 1804, 1841-9	12
1270	Electrophoresis of neutral oil in water. 2010 , 352, 223-31	23
1269	The morphology of integrated self-assembled monolayers and their impact on devices \square computational and experimental approach. 2010 , 11, 1476-1482	42
1268	Structural comparison of mu-opioid receptor selective peptides confirmed four parameters of bioactivity. 2010 , 28, 495-505	35
1267	Ensemble-based virtual screening reveals dual-inhibitors for the p53-MDM2/MDMX interactions. 2010 , 28, 555-68	50
1266	An evaluation of the GLYCAM06 and MM3 force fields, and the PM3-D* molecular orbital method for modelling prototype carbohydrate-aromatic interactions. 2010 , 29, 321-5	13
1265	QM methods in structure based design: utility in probing protein-ligand interactions. 2010 , 29, 507-17	5
1264	Study of the inclusion of the (R)- and (S)-camphor enantiomers in alpha-cyclodextrin by X-ray crystallography and molecular dynamics. 2010 , 345, 1034-40	15
1263	A synthetic and in silico study on the highly regioselective Diels-Alder reaction of the polyenic antifungal antibiotics natamycin and flavofungin. 2010 , 51, 4968-4971	2
1262	A comparative molecular dynamics study on the complexation of alkali metal cations by a poly-ethylene-glycol type podand in water and in dichloromethane. 2010 , 946, 77-82	8
1261	Examining the potency of suggested inhibitors for the phosphatase activity of the human soluble epoxide hydrolase by molecular dynamics simulations. 2010 , 944, 97-104	2
1260	Small-molecule ligands of GD2 ganglioside, designed from NMR studies, exhibit induced-fit binding and bioactivity. 2010 , 17, 183-94	11
1259	A harmonic approximation of intramolecular vibrations in a mixed quantum-classical methodology: Linear absorbance of a dissolved Pheophorbid-a molecule as an example. 2010 , 377, 10-14	15

1258	Pyrazolone-fused combretastatins and their precursors: synthesis, cytotoxicity, antitubulin activity and molecular modeling studies. 2010 , 18, 2375-87	34
1257	On the inhibition of histone deacetylase 8. 2010 , 18, 4103-10	70
1256	Synthesis, DNA-binding ability and anticancer activity of benzothiazole/benzoxazole-pyrrolo[2,1-c][1,4]benzodiazepine conjugates. 2010 , 18, 4747-61	91
1255	Formation of Schiff-base for photoreaction mechanism of red shift of GFP spectra. 2010 , 147, 140-5	5
1254	GROMOS96 43a1 performance in predicting oligosaccharide conformational ensembles within glycoproteins. 2010 , 345, 663-71	44
1253	Parameter determination for the charge equilibration method including third- and fourth-order terms applied to non-metallic compounds. 2010 , 495, 155-159	6
1252	Phase solubility, ¹ H NMR and molecular modelling studies of bupivacaine hydrochloride complexation with different cyclodextrin derivatives. 2010 , 500, 347-354	20
1251	Molecular modeling study of binding site selectivity of TQMP to G-quadruplex DNA. 2010 , 45, 983-91	15
1250	Investigation and improvement of DNA cleavage models of polyamide + Cu(II) nuclease + OOH-ligands bound to DNA. 2010 , 10, 35	3
1249	T-cell epitope prediction and immune complex simulation using molecular dynamics: state of the art and persisting challenges. 2010 , 6 Suppl 2, S4	22
1248	Computational Modeling of Human Paraoxonase 1: Preparation of Protein Models, Binding Studies, and Mechanistic Insights. 2010 , 23, 357-369	17
1247	Application of nonlinear dimensionality reduction to characterize the conformational landscape of small peptides. 2010 , 78, 223-35	47
1246	Improving computational protein design by using structure-derived sequence profile. 2010 , 78, 2338-48	20
1245	Structural facets of disease-linked human prion protein mutants: a molecular dynamic study. 2010 , 78, 3270-80	41
1244	Predicting the binding affinity of epitope-peptides with HLA-A*0201 by encoding atom-pair non-covalent interaction information between receptor and ligands. 2010 , 75, 597-606	5
1243	Molecular dynamics simulations of 2-amino-6-arylsulphonylbenzotrioles analogues as HIV inhibitors: interaction modes and binding free energies. 2010 , 76, 518-26	35
1242	Atomic force field FFsol for calculating molecular interactions in water environment. 2010 , 44, 303-316	6
1241	GUI-BioPASED: A program for molecular dynamics simulations of biopolymers with a graphical user interface. 2010 , 44, 648-654	21

1240	Lead generation and optimization based on protein-ligand complementarity. 2010 , 15, 4382-400	7
1239	Insights in 17beta-HSD1 enzyme kinetics and ligand binding by dynamic motion investigation. 2010 , 5, e12026	18
1238	Free-energy calculations in structure-based drug design. 61-86	58
1237	Impact of the DRY motif and the missing "ionic lock" on constitutive activity and G-protein coupling of the human histamine H4 receptor. 2010 , 333, 382-92	48
1236	GPU acceleration of Dock6's Amber scoring computation. 2010 , 680, 497-511	7
1235	Combination of V106I and V179D polymorphic mutations in human immunodeficiency virus type 1 reverse transcriptase confers resistance to efavirenz and nevirapine but not etravirine. 2010 , 54, 1596-602	21
1234	QM and QM/MM Approaches to Evaluating Binding Affinities. 2010 , 725-752	1
1233	A crystallographic and modelling study of a human telomeric RNA (TERRA) quadruplex. 2010 , 38, 5569-80	179
1232	Stapled peptides in the p53 pathway: computer simulations reveal novel interactions of the staples with the target protein. 2010 , 9, 4560-8	43
1231	Molecular determinants of ligand binding to H4R species variants. 2010 , 77, 734-43	50
1230	Microscopic structures and dynamics of high- and low-density liquid trans-1,2-dichloroethylene. 2010 , 81,	14
1229	New potent dual inhibitors of CK2 and Pim kinases: discovery and structural insights. 2010 , 24, 3171-85	47
1228	Theoretical studies on the interaction of guanine riboswitch with guanine and its closest analogues. 2010 , 36, 929-938	4
1227	X-ray structure and mechanism of RNA polymerase II stalled at an antineoplastic monofunctional platinum-DNA adduct. 2010 , 107, 9584-9	105
1226	DOCKING AND MD SIMULATIONS OF THE INTERACTION OF THE POTASSIUM-SPARING DIURETIC AGENT AMILORIDE WITH THE hASIC1a CHANNEL USING A HOMOLGY MODEL. 2010 , 09, 365-378	2
1225	A Bayesian Optimization Algorithm for De Novo ligand design based docking running over GPU. 2010 ,	1
1224	Theory of docking scores and its application to a customizable scoring function. 2010 , 21, 547-58	6
1223	Molecular dynamics simulations of Ac-3Aib-Cage-3Aib-NHMe. 2010 , 36, 1035-1044	9

1222	Conformational transitions upon ligand binding: holo-structure prediction from apo conformations. 2010 , 6, e1000634	85
1221	The role of oligomerization and cooperative regulation in protein function: the case of tryptophan synthase. 2010 , 6, e1000994	31
1220	Functional rotation of the transporter AcrB: insights into drug extrusion from simulations. 2010 , 6, e1000806	70
1219	Hydration of cyanin dyes. 2010 , 132, 114304	8
1218	Quantum mechanics based force field for carbon (QMFF-Cx) validated to reproduce the mechanical and thermodynamics properties of graphite. 2010 , 133, 134114	16
1217	Dynamical effects in ab initio NMR calculations: classical force fields fitted to quantum forces. 2010 , 133, 084109	35
1216	Watching solvent friction impede ultrafast barrier crossings: a direct test of Kramers theory. 2010 , 133, 174506	44
1215	Activation of integrins by urea in perfused rat liver. 2010 , 285, 29348-56	13
1214	Characterisation of the effect of electrostatic interaction on the structure of Trp-cage using molecular dynamics simulation. 2010 , 36, 1086-1095	
1213	Deciphering the role of glucosamine-6-phosphate in the riboswitch action of glmS ribozyme. 2010 , 16, 2455-63	42
1212	Accurate calculations of the hydration free energies of druglike molecules using the reference interaction site model. 2010 , 133, 044104	43
1211	Studies of benzothiadiazine derivatives as hepatitis C virus NS5B polymerase inhibitors using 3D-QSAR, molecular docking and molecular dynamics. 2010 , 17, 2788-803	37
1210	Towards accurate free energy calculations in ligand protein-binding studies. 2010 , 17, 767-85	116
1209	Computational study of the resistance shown by the subtype B/HIV-1 protease to currently known inhibitors. 2010 , 49, 4283-95	18
1208	Postprocessing of protein-ligand docking poses using linear response MM-PB/SA: application to Wee1 kinase inhibitors. 2010 , 50, 1574-88	26
1207	Grand canonical Monte Carlo studies of CO ₂ and CH ₄ adsorption in p-tert-butylcalix[4]arene. 2010 , 114, 5764-8	6
1206	Molecular Dynamics: Further Topics. 2010 , 463-517	0
1205	Diarylaniline derivatives as a distinct class of HIV-1 non-nucleoside reverse transcriptase inhibitors. 2010 , 53, 4906-16	38

1204	Structure and dynamics of the protic ionic liquid monomethylammonium nitrate ([CH ₃ NH ₃][NO ₃]) from ab initio molecular dynamics simulations. 2010 , 132, 124506	106
1203	Binding modes of flavones to human serum albumin: insights from experimental and computational studies. 2010 , 114, 12938-47	55
1202	Iterative saturation mutagenesis accelerates laboratory evolution of enzyme stereoselectivity: rigorous comparison with traditional methods. 2010 , 132, 9144-52	180
1201	Low Inhibiting Power of N ^ω -Methyl-L-tyrosine Based Peptidomimetic Compounds against HIV-1 Protease: Insights from a QM/MM Study. 2010 , 6, 1369-1379	8
1200	Accelerating Docking Amber Scoring with Graphic Processing Unit. 2010 , 404-415	1
1199	Systematic Derivation of AMBER Force Field Parameters Applicable to Zinc-Containing Systems. 2010 , 6, 1852-70	87
1198	Solvatochromic shift of phenol blue in water from a combined Car-Parrinello molecular dynamics hybrid quantum mechanics-molecular mechanics and ZINDO approach. 2010 , 132, 234508	24
1197	In silico identification of the potential drug resistance sites over 2009 influenza A (H1N1) virus neuraminidase. 2010 , 7, 894-904	55
1196	Synthesis, in vitro activity, and three-dimensional quantitative structure-activity relationship of novel hydrazine inhibitors of human vascular adhesion protein-1. 2010 , 53, 6301-15	23
1195	Molecular dynamics study on the interactions of porphyrin with two antiparallel human telomeric quadruplexes. 2010 , 114, 6216-24	15
1194	Improved united-atom force field for 1-alkyl-3-methylimidazolium chloride. 2010 , 114, 4572-82	68
1193	Benzimidazole derivatives as new serotonin 5-HT ₆ receptor antagonists. Molecular mechanisms of receptor inactivation. 2010 , 53, 1357-69	50
1192	Atomistic simulation of water percolation and proton hopping in Nafion fuel cell membrane. 2010 , 114, 13681-90	108
1191	Structural and dynamical properties of the porins OmpF and OmpC: insights from molecular simulations. 2010 , 22, 454125	28
1190	Charge transport simulations in conjugated dendrimers. 2010 , 114, 4388-93	37
1189	Backbone flexibility controls the activity and specificity of a protein-protein interface: specificity in snake venom metalloproteases. 2010 , 132, 10330-7	40
1188	Permeability of drugs and hormones through a lipid bilayer: insights from dual-resolution molecular dynamics. 2010 , 6, 3797	118
1187	Docking validation resources: protein family and ligand flexibility experiments. 2010 , 50, 1986-2000	120

- 1186 Arginine-assisted solubilization system for drug substances: solubility experiment and simulation. **2010**, 114, 13455-62 69
- 1185 Molecular Design of High Capacity, Low Viscosity, Chemically Tunable Ionic Liquids for CO₂ Capture. **2010**, 1, 3494-3499 335
- 1184 Flexibility of Catalytic Zinc Coordination in Thermolysin and HDAC8: A Born-Oppenheimer ab initio QM/MM Molecular Dynamics Study. **2009**, 6, 337 74
- 1183 Statistics and physical origins of pK and ionization state changes upon protein-ligand binding. **2010**, 98, 872-80 38
- 1182 Accounting for ligand conformational restriction in calculations of protein-ligand binding affinities. **2010**, 98, 901-10 37
- 1181 Mapping spatial relationships between residues in the ligand-binding domain of the 5-HT₃ receptor using a molecular ruler. **2010**, 98, 1847-55 9
- 1180 IGERS: inferring Gibbs energy changes of biochemical reactions from reaction similarities. **2010**, 98, 2478-86 11
- 1179 Long-timescale molecular-dynamics simulations of the major urinary protein provide atomistic interpretations of the unusual thermodynamics of ligand binding. **2010**, 99, 218-26 23
- 1178 Analysis of the bacterial luciferase mobile loop by replica-exchange molecular dynamics. **2010**, 99, 4012-9 18
- 1177 Dispersion dominated halogen- π interactions: energies and locations of minima. **2010**, 12, 14941-9 69
- 1176 The effects of perfluorination on carbohydrate- π interactions: computational studies of the interaction of benzene and hexafluorobenzene with fucose and cyclodextrin. **2010**, 12, 7959-67 23
- 1175 1-Alkyl-4-phenyl-6-alkoxy-1H-quinazolin-2-ones: a novel series of potent calcium-sensing receptor antagonists. **2010**, 53, 2250-63 28
- 1174 3'-[4-Aryl-(1,2,3-triazol-1-yl)]-3'-deoxythymidine analogues as potent and selective inhibitors of human mitochondrial thymidine kinase. **2010**, 53, 2902-12 30
- 1173 Oil/water transfer is partly driven by molecular shape, not just size. **2010**, 132, 234-40 41
- 1172 Cholic acid micelles--controlling the size of the aqueous cavity by PEGylation. **2010**, 12, 1589-94 12
- 1171 Accurate ensemble molecular dynamics binding free energy ranking of multidrug-resistant HIV-1 proteases. **2010**, 50, 890-905 70
- 1170 Molecular dynamics study of secretory phospholipase A₂ of Russell's viper and bovine pancreatic sources. **2010**, 114, 13463-72 8
- 1169 Role of aromatic rings in the molecular recognition of aminoglycoside antibiotics: implications for drug design. **2010**, 132, 12074-90 49

1168	Effects of structural fluctuations on two-photon absorption activity of interacting dipolar chromophores. 2010 , 114, 10814-20	19
1167	Computing Relative Free Energies of Solvation using Single Reference Thermodynamic Integration Augmented with Hamiltonian Replica Exchange. 2010 , 6, 3427-3441	20
1166	Crucial roles of the subnanosecond local dynamics of the flap tips in the global conformational changes of HIV-1 protease. 2010 , 114, 3060-9	26
1165	Finding a needle in the haystack: computational modeling of Mg ²⁺ binding in the active site of protein farnesyltransferase. 2010 , 49, 9658-66	15
1164	Interaction and dimerization energies in methyl-blocked alpha,gamma-peptide nanotube segments. 2010 , 114, 4973-83	31
1163	Modeling, preparation, and characterization of a dipole moment switch driven by Z/E photoisomerization. 2010 , 132, 9310-9	46
1162	Nonpolar Solvation Free Energies of Protein-Ligand Complexes. 2010 , 6, 3558-68	21
1161	Absolute binding free energy calculations of sparsomycin analogs to the bacterial ribosome. 2010 , 114, 9525-39	45
1160	Catalysis in the oil droplet/water interface for aromatic claisen rearrangement. 2010 , 114, 4325-33	21
1159	Determination of energies and sites of binding of PFOA and PFOS to human serum albumin. 2010 , 114, 14860-74	80
1158	Structural and energetic analysis on the complexes of clinically isolated subtype C HIV-1 proteases and approved inhibitors by molecular dynamics simulation. 2010 , 114, 521-30	29
1157	Molecular Dynamics of Methyl Viologen-Cucurbit[n]uril Complexes in Aqueous Solution. 2010 , 6, 984-992	40
1156	Using molecular dynamics to probe the structural basis for enhanced stability in thermal stable cytochromes P450. 2010 , 49, 6680-6	23
1155	Computational approach for understanding the interactions of UV-degradable dendrons with DNA and siRNA. 2010 , 114, 5686-93	35
1154	Carbamate transport in carbamoyl phosphate synthetase: a theoretical and experimental investigation. 2010 , 132, 3870-8	11
1153	Nitrile bonds as infrared probes of electrostatics in ribonuclease S. 2010 , 114, 13536-44	81
1152	Nuclear magnetic resonance structure of the prohead RNA E-loop hairpin. 2010 , 49, 5989-97	13
1151	Glutathione transferase classes alpha, pi, and mu: GSH activation mechanism. 2010 , 114, 12972-80	14

1150	Dominant conformation of valsartan in sodium dodecyl sulfate micelle environment. 2010 , 114, 2719-27	11
1149	Halogen-Ionic Bridges: Do They Exist in the Biomolecular World?. 2010 , 6, 2225-41	19
1148	Quantum mechanical pairwise decomposition analysis of protein kinase B inhibitors: validating a new tool for guiding drug design. 2010 , 50, 651-61	15
1147	Rare casbane diterpenoids from the Hainan soft coral <i>Sinularia depressa</i> . 2010 , 73, 133-8	62
1146	Magnetic resonance studies of a redox probe in a reverse sodium bis(2-ethylhexyl)sulfosuccinate/octane/water microemulsion. 2010 , 114, 12558-64	11
1145	Ion selectivity of alpha-hemolysin with beta-cyclodextrin adapter. II. Multi-ion effects studied with grand canonical Monte Carlo/Brownian dynamics simulations. 2010 , 114, 2901-9	36
1144	Modeling the adsorption behavior of linear end-functionalized poly(ethylene glycol) on an ionic substrate by a coarse-grained Monte Carlo approach. 2010 , 26, 15814-23	6
1143	Linear relationship between deformability and thermal stability of 2'-O-modified RNA hetero duplexes. 2010 , 114, 2517-24	17
1142	Unexpected binding modes of nitric oxide synthase inhibitors effective in the prevention of a cerebral palsy phenotype in an animal model. 2010 , 132, 5437-42	46
1141	Computational mutation scanning and drug resistance mechanisms of HIV-1 protease inhibitors. 2010 , 114, 9663-76	34
1140	Molecular Dynamics Study of Ionomer and Water Adsorption at Carbon Support Materials. 2010 , 114, 13739-13745	59
1139	Interfacial molecular organization at aqueous solution surfaces of atmospherically relevant dimethyl sulfoxide and methanesulfonic Acid using sum frequency spectroscopy and molecular dynamics simulation. 2010 , 114, 15546-53	32
1138	Nonadditive empirical force fields for short-chain linear alcohols: methanol to butanol. Hydration free energetics and Kirkwood-Buff analysis using charge equilibration models. 2010 , 114, 11076-92	42
1137	Molecular dynamics study of congruent melting of the equimolar ionic liquid-benzene inclusion crystal [emim][NTf(2)].C(6)H(6). 2010 , 132, 044507	11
1136	Selection of in silico drug screening results by using universal active probes (UAPs). 2010 , 50, 1233-40	7
1135	Conformational preferences of proline analogues with a fused benzene ring. 2010 , 114, 11761-70	15
1134	Amino-alcohol ligands: synthesis and structure of N,N'-bis(2-hydroxycyclopentyl)ethane-1,2-diamine and its salts, and an assessment of its fitness and that of related ligands for complexing metal ions. 2010 , 49, 8003-11	5
1133	Comparison of entropic contributions to binding in a "hydrophilic" versus "hydrophobic" ligand-protein interaction. 2010 , 132, 8682-9	41

1132	Transport Properties of Aqueous Solutions of (1R,2S)-(-) and (1S,2R)-(+)-Ephedrine Hydrochloride at Different Temperatures. 2010 , 55, 1145-1152	10
1131	Bovine chymosin: a computational study of recognition and binding of bovine kappa-casein. 2010 , 49, 2563-73	21
1130	Energetics of intercavity diffusion in a simple model of a low-density p-tert-butylcalix[4]arene crystal. 2010 , 132, 10996-7	7
1129	Electrostatic polarization makes a substantial contribution to the free energy of avidin-biotin binding. 2010 , 132, 5137-42	97
1128	Class I phospho-inositide-3-kinases (PI3Ks) isoform-specific inhibition study by the combination of docking and molecular dynamics simulation. 2010 , 50, 136-45	25
1127	Potent arylsulfonamide inhibitors of tumor necrosis factor-alpha converting enzyme able to reduce activated leukocyte cell adhesion molecule shedding in cancer cell models. 2010 , 53, 2622-35	35
1126	Ion selectivity of alpha-hemolysin with a beta-cyclodextrin adapter. I. Single ion potential of mean force and diffusion coefficient. 2010 , 114, 952-8	34
1125	Automated force field optimisation of small molecules using a gradient-based workflow package. 2010 , 36, 1182-1196	20
1124	Structural and conformational requisites in DNA quadruplex groove binding: another piece to the puzzle. 2010 , 132, 6425-33	102
1123	Molecular order in a chromonic liquid crystal: a molecular simulation study of the anionic azo dye sunset yellow. 2010 , 132, 7794-802	108
1122	Understanding the interactions of cellulose with ionic liquids: a molecular dynamics study. 2010 , 114, 4293-301	269
1121	Comparative Study of Force Fields for Molecular Dynamics Simulations of Glycine Crystal Growth from Solution. 2010 , 10, 5146-5158	40
1120	The R.E.D. tools: advances in RESP and ESP charge derivation and force field library building. 2010 , 12, 7821-39	631
1119	Light activation of rhodopsin: insights from molecular dynamics simulations guided by solid-state NMR distance restraints. 2010 , 396, 510-27	50
1118	Homology-modelling protein-ligand interactions: allowing for ligand-induced conformational change. 2010 , 399, 645-61	21
1117	Structural requirement for PPARgamma binding revealed by a meta analysis of holo-crystal structures. 2010 , 92, 499-506	4
1116	Genome scanning of Amazonian Plasmodium falciparum shows subtelomeric instability and clindamycin-resistant parasites. 2010 , 20, 1534-44	48
1115	Molecular Dynamics Simulations: Difficulties, Solutions and Strategies for Treating Metalloenzymes. 2010 , 299-330	10

1114	Rapid Prediction of Solvation Free Energy. 2. The First-Shell Hydration (FiSH) Continuum Model. 2010 , 6, 1622-37	27
1113	Rapid Prediction of Solvation Free Energy. 1. An Extensive Test of Linear Interaction Energy (LIE). 2010 , 6, 1608-21	12
1112	Tritopic phenanthroline and pyridine tail-tied aza-scorpiaids. 2010 , 8, 2367-76	19
1111	Accounting for polarization cost when using fixed charge force fields. II. Method and application for computing effect of polarization cost on free energy of hydration. 2010 , 114, 8631-45	29
1110	New insights into the structures of ligand-quadruplex complexes from molecular dynamics simulations. 2010 , 114, 15301-10	35
1109	Molecular characterization of the interaction between siRNA and PAMAM G7 dendrimers by SAXS, ITC, and molecular dynamics simulations. 2010 , 11, 3571-7	70
1108	An o-aminoanilide analogue of 1 α ,25-dihydroxyvitamin D(3) functions as a strong vitamin D receptor antagonist. 2010 , 53, 7461-5	21
1107	Probing interaction requirements in PTP1B inhibitors: a comparative molecular dynamics study. 2010 , 50, 1147-58	26
1106	A proton-shuttle reaction mechanism for histone deacetylase 8 and the catalytic role of metal ions. 2010 , 132, 9471-9	103
1105	Triplet Excitation Energy Transfer through Fluorene π Stack. 2010 , 114, 20236-20239	12
1104	Self-assembly of structurally persistent micelles is controlled by specific-ion effects and hydrophobic guests. 2010 , 26, 10460-6	21
1103	On the Validation of Molecular Dynamics Simulations of Saturated and cis-Monounsaturated Phosphatidylcholine Lipid Bilayers: A Comparison with Experiment. 2010 , 6, 325-36	232
1102	A reliable docking/scoring scheme based on the semiempirical quantum mechanical PM6-DH2 method accurately covering dispersion and H-bonding: HIV-1 protease with 22 ligands. 2010 , 114, 12666-78	103
1101	Computational identification of uncharacterized cruzain binding sites. 2010 , 4, e676	34
1100	Correlation analyses on binding affinity of sialic acid analogues with influenza virus neuraminidase-1 using ab initio MO calculations on their complex structures. 2010 , 50, 1796-805	35
1099	Free-energy-based methods for binding profile determination in a congeneric series of CDK2 inhibitors. 2010 , 114, 9516-24	40
1098	Affinity of sulfamates and sulfamides to carbonic anhydrase II isoform: experimental and molecular modeling approaches. 2010 , 50, 1113-22	12
1097	Detailed molecular dynamics simulations of a model NaPSS in water. 2010 , 114, 9391-9	46

1096	A substrate selectivity and inhibitor design lesson from the PDE10-cAMP crystal structure: a computational study. 2010 , 114, 5154-60	5
1095	Molecular dynamics study of thermodynamic scaling of the glass-transition dynamics in ionic liquids over wide temperature and pressure ranges. 2010 , 114, 3902-11	22
1094	Assignment of UV-vis spectrum of (3,3')-diindolylmethane, a Leishmania donovani topoisomerase IB inhibitor and a candidate DNA minor groove binder. 2010 , 114, 7121-6	6
1093	Advances in Computational Biology. 2010 ,	2
1092	Sequence-dependent configurational entropy change of DNA upon intercalation. 2010 , 114, 13446-54	27
1091	Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology. 2010 , 6, 2566-2580	41
1090	A new battery-charging method suggested by molecular dynamics simulations. 2010 , 12, 2740-3	16
1089	Molecular dynamics simulations of pentacene thin films: The effect of surface on polymorph selection. 2010 , 20, 10397	40
1088	Energy landscapes associated with macromolecular conformational changes from endpoint structures. 2010 , 132, 17570-7	13
1087	Decomposing the energetic impact of drug resistant mutations in HIV-1 protease on binding DRV. 2010 , 6, 1358-1368	40
1086	Sodium bis(2-ethylhexyl)sulfosuccinate self-aggregation in vacuo: molecular dynamics simulation. 2010 , 12, 4694-703	22
1085	Fatty acid hydroxytyrosyl esters: structure/antioxidant activity relationship by ABTS and in cell-culture DCF assays. 2010 , 58, 5292-9	64
1084	Modeling the structure and absorption spectra of stilbazolium merocyanine in polar and nonpolar solvents using hybrid QM/MM techniques. 2010 , 114, 13349-57	51
1083	Ion specificity at the peptide bond: molecular dynamics simulations of N-methylacetamide in aqueous salt solutions. 2010 , 114, 1213-20	95
1082	Effect of a monomeric sequence on the structure of hydrated Nafion in the sandwich model and solvent dynamics in nano-channels: a molecular dynamic study. 2010 , 108, 3393-3404	2
1081	G-Quadruplex DNA. 2010 ,	8
1080	DNA binding characteristics of mithramycin and chromomycin analogues obtained by combinatorial biosynthesis. 2010 , 49, 10543-52	46
1079	Towards a universal method for calculating hydration free energies: a 3D reference interaction site model with partial molar volume correction. 2010 , 22, 492101	89

1078	Modeling Protein-Ligand Binding by Mining Minima. 2010 , 6, 3540-3557	50
1077	Quantifying interactions between G-quadruplex DNA and transition-metal complexes. 2010 , 608, 223-55	6
1076	The thermodynamics of charge transfer in DNA photolyase: using thermodynamic integration calculations to analyse the kinetics of electron transfer reactions. 2010 , 12, 9516-25	28
1075	Less is more [multiscale modelling of self-assembling multivalency and its impact on DNA binding and gene delivery. 2010 , 1, 393	71
1074	Structure and dynamics of electrical double layers in organic electrolytes. 2010 , 12, 5468-79	84
1073	A comparative study of the binding of QSY 21 and Rhodamine 6G fluorescence probes to DNA: structure and dynamics. 2010 , 12, 9677-84	16
1072	Importance of loop dynamics in the neocarzinostatin chromophore binding and release mechanisms. 2010 , 12, 3443-9	4
1071	Specific interactions of ammonium functionalities in amino acids with aqueous fluoride and iodide. 2010 , 114, 13853-60	18
1070	On the role of water in peroxidase catalysis: a theoretical investigation of HRP compound I formation. 2010 , 114, 5161-9	75
1069	Single-molecule pulling simulations can discern active from inactive enzyme inhibitors. 2010 , 132, 7361-71	153
1068	Differential binding of p53 and nutlin to MDM2 and MDMX: computational studies. 2010 , 9, 1167-81	78
1067	Modelling the binding of HIV-reverse transcriptase and nevirapine: an assessment of quantum mechanical and force field approaches and predictions of the effect of mutations on binding. 2010 , 12, 7117-25	26
1066	Tackling the challenges posed by target flexibility in drug design. 2010 , 5, 347-59	35
1065	OGOLEM: Global cluster structure optimisation for arbitrary mixtures of flexible molecules. A multiscaling, object-oriented approach. 2010 , 108, 279-291	85
1064	Clipping and stoppering anion templated synthesis of a [2]rotaxane host system. 2011 , 40, 12180-90	9
1063	Redistribution of electron density in pyridinium and pyrazinium guests induced by complexation with cucurbit[6]uril. 2011 , 35, 2854	8
1062	Solvent dependence of structure, charge distribution, and absorption spectrum in the photochromic merocyanine-spiropyran pair. 2011 , 115, 4025-32	36
1061	Photosynthetic light-harvesting is tuned by the heterogeneous polarizable environment of the protein. 2011 , 133, 3078-84	110

1060	Catalytic roles of active-site residues in 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase: an ONIOM/DFT study. 2011 , 115, 1918-26	20
1059	A new method for screening potential sII and sH hydrogen clathrate hydrate promoters with model potentials. 2011 , 13, 13410-20	16
1058	Computational evidence for the substrate-assisted catalytic mechanism of O-GlcNAcase. A DFT investigation. 2011 , 13, 9568-77	12
1057	An atomistic simulation of the liquid-crystalline phases of sexithiophene. 2011 , 21, 125-133	55
1056	R.E.D. Server: a web service for deriving RESP and ESP charges and building force field libraries for new molecules and molecular fragments. 2011 , 39, W511-7	508
1055	Internal structure, hygroscopic and reactive properties of mixed sodium methanesulfonate-sodium chloride particles. 2011 , 13, 11846-57	24
1054	Hybrid density functional theory/molecular mechanics calculations of two-photon absorption of dimethylamino nitro stilbene in solution. 2011 , 13, 12506-16	58
1053	The role of CH \cdots interaction in the charge transfer properties in tris(8-hydroxyquinolinato)aluminium(III). 2011 , 13, 20704-13	14
1052	Conjugation of organic-metallic hybrid polymers and calf-thymus DNA. 2011 , 13, 4839-41	29
1051	A molecular dynamics study of structure, stability and fragmentation patterns of sodium bis(2-ethylhexyl)sulfosuccinate positively charged aggregates in vacuo. 2011 , 13, 21423-31	13
1050	The importance of solvation in the design of ligands targeting membrane proteins. 2011 , 2, 160	11
1049	Coenzyme A binding to the aminoglycoside acetyltransferase (3)-IIIb increases conformational sampling of antibiotic binding site. 2011 , 50, 10559-65	10
1048	Probing the steric space at the floor of the D1 dopamine receptor orthosteric binding domain: 7 μ M, 8 μ M and 8 μ M methyl substituted dihydroxidine analogues. 2011 , 54, 5508-21	14
1047	Density functional theory/molecular mechanics approach for electronic g-tensors of solvated molecules. 2011 , 115, 4350-8	19
1046	Modeling solvatochromism of a quinolinium betaine dye in water solvent using sequential hybrid QM/MM and semicontinuum approach. 2011 , 115, 1056-61	14
1045	Physicochemical conjugation with deoxycholic acid and dimethylsulfoxide for heparin oral delivery. 2011 , 22, 1451-8	19
1044	Nonadiabatic QM/MM simulations of fast charge transfer in Escherichia coli DNA photolyase. 2011 , 115, 9846-63	69
1043	Dual-resolution molecular dynamics simulation of antimicrobials in biomembranes. 2011 , 8, 826-41	49

1042	Transplant-insert-constrain-relax-assemble (TICRA): protein-ligand complex structure modeling and application to kinases. 2011 , 51, 52-60	1
1041	Experimental and theoretical study on the intermolecular complex formation between trehalose and benzene compounds in aqueous solution. 2011 , 115, 9823-30	19
1040	Molecular dynamics simulations of CXCL-8 and its interactions with a receptor peptide, heparin fragments, and sulfated linked cyclitols. 2011 , 51, 335-58	29
1039	Formation mechanism and structure of a guanine-uracil DNA intrastrand cross-link. 2011 , 24, 2189-99	14
1038	Small Molecule Solvation Free Energy: Enhanced Conformational Sampling Using Expanded Ensemble Molecular Dynamics Simulation. 2011 , 7, 2910-8	37
1037	Formal Estimation of Errors in Computed Absolute Interaction Energies of Protein-ligand Complexes. 2011 , 7, 790-797	116
1036	Computational study of hydrocarbon adsorption in metal-organic framework Ni ₂ (dhtp). 2011 , 115, 2842-9	12
1035	A Classical Potential to Model the Adsorption of Biological Molecules on Oxidized Titanium Surfaces. 2011 , 7, 473-84	50
1034	Mechanism of concerted hydrogen bond reorientation in clathrates of Dianin's compound and hydroquinone. 2011 , 133, 18880-8	18
1033	Insights on the mechanism of amine oxidation catalyzed by D-arginine dehydrogenase through pH and kinetic isotope effects. 2011 , 133, 18957-65	15
1032	Importance of polar solvation for cross-reactivity of antibody and its variants with steroids. 2011 , 115, 7661-9	32
1031	Inhibition of Myosin ATPase activity by halogenated pseudilins: a structure-activity study. 2011 , 54, 3675-85	36
1030	On the role of London dispersion forces in biomolecular structure determination. 2011 , 115, 8038-46	35
1029	L-arginine binding to human inducible nitric oxide synthase: an antisymmetric funnel route toward isoform-specific inhibitors?. 2011 , 51, 1325-35	2
1028	Exploring the intermediate states of ADP-ATP exchange: a simulation study on Eg5. 2011 , 115, 784-95	13
1027	Binding affinities of factor Xa inhibitors estimated by thermodynamic integration and MM/GBSA. 2011 , 51, 947-58	59
1026	Behavior of β -amyloid 1-16 at the air-water interface at varying pH by nonlinear spectroscopy and molecular dynamics simulations. 2011 , 115, 5873-80	7
1025	A highly C70 selective shape-persistent rectangular prism constructed through one-step alkyne metathesis. 2011 , 133, 20995-1001	218

1024	Theoretical studies on the interactions and interferences of HIV-1 glycoprotein gp120 and its coreceptor CCR5. 2011 , 51, 359-69	10
1023	Urea and guanidinium induced denaturation of a Trp-cage miniprotein. 2011 , 115, 8910-24	54
1022	Structure of the HIV-1 frameshift site RNA bound to a small molecule inhibitor of viral replication. 2011 , 6, 857-64	48
1021	Postprocessing of docked protein-ligand complexes using implicit solvation models. 2011 , 51, 267-82	39
1020	Rational design of new class of BH3-mimetics as inhibitors of the Bcl-xL protein. 2011 , 51, 1249-58	17
1019	Solvent interaction energy calculations on molecular dynamics trajectories: increasing the efficiency using systematic frame selection. 2011 , 51, 2680-9	20
1018	Entropy Balance in the Intercalation Process of an Anti-Cancer Drug Daunomycin. 2011 , 2, 3021-3026	33
1017	Designing a new Diels-Alderase: a combinatorial, semirational approach including dynamic optimization. 2011 , 51, 1906-17	11
1016	First Principles-Based Calculations of Free Energy of Binding: Application to Ligand Binding in a Self-Assembling Superstructure. 2011 , 7, 1102-8	17
1015	Helix stabilization of poly(ethylene glycol)-peptide conjugates. 2011 , 12, 2729-34	49
1014	Vibrational energy relaxation in liquid HCl and DCl via the linearized semiclassical method: electrostriction versus quantum delocalization. 2011 , 115, 9775-81	19
1013	Generation of human chiral metabolites of simvastatin and lovastatin by bacterial CYP102A1 mutants. 2011 , 39, 140-50	33
1012	Predicting the Solubility of the Sparingly Soluble Solids 1,2,4,5-Tetramethylbenzene, Phenanthrene, and Fluorene in Various Organic Solvents by Molecular Simulation. 2011 , 56, 1587-1595	15
1011	Novel hydrazine molecules as tools to understand the flexibility of vascular adhesion protein-1 ligand-binding site: toward more selective inhibitors. 2011 , 54, 2143-54	20
1010	Catalytic mechanism of cytochrome P450 for 5'-hydroxylation of nicotine: fundamental reaction pathways and stereoselectivity. 2011 , 133, 7416-27	105
1009	Comparison of Methods to Obtain Force-Field Parameters for Metal Sites. 2011 , 7, 2452-63	83
1008	A molecular dynamics study of water mass accommodation on condensed phase water coated by fatty acid monolayers. 2011 , 116,	43
1007	Alzheimer's disease drug candidates stabilize A β protein native structure by interacting with the hydrophobic core. 2011 , 100, 1076-82	27

1006	Reengineering rate-limiting, millisecond enzyme motions by introduction of an unnatural amino acid. 2011 , 101, 411-20	13
1005	Three-dimensional models of 14 β -sterol demethylase (Cyp51A) from <i>Aspergillus lentulus</i> and <i>Aspergillus fumigatus</i> : an insight into differences in voriconazole interaction. 2011 , 38, 426-34	20
1004	Toward a universal model to calculate the solvation thermodynamics of druglike molecules: the importance of new experimental databases. 2011 , 8, 1423-9	36
1003	Molecular dynamics studies of native and substituted cyclodextrins in different media: 1. Charge derivation and force field performances. 2011 , 13, 15103-21	78
1002	Thermodynamics of liquids: standard molar entropies and heat capacities of common solvents from 2PT molecular dynamics. 2011 , 13, 169-81	113
1001	Computational modeling of the catalytic mechanism of human placental alkaline phosphatase (PLAP). 2011 , 51, 2538-48	11
1000	Halogen bonding in ligand-receptor systems in the framework of classical force fields. 2011 , 13, 19508-16	72
999	Performance assessment of semiempirical molecular orbital methods in describing halogen bonding: quantum mechanical and quantum mechanical/molecular mechanical-molecular dynamics study. 2011 , 51, 2549-59	31
998	Tautomerism in 7-hydroxyquinoline: a combined experimental and theoretical study in water. 2011 , 115, 4195-201	28
997	Assessing the performance of the MM/PBSA and MM/GBSA methods. 1. The accuracy of binding free energy calculations based on molecular dynamics simulations. 2011 , 51, 69-82	1511
996	Quantum Instanton Evaluation of the Kinetic Isotope Effects and of the Temperature Dependence of the Rate Constant. 2011 , 67-92	
995	Theoretical Investigation on Triplet Excitation Energy Transfer in Fluorene Dimer. 2011 , 24, 538-546	5
994	Comparison of virtual high-throughput screening methods for the identification of phosphodiesterase-5 inhibitors. 2011 , 51, 1353-63	23
993	Surface supramolecular organization of a terbium(III) double-decker complex on graphite and its single molecule magnet behavior. 2011 , 133, 6603-12	171
992	Synthesis, biological evaluation, and automated docking of constrained analogues of the opioid peptide H-Dmt-D-Ala-Phe-Gly-NH ₂ using the 4- or 5-methyl substituted 4-amino-1,2,4,5-tetrahydro-2-benzazepin-3-one scaffold. 2011 , 54, 6538-47	12
991	Improved classical united-atom force field for imidazolium-based ionic liquids: tetrafluoroborate, hexafluorophosphate, methylsulfate, trifluoromethylsulfonate, acetate, trifluoroacetate, and bis(trifluoromethylsulfonyl)amide. 2011 , 115, 10027-40	121
990	Araiosamines A-D: tris-bromoindole cyclic guanidine alkaloids from the marine sponge <i>Clathria</i> (<i>Thalysias</i>) <i>araiosa</i> . 2011 , 76, 5515-23	30
989	Molecular dynamics simulation, free energy calculation and structure-based 3D-QSAR studies of B-RAF kinase inhibitors. 2011 , 51, 680-92	64

988	Efficient Solvation Free Energy Calculations of Amino Acid Analogs by Expanded Ensemble Molecular Simulation. 2011 , 7, 1394-403	26
987	Computational ligand-based rational design: Role of conformational sampling and force fields in model development. 2011 , 2, 356-370	58
986	Modeling the tetraphenylalanine-PEG hybrid amphiphile: from DFT calculations on the peptide to molecular dynamics simulations on the conjugate. 2011 , 115, 8937-46	21
985	A simple QM/MM approach for capturing polarization effects in protein-ligand binding free energy calculations. 2011 , 115, 4911-26	83
984	A Transferable Non-bonded Pairwise Force Field to Model Zinc Interactions in Metalloproteins. 2011 , 7, 433-443	43
983	Origin of chiral selectivity in gas-phase serine tetramers. 2011 , 13, 877-85	8
982	A theoretical investigation of inositol 1,3,4,5-tetrakisphosphate. 2011 , 13, 1070-81	7
981	AADS--an automated active site identification, docking, and scoring protocol for protein targets based on physicochemical descriptors. 2011 , 51, 2515-27	95
980	Anisotropic Thermal Transport in Organic Molecular Crystals from Nonequilibrium Molecular Dynamics Simulations. 2011 , 115, 5940-5946	39
979	Computational screening and design of DNA-linked molecular nanowires. 2011 , 11, 604-8	4
978	Investigation of ligand exchange reactions in aqueous uranyl carbonate complexes using computational approaches. 2011 , 13, 11402-11	37
977	Thermodynamic properties for applications in chemical industry via classical force fields. 2012 , 307, 201-49	21
976	Covalent inhibitors of fatty acid amide hydrolase: a rationale for the activity of piperidine and piperazine aryl ureas. 2011 , 54, 6612-23	33
975	Molecular dynamics simulation of NMR powder lineshapes of linear guests in structure I clathrate hydrates. 2011 , 13, 2367-77	8
974	Effect of water/ethanol content on the structure of Nafion in the sandwich model and solvent dynamics in nano-channels; a molecular dynamics study. 2011 , 109, 709-724	16
973	Using free energy of binding calculations to improve the accuracy of virtual screening predictions. 2011 , 51, 1648-55	20
972	Nonequilibrium water transport in a nonionic microemulsion system. 2011 , 115, 6503-8	1
971	Insights into Ligand-Protein Binding from Local Mechanical Response. 2011 , 7, 3368-3378	14

970	Using molecular dynamics and quantum mechanics calculations to model fluorescence observables. 2011 , 115, 3997-4008	30
969	Free-Energy Simulations of Hydrogen Bonding versus Stacking of Nucleobases on a Graphene Surface. 2011 , 115, 19455-19462	23
968	Vibrational spectroscopy of water in hydrated lipid multi-bilayers. I. Infrared spectra and ultrafast pump-probe observables. 2011 , 135, 075101	48
967	Accelerated convergence of molecular free energy via superposition approximation-based reference states. 2011 , 134, 134107	4
966	Modeling the chemical step utilized by human alkyladenine DNA glycosylase: a concerted mechanism AIDS in selectively excising damaged purines. 2011 , 133, 16258-69	31
965	Structural determinants of CX-4945 derivatives as protein kinase CK2 inhibitors: a computational study. 2011 , 12, 7004-21	12
964	Development of the CHARMM Force Field for Lipids. 2011 , 2, 1526-1532	240
963	Modeling of hyperbranched polyesters as hosts for the multifunctional bioactive agent Shikonin. 2011 , 13, 10808-17	15
962	Accurate predictions of nonpolar solvation free energies require explicit consideration of binding-site hydration. 2011 , 133, 13081-92	53
961	Pocket-space maps to identify novel binding-site conformations in proteins. 2011 , 51, 2666-79	37
960	Probing the dynamic nature of water molecules and their influences on ligand binding in a model binding site. 2011 , 51, 2581-94	18
959	Resolution of discordant HIV-1 protease resistance rankings using molecular dynamics simulations. 2011 , 51, 2636-49	10
958	Selection of in silico drug screening results for G-protein-coupled receptors by using universal active probes. 2011 , 51, 2398-407	19
957	A Multibox Splitting Scheme: Robust Approximation For ab Initio Molecular Dynamics. 2011 , 7, 3872-83	2
956	Calculation of the Absolute Free Energy of Binding and Related Entropies with the HSMD-TI Method: The FKBP12-L8 Complex. 2011 , 7, 4196-4207	7
955	Improved Binding Free Energy Predictions from Single-Reference Thermodynamic Integration Augmented with Hamiltonian Replica Exchange. 2011 , 7, 3001-3011	35
954	Dynamic Behavior of Carbon Nanotube and Bio-/Artificial Surfactants Complexes in an Aqueous Environment. 2011 , 115, 19659-19667	16
953	Biomolecular modeling and simulation: a field coming of age. 2011 , 44, 191-228	119

952	Normal mode analysis with molecular geometry restraints: bridging molecular mechanics and elastic models. 2011 , 508, 64-71	10
951	What is the effective dielectric constant in a β -cyclodextrin cavity? Insights from Molecular Dynamics simulations and QM/MM calculations. 2011 , 968, 71-76	7
950	Binding properties and conformational dynamics of reversible amidines with DNA from a theoretical view. 2011 , 977, 188-194	4
949	Synthesis, biological evaluation, and molecular modeling of donepezil and N-[(5-(benzyloxy)-1-methyl-1H-indol-2-yl)methyl]-N-methylprop-2-yn-1-amine hybrids as new multipotent cholinesterase/monoamine oxidase inhibitors for the treatment of Alzheimer's disease. 2011 , 54, 8251-70	178
948	Indolylarylsulfones as HIV-1 non-nucleoside reverse transcriptase inhibitors: new cyclic substituents at indole-2-carboxamide. 2011 , 54, 1587-98	112
947	Solvated interaction energy (SIE) for scoring protein-ligand binding affinities. 2. Benchmark in the CSAR-2010 scoring exercise. 2011 , 51, 2066-81	37
946	Role of water during the extrusion of substrates by the efflux transporter AcrB. 2011 , 115, 8278-87	35
945	Bioreductive molecular probe: fluorescence signalling upon reduction of an azo group. 2011 , 35, 701	6
944	Chapter 4:Polymorph Prediction of Small Organic Molecules, Co-crystals and Salts. 2011 , 44-88	1
943	Comparison of computational methods to model DNA minor groove binders. 2011 , 51, 558-71	57
942	Molecular Simulations of PIM-1-like Polymers of Intrinsic Microporosity. 2011 , 44, 6944-6951	141
941	Effects of Biomolecular Flexibility on Alchemical Calculations of Absolute Binding Free Energies. 2011 , 7, 2224-2232	16
940	Incorporation of charge transfer into the explicit polarization fragment method by grand canonical density functional theory. 2011 , 135, 084107	14
939	Computational investigation of the substrate recognition mechanism of protein D-aspartyl (L-isoaspartyl) O-methyltransferase by docking and molecular dynamics simulation studies and application to interpret size exclusion chromatography data. 2011 , 879, 3310-6	6
938	Exploration of the binding of benzimidazole-biphenyl derivatives to hemoglobin using docking and molecular dynamics simulation. 2011 , 48, 20-6	9
937	Use of the parmbsc0 force field and trajectory analysis to study the binding of netropsin to the DNA fragment (5'CCAATTGG)(2) in the presence of excess NaCl salt in aqueous solution. 2011 , 48, 531-9	5
936	The recognition specificity of the CHD1 chromodomain with modified histone H3 peptides. 2011 , 406, 527-41	9
935	A concerted mechanism for opening the GDP binding pocket and release of the nucleotide in hetero-trimeric G-proteins. 2011 , 411, 298-312	26

934	Arg149 is involved in switching the low affinity, open state of the binding protein AfProX into its high affinity, closed state. 2011 , 411, 36-52	22
933	Molecular dynamics simulations of the effect of the G-protein and diffusible ligands on the β -adrenergic receptor. 2011 , 414, 611-23	29
932	Spiral Growth Model for Faceted Crystals of Non-Centrosymmetric Organic Molecules Grown from Solution. 2011 , 11, 2780-2802	59
931	Structural Characterization of a Polymer of Intrinsic Microporosity: X-ray Scattering with Interpretation Enhanced by Molecular Dynamics Simulations. 2011 , 44, 14-16	63
930	A water-swap reaction coordinate for the calculation of absolute protein-ligand binding free energies. 2011 , 134, 054114	53
929	A molecular dynamics investigation of the structural and dynamic properties of the ionic liquid 1-n-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide. 2011 , 135, 124507	149
928	Water in the active site of ketosteroid isomerase. 2011 , 50, 6689-700	7
927	Understanding the effect of polylysine architecture on DNA binding using molecular dynamics simulations. 2011 , 12, 3870-9	69
926	A Comparative Study for Molecular Dynamics Simulations of Liquid Benzene. 2011 , 7, 2240-52	53
925	Impact of planarity of unfused aromatic molecules on G-quadruplex binding: learning from isaindigotone derivatives. 2011 , 9, 6422-36	32
924	Molecular dynamics simulations of the Salmonella typhi Vi antigenic polysaccharide and effects of the introduction of a zwitterionic motif. 2011 , 9, 5554-9	2
923	On the origin of the stronger binding of PIB over thioflavin T to protofibrils of the Alzheimer amyloid- β peptide: a molecular dynamics study. 2011 , 100, 1316-24	74
922	Quantum mechanical/molecular mechanical analysis of mechanisms of enzyme action. Human acetylcholinesterase. 2011 , 60, 2196-2204	1
921	Application of Molecular Dynamics Simulations in Molecular Property Prediction I: Density and Heat of Vaporization. 2011 , 7, 2151-2165	85
920	Solution structure of a DNA duplex containing the potent anti-poxvirus agent cidofovir. 2011 , 133, 2264-74	23
919	Correlation analyses on binding affinity of sialic acid analogues and anti-influenza drugs with human neuraminidase using ab initio MO calculations on their complex structures--LERE-QSAR analysis (IV). 2011 , 51, 2706-16	33
918	Elucidating the energetics of entropically driven protein-ligand association: calculations of absolute binding free energy and entropy. 2011 , 115, 11902-10	37
917	Computational Biology, Protein Engineering, and Biosensor Technology: a Close Cooperation for Herbicides Monitoring. 2011 ,	3

- 916 An introduction to quantum chemical methods applied to drug design. **2011**, 3, 1061-78
- 915 Insights into the complex formed by matrix metalloproteinase-2 and alloxan inhibitors: molecular dynamics simulations and free energy calculations. **2011**, 6, e25597 12
- 914 Elucidation of the ATP7B N-domain Mg²⁺-ATP coordination site and its allosteric regulation. **2011**, 6, e26245 1
- 913 Farnesyl pyrophosphate regulates adipocyte functions as an endogenous PPAR α agonist. **2011**, 438, 111-9 43
- 912 Modeling of HIV-1 TAR RNA-ligand complexes. **2011**, 7, 301-8 2
- 911 Molecular Dynamics Simulation for Irreversibility of Green Fluorescent Protein before and after Photoactivation. **2011**, 40, 476-477
- 910 Steric and allosteric effects of fatty acids on the binding of warfarin to human serum albumin revealed by molecular dynamics and free energy calculations. **2011**, 59, 860-7 27
- 909 Molecular Dynamics Study on Evaporation Coefficient of Long-Chain Molecules. **2011**, 77, 1826-1833 2
- 908 Structure-based drug design of a new chemical class of small molecules active against influenza A nucleoprotein in vitro and in vivo. **2011**, 3, RRN1253 21
- 907 Structural and functional analyses of a saturated acyl ACP thioesterase, type B from immature seed tissue of *Jatropha curcas*. **2011**, 13, 453-61 13
- 906 Catalytic mechanism of the primary human prostaglandin F₂ synthase, aldo-keto reductase 1B1--prostaglandin D₂ synthase activity in the absence of NADP(H). **2011**, 278, 1288-98 22
- 905 Characterization of the PLP-dependent aminotransferase NikK from *Streptomyces tendae* and its putative role in nikkomycin biosynthesis. **2011**, 278, 4122-35 16
- 904 Drug resistant mechanism of diaryltriazine analog inhibitors of HIV-1 reverse transcriptase using molecular dynamics simulation and 3D-QSAR. **2011**, 77, 63-74 3
- 903 Docking, synthesis, and in vitro evaluation of antimetabolic estrone analogs. **2011**, 77, 173-81 44
- 902 Assessing protein kinase selectivity with molecular dynamics and mm-pbsa binding free energy calculations. **2011**, 78, 252-9 26
- 901 Investigation of formate transport through the substrate channel of formate dehydrogenase by steered molecular dynamics simulations. **2011**, 76, 172-4 3
- 900 Molecular dynamics method for proteins with ionization-conformation coupling and equilibrium titration. **2011**, 45, 309-317
- 899 The hidden energetics of ligand binding and activation in a glutamate receptor. **2011**, 18, 283-7 99

898	Computational characterization of reaction intermediates in the photocycle of the sensory domain of the AppA blue light photoreceptor. 2011 , 87, 564-73	23
897	Structural model and trans-interaction of the entire ectodomain of the olfactory cell adhesion molecule. 2011 , 19, 203-11	22
896	Computer simulations of water flux and salt permeability of the reverse osmosis FT-30 aromatic polyamide membrane. 2011 , 384, 1-9	69
895	Solvent penetration in photoactive yellow protein R52Q mutant: A theoretical study. 2011 , 164, 120-122	4
894	Hydration of acetic acid and acetate ion in water studied by 1D-RISM theory. 2011 , 164, 201-206	46
893	Computational insights into the different catalytic activities of CYP2A13 and CYP2A6 on NNK. 2011 , 30, 1-9	12
892	QM and QM/MD simulations of the Vinca alkaloids docked to tubulin. 2011 , 30, 54-66	2
891	Molecular modeling and molecular dynamics simulation studies on pyrrolopyrimidine-based α -helix mimetic as dual inhibitors of MDM2 and MDMX. 2011 , 30, 167-78	16
890	Atomic-scale characterization of conformational changes in the preQ1 riboswitch aptamer upon ligand binding. 2011 , 30, 179-85	16
889	HBonanza: a computer algorithm for molecular-dynamics-trajectory hydrogen-bond analysis. 2011 , 31, 5-9	59
888	Protein-ligand docking guided by ligand pharmacophore-mapping experiment by NMR. 2011 , 31, 20-7	12
887	Preparation and characterization of new hybrid nanostructured thin films for biosensors design. 2011 , 65, 2032-2035	9
886	A new polymorph (IV) of benzamide: Structural characterization and mechanism of the I \rightarrow IV phase transition. 2011 , 514, 274-277	9
885	Molecular modeling of the inhibition of protein-protein interactions with small molecules: The IL2R β case. 2011 , 517, 217-222	6
884	Agonist-dependent effects of mutations in the sphingosine-1-phosphate type 1 receptor. 2011 , 667, 105-12	13
883	Conformations of the Huntingtin N-term in aqueous solution from atomistic simulations. 2011 , 585, 3086-9	20
882	A theoretical investigation of the functional role of the axial methionine ligand of the Cu(A) site in cytochrome c oxidase. 2011 , 1807, 1314-27	4
881	Synthesis, structural, and biological evaluation of bis-heteroarylmaleimides and bis-heterofused imides. 2011 , 19, 5291-9	23

880	Novel human mPGES-1 inhibitors identified through structure-based virtual screening. 2011 , 19, 6077-86	44
879	Molecular dynamics simulations and MM/GBSA methods to investigate binding mechanisms of aminomethylpyrimidine inhibitors with DPP-IV. 2011 , 21, 6630-5	12
878	Identification of nonplanar small molecule for G-quadruplex grooves: molecular docking and molecular dynamic study. 2011 , 21, 6969-72	18
877	Adsorption behavior of 17 β -ethynylestradiol onto soils followed by fluorescence spectral deconvolution. 2011 , 84, 1072-8	22
876	Structure and orientation of water molecules at model hydrophobic surfaces with curvature: From graphene sheets to carbon nanotubes and fullerenes. 2011 , 388, 47-56	35
875	Semiempirical quantum mechanical method PM6-DH2X describes the geometry and energetics of CK2-inhibitor complexes involving halogen bonds well, while the empirical potential fails. 2011 , 115, 8581-9	75
874	A New Approach for Investigating the Molecular Recognition of Protein: Toward Structure-Based Drug Design Based on the 3D-RISM Theory. 2011 , 7, 3803-15	39
873	Structure-reactivity relationship of piperidine nitroxide: electrochemical, ESR and computational studies. 2011 , 76, 435-40	61
872	An Automated Force Field Topology Builder (ATB) and Repository: Version 1.0. 2011 , 7, 4026-37	1030
871	Molecular dynamics simulation and free energy calculation studies of the binding mechanism of allosteric inhibitors with p38 β MAP kinase. 2011 , 51, 3235-46	63
870	Role of a mutated residue at the entrance of the substrate access channel in cytochrome p450 engineered for vitamin D(3) hydroxylation activity. 2011 , 50, 8302-10	11
869	Recent development in computer simulations of lipid bilayers. 2011 , 7, 25-39	122
868	Biophysical probes reveal a "compromise" nature of the methyl-lysine binding pocket in L3MBTL1. 2011 , 133, 5357-62	32
867	A molecular dynamics investigation of structure and dynamics of SDS and SDBS micelles. 2011 , 7, 9148	83
866	Promiscuity of carbonic anhydrase II. Unexpected ester hydrolysis of carbohydrate-based sulfamate inhibitors. 2011 , 133, 18452-62	37
865	Ligand conformational and solvation/desolvation free energy in protein-ligand complex formation. 2011 , 115, 4718-24	22
864	Theoretical studies on the interaction of partial agonists with the 5-HT _{2A} receptor. 2011 , 25, 51-66	16
863	Molecular and structural determinants of adamantyl susceptibility to HLA-DRs allelic variants: an in silico approach to understand the mechanism of MLEs. 2011 , 25, 81-101	20

862	The molecular mechanism studies of chirality effect of PHA-739358 on Aurora kinase A by molecular dynamics simulation and free energy calculations. 2011 , 25, 171-80	19
861	Structure-activity relationships of diphenyl-ether as protoporphyrinogen oxidase inhibitors: insights from computational simulations. 2011 , 25, 213-22	16
860	Transferable scoring function based on semiempirical quantum mechanical PM6-DH2 method: CDK2 with 15 structurally diverse inhibitors. 2011 , 25, 223-35	46
859	Towards a rational spacer design for bivalent inhibition of estrogen receptor. 2011 , 25, 253-62	13
858	A QM/MM study of the binding of RAPTA ligands to cathepsin B. 2011 , 25, 729-42	34
857	Computational investigation of the binding mode of bis(hydroxyphenyl)arenes in 17β-HSD1: molecular dynamics simulations, MM-PBSA free energy calculations, and molecular electrostatic potential maps. 2011 , 25, 795-811	16
856	Binding of novel fullerene inhibitors to HIV-1 protease: insight through molecular dynamics and molecular mechanics Poisson-Boltzmann surface area calculations. 2011 , 25, 959-76	41
855	Molecular dynamics of Mycobacterium tuberculosis KasA: implications for inhibitor and substrate binding and consequences for drug design. 2011 , 25, 1053-69	5
854	MM/GBSA and LIE estimates of host-guest affinities: dependence on charges and solvation model. 2011 , 25, 1085-93	21
853	Binding free energy calculation with QM/MM hybrid methods for Abl-Kinase inhibitor. 2011 , 37, 69-78	29
852	Physical Modeling of Aqueous Solvation. 2011 , 145, 209-226	35
851	Molecular dynamics directed CoMFA studies on carbocyclic neuraminidase inhibitors. 2011 , 15, 979-87	8
850	Structural and functional role of nickel ions in urease by molecular dynamics simulation. 2011 , 16, 125-35	5
849	Docking study and binding free energy calculation of poly (ADP-ribose) polymerase inhibitors. 2011 , 17, 383-9	7
848	Computational simulations of structural role of the active-site W374C mutation of acetyl-coenzyme-A carboxylase: multi-drug resistance mechanism. 2011 , 17, 495-503	18
847	Molecular dynamics simulation of oseltamivir resistance in neuraminidase of avian influenza H5N1 virus. 2011 , 17, 587-92	18
846	Studying the mechanism that enables paullones to selectively inhibit glycogen synthase kinase 3 rather than cyclin-dependent kinase 5 by molecular dynamics simulations and free-energy calculations. 2011 , 17, 795-803	15
845	Computational design of a lipase for catalysis of the Diels-Alder reaction. 2011 , 17, 833-49	12

844	Identification of ligand binding site on RXR α using molecular docking and dynamics methods. 2011 , 17, 1259-65	2
843	Coupling between the BLUF and EAL domains in the blue light-regulated phosphodiesterase BlrP1. 2011 , 17, 1579-86	15
842	Insights into scFv:drug binding using the molecular dynamics simulation and free energy calculation. 2011 , 17, 1919-26	11
841	Effect of the SH3-SH2 domain linker sequence on the structure of Hck kinase. 2011 , 17, 1927-34	3
840	Prediction of zanamivir efficiency over the possible 2009 influenza A (H1N1) mutants by multiple molecular dynamics simulations and free energy calculations. 2011 , 17, 2465-73	21
839	Molecular dynamics simulations and binding free energy analysis of DNA minor groove complexes of curcumin. 2011 , 17, 2805-16	21
838	A comparative study of HIV-1 and HTLV-I protease structure and dynamics reveals a conserved residue interaction network. 2011 , 17, 2693-705	7
837	Coarse-grained modeling study of nonpeptide RGD ligand density and PEG molecular weight on the conformation of poly(β -glutamyl-glutamate) paclitaxel conjugates. 2011 , 17, 2973-87	5
836	Why OppA protein can bind sequence-independent peptides? A combination of QM/MM, PB/SA, and structure-based QSAR analyses. 2011 , 40, 493-503	37
835	MD studies on neuraminidase for probing binding pose of its inhibitors. 2011 , 20, 1680-1686	1
834	Predicting binding energies of CDK6 inhibitors in the hit-to-lead process. 2011 , 128, 807-823	6
833	Simulations of ^{129}Xe NMR chemical shift of atomic xenon dissolved in liquid benzene. 2011 , 129, 677-684	20
832	Reaction path optimization and vibrational frequency analysis via ab initio QM/MM free energy gradient (FEG) method: application to isomerization process of glycine in aqueous solution. 2011 , 130, 215-226	26
831	Towards a synthetic avidin mimic. 2011 , 400, 1397-404	8
830	Rational design of biomimetic molecularly imprinted materials: theoretical and computational strategies for guiding nanoscale structured polymer development. 2011 , 400, 1771-86	69
829	How do carbon nanotubes serve as carriers for gemcitabine transport in a drug delivery system?. 2011 , 29, 591-6	109
828	Relaxed complex scheme suggests novel inhibitors for the lyase activity of DNA polymerase beta. 2011 , 29, 702-16	31
827	Effect of CpG methylation on DNA binding protein: molecular dynamics simulations of the homeodomain PITX2 bound to the methylated DNA. 2011 , 29, 920-7	5

826	Resistant mechanism against nelfinavir of subtype C human immunodeficiency virus type 1 proteases. 2011 , 986, 30-38	3
825	Computer- and structure-based lead design for epigenetic targets. 2011 , 19, 3605-15	18
824	Intramolecular hydrogen bonding in artocaine can be related to superior bone tissue penetration: a molecular dynamics study. 2011 , 154, 18-25	29
823	Structural properties of hydroxyl-substituted alkyl benzenesulfonates at the water/vapor and water/decane interfaces. 2011 , 54, 1078-1085	10
822	Molecular dynamics simulations and drug discovery. 2011 , 9, 71	615
821	Open Babel: An open chemical toolbox. 2011 , 3, 33	3717
820	Virtual screening using molecular simulations. 2011 , 79, 1940-51	128
819	Binding to the open conformation of HIV-1 protease. 2011 , 79, 2282-90	12
818	A mixed molecular modeling-robotics approach to investigate lipase large molecular motions. 2011 , 79, 2517-29	16
817	Molecular dynamics study of small molecule inhibitors of the Bcl-2 family. 2011 , 79, 2624-36	24
816	Statistical mechanics-based method to extract atomic distance-dependent potentials from protein structures. 2011 , 79, 2648-61	43
815	Factors determining electrostatic fields in molecular dynamics simulations of the Ras/effector interface. 2011 , 79, 3511-24	17
814	Predicting large-scale conformational changes in proteins using energy-weighted normal modes. 2011 , 79, 2778-93	6
813	Separation of chemical reaction intermediates by metal-organic frameworks. 2011 , 7, 2356-64	40
812	Modeling solvatochromism of Nile red in water. 2011 , 111, 1521-1530	20
811	Amylose's recognition of chirality in polylactides on formation of inclusion complexes in vine-twining polymerization. 2011 , 11, 1407-15	26
810	Design of novel ligands of CDP-methylerythritol kinase by mimicking direct protein-protein and solvent-mediated interactions. 2011 , 24, 71-80	4
809	Characterization of molecular recognition of STAT3 SH2 domain inhibitors through molecular simulation. 2011 , 24, 254-65	33

808	Structural analysis of zinc-finger (TTK) + [Cu(BPA)] ²⁺ / [Cu(IDB)] ²⁺ + DNA complexes: an investigation by molecular dynamics simulation. 2011 , 24, 981-94		5
807	Docking and Molecular Dynamics Calculations of Pyrrolidinone Analog MMK16 Bound to COX and LOX Enzymes. 2011 , 30, 473-86		8
806	Conformational Properties and Energetic Analysis of Aliskiren in Solution and Receptor Site. 2011 , 30, 973-85		11
805	Affinity of vitamin E analogues for the ubiquinone complex II site correlates with their toxicity to cancer cells. 2011 , 55, 1543-51		8
804	Asymmetric Synthesis of New β -Lactam Lipopeptides as Bacterial Signal Peptidase I Inhibitors. 2011 , 2011, 3437-3449		6
803	Evaluation of the separation mechanism of electrokinetic chromatography with a microemulsion and cyclodextrins using NMR and molecular modeling. 2011 , 32, 3062-9		12
802	Is the pig a good umami sensing model for humans? A comparative taste receptor study. 2011 , 26, 282-285		19
801	New huprine derivatives functionalized at position 9 as highly potent acetylcholinesterase inhibitors. 2011 , 6, 876-88		28
800	Mapping the catechol binding site in dopamine D ₁ receptors: synthesis and evaluation of two parallel series of bicyclic dopamine analogues. 2011 , 6, 1024-40		17
799	Asymmetric synthesis and conformational analysis by NMR spectroscopy and MD of Aba- and β -MeAba-containing dermorphin analogues. 2011 , 6, 2035-47		8
798	Structure-based discovery of allosteric modulators of two related class B G-protein-coupled receptors. 2011 , 6, 2159-69		57
797	A mixed quantum-classical description of excitation energy transfer in supramolecular complexes: F ₀ theory and beyond. 2011 , 12, 645-56		31
796	Revisiting the lipase from <i>Pseudomonas aeruginosa</i> : directed evolution of substrate acceptance and enantioselectivity using iterative saturation mutagenesis. 2011 , 12, 1550-7		28
795	A comparison of different initialization protocols to obtain statistically independent molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , 2011 , 32, 187-95	3.5	54
794	Interaction identification of Zif268 and TATA(ZF) proteins with GC-/AT-rich DNA sequence: A theoretical study. <i>Journal of Computational Chemistry</i> , 2011 , 32, 416-28	3.5	25
793	Assessing the performance of the molecular mechanics/Poisson Boltzmann surface area and molecular mechanics/generalized Born surface area methods. II. The accuracy of ranking poses generated from docking. <i>Journal of Computational Chemistry</i> , 2011 , 32, 866-77	3.5	484
792	A fast empirical GAFF compatible partial atomic charge assignment scheme for modeling interactions of small molecules with biomolecular targets. <i>Journal of Computational Chemistry</i> , 2011 , 32, 893-907	3.5	40
791	Vibrational spectral signatures of peptide secondary structures: N-methylation and side chain hydrogen bond in cyclosporin A. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1500-18	3.5	2

790	A challenging system: free energy prediction for factor Xa. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1743-52	3.5	55
789	An ab initio molecular orbital study of intramolecular hydrogen bonding in ortho-substituted arylamides: implications for the parameterization of molecular mechanics force fields. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1846-58	3.5	13
788	Role of bridging water molecules in GSK3 β inhibitor complexes: insights from QM/MM, MD, and molecular docking studies. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1907-18	3.5	31
787	SwissParam: a fast force field generation tool for small organic molecules. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2359-68	3.5	1025
786	Molecular mechanical study of halogen bonding in drug discovery. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2564-74	3.5	171
785	Theoretical modulation of the color of light emitted by firefly oxyluciferin. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2654-63	3.5	28
784	Ab initio prediction of protein-ligand binding structures by replica-exchange umbrella sampling simulations. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2810-21	3.5	48
783	Computational protocols for prediction of solute NMR relative chemical shifts. a case study of L-tryptophan in aqueous solution. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2853-64	3.5	23
782	Surveying implicit solvent models for estimating small molecule absolute hydration free energies. <i>Journal of Computational Chemistry</i> , 2011 , 32, 2909-23	3.5	58
781	Soft-core potentials in thermodynamic integration: comparing one- and two-step transformations. <i>Journal of Computational Chemistry</i> , 2011 , 32, 3253-63	3.5	137
780	Peptoid conformational free energy landscapes from implicit-solvent molecular simulations in AMBER. 2011 , 96, 639-50		43
779	Silver baits for the "miraculous draught" of amphiphilic lanthanide helicates. 2011 , 17, 184-95		12
778	Carbohydrate recognition at the minor-groove of the self-complementary duplex d(CGCGAATTCGCG) ₂ by a synthetic glyco-oligoamide. 2011 , 17, 4561-70		10
777	Investigating the imidazolium π anion interaction through the anion-templated construction of interpenetrated and interlocked assemblies. 2011 , 17, 12955-66		30
776	Molecular recognition of β -O-GlcNAc glycopeptides by a lectin-like receptor: binding modulation by the underlying Ser or Thr amino acids. 2011 , 12, 110-7		15
775	Conformational analysis of bivalent estrogen receptor ligands: from intramolecular to intermolecular binding. 2011 , 12, 2587-98		27
774	Chemical screens against a reconstituted multiprotein complex: myricetin blocks DnaJ regulation of DnaK through an allosteric mechanism. 2011 , 18, 210-21		80
773	Cytotoxic 3,6-bis((imidazolidinone)imino)acridines: synthesis, DNA binding and molecular modeling. 2011 , 19, 1790-801		74

772	Potential of mean force for separation of the repeating units in cellulose and hemicellulose. 2011 , 346, 867-71	9
771	Curcumin analogues as possible anti-proliferative & anti-inflammatory agents. 2011 , 46, 2722-35	66
770	Topology and dynamics of the interaction between 5-nitroimidazole radiosensitizers and duplex DNA studied by a combination of docking, molecular dynamic simulations and NMR spectroscopy. 2011 , 992, 65-71	13
769	Exploring the conformational changes of the ATP binding site of gyrase B from Escherichia coli complexed with different established inhibitors by using molecular dynamics simulation: protein-ligand interactions in the light of the alanine scanning and free energy decomposition methods. 2011 , 29, 726-39	33
768	Insight into analysis of interactions of GW9508 to wild-type and H86F and H137F GPR40: a combined QM/MM study and pharmacophore modeling. 2011 , 29, 818-25	7
767	Novel ligands that target the mitochondrial membrane protein mitoNEET. 2011 , 29, 965-73	24
766	Theoretical study of the reversible photoconversion mechanism in Dronpa. 2011 , 4, 251-260	4
765	Electro-osmotic drag coefficient of Nafion membrane with low water Content for Proton exchange membrane fuel cells. 2022 , 8, 598-612	0
764	Molecular insight into the polymorphism-dependent organic phosphorescence. 2022 , 208, 110853	0
763	Antagonistic mechanisms of bisphenol analogues on the estrogen receptor in zebrafish embryos: Experimental and computational studies. 2023 , 857, 159259	0
762	Thyroid hormone activities of neutral and anionic hydroxylated polybrominated diphenyl ethers to thyroid receptor α : A molecular dynamics study. 2023 , 311, 136920	0
761	Exploring the separation mechanism of Gemini surfactant in scheelite froth flotation at low temperatures: Surface characterization, DFT calculations and kinetic simulations. 2023 , 305, 122358	0
760	Some things old, new and borrowed: Delivery of dabrafenib and vemurafenib to melanoma cells via self-assembled nanomicelles based on an amphiphilic dendrimer. 2023 , 180, 106311	0
759	Spectroscopic methods to study the thermodynamics of biomolecular interactions. 2023 , 375-413	1
758	Demystifying viscous isoalkanes as the organic solvent in interfacial polymerization for manufacturing desalination membranes. 2023 , 545, 116166	0
757	Solvent interaction and dynamics of neurotransmitters -aspartic acid and -glutamic acid with water and ethanol. 2023 , 1273, 134347	1
756	Linear response properties of solvated systems: a computational study.	0
755	VR-MD: A Smartphone VR Application of Molecular Dynamics Simulation for Chemical Education. 2022 , 21, 43-44	0

- 754 Ion formation mechanism of cortisone molecules and clusters in charged nanodroplets. 0
- 753 How general is the effect of the bulkiness of organic ligands on the basicity of metalorganic catalysts? H₂-evolving Mo oxides/sulphides as case studies. 0
- 752 Theoretical study on the origin of the dual phosphorescence emission from organic aggregates at room temperature. **2023**, 287, 122077 0
- 751 Insights into the molecular interaction of cyclodextran with a guest molecule: A computational study. **2023**, 301, 120315 0
- 750 The impact of simulation time in predicting binding free energies using end-point approaches. **2022**, 20, 1 1
- 749 Influence of alkali metals on water dynamics inside imidazolium-based ionic liquid nano-domains. 10, 0
- 748 Glass transition of random heteropolymers: A molecular dynamics simulation study in melt, in water, and in vacuum. **2022**, 125503 2
- 747 Dimethylmyricacene: An In Vitro and In Silico Study of a Semisynthetic Non-Camptothecin Derivative Compound, Targeting Human DNA Topoisomerase 1B. **2022**, 11, 3486 0
- 746 RadonPy: automated physical property calculation using all-atom classical molecular dynamics simulations for polymer informatics. **2022**, 8, 0
- 745 Role of Chemical Linkage in Solvation of Polyurethanes in Organic Solvents Studied by Explicit Molecular Dynamics Simulations. **2022**, 61, 16883-16894 0
- 744 Insights into the mechanism of phospholipid hydrolysis by plant non-specific phospholipase C. 0
- 743 Computational Analysis of SAM Analogs as Methyltransferase Inhibitors of nsp16/nsp10 Complex from SARS-CoV-2. **2022**, 23, 13972 0
- 742 Molecular Insights Into the Physics of Poly(amidoamine)-Dendrimer-Based Supercapacitors. **2022**, 18, 0
- 741 MD simulations explain the excess molar enthalpies in pseudo-binary mixtures of a choline chloride-based deep eutectic solvent with water or methanol. 10, 0
- 740 pH Regulates Ligand Binding to an Enzyme Active Site by Modulating Intermediate Populations. 0
- 739 Cryo-EM structure of the agonist-bound Hsp90-XAP2-AHR cytosolic complex. **2022**, 13, 1 1
- 738 Computational modeling studies reveal the origin of the binding preference of 3-(3,4-dihydroisoquinolin-2(1H)-ylsulfonyl)benzoic acids for AKR1C3 over its isoforms. 0
- 737 Molecular Insights into the Heterotropic Allosteric Mechanism in Cytochrome P450 3A4-Mediated Midazolam Metabolism. 0

- 736 Binding Kinetics Toolkit for Analyzing Transient Molecular Conformations and Computing Free Energy Landscapes. ○
- 735 (Un)coupling the factors contributing to the interfacial activation of *Streptomyces rimosus* lipase: computational and spectrophotometric study. 1-11 ○
- 734 Building a Torsional Potential between Thiophene Rings to Illustrate the Basics of Molecular Modeling. ○
- 733 Binding site plasticity regulation of the FimH catch-bond mechanism. ○
- 732 Computational design, synthesis and biological evaluation of PDE5 inhibitors based on N2,N4-diaminoquinazoline and N2,N6-diaminopurine scaffolds. **2022**, 117092 ○
- 731 Enabling Donor:Acceptor Bicontinuous Networks via Short Contacts in Double-Cable Polymers with Pendant Rylene Diimides. ○
- 730 Libra: A modular software library for quantum nonadiabatic dynamics. **2022**, 100445 ○
- 729 Conserved Water Networks Identification for Drug Design Using Density Clustering Approaches on Positional and Orientational Data. ○
- 728 Volatile compounds of *Bacillus pseudomycooides* induce growth and drought tolerance in wheat (*Triticum aestivum* L.). **2022**, 12, ○
- 727 Estimation of Drug-Target Residence Time by Targeted Molecular Dynamics Simulations. ○
- 726 Practical Design of 3,6-Di-tert-butylidiphenyldibenzofulvene Derivatives with Enhanced Aggregation-Induced Emission. ○
- 725 Probing New Antileukemia Agents That Target FLT3 and BCL-2 from Traditional Concoctions through a Combination of Mass Spectrometry Analysis and Consensus Docking Methods. **2022**, 12, 11611 ○
- 724 Hydrophobicity Effects of β -Glutamyl Transpeptidase-Responsive Polymers on the Catalytic Activity and Transcytosis Efficacy. **2022**, 33, 2132-2142 ○
- 723 Ion-Exchanging Graphenic Nanochannels for Macroscopic Osmotic Energy Harvesting. ○
- 722 Selectivity and ranking of tight-binding JAK-STAT inhibitors using Markovian milestoning with Voronoi tessellations. ○
- 721 Identification of Active Compounds against Melanoma Growth by Virtual Screening for Non-Classical Human DHFR Inhibitors. **2022**, 23, 13946 ○
- 720 Enhanced Thermostability and Molecular Insights for L-Asparaginase from *Bacillus licheniformis* via Structure- and Computation-Based Rational Design. **2022**, 70, 14499-14509 ○
- 719 Molecular Dynamics Simulations of Self-Assembling Colloids in Fed-State Human Intestinal Fluids and Their Solubilization of Lipophilic Drugs. 1

718	Effect of hydrophobic groups on adsorption of arginine-based amino acids to solid surfaces in water.	0
717	Clustering conformational ensembles of intrinsically disordered proteins with t-distributed stochastic neighbor embedding.	1
716	Glycolytic flux control by drugging phosphoglycolate phosphatase. 2022 , 13,	0
715	SARS-CoV-2 Variants of Concern and Variations within Their Genome Architecture: Does Nucleotide Distribution and Mutation Rate Alter the Functionality and Evolution of the Virus?. 2022 , 14, 2499	0
714	Binding selectivity-dependent molecular mechanism of inhibitors towards CDK2 and CDK6 investigated by multiple short molecular dynamics and free energy landscapes. 2023 , 38, 84-99	3
713	Dynamic and thermodynamic impact of L94A, W100A, and W100L mutations on the D2 dopamine receptor bound to risperidone.	0
712	Comprehensive evaluation of end-point free energy techniques in carboxylated-pillar[6]arene host-guest binding: II. regression and dielectric constant.	2
711	CADD, AI and ML in Drug Discovery: A Comprehensive Review. 2022 , 106324	2
710	Ureas derived from camphor and fenchone reveal enantiomeric preference of human soluble epoxide hydrolase. 2022 , 100653	0
709	Supramolecular Combination Chemotherapy: Cucurbit[8]uril Complex Enhanced Platinum Drug Infiltration and Modified Nanomechanical Property of Colorectal Cancer Cells.	0
708	What drives chorismate mutase to top performance? Insights from a combined in silico and in vitro study.	0
707	Identification of Selective BRD9 Inhibitor via Integrated Computational Approach. 2022 , 23, 13513	0
706	Examining the Effect of Polymer Extension on Protein-Polymer Interactions That Occur during Formulation of Protein-Loaded Poly(lactic acid-co-glycolic acid)-polyethylene Glycol Nanoparticles. 2022 , 14, 4730	0
705	Study of the dynamics of the interaction of glycine and GABA with water and ethanol using theoretical tools. 2022 , 368, 120721	1
704	Mechanistic insight into separation of benzene and cyclohexane by extractive distillation using deep eutectic solvent as entrainer. 2022 , 368, 120780	0
703	Understanding the Hydration Thermodynamics of Cationic Quaternary Ammonium and Charge-Neutral Amine Surfactants.	0
702	Finding inhibitors and deciphering inhibitor-induced conformational plasticity in the Janus kinase via multiscale simulations. 1-27	0
701	Interactions of Proteins with Small Molecules, Allosteric Effects. 2022 , 315-332	0

- 700 Discovery and Optimization of N-Acyl-6-sulfonamide-tetrahydroquinoline Derivatives as Novel Non-Steroidal Selective Glucocorticoid Receptor Modulators. ○
- 699 Probing Phase Transitions in Organic Crystals Using Atomistic MD Simulations. ○
- 698 Nontoxic Artificial Chloride Channel Formation in Epithelial Cells by Isophthalic Acid-Based Small Molecules. ○
- 697 In silico molecular docking, dynamics simulation and repurposing of some VEGFR-2 inhibitors based on the SARS-CoV-2-main-protease inhibitor N3. 1-15 1
- 696 Novel Ascorbic Acid Co-Crystal Formulations for Improved Stability. **2022**, 27, 7998 ○
- 695 Molecular Simulations of Liquid Aliphatic Carboxylic Acids (C1-C6) using the 3D-RISM-KH Molecular Solvation Theory. **2022**, 120825 ○
- 694 The vitamin D receptor as a potential target for the toxic effects of per- and polyfluoroalkyl substances (PFASs): An in-silico study. **2022**, 114832 ○
- 693 Controlling the Polymorphism of Indomethacin with Poloxamer 407 in a Gas Antisolvent Crystallization Process. ○
- 692 Open Binding Pose Metadynamics: An Effective Approach for the Ranking of Protein-Ligand Binding Poses. ○
- 691 The binding affinity of human pediatric respiratory syncytial virus Phosphoprotein's C-terminal tail to nucleocapsid can be improved by a rationally designed halogen-bonded system. **2023**, 118, 108374 ○
- 690 Hydrolysis and aminolysis of aldehydes catalyzed by water and amines: Formation of diols/aminol and the implication to atmospheric particle formation. **2023**, 294, 119462 ○
- 689 Computational and experimental therapeutic efficacy analysis of andrographolide phospholipid complex self-assembled nanoparticles against Neuro2a cells. **2022**, 130283 1
- 688 Exploration of thiazolidine-2,4-diones as tyrosine kinase inhibitors: Design, synthesis, ADMET, docking, and antiproliferative evaluations. 1
- 687 Intermolecular noncovalent interactions with carbon in solution. **2022**, 13, 14327-14335 1
- 686 Optimization of potential non-covalent inhibitors for the SARS-CoV-2 main protease inspected by a descriptor of the subpocket occupancy. **2022**, 24, 29940-29951 ○
- 685 Dynamic and thermodynamic impact of L94A, W100A, and W100L mutations on the D2 dopamine receptor bound to risperidone. **2022**, 12, 34359-34368 ○
- 684 Basics of Quantum Chemical Calculation. **2022**, 217-241 ○
- 683 A direct approach toward investigating DNA-ligand interactions via surface-enhanced Raman spectroscopy combined with molecular dynamics simulations. ○

- 682 Discovery of allosteric SHP2 inhibitors through ensemble-based consensus molecular docking, endpoint and absolute binding free energy calculations. **2023**, 152, 106442 ○
- 681 Neuroprotective potential of cinnamoyl derivatives against Parkinson's disease indicators in *Drosophila melanogaster* and in silico models. **2023**, 94, 147-157 ○
- 680 Oleochemical carbonates: A comprehensive characterization of an emerging class of organic compounds. **2023**, 369, 120854 1
- 679 Structure-based drug design of novel *M. tuberculosis* InhA inhibitors based on fragment molecular orbital calculations. **2023**, 152, 106434 ○
- 678 Evaluation of ZIF-8 flexible force fields for structural and mechanical properties. **2023**, 348, 112406 ○
- 677 On the not so anomalous water-induced structural transformations of choline chloride-urea (reline) deep eutectic system. **2022**, 25, 439-454 ○
- 676 Investigation of structure and properties of polymerizable deep eutectic solvent based on choline chloride and acrylic acid. **2023**, 370, 121030 ○
- 675 Accurately predicting solvation free energy in aqueous and organic solvents beyond 298 K by combining deep learning and the 1D reference interaction site model. 1
- 674 Local conformations and heterogeneities in structures and dynamics of isotactic polypropylene adsorbed onto carbon fiber. **2023**, 265, 125584 ○
- 673 Molecular dynamics simulations and kinetic measurements provide insights into the structural requirements of substrate size-dependent specificity of oligogalacturonide oxidase 1 (OGOX1). **2023**, 194, 315-325 ○
- 672 Improving the thermostability of glycosyltransferase YojK by targeting mutagenesis for highly efficient biosynthesis of rebaudioside D. **2023**, 535, 112898 ○
- 671 A theoretical framework for the design of molecular crystal engines. ○
- 670 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 ○
- 669 Understanding the role of host-guest interactions in enhancing oil recovery through β -cyclodextrin and adamantane modified copolymer. **2023**, 369, 120841 ○
- 668 Internal acylation-induced AIE/AIEE switch of pyrimido[2,1-b][1,3]benzothiazoles (PBTs): Restriction of access to dark state caused by distortion of 4H-pyrimidine ring. **2023**, 210, 110982 ○
- 667 Design, synthetic approach, in silico molecular docking and antibacterial activity of quinazolin-2,4-dione hybrids bearing bioactive scaffolds. **2022**, 13, 292-308 ○
- 666 A photodecarboxylase from *Micractinium conductrix* active on medium and short-chain fatty acids. **2023**, 44, 160-170 ○
- 665 Liquid-liquid equilibrium experiment and mechanism analysis of menthol-based deep eutectic solvents extraction for separation of fuel additive tert-butanol. **2023**, 218, 115043 ○

- 664 Study of potential inhibition of the estrogen receptor by cannabinoids using an in silico approach: Agonist vs antagonist mechanism. **2023**, 152, 106403 ○
- 663 Efficient regulation of active layer morphology and interfacial charge-transfer process by porphyrin-based additive in organic solar cells. **2023**, 659, 130818 ○
- 662 Distinct binding pattern of nor-NOHA inhibitor to liver arginase in aqueous solution [Perspectives from molecular dynamics simulations. **2023**, 371, 121014 ○
- 661 An in-silico study to gain a comprehensive understanding of the effects of glucosylation on quercetin properties. **2023**, 1220, 113981 ○
- 660 Combined experimental and computational study on the effect of solvent structure on developing CO₂ biphasic absorbents. **2023**, 308, 122856 ○
- 659 In silico guided designing of optimized benzochalcones derivatives as potent CYP1B1 inhibitors: An integrated in vitro and ONIOM study. **2023**, 119, 108390 ○
- 658 Role of supramolecular steric compression during photoinduced intramolecular hydrogen abstraction reactions of ketones and thioketones. **2023**, 437, 114442 ○
- 657 Synthesis, biological evaluation and molecular docking study of benzimidazole derivatives as α-glucosidase inhibitors and anti-diabetes candidates. **2023**, 1276, 134774 ○
- 656 One-step production of biodiesel by wet Escherichia coli cells expressing a non-specific and methanol-resistant lipase. **2023**, 125, 75-83 ○
- 655 Heptakis(2,6-di-O-methyl)-β-CD as a host of olanzapine: Experimental and computational study. **2023**, 1276, 134812 ○
- 654 Inhibitory mechanism of phenolic compounds in rapeseed oil on α-amylase and α-glucosidase: Spectroscopy, molecular docking, and molecular dynamic simulation. **2023**, 289, 122251 ○
- 653 Integrated investigation for extractive denitrogenation of fuel oils with Eco-friendly Piperazine-Based ionic liquids. **2023**, 337, 127187 ○
- 652 Structural basis of Nrf2 activation by flavonolignans from silymarin. **2023**, 119, 108393 ○
- 651 Combined QM (MS-CASPT2)/MM studies on photocyclization and photoisomerization of a fulgide derivative in toluene solution. **2022**, 24, 29918-29926 ○
- 650 The effect of electric field on the structural order of water molecules around chitosan between nano gold plates determined by molecular dynamics simulations. **2022**, 24, 30035-30043 ○
- 649 Photochemistry of Biological Systems: Excited-State Electronic Structure Calculations and Nonadiabatic Dynamics Simulations with QM/MM Methods. **2022**, ○
- 648 Structural and conformational dynamics of human milk oligosaccharides, lacto-N-fucopentaose I and II, through molecular dynamics simulation. **2022**, 41, 385-404 ○
- 647 Reflections on a Career of Physical Chemistry Research at Undergraduate Liberal Arts Colleges: Overview of Research and Advice to Emerging Researchers. 1-18 ○

646	Facet Selectivity of Cetyltrimethyl Ammonium Bromide Surfactants on Gold Nanoparticles Studied Using Molecular Simulations. 2022 , 126, 10249-10255	0
645	Molecular Dynamics Simulations of Rhodamine B Zwitterion Diffusion in Polyelectrolyte Solutions. 2022 , 126, 10256-10272	0
644	TransRot: A Portable Software Package for Simulated Annealing Monte Carlo Geometry Optimization of Atomic and Molecular Clusters. 19-38	0
643	Structural basis of synthetic agonist activation of the nuclear receptor REV-ERB. 2022 , 13,	1
642	Accelerating cryptic pocket discovery using AlphaFold.	1
641	Orthogonal glycolytic pathway enables directed evolution of noncanonical cofactor oxidase. 2022 , 13,	0
640	Diffusion theory of molecular liquids in the energy representation and application to solvation dynamics.	0
639	Computer simulation of molecular recognition in biomolecular system: from in silico screening to generalized ensembles.	1
638	The Signature C=C=O Stretch of Propenylketenes and Ketene Clusters. 53-67	0
637	Investigating the Dynamic Binding Behavior of PMX53 Cooperating with Allosteric Antagonist NDT9513727 to C5a Anaphylatoxin Chemotactic Receptor 1 through Gaussian Accelerated Molecular Dynamics and Free-Energy Perturbation Simulations. 2022 , 13, 3502-3511	2
636	Design Two Novel Tetrahydroquinoline Derivatives against Anticancer Target LSD1 with 3D-QSAR Model and Molecular Simulation. 2022 , 27, 8358	0
635	QM/MM Investigation to Identify the Hallmarks of Superior PET Biodegradation Activity of PETase over Cutinase. 2022 , 10, 15857-15868	0
634	Computer-Aided Drug Design: An Update. 2023 , 123-152	1
633	Molecular modelling of SdiA protein by selected flavonoid and terpenes compounds to attenuate virulence in <i>Klebsiella pneumoniae</i> . 1-19	0
632	Insights into the Interactions of Peptides with Monolayer-Protected Metal Nanoclusters.	0
631	ES-Screen: A Novel Electrostatics-Driven Method for Drug Discovery Virtual Screening. 2022 , 23, 14830	0
630	Decoding the Identification Mechanism of an SAM-III Riboswitch on Ligands through Multiple Independent Gaussian-Accelerated Molecular Dynamics Simulations. 2022 , 62, 6118-6132	10
629	Computational Analysis of the Structure of the Kappa-Opioid Receptor for the Development of Selective Antagonists. 99-122	0

628	Title, Copyright, Foreword. i-v	0
627	Using Modified Long Chain Fatty Acids to Explore Protein Dynamics in an Intracellular-Lipid Binding Protein. 145-156	0
626	Bergman Cyclization of Maleimide-Based Eneidyne. 157-175	0
625	Potential SARS-CoV-2 RdRp inhibitors of cytidine derivatives: Molecular docking, molecular dynamic simulations, ADMET, and POM analyses for the identification of pharmacophore sites. 2022 , 17, e0273256	1
624	Cooling-Rate Computer Simulations for the Description of Crystallization of Organic Phase-Change Materials. 2022 , 23, 14576	1
623	DeepPROTACs is a deep learning-based targeted degradation predictor for PROTACs. 2022 , 13,	2
622	Computational Study of Helicase from SARS-CoV-2 in RNA-Free and Engaged Form. 2022 , 23, 14721	0
621	Evolution of drug resistance drives progressive destabilizations in functionally conserved molecular dynamics of the flap region of the HIV-1 protease.	0
620	Osmotic Contribution of Synthesized Betaine by Choline Dehydrogenase Using In Vivo and In Vitro Models of Post-traumatic Syringomyelia.	0
619	Confining donor conformation distributions for efficient thermally activated delayed fluorescence with fast spin-flipping.	0
618	Resolving the Impact of Hydrogen Bonding on the Phylloquinone Cofactor through Two-Dimensional Infrared Spectroscopy. 2022 , 126, 10120-10135	0
617	The Infrared Spectrum of Matrix-Isolated Ethanethiol. 85-98	0
616	Building a Successful Computational Chemistry Laboratory. 69-83	0
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613	Physical Chemistry Research at Undergraduate Institutions: Innovative and Impactful Approaches, Volume 1.	0
612	Toward Reliable and Insightful Entropy Calculations on Flexible Molecules. 2022 , 18, 7166-7178	0
611	A Comparison of Methods for Computing Relative Anhydrous Hydrate Stability with Molecular Simulation.	0

610	Deciphering the active constituents of Dabushen decoction of ameliorating osteoarthritis via PPAR α preservation by targeting DNMT1. 13,	0
609	AMBER Drug Discovery Boost Tools: Automated Workflow for Production Free-Energy Simulation Setup and Analysis (ProFESSA). 2022 , 62, 6069-6083	0
608	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
607	Obtaining and Characterizing Stable Bicontinuous Cubic Morphologies and Their Nanochannels in Lyotropic Liquid Crystal Membranes. 2022 , 126, 10098-10110	0
606	Preface. ix-x	0
605	Subject Index. 193-195	0
604	Screening and Molecular Mechanisms of Novel ACE-Inhibitory Peptides from Gracilariopsis lemneiformis. 2022 , 23, 14850	0
603	Efficient Computation of the Interaction Energies of Very Large Non-covalently Bound Complexes.	0
602	Mechanism of Action of Flavin-Dependent Halogenases. 2022 , 12, 15352-15360	0
601	Theoretical Studies of Leu-Pro-Arg-Asp-Ala Pentapeptide (LPRDA) Binding to Sortase A of Staphylococcus aureus. 2022 , 27, 8182	0
600	Synthesis of indole derivatives as Alzheimer inhibitors and their molecular docking study. 1-14	0
599	Potential Competitive Inhibitors of SHP-2 Identified by Structure-Based Virtual Screening and Molecular Dynamics Simulation. 123-143	0
598	Embracing Modern Software Development Best Practices in an Undergraduate Research Setting: A Case Study with the WPTherml Software Package. 39-52	0
597	Inhibition of VMAT2 by α -adrenergic agonists, antagonists, and the atypical antipsychotic ziprasidone. 2022 , 5,	0
596	Collaborative Assessment of Molecular Geometries and Energies from the Open Force Field. 2022 , 62, 6094-6104	0
595	Evaluation of interactions between the hepatitis C virus NS3/4A and sulfonamidobenzamide based molecules using molecular docking, molecular dynamics simulations and binding free energy calculations.	0
594	Realistic simulation of thermoelectric characteristics of organic semiconductors based on electronic structure calculations.	0
593	A Molecular Dynamics Study on the Tribological Performance of ImidazoliumBased Ionic Liquids Mixed with Oil in Comparison to Pure Liquids. 2022 , 7, 384	0

592	Endophytic bacteria of <i>Fagonia indica</i> Burm. f revealed to harbour rich secondary antibacterial metabolites. 2022 , 17, e0277825	1
591	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
590	The SARS-CoV-2 spike protein binds and modulates estrogen receptors. 2022 , 8,	2
589	Anticancer Activity, Reduction Mechanism and G-Quadruplex DNA Binding of a Redox-Activated Platinum(IV)Salphen Complex. 2022 , 23, 15579	1
588	α-amino carbonyl derivatives: Synthesis, Molecular Docking, ADMET, Molecular Dynamic and Herbicidal studies.. 2022 , 7,	3
587	Fluorination of Terminal Groups Promoting Electron Transfer in Small Molecular Acceptors of Bulk Heterojunction Films. 2022 , 27, 9037	0
586	Shorter Alkanesulfonate Carbon Chains Destabilize the Active Site Architecture of SsuD for Desulfonation.	0
585	Novel Peptide Inhibitor of Human Tumor Necrosis Factor- α has Antiarthritic Activity.	0
584	Protein-Ligand Binding Free-Energy Calculations with ARROW-A Purely First-Principles Parameterized Polarizable Force Field. 2022 , 18, 7751-7763	0
583	Arf GTPase activates the WAVE regulatory complex through a distinct binding site. 2022 , 8,	0
582	(-)-Epigallocatechin-3-gallate Directly Binds Cyclophilin D: A Potential Mechanism for Mitochondrial Protection. 2022 , 27, 8661	0
581	Using machine learning to detect coronaviruses potentially infectious to humans.	0
580	Molecular Dynamics Simulation of Poly(Ether Ether Ketone) (PEEK) Polymer to Analyze Intermolecular Ordering by Low Wavenumber Raman Spectroscopy and X-ray Diffraction. 2022 , 14, 5406	0
579	Water Networks in Complexes between Proteins and FDA-Approved Drugs.	0
578	Machine learning in accelerating microsphere formulation development.	0
577	Biodegradation of 2,5-Dihydropyridine by 2,5-Dihydropyridine Dioxygenase and Its Mutants: Insights into O-D Bond Activation and Flexible Reaction Mechanisms from QM/MM Simulations. 2022 , 61, 20501-20512	0
576	Structures of the Inhibitory Receptor Siglec-8 in Complex with a High-Affinity Sialoside Analogue and a Therapeutic Antibody.	0
575	SARS-CoV-2 proteases Mpro and PLpro: Design of inhibitors with predicted high potency and low mammalian toxicity using artificial neural networks, ligand-protein docking, molecular dynamics simulations, and ADMET calculations. 2022 , 106449	1

- 574 Engineering a Medium-chain Alcohol Dehydrogenase for Efficient Synthesis of (S)-N-Boc-3-pyrrolidinol by Adjusting the Conformational Dynamics of Loops. ○
- 573 Conformational Flexibility Is a Key Determinant for the Lytic Activity of the Pore-Forming Protein, Cytolysin A. ○
- 572 Molecular Basis for Non-Covalent, Non-Competitive FAAH Inhibition. **2022**, 23, 15502 ○
- 571 Role of Monovalent Ions in the NKCC1 Inhibition Mechanism Revealed through Molecular Simulations. **2022**, 23, 15439 ○
- 570 A Density Functional Theory and Molecular Dynamics Study of Antifolate Molecules under Physiological Conditions. **2022**, 7, ○
- 569 Mechanistic investigation of SARS-CoV-2 main protease to accelerate design of covalent inhibitors. **2022**, 12, 1 ○
- 568 Overcoming pancreatic cancer immune resistance by codelivery of CCR2 antagonist using a STING-activating gemcitabine-based nanocarrier. **2022**, ○
- 567 Effects of Salinity and Temperature on the Flexibility and Function of a Polyextremophilic Enzyme. **2022**, 23, 15620 ○
- 566 An Efficient Approach to Large-Scale Ab Initio Conformational Energy Profiles of Small Molecules. **2022**, 27, 8567 ○
- 565 Guanidino acid hydrolysis by the human enzyme annotated as agmatinase. **2022**, 12, ○
- 564 Virtual screening for finding inhibitor against the main protease of SARS-Cov-2 from the FDA-approved drugs database. **2022**, ○
- 563 Molecular dynamics-based insight of VEGFR-2 kinase domain: a combined study of pharmacophore modeling and molecular docking and dynamics. **2023**, 29, ○
- 562 Perturbation of Lipid Bilayers by Biomimetic Photoswitches Based on Cyclocurcumin. ○
- 561 Quinoxalinones as A Novel Inhibitor Scaffold for EGFR (L858R/T790M/C797S) Tyrosine Kinase: Molecular Docking, Biological Evaluations, and Computational Insights. **2022**, 27, 8901 ○
- 560 Evolutionary and cellular analysis of the 'dark' pseudokinase PSKH2. ○
- 559 Virtual Screening of FDA-Approved Drugs for Enhanced Binding with Mitochondrial Aldehyde Dehydrogenase. **2022**, 27, 8773 ○
- 558 Microsecond-long simulation reveals the molecular mechanism for the dual inhibition of falcipain-2 and falcipain-3 by antimalarial lead compounds. 9, ○
- 557 Understanding the Allosteric Modulation of PTH1R by a Negative Allosteric Modulator. **2023**, 12, 41 ○

- 556 Design, Synthesis, Inhibitory Activity, and Molecular Modeling of Novel Pyrazole-Furan/Thiophene Carboxamide Hybrids as Potential Fungicides Targeting Succinate Dehydrogenase. ○
- 555 Novel Camphor Sulfonylhydrazide and Sulfonamide Derivatives as Potential Succinate Dehydrogenase Inhibitors against Phytopathogenic Fungi/Oomycetes. ○
- 554 Comparative antibacterial analysis of the anthraquinone compounds based on the AIM theory, molecular docking, and dynamics simulation analysis. **2023**, 29, ○
- 553 Identification of new potent agonists for toll-like receptor 8 by virtual screening methods, molecular dynamics simulation, and MM-GBSA. 1-11 ○
- 552 HIF-1 signalling pathway was identified as a potential new pathway for Icaritin treatment against Alzheimer's disease based on preclinical evidence and bioinformatics. 13, ○
- 551 Rational enzyme design for enabling biocatalytic Baldwin cyclization and asymmetric synthesis of chiral heterocycles. **2022**, 13, ○
- 550 Ligand Gaussian accelerated molecular dynamics 2 (LiGaMD2): Improved calculations of ligand binding thermodynamics and kinetics with closed protein pocket. ○
- 549 Benchmarking biomolecular force field-based Zn²⁺ for mono- and bimetallic ligand binding sites. 2
- 548 SARS-CoV-2 induces cytokine storm/hyperinflammatory responses in RA patients through pyroptosis. 13, ○
- 547 Cumulative Millisecond-Long Sampling for a Comprehensive Energetic Evaluation of Aqueous Ionic Liquid Effects on Amino Acid Interactions. ○
- 546 DeePKS + ABACUS as a Bridge between Expensive Quantum Mechanical Models and Machine Learning Potentials. **2022**, 126, 9154-9164 ○
- 545 Modeling Impurity-Mediated Crystal Growth and Morphologies of Centrosymmetric Molecules. ○
- 544 N-Substituted piperidine-3-carbohydrazide-hydrazones against Alzheimer's disease: Synthesis and evaluation of cholinesterase, beta-amyloid inhibitory activity, and antioxidant capacity. ○
- 543 Structural and binding studies of 2'- and 3-fucosyllactose and its complexes with norovirus capsid protein by molecular dynamics simulations. 1-14 ○
- 542 Prediction of Water Diffusion in Wide Varieties of Polymers with All-Atom Molecular Dynamics Simulations and Deep Generative Models. ○
- 541 Unraveling the Abnormal Molecular Mechanism of Suicide Inhibition of Cytochrome P450 3A4. **2022**, 62, 6172-6181 ○
- 540 Thermally Controlled Exciplex Fluorescence in a Dynamic Homo[2]catenane. ○
- 539 Simulation Reveals the Chameleonic Behavior of Macrocycles. ○

- 538 Preclinical Studies and Drug Combination of Low-Cost Molecules for Chagas Disease. **2023**, 16, 20 ○
- 537 Macrophage ferroportin serves as a therapeutic target against bacteria-induced acute lung injury by promoting barrier restoration. **2022**, 25, 105698 ○
- 536 Blue Fluorescence of Cyano-tryptophan Predicts Local Electrostatics and Hydrogen Bonding in Biomolecules. **2022**, 126, 10732-10740 ○
- 535 Predicting the Electronic Absorption Band Shape of Azobenzene Photoswitches. **2023**, 24, 25 ○
- 534 Activation Mechanism of RhoA Caused by Constitutively Activating Mutations G14V and Q63L. **2022**, 23, 15458 ○
- 533 Carbonyl-Containing Solid Polymer Electrolyte Host Materials: Conduction and Coordination in Polyketone, Polyester, and Polycarbonate Systems. **2022**, 55, 10940-10949 2
- 532 MoBioTools : A toolkit to setup quantum mechanics/molecular mechanics calculations. ○
- 531 Purine 5Ribonucleotide- l -Glutamate Hybrids As Potential Tools To Investigate The Mechanism Of Umami Taste Reception. **2022**, 7, ○
- 530 Chemoenzymatic synthesis of sulfur-linked sugar polymers as heparanase inhibitors. **2022**, 13, ○
- 529 Building Quantitative Bridges between Dynamics and Sequences of SARS-CoV-2 Main Protease and a Diverse Set of Thirty-Two Proteins. ○
- 528 Computational Prediction of Resistance Induced Alanine-Mutation in ATP Site of Epidermal Growth Factor Receptor. **2022**, 23, 15828 ○
- 527 Enhanced mechanical, barrier and antioxidant properties of rice protein/sodium alginate-based films by incorporating cellulose nanocrystals and rosemary extract. **2022**, 34, 101000 ○
- 526 In Vitro Study of Cytotoxic Mechanisms of Alkylphospholipids and Alkyltriazoles in Acute Lymphoblastic Leukemia Models. **2022**, 27, 8633 ○
- 525 Total enzymatic synthesis of cis- β -trone from a simple carbon source. **2022**, 13, ○
- 524 Identification of potential inhibitors of omicron variant of SARS-Cov-2 RBD based virtual screening, MD simulation, and DFT. 10, ○
- 523 Comparison of Conformational Analyses of Naturally Occurring Flavonoid-O-Glycosides with Unnatural Flavonoid-CF2-Glycosides Using Molecular Modeling. ○
- 522 MM/PB(GB)SA benchmarks on soluble proteins and membrane proteins. 13, ○
- 521 Improved docking of peptides and small molecules in iMOLSDOCK. **2023**, 29, 1

- 520 Phase Equilibria and Mechanism Insights into the Separation of Isopropyl Acetate and Methanol by Deep Eutectic Solvents. ○
- 519 Design of new chemical entities targeting both native and H275Y mutant influenza a virus by deep reinforcement learning. 1-15 ○
- 518 Cofactor-Free Dioxygenases-Catalyzed Reaction Pathway via Proton-Coupled Electron Transfer. ○
- 517 Evolutionary divergence in the conformational landscapes of Tyrosine vs Serine/Threonine Kinases. 11, ○
- 516 Novel quinolin-2(1H)-one analogous as potential fungicides targeting succinate dehydrogenase: design, synthesis, inhibitory evaluation and molecular modeling. ○
- 515 Molecular Dynamics Study on the Structure-Property Relationship of Self-Assembled Gear-Shaped Amphiphile Molecules with/without Methyl Groups. ○
- 514 Insights from incorporating quantum computing into drug design workflows. ○
- 513 Efficient Antibacterial/Antifungal Activities: Synthesis, Molecular Docking, Molecular Dynamics, Pharmacokinetic, and Binding Free Energy of Galactopyranoside Derivatives. **2023**, 28, 219 4
- 512 Conformational switch and multiple supramolecular structures of a newly identified self-assembling protein-mimetic peptide from *Pseudomonas aeruginosa* YeaZ protein. 10, ○
- 511 In silico and in vitro studies of potential inhibitors against Dengue viral protein NS5 Methyl Transferase from Ginseng and Notoginseng. **2022**, ○
- 510 Ligands-Induced Open-Close Conformational Change during DapE Catalysis: Insights from Molecular Dynamics Simulations. ○
- 509 Strain data augmentation enables machine learning of inorganic crystal geometry optimization. **2023**, 100663 ○
- 508 AMBER Free Energy Tools: A New Framework for the Design of Optimized Alchemical Transformation Pathways. 1
- 507 Identification of an Evolutionarily Conserved Allosteric Network in Steroid Receptors. ○
- 506 Coenzyme corona formation on carbon nanotubes leads to disruption of the redox balance in metabolic reactions. ○
- 505 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 ○
- 504 Cryo-EM Structures of AcrD Illuminate a Mechanism for Capturing Aminoglycosides from Its Central Cavity. ○
- 503 Regularized by Physics: Graph Neural Network Parametrized Potentials for the Description of Intermolecular Interactions. ○

- 502 Computer-aided structure-based optimization of 4,5,6,7-tetrahydrobenzo[d]thiazole-2,6-diamine derivatives as DNA gyrase B inhibitors. ○
- 501 Computationally guided discovery of novel non-steroidal AR-GR dual antagonists demonstrating potency against antiandrogen resistance. 1
- 500 MemCross: Accelerated Weight Histogram method to assess membrane permeability. **2023**, 184120 ○
- 499 Conformational Search for the Building Block of Proteins Based on the Gradient Gravitational Search Algorithm (ConfGGS) Using Force Fields: CHARMM, AMBER, and OPLS-AA. ○
- 498 *Klebsiella Pneumoniae* Volatile Organic Compounds (VOCs) Protect *Artemia salina* from Fish Pathogen *Aeromonas* sp.: A Combined In Vitro, In Vivo, and In Silico Approach. **2023**, 11, 172 ○
- 497 The effect of solvent on determining highest occupied molecular orbital energies of semiconducting organic molecules: Insight from a combined computational approach. ○
- 496 Molecular Modelling of Ionic Liquids: Situations When Charge Scaling Seems Insufficient. **2023**, 28, 800 ○
- 495 Modus Operandi of a Pedalo-Type Molecular Switch: Insight from Dynamics and Theoretical Spectroscopy. **2023**, 28, 816 ○
- 494 Chetomin, a SARS-CoV-2 3C-like Protease (3CLpro) Inhibitor: In Silico Screening, Enzyme Docking, Molecular Dynamics and Pharmacokinetics Analysis. **2023**, 15, 250 ○
- 493 Novel Lennard-Jones Parameters for Cysteine and Selenocysteine in the AMBER Force Field. 1
- 492 Citrus, Milk Thistle, and Propolis Extracts Improved the Intestinal Permeability of Curcuminoids from Turmeric Extract- an In Silico and In Vitro Permeability Caco-2 Cells Approach. ○
- 491 Approaching the Dimerization Mechanism of Small Molecule Inhibitors Targeting PD-L1 with Molecular Simulation. **2023**, 24, 1280 1
- 490 Reentrant 2D Nanostructured Liquid Crystals by Competition between Molecular Packing and Conformation: Potential Design for Multistep Switching of Ionic Conductivity. ○
- 489 Small-Molecule Inhibitor of Flaviviral NS3-NS5 Interaction with Broad-Spectrum Activity and Efficacy In Vivo. ○
- 488 An NmrA-like enzyme-catalysed redox-mediated Diels-Alder cycloaddition with anti-selectivity. ○
- 487 Mechanistic Investigation of the Androgen Receptor DNA-Binding Domain and Modulation via Direct Interactions with DNA Abasic Sites: Understanding the Mechanisms Involved in Castration-Resistant Prostate Cancer. **2023**, 24, 1270 ○
- 486 Additive energetic contributions of multiple peptide positions determine the relative promiscuity of viral and human sequences for PDZ domain targets. ○
- 485 How Does Multiple Substrate Binding Lead to Substrate Inhibition of CYP2D6 Metabolizing Dextromethorphan? A Theoretical Study. ○

- 484 Discovery of Novel Drug-like PHGDH Inhibitors to Disrupt Serine Biosynthesis for Cancer Therapy. **2023**, 66, 285-305 ○
- 483 Quasi-static Deformation Simulations of Molecular Crystals. ○
- 482 Catalytic mechanism for Renilla-type luciferases. 1
- 481 Assessment of host-guest molecular encapsulation of eugenol using β -cyclodextrin. 10, ○
- 480 An ensemble docking-based virtual screening according to different TRPV1 pore states toward identifying phytochemical activators. ○
- 479 Study on endogenous inhibitors against PD-L1: cAMP as a potential candidate. **2023**, 123266 ○
- 478 Treating Polarization Effects in Charged and Polar Bio-Molecules Through Variable Electrostatic Parameters. 1
- 477 Investigating the Solvent Effects on Binding Affinity of PAHs-Box4+ Complexes: An Alchemical Approach. **2023**, 127, 249-260 ○
- 476 Direct detection of a single [4Fe-4S] cluster in a tungsten-containing enzyme: Electrochemical conversion of CO₂ into formate by formate dehydrogenase. ○
- 475 Substrate selectivity and inhibition of histidine JmjC hydroxylases MINA53 and NO66. ○
- 474 Computational studies on potential small molecule inhibitors of Leishmania pteridine reductase 1. 1-14 ○
- 473 Inhibition of Iron Release from Donkey Spleen Ferritin through Malt-Derived Protein Zherulic Acid Interactions. **2023**, 12, 234 ○
- 472 In silico Assessment of Dipeptidyl Peptidase 4 (DPP-4) Inhibiting Potential of a few Bioactive Compounds Present in Black Rice Bran for Effective Management of Postprandial Hyperglycemia. ○
- 471 Adsorption of water and organic solvents on the calcite [101 $\bar{4}$] surface: implications for marble conservation treatments. **2023**, 156438 ○
- 470 Effect of Conformational Equilibrium on Solvation Properties of 1,2-DCE in Water: A Solvation Thermodynamics and 3D-RISM Study. ○
- 469 Development of fluorophore labeled or biotinylated anticancer small molecule NSC243928. **2023**, 117171 ○
- 468 Predictions of the Poses and Affinity of a Ligand over the Entire Surface of a NEET Protein: The Case of Human MitoNEET. ○
- 467 Modulating membrane shape and mechanics of minimal cells by light: area increase, softening and interleaflet coupling of membrane models doped with azobenzene-lipid photoswitches. ○

- 466 4-Cyanotryptophan as a Sensitive Fluorescence Probe of Local Electric Field of Proteins. ○
- 465 Discovery and Computational Studies of Potent Covalent Kinase Inhibitors with π -Substituent Electrophiles Targeting Cysteine. ○
- 464 Seleno-Analogs of Scaffolds Resembling Natural Products a Novel Warhead toward Dual Compounds. **2023**, 12, 139 1
- 463 Is the Triggering of PD-L1 Dimerization a Potential Mechanism for Food-Derived Small Molecules in Cancer Immunotherapy? A Study by Molecular Dynamics. **2023**, 24, 1413 ○
- 462 In Silico Discovery of Aptamers with An Enhanced Library Design Strategy. **2023**, ○
- 461 Molecular dynamics simulation study on the inhibitory mechanism of RIPK1 by 4,5-dihydropyrazole derivatives. ○
- 460 Anti-colorectal cancer of *Ardisia gigantifolia* Stapf. and targets prediction via network pharmacology and molecular docking study. **2023**, 23, ○
- 459 ACES: Optimized Alchemically Enhanced Sampling. ○
- 458 Probing DNA structural heterogeneity by identifying conformational subensembles of a bicovalently bound cyanine dye. **2023**, 158, 035101 ○
- 457 Selective modification of diclofenac to reduce the adverse effects; A computer-aided drug design approach. **2023**, 36, 101159 ○
- 456 Determining interchromophore effects for energy transport in molecular networks using machine-learning algorithms. ○
- 455 Reproduction of super-multicomponent self-assembled structures and their functionality using coarse-grained molecular simulation - the example of cleansing foams. ○
- 454 State averaged CASSCF in AMOEBA polarizable water model for simulating nonadiabatic molecular dynamics with nonequilibrium solvation effects. **2023**, 158, 014101 ○
- 453 Synthesis, Biological Evaluation and Molecular Modeling Studies of Naphthoquinone Sulfonamides and Sulfonate Ester Derivatives as P2X7 Inhibitors. **2023**, 28, 590 ○
- 452 gmak: A Parameter-Space Mapping Strategy for Force-Field Calibration. ○
- 451 Structural Analysis, Multi-Conformation Virtual Screening and Molecular Simulation to Identify Potential Inhibitors Targeting pS273R Proteases of African Swine Fever Virus. **2023**, 28, 570 ○
- 450 Use of Apatinib as a Bait to Fish Its Unexpected Kinase Targets from the Hepatocellular Carcinoma Druggable Kinome. ○
- 449 Diameter-Selective Sorting of Single-Walled Carbon Nanotubes Using π -Molecular Tweezers for Energy Materials. ○

- 448 Enzymatic (2 R ,4 R)-Pentanediol Synthesis [Putting a Bottle on the Table] ○
- 447 Interaction of Chondroitin and Hyaluronan Glycosaminoglycans with Surfaces of Carboxylated Carbon Nanotubes Studied Using Molecular Dynamics Simulations. **2023**, 28, 826 ○
- 446 Amino acid-driven adsorption of emerging contaminants in water by modified graphene oxide nanosheets. ○
- 445 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 ○
- 444 Discovery of Novel Chinese Medicine Compounds Targeting 3CL Protease by Virtual Screening and Molecular Dynamics Simulation. **2023**, 28, 937 ○
- 443 Bio-inspired polydopamine nanofiltration membranes modulated by spiro-piperazine. **2023**, 3, 100059 ○
- 442 An Imbalance in the Force: The Need for Standardized Benchmarks for Molecular Simulation. ○
- 441 Discovery of aromatic 2-(3-(methylcarbamoyl) guanidino)-N-acylacetamides as highly potent chitinase inhibitors. **2023**, 117172 ○
- 440 Insights into the mechanism of phospholipid hydrolysis by plant non-specific phospholipase C. **2023**, 14, ○
- 439 Integrating physics in deep learning algorithms: A force field as a PyTorch module. ○
- 438 Identification of Potential Druggable Targets and Structure-Based Virtual Screening for Drug-like Molecules against the Shrimp Pathogen *Enterocytozoon hepatopenaei*. **2023**, 24, 1412 ○
- 437 Repurposing Ponatinib as a PD-L1 Inhibitor Revealed by Drug Repurposing Screening and Validation by In Vitro and In Vivo Experiments. ○
- 436 [4Fe4S]-Mediated Proton-Coupled Electron Transfer Enables the Efficient Degradation of Chloroalkenes by Reductive Dehalogenases. 1173-1185 ○
- 435 Identifying Systematic Force Field Errors Using a 3D-RISM Element Counting Correction. **2023**, 28, 925 1
- 434 Critical Assessment of Methods for Predicting the 3D Structure of Proteins and Protein Complexes. **2023**, 52, ○
- 433 In Silico and In Vitro Study of Janus Kinases Inhibitors from Naphthoquinones. **2023**, 28, 597 ○
- 432 Computational Study of the Inhibition of RgpB Gingipain, a Promising Target for the Treatment of Alzheimer's Disease. ○
- 431 α -5 Helices on Surface of KRAS Can Accommodate Small Compounds That Increase KRAS Signaling While Inducing CRC Cell Death. **2023**, 24, 748 1

- 430 1,2-Dibenzoylhydrazine as a Multi-Inhibitor Compound: A Morphological and Docking Study. **2023**, 24, 1425 1
- 429 Active Learning Guided Drug Design Lead Optimization Based on Relative Binding Free Energy Modeling. 0
- 428 Molecular dynamics study on the behavior and binding mechanism of target protein Transgelin-2 with its agonist TSG12 for anti-asthma drug discovery. **2023**, 153, 106515 0
- 427 Highly triple-effective synergy based on tetrahedral DNA nanostructure-induced tumor vaccines for cancer therapy. **2023**, 226, 111584 0
- 426 Spiral donor-based host materials for highly efficient blue thermally activated delayed fluorescence OLEDs. **2023**, 458, 141416 0
- 425 Discovery of inhibitors against SARS-CoV-2 main protease using fragment-based drug design. **2023**, 371, 110352 0
- 424 HTPolyNet: A general system generator for all-atom molecular simulations of amorphous crosslinked polymers. **2023**, 21, 101303 0
- 423 Computer-aided identification, synthesis, and biological evaluation of DNA polymerase α inhibitors for the treatment of cancer. **2023**, 248, 115044 0
- 422 Revealing the critical role of Leucine145 of β -glucosidase AgIA for enhancing β -arbutin production. **2023**, 537, 112943 0
- 421 Non-classical digestive lipase BmTGL selected by gene amplification reduces the effects of mulberry inhibitor during silkworm domestication. **2023**, 229, 589-599 0
- 420 Covalent polyphenol modification of a reactive cysteine in the major apple allergen Mal d 1. **2023**, 410, 135374 0
- 419 Understanding the pH-dependent interaction of anthocyanin with two food-derived transferrins. **2023**, 410, 135473 0
- 418 High-Throughput Prediction of the Impact of Genetic Variability on Drug Sensitivity and Resistance Patterns for Clinically Relevant Epidermal Growth Factor Receptor Mutations from Atomistic Simulations. **2023**, 63, 321-334 0
- 417 Mechanism of β -hairpin formation in AzoChignolin and Chignolin. 0
- 416 Insights into pralsetinib resistance to the non-gatekeeper RET kinase G810C mutation through molecular dynamics simulations. **2023**, 29, 0
- 415 Theoretical Computational Analysis Predicts Interaction Changes Due to Differences of a Single Molecule in DNA. **2023**, 13, 510 0
- 414 StructureDynamics Interrelation Governing Charge Transport in Cosolvated Acetonitrile/LiTFSI Solutions. **2023**, 127, 308-320 0
- 413 Cooperation of structural motifs controls drug selectivity in cyclin-dependent kinases: an advanced theoretical analysis. **2023**, 24, 0

- 4¹² Monocarbonyl Curcumin Analogues as Potent Inhibitors against Human Glutathione Transferase P1-1. **2023**, 12, 63 5
- 4¹¹ Charge Transport Measured Using the EGaIn Junction through Self-Assembled Monolayers Immersed in Organic Liquids. **2023**, 127, 407-424 0
- 4¹⁰ Influence of polymer compatibility and layer thickness on the structural and thermophysical properties of polymer multilayer films. 0
- 4⁰⁹ Elucidating the Hydrotropic Mechanism of the Antagonistic Salt PPh₄Cl. **2023**, 127, 996-1012 0
- 4⁰⁸ Antiproliferative Noscapiroids Bearing an Amidothiadiazole Scaffold as Apoptosis Inducers: Design, Synthesis and Molecular Docking. 0
- 4⁰⁷ Molecular Epidemiology of SARS-CoV-2: The Dominant Role of Arginine in Mutations and Infectivity. **2023**, 15, 309 0
- 4⁰⁶ Quantitative Target-specific Toxicity Prediction Modeling (QTTPM): Coupling Machine Learning with Dynamic ProteinLigand Interaction Descriptors (DyPLIDs) to Predict Androgen Receptor-mediated Toxicity. **2023**, 263-295 0
- 4⁰⁵ (Pyridylamido)Hf(IV)-Catalyzed 1-Octene Polymerization Reaction Interwoven with the Structural Dynamics of the Ion-Pair-Active Species: Bridging from Microscopic Simulation to Chemical Kinetics with the Red Moon Method. **2023**, 127, 1209-1218 0
- 4⁰⁴ Using machine learning to detect coronaviruses potentially infectious to humans. 0
- 4⁰³ Anisotropy and Hybrid Heterosurface-Modulated Two-Dimensional Hydrogen Bond Network of Water. **2023**, 127, 2544-2557 0
- 4⁰² The nuclear receptor LRH-1 discriminates between ligands using distinct allosteric signaling circuits. 0
- 4⁰¹ Ligand Gaussian Accelerated Molecular Dynamics 2 (LiGaMD2): Improved Calculations of Ligand Binding Thermodynamics and Kinetics with Closed Protein Pocket. 0
- 4⁰⁰ Computer-Aided Drug Design towards New Psychotropic and Neurological Drugs. **2023**, 28, 1324 0
- 3⁹⁹ The *Mythimna separata* general odorant binding protein 2 (MsepGOBP2) is involved in the larval detection of the sex pheromone (Z)-11-hexadecenal. 0
- 3⁹⁸ An Inorganic Fluorescent Chemosensor: Rational Design and Selective Mg²⁺ Detection. **2023**, 8, 3835-3841 0
- 3⁹⁷ Special structural and dynamical interplay of cyano-based novel deep eutectic solvent. 0
- 3⁹⁶ A Low-Concentration and High Ionic Conductivity Aqueous Electrolyte toward Ultralow-Temperature Zinc-Ion Hybrid Capacitors. 2200345 0
- 3⁹⁵ Peptide valence-induced breaks in plasmonic coupling. 0

- 394 The application of QM/MM simulations in heterogeneous catalysis. ○
- 393 What Drives Chorismate Mutase to Top Performance? Insights from a Combined In Silico and In Vitro Study. **2023**, 62, 782-796 ○
- 392 Efficient polyethylene terephthalate degradation at moderate temperature: a protein engineering study of LC -cutinase highlights the key role of residue 243. 1
- 391 Molecular dynamics simulations depict structural motions of the whole human aryl hydrocarbon receptor influencing its binding of ligands and HSP90. 1-16 ○
- 390 Surrogate Based Genetic Algorithm Method for Efficient Identification of Low-Energy Peptide Structures. ○
- 389 Calculation of Protein Folding Thermodynamics using Molecular Dynamics Simulations. ○
- 388 Loading and Co-Solvent-Triggered Release of Okanin, a C4 Plant Key Enzyme Inhibitor, into/from Functional Microgels. **2023**, 141631 ○
- 387 HuR modulation with tanshinone mimics impairs LPS response in murine macrophages. ○
- 386 BH₃ and CH₃ interactions in protein-ligand complexes: carbonic anhydrase II inhibition by carborane sulfonamides. **2023**, 25, 1728-1733 ○
- 385 Molecular Modeling Study of a Receptor-Orthosteric Ligand-Allosteric Modulator Signaling Complex. **2023**, 14, 418-434 ○
- 384 Effect of Solvent on the Emulsion and Morphology of Polyfluorene Films: All-atom molecular dynamics approach. 1
- 383 Deep Learning Dynamic Allostery of G-Protein-Coupled Receptors. ○
- 382 MD Investigation on the Interaction between Carbamazepine and Two CYP Isoforms, CYP3A4 and CYP3A5. **2023**, 24, 2188 ○
- 381 Synthesis, Molecular Dynamics Simulation, and In-vitro Antitumor Activity of Quinazoline-2,4,6-triamine Derivatives as Novel EGFR Tyrosine Kinase Inhibitors. **2023**, 21, ○
- 380 Dual Anta-Inhibitors of the A_{2A} Adenosine Receptor and Casein Kinase CK1delta: Synthesis, Biological Evaluation, and Molecular Modeling Studies. **2023**, 16, 167 ○
- 379 Application of Molecular Simulation Methods in Food Science: Status and Prospects. ○
- 378 Highlights in TMPRSS2 inhibition mechanism with guanidine derivatives approved drugs for COVID-19 treatment. 1-15 ○
- 377 Influencing Molecular Dynamics Simulations of Ion-Exchange Membranes by Considering Comonomer Propagation. ○

- 376 Molecular Dynamics and Raman Optical Activity Spectra Reveal Nucleotide Conformation Ratios in Solution. ○
- 375 Atomistic simulations of pristine and nanoparticle reinforced hydrogels: A review. ○
- 374 Voriconazole Eye Drops: Enhanced Solubility and Stability through Ternary Voriconazole/Sulfobutyl Ether β -Cyclodextrin/Polyvinyl Alcohol Complexes. **2023**, 24, 2343 ○
- 373 Sum-frequency vibrational spectroscopy of centrosymmetric molecule at interfaces. ○
- 372 One-pot two-component synthesis of halogenated xanthone, 3-o substituted xanthone, and prenylated xanthone derivatives as aromatase inhibitors. **2023**, 5, 100789 ○
- 371 GPU-Enhanced DFTB Metadynamics for Efficiently Predicting Free Energies of Biochemical Systems. **2023**, 28, 1277 ○
- 370 Effect of Charge State on the Equilibrium and Kinetic Properties of Mechanically Interlocked [5]Rotaxane: A Molecular Dynamics Study. **2023**, 127, 1254-1263 ○
- 369 Effect of the QM Size, Basis Set, and Polarization on QM/MM Interaction Energy Decomposition Analysis. 1
- 368 Tackling hysteresis in conformational sampling [how to be forgetful with MEMENTO]. ○
- 367 Catalytic deAMPylation in AMPylation-inhibitory/assistant forms of FICD protein. 11, ○
- 366 Understanding the Key Roles of pH Buffer in Accelerating Lignin Degradation by Lignin Peroxidase. ○
- 365 Quinate-based ligands for irreversible inactivation of the bacterial virulence factor DHQ1 enzyme: A molecular insight [10], ○
- 364 Coenzyme Engineering of Glucose-6-phosphate Dehydrogenase on a Nicotinamide-Based Biomimic and Its Application as a Glucose Biosensor. **2023**, 13, 1983-1998 ○
- 363 Molecular Dynamics Simulations of Asphaltene Aggregation: Machine-Learning Identification of Representative Molecules, Molecular Polydispersity, and Inhibitor Performance. **2023**, 8, 4862-4877 ○
- 362 Molecular Dynamics Simulation Study of Organic Solvents Confined in PIM-1 and P84 Polyimide Membranes. **2023**, 127, 1237-1243 ○
- 361 Click-designed vanilloid-triazole conjugates as dual inhibitors of AChE and A β aggregation. **2023**, 13, 2871-2883 ○
- 360 Enhanced Grand Canonical Sampling of Occluded Water Sites Using Nonequilibrium Candidate Monte Carlo. ○
- 359 Can molecular dynamics simulations improve predictions of protein-ligand binding affinity with machine learning?. 1

- 358 Monomer morphology selection rules for an accurate design of bulk heterojunction: An updated theoretical account. ○
- 357 Understanding FABP7 binding to fatty acid micelles and membranes. **2023**, ○
- 356 Mechanistic Basis for Enhanced Strigolactone Sensitivity in KAI2 Triple Mutant. ○
- 355 Theoretical and Experimental Study of Molecular Interactions of Fluralaner with Lipid Membranes. **2023**, 71, 2134-2142 ○
- 354 Learning local equivariant representations for large-scale atomistic dynamics. **2023**, 14, 1
- 353 Roxadustat and its failure: A comparative dynamic study. **2023**, 120, 108422 ○
- 352 Interaction of bioactive kaempferol with HMGB1: Investigation by multi-spectroscopic and molecular simulation methods. **2023**, 292, 122360 ○
- 351 Role of hinge motion and ATP dynamics in factors for inversion stimulation FIS protein deduced while targeting drug resistant *Orientia tsutsugamushi*. **2023**, 120, 108425 ○
- 350 Synergistic effect of lecithin and alginate, CMC, or PVP in stabilizing curcumin and its potential mechanism. **2023**, 413, 135634 ○
- 349 Carboxyl PEGylation of magnetic nanoparticles as antithrombotic and thrombolytic agents by calcium binding. **2023**, 638, 672-685 ○
- 348 Solvation entropy, enthalpy and free energy prediction using a multi-task deep learning functional in 1D-RISM. **2023**, 25, 6944-6954 ○
- 347 The substrate specificity in the O-demethylation of 4-alkylguaiacols by cytochrome P450 AgcAP450. **2023**, 13, 2070-2079 ○
- 346 Binding modes of GDP, GTP and GNP to NRAS deciphered by using Gaussian accelerated molecular dynamics simulations. **2023**, 34, 65-89 3
- 345 Visualization Analysis of Weak Interactions in Chemical Systems. **2023**, ○
- 344 Molecular Dynamics Simulation Study of Chitosan-Zinc Chloride Complex Model. **2023**, 79, 24-31 ○
- 343 Coumarin-based derivatives targeting *Trypanosoma cruzi* cruzain and *Trypanosoma brucei* cathepsin L-like proteases. ○
- 342 Thermal Titration Molecular Dynamics (TTMD): Not Your Usual Post-Docking Refinement. **2023**, 24, 3596 1
- 341 Theoretical Study on Thermal Structural Fluctuation Effects of Intermolecular Configurations on Singlet Fission in Pentacene Crystal Models. **2023**, 127, 1883-1893 ○

- 340 Identifying Mutational Hotspots using Differences in Atomic Fluctuations combined with Positional Variability. ○
- 339 Integrated Computational Approaches for Inhibiting Sex Hormone-Binding Globulin in Male Infertility by Screening Potent Phytochemicals. **2023**, 13, 476 ○
- 338 Molecular Dynamics Simulation of Adsorption and Absorption Behavior of Shale Oil in Realistic Kerogen Slits. **2023**, 37, 3654-3671 ○
- 337 Cooperative Substrate Binding Controls Catalysis in Bacterial Cytochrome P450terp (CYP108A1). ○
- 336 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 ○
- 335 Impact of the Force Field on the Calculation of Density and Surface Tension of Epoxy Resins. **2023**, 127, 2617-2628 ○
- 334 Screening and Analysis for Inhibitors of SHMT2 Enzyme Protein. ○
- 333 Magnesium ions mediate ligand binding and conformational transition of the SAM/SAH riboswitch. ○
- 332 Coumarin-Based Compounds as Inhibitors of Tyrosinase/Tyrosine Hydroxylase: Synthesis, Kinetic Studies, and In Silico Approaches. **2023**, 24, 5216 ○
- 331 Molecular recognition of SARS-CoV-2 spike protein with three essential partners: exploring possible immune escape mechanisms of viral mutants. **2023**, 29, ○
- 330 Imidazole/Monoethanolamine-Based Deep Eutectic Solvent for Carbon Dioxide Capture: A Combined Experimental and Molecular Dynamics Investigation. ○
- 329 Structural mechanism of a drug-binding process involving a large conformational change of the protein target. **2023**, 14, ○
- 328 Why Does Synergistic Activation of WASP, but Not N-WASP, by Cdc42 and PIP2 Require Cdc42 Prenylation?. **2023**, 435, 168035 ○
- 327 Solidified Methane Storage Using an Efficient Class of Anionic Surfactants under Dynamic and Static Conditions: An Experimental and Computational Investigation. ○
- 326 Contribution of air-water interface in removing PFAS from drinking water: adsorption, stability, interaction and machine learning studies. **2023**, 119947 ○
- 325 A green and novel strategy based on CO₂-responsive surfactant-functionalized multi-walled carbon nanotubes with microwave-ultrasound assistant to improve extraction and enrichment of phytochemicals from plant waste. **2023**, 194, 116294 ○
- 324 N²-Phenylacetohydrazide Derivatives as Potent Ebola Virus Entry Inhibitors with an Improved Pharmacokinetic Profile. ○
- 323 Dipole alignment of water molecules flowing through a carbon nanotube. **2023**, 107, ○

- 322 Constrained catecholamines gain β AR selectivity through allosteric effects on pocket dynamics. **2023**, 14, ○
- 321 Active and stable alcohol dehydrogenase-assembled hydrogels via synergistic bridging of triazoles and metal ions. **2023**, 14, ○
- 320 Embedding Beyond Electrostatics: The Extended Polarizable Density Embedding Model. **2023**, 127, 3248-3256 ○
- 319 Silica In Silico: A Molecular Dynamics Characterization of the Early Stages of Protein Embedding for Atom Probe Tomography. **2023**, 3, 276-287 ○
- 318 Proposal of novel ApoE4 inhibitors from the natural spice Cinnamon for the treatment of Alzheimer's disease: Ab initio molecular simulations. **2023**, 296, 106990 ○
- 317 Conformers of 1,4-dioxane and their hydrogen bond complexation with methanol. **2023**, 126, 103519 ○
- 316 Investigation of hexacyanoferrate(II)/(III) charge-dependent interactions with bovine and human serum albumins. **2023**, 293, 122505 ○
- 315 Atomic insights into the mechanism of trace water influence on lipase catalysis in organic media. **2023**, 464, 142610 ○
- 314 Computational design of cyclic peptides to inhibit protein-peptide interactions. **2023**, 296, 106987 ○
- 313 Click chemistry-initiated highly uniform semi-interpenetrating polymer electrolyte with dual salts for high-performance lithium metal batteries. **2023**, 565, 232884 ○
- 312 Molecular modelling of ionic liquids: Perfluorinated anionic species with enlarged halogen substitutions. **2023**, 378, 121599 ○
- 311 Aqueous solutions of chiral ionic liquids based on (1)-menthol: An experimental and computational study of volumetric and transport properties. **2023**, 378, 121591 ○
- 310 Novel multiscale simulations on the membrane formation via hybrid induced phase separation process based on dissipative particle dynamics. **2023**, 314, 123614 ○
- 309 Effect of water content on transport properties and interactions of amino-functionalized ionic liquids. **2023**, 569, 111852 ○
- 308 Selective recovery of lithium from mother liquor of Li_2CO_3 by synergistic hydrophobic deep eutectic solvents: Performance and mechanistic insight. **2023**, 313, 123353 ○
- 307 Discovery of the new alpha-glucosidase inhibitor with therapeutic potential in type 2 diabetes mellitus by a novel high-throughput virtual screening and free energy evaluation. **2023**, 121, 108447 ○
- 306 Design and structure optimization of novel butenolide derivatives as low bee-toxicity candidates. **2023**, 1282, 135257 ○
- 305 Molecular insights into the inhibition mechanism of harringtonine against essential proteins associated with SARS-CoV-2 entry. **2023**, 240, 124352 ○

- 304 Biochemical interaction of human hemoglobin with ionic liquids of noscapinoids: Spectroscopic and computational approach. **2023**, 239, 124227
- 303 Computational study on the encapsulation of glucosamine anomers by cucurbit[6]uril and cucurbit[8]uril in aqueous solution. **2023**, 16, 104779
- 302 Design, synthesis and biological evaluation of novel thiosemicarbazones as cruzipain inhibitors. **2023**, 254, 115345
- 301 Molecular dynamics simulation study on interfacial behaviors of betaines and extended surfactants. **2023**, 666, 131323
- 300 Structure-based virtual screening for potent inhibitors of GH-20 β -N-acetylglucosaminidase: Classical and machine learning scoring functions, and molecular dynamics simulations. **2023**, 104, 107856
- 299 Selective adsorption and transport of CO₂/H₄ mixture under nano-confinement. **2023**, 273, 127224
- 298 Cucurbit[7]uril complexes with gabapentin: Effect on lactamization. **2023**, 380, 121716
- 297 Rational engineering of glycosaminoglycan-based Dickkopf-1 scavengers to improve bone regeneration. **2023**, 297, 122105
- 296 Separation of butyl acetate and propyl acetate from wastewater by liquid-liquid extraction and molecular dynamics simulation. **2023**, 379, 121699
- 295 Computational insight into stability-enhanced systems of anthocyanin with protein/peptide. **2023**, 6, 100168
- 294 New insights into the pH dependence of anthocyanin-protein interactions by a case study of cyanidin-3-O-glucoside and bovine serum albumin. **2023**, 140, 108649
- 293 Composite electrolytes engineered by anion acceptors for boosted high-voltage solid-state lithium metal batteries. **2023**, 642, 330-339
- 292 Molecular dynamics simulations of the nickel removal from crude oil by neutral and charged spherical polymer brushes. **2023**, 345, 128179
- 291 A molecular dynamics study on polybenzimidazole based proton exchange membrane with dual proton conductors. **2023**, 677, 121618
- 290 Molecular simulations of adsorption of surfactant micelles on partially and fully covered iron surfaces. **2023**, 379, 121685
- 289 Synthesis, Insecticidal Activity and Computational Studies of Eugenol-Based Insecticides.
- 288 Emerging Trends of Computational Chemistry and Molecular Modeling in Froth Flotation: A Review.
- 287 What Makes a Good Protein-Protein Interaction Stabilizer: Analysis and Application of the Dual-Binding Mechanism.

- 286 Adsorption of emerging contaminants by graphene related materials and their alginate composite hydrogels. **2023**, 11, 109566 ○
- 285 Multi-state Model-Based Identification of Cryptic Allosteric Sites on Human Serotonin Transporter. ○
- 284 Towards a cost-effective modeling of fluorescence in the condensed phase. **2023**, 215, 111227 ○
- 283 Computational insights into the antioxidant and antidiabetic mechanisms of cannabidiol: An in vitro and in silico study. **2023**, 16, 104842 ○
- 282 Effect of molecular dynamics water models on flux, diffusivity, and ion dynamics for polyamide membrane simulations. **2023**, 678, 121630 ○
- 281 Solute structure effect on aromatics-alkanes extractive separation toward rational LCO upgrading. **2023**, 310, 123213 ○
- 280 Galantamine Based Novel Acetylcholinesterase Enzyme Inhibitors: A Molecular Modeling Design Approach. **2023**, 28, 1035 1
- 279 Revealing the supramolecular interactions of the bis(azopyrenyl) dibenzo-18-crown-6-ether system. **2023**, 374, 121298 ○
- 278 Evaluating the active site-substrate interplay between x-ray crystal structure and molecular dynamics in chorismate mutase. **2023**, 158, 065101 ○
- 277 BitTo lead optimization and chemoinformatic studies for a new series of Autotaxin inhibitors. **2023**, 249, 115130 ○
- 276 Distant sequence regions of JBP1 contribute to J-DNA binding. ○
- 275 Turning thermostability of *Aspergillus terreus* (R)-selective transaminase At-ATA by synthetic shuffling. **2023**, 364, 66-74 ○
- 274 N-terminal domain of tyrosyl-DNA phosphodiesterase I regulates topoisomerase I-induced toxicity in cells. **2023**, 13, ○
- 273 Role of Nanoscale Morphology on the Efficiency of Solvent-Based Desalination Method. **2023**, 3, 400-409 ○
- 272 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 ○
- 271 On the Behavior of the Ethylene Glycol Components of Polydisperse Polyethylene Glycol PEG200. **2023**, 127, 1178-1196 ○
- 270 UV light-driven late-stage skeletal reorganization to diverse limonoid frameworks: A proof of concept for photobiosynthesis. **2023**, 9, ○
- 269 Theoretical and experimental studies of chitin nanocrystals treated with ionic liquid or deep eutectic solvent to afford nanochitosan sheets. **2023**, 375, 121350 ○

- 268 Binding Affinity and Mechanisms of Antagonists Targeting Human NMDA Receptors. ○
- 267 Simulating dynamic interaction between diazepam and ethanol targeting the GABAA receptor via in silico model. **2023**, 95, 136-143 ○
- 266 CHARMM-GUI PDB Manipulator: Various PDB Structural Modifications for Biomolecular Modeling and Simulation. **2023**, 167995 ○
- 265 Molecular Modeling to Predict the Optimal Mineralogy of Smectites as Binders of Aflatoxin. ○
- 264 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 ○
- 263 A short blanket dilemma for a state-of-the-art neural network potential for water: Reproducing experimental properties or the physics of the underlying many-body interactions?. **2023**, 158, 084111 1
- 262 Hydration of the neurotransmitter β -aminobutyric acid and its isomer δ -aminobutyric acid. **2023**, 375, 121363 ○
- 261 New Glucosamine-Based TLR4 Agonists: Design, Synthesis, Mechanism of Action, and In Vivo Activity as Vaccine Adjuvants. **2023**, 66, 3010-3029 1
- 260 Substrate binding and lipid-mediated allostery in the human organic anion transporter 1 at the atomic-scale. **2023**, 160, 114342 ○
- 259 Multi-Hydration Induced Zwitterionic Hydrogel with Open Environment Stability for Chemical Sensing. 2200061 ○
- 258 On the interplay between lipids and asymmetric dynamics of an NBS degenerate ABC transporter. **2023**, 6, ○
- 257 An Insight into the Metabolism of 2,5-Disubstituted Monotetrazole Bearing Bisphenol Structures: Emerging Bisphenol A Structural Congeners. **2023**, 28, 1465 ○
- 256 Degradation and lifetime prediction of thermoplastic polyurethane encapsulants in seawater for underwater acoustic sensor applications. **2023**, 209, 110281 ○
- 255 Evidence That Less Can Be More for Transferable Force Fields. **2023**, 63, 1188-1195 ○
- 254 Antiplasmodial activity of coumarins isolated from Polygala boliviensis: in vitro and in silico studies. 1-21 ○
- 253 Dynamic density functional theory of multicomponent cellular membranes. **2023**, 5, ○
- 252 Thermal site energy fluctuations in photosystem I: new insights from MD/QM/MM calculations. **2023**, 14, 3117-3131 ○
- 251 Hydration Structure of Diamondoids from Reactive Force Fields. **2023**, 127, 3217-3227 ○

- 250 In silico drug discovery of SIRT2 inhibitors from natural source as anticancer agents. **2023**, 13, ○
- 249 A combined computational-biophysical approach to understanding fatty acid binding to FABP7. **2023**, 122, 741-752 ○
- 248 Supramolecular Study of the Interactions between Malvidin-3-O-Glucoside and Wine Phenolic Compounds: Influence on Color. ○
- 247 Ensemble-based virtual screening of human PI4KIII α inhibitors toward the Hepatitis C virus. **2023**, 815, 140354 ○
- 246 Drug Repurposing and Systems Biology approaches of Enzastaurin can target potential biomarkers and critical pathways in Colorectal Cancer. **2023**, 155, 106630 ○
- 245 Discovery of New Quinoline-Based Diarylamides as Potent B-RAFV600E/C-RAF Kinase Inhibitors Endowed with Promising In Vitro Anticancer Activity. **2023**, 24, 3216 ○
- 244 Foregrounding the Code: Computational Chemistry Instructional Activities Using a Highly Readable Fluid Simulation Code. **2023**, 100, 1155-1163 ○
- 243 Can Resveratrol Influence the Activity of 11 β -Hydroxysteroid Dehydrogenase Type 1? A Combined In Silico and In Vivo Study. **2023**, 16, 251 ○
- 242 Identification of potential ATP-competitive cyclin-dependent kinase 1 inhibitors: De novo drug generation, molecular docking, and molecular dynamics simulation. **2023**, 155, 106645 ○
- 241 Molecular interaction of a putative inhibitor with bacterial SHV, an enzyme associated with antibiotic resistance. **2023**, 10, 1 ○
- 240 Molecular Mechanism of Conformational Crossover of Mefenamic Acid Molecules in scCO₂. **2023**, 16, 1403 ○
- 239 In-silico drug design for the novel Karachi-NF001 strain of brain-eating amoeba: Naegleria fowleri. 10, ○
- 238 Construction of a Gaussian Process Regression Model of Formamide for Use in Molecular Simulations. **2023**, 127, 1702-1714 ○
- 237 Interaction of Some Asymmetrical Porphyrins with U937 Cell Membranes In Vitro and In Silico Studies. **2023**, 28, 1640 ○
- 236 Toward Accurate Prediction of Ion Mobility in Organic Semiconductors by Atomistic Simulation. **2023**, 19, 1517-1528 ○
- 235 A general force field by machine learning on experimental crystal structures. Calculations of intermolecular Gibbs energy with FlexCryst. **2023**, 79, 132-144 ○
- 234 Design, synthesis, and biological evaluation of some novel naphthoquinone-glycine / Alanine anilide derivatives as noncovalent proteasome inhibitors. ○
- 233 A Combined in Silico and Structural Study Opens New Perspectives on Aliphatic Sulfonamides, a Still Poorly Investigated Class of CA Inhibitors. **2023**, 12, 281 ○

- 232 Insertion of an Amphipathic Linker in a Tetrapodal Tryptophan Derivative Leads to a Novel and Highly Potent Entry Inhibitor of Enterovirus A71 Clinical Isolates. **2023**, 24, 3539 ○
- 231 Mechanistic Modeling of Lys745 Sulfonylation in EGFR C797S Reveals Chemical Determinants for Inhibitor Activity and Discriminates Reversible from Irreversible Agents. **2023**, 63, 1301-1312 ○
- 230 Modulating structural dynamics of dual drugs for CDK4 complex addressing prostate cancer. **2023**, 376, 121454 ○
- 229 HNRNPA2B1 as a potential therapeutic target for thymic epithelial tumor recurrence: An integrative network analysis. **2023**, 155, 106665 ○
- 228 Effect of TiO₂ nanoparticles on the mass transfer process of absorption of toluene: Experimental investigation and molecular dynamics simulation. **2023**, 11, 109474 ○
- 227 Small molecule inhibitors of 15-PGDH exploit a physiologic induced-fit closing system. **2023**, 14, ○
- 226 An Efficient Multilayer Approach to Model DNA-Based Nanobiosensors. **2023**, 127, 1513-1525 ○
- 225 Development and Implementation of Atomically Anisotropic First-Principles Force Fields: A Benzene Case Study. **2023**, 127, 1736-1749 ○
- 224 Ab Initio Study of Adsorption of Polymers on Metal-Organic Framework Surfaces. **2023**, 127, 3715-3725 ○
- 223 Revealing Structural and Physical Properties of Polylactide: What Simulation Can Do beyond the Experimental Methods. 1-39 ○
- 222 Flexural behavior and microstructural material properties of sandwich foam core under arctic temperature conditions. 109963622311570 ○
- 221 Molecular Dynamics and Multi-Spectroscopic of the Interaction Behavior between Bladder Cancer Cells and Calf Thymus DNA with Rebeccamycin: Apoptosis through the Down Regulation of PI3K/AKT Signaling Pathway. ○
- 220 Inviting C5-Trifluoromethylated Pseudoprolines into Collagen Mimetic Peptides. **2023**, 24, 1555-1562 ○
- 219 Exploring the Effects of Mutagenesis on FusionRed by Using Excited-State QM/MM Dynamics and Classical Force Field Simulations. ○
- 218 Therapeutic phosphorodiamidate morpholino oligonucleotides: Physical properties, solution structures, and folding thermodynamics. **2023**, 31, 631-647 ○
- 217 Novel Inhibitory Role of Fenofibric Acid by Targeting Cryptic Site on the RBD of SARS-CoV-2. **2023**, 13, 359 ○
- 216 Insights into the Degradation of Polymer-Drug Conjugates by an Overexpressed Enzyme in Cancer Cells. **2023**, 66, 2761-2772 ○
- 215 Ligand binding free energy evaluation by Monte Carlo Recursion. **2023**, 103, 107830 ○

- 214 Influence of gelation temperature on physicochemical properties of cellulose hydrogels prepared from ionic liquid/DMSO solution. **2023**, 376, 121465 ○
- 213 Enhancing the Activity of an Alcohol Dehydrogenase by Using Aromatic Residue Scanning at Potential Plasticity Sites. ○
- 212 MoSDeF-GOMC: Python Software for the Creation of Scientific Workflows for the Monte Carlo Simulation Engine GOMC. **2023**, 63, 1218-1228 1
- 211 Molecular dynamics simulations of the interactions between CO₂ and branched unreacted and reacted polyethylenimine films. **2023**, 111, 204928 ○
- 210 Silk Assembly against Hydrophobic Surfaces-Modeling and Imaging of Formation of Nanofibrils. **2023**, 6, 1011-1018 ○
- 209 Non-active Site Residue in Loop L4 Alters Substrate Capture and Product Release in d-Arginine Dehydrogenase. **2023**, 62, 1070-1081 ○
- 208 Effect of histidine covalent modification on strigolactone receptor activation and selectivity. **2023**, 122, 1219-1228 ○
- 207 How ractopamine binds to bovine serum albumin at the drug site 1. **2023**, 49, 599-607 ○
- 206 Stability Mechanism of Menthol and Fatty Acid Based Hydrophobic Eutectic Solvents: Insights from Nonbonded Interactions. **2023**, 11, 3539-3556 ○
- 205 Conformational analysis of amphetamine and methamphetamine: a comprehensive approach by vibrational and chiroptical spectroscopy. **2023**, 148, 1337-1348 ○
- 204 Thermal batteries based on inverse barocaloric effects. **2023**, 9, ○
- 203 Integrative network pharmacology and in silico analyses identify the anti-omicron SARS-CoV-2 potential of eugenol. **2023**, 9, e13853 ○
- 202 Unraveling topoisomerase IA gate dynamics in presence of PPEF and its preclinical evaluation against multidrug-resistant pathogens. **2023**, 6, ○
- 201 Deep Learning Dynamic Allosteric of G-Protein-Coupled Receptors. ○
- 200 Theoretical prediction of nanomolar and sequence-selective binding of synthetic supramolecular cucurbit[7]uril to N-terminal Leu-containing tripeptides. **2023**, 25, 7893-7900 ○
- 199 A review on shale oil and gas characteristics and molecular dynamics simulation for the fluid behavior in shale pore. **2023**, 376, 121507 ○
- 198 Physiological Buffer Effects in Drug Supersaturation - A Mechanistic Study of Hydroxypropyl Cellulose as Precipitation Inhibitor. **2023**, ○
- 197 Selective Targeting of Cancer-Related G-Quadruplex Structures by the Natural Compound Dicentrine. **2023**, 24, 4070 ○

- 196 Molecular Dynamics Simulation of the Complex of PDE5 and Evodiamine. **2023**, 13, 578 ○
- 195 Molecular Dynamic Studies of Dye-Dye and Dye-DNA Interactions Governing Excitonic Coupling in Squaraine Aggregates Templated by DNA Holliday Junctions. **2023**, 24, 4059 ○
- 194 The chemosensory protein 1 contributes to indoxacarb resistance in *Plutella xylostella* (L.). ○
- 193 Modelling shear thinning of Imidazolium-based ionic liquids. **2023**, 816, 140387 ○
- 192 Conformational landscapes of artificial peptides predicted by various force fields: are we ready to simulate amino acids?. **2023**, 25, 7466-7476 ○
- 191 Ligand-Triggered Self-Assembly of Flexible Carbon Dot Nanoribbons for Optoelectronic Memristor Devices and Neuromorphic Computing. 2207688 ○
- 190 Evaluation of polyanionic cyclodextrins as high affinity binding scaffolds for fentanyl. **2023**, 13, ○
- 189 Templated Enzymatic Synthesis of β -Cyclodextrin. **2023**, 145, 4882-4891 ○
- 188 AI-Accelerated Design of Targeted Covalent Inhibitors for SARS-CoV-2. **2023**, 63, 1438-1453 1
- 187 Development and test of highly accurate endpoint free energy methods. 1: Evaluation of ABCG2 charge model on solvation free energy prediction and optimization of atom radii suitable for more accurate solvation-free energy prediction by the PBSA method. ○
- 186 Allosteric regulation of reaction stage I in tryptophan synthase upon the ligand binding. **2023**, 158, 115101 ○
- 185 A multiple-step screening protocol to identify norepinephrine and dopamine reuptake inhibitors for depression. **2023**, 25, 8341-8354 ○
- 184 Venetoclax analogs as promising anticancer therapeutics via targeting Bcl-2 protein: in-silico drug discovery study. 1-17 ○
- 183 In Vitro and In Silico Study on the Molecular Encapsulation of Tocopherol in a Large-Ring Cyclodextrin. **2023**, 24, 4425 ○
- 182 Unbiased molecular dynamics simulation of a first-in-class small molecule inhibitor binds to oncostatin M. **2023**, 155, 106709 ○
- 181 Phenotypic Discovery of Thiocarbohydrazone with Anticancer Properties and Catalytic Inhibition of Human DNA Topoisomerase II. **2023**, 16, 341 ○
- 180 Deformation constraints of graphene oxide nanochannels under reverse osmosis. **2023**, 14, ○
- 179 Ground-state heterogeneity and vibrational energy redistribution in bacterial phytochrome observed with femtosecond 2D IR spectroscopy. **2023**, 158, 085103 ○

- 178 Nanoscale and Real-Time Nuclear Electronic Dynamics Simulation Study of Charge Transfer at the Donor-Acceptor Interface in Organic Photovoltaics. **2023**, 14, 2292-2300 ○
- 177 Molecular effects of site-specific phosphate-methylated primer on the structure and motions of Taq DNA polymerase. **2023**, 21, 1820-1827 ○
- 176 Tween-80 on Water/Oil Interface: Structure and Interfacial Tension by Molecular Dynamics Simulations. **2023**, 39, 3255-3265 ○
- 175 What is the Optimal Dipole Moment for Nonpolarizable Models of Liquids?. **2023**, 19, 1790-1804 ○
- 174 Structure-Based Virtual Screening of Furan-1,3,4-Oxadiazole Tethered N-phenylacetamide Derivatives as Novel Class of hTYR and hTYRP1 Inhibitors. **2023**, 16, 344 ○
- 173 Machine learning combines atomistic simulations to predict SARS-CoV-2 Mpro inhibitors from natural compounds. ○
- 172 Modeling the zinc effect on OsASR5- STAR1 promoter interaction by molecular dynamics. ○
- 171 GAFF-AIC: reoptimisation of the GAFF force field for realistic densities and viscosities in aromatic isocyanates. **2023**, 49, 576-588 ○
- 170 Design, synthesis and characterisation of a novel type II B-RAF paradox breaker inhibitor. **2023**, 250, 115231 ○
- 169 Polyethylene glycol regulated carnallite decomposition-crystallization: Experimental and theoretical analysis. **2023**, 195, 108021 ○
- 168 Chelation Behaviors of 3,4,3-LI(1,2-HOPO) with Lanthanides and Actinides Implicated by Molecular Dynamics Simulations. **2023**, 62, 4304-4313 ○
- 167 Million-atom molecular dynamics simulations reveal the interfacial interactions and assembly of plant PSII-LHCII supercomplex. **2023**, 13, 6699-6712 ○
- 166 Heparan sulfate glycomimetics via iterative assembly of clickable disaccharides. **2023**, 14, 3514-3522 ○
- 165 Carbosilane ruthenium metallodendrimer as alternative anti-cancer drug carrier in triple negative breast cancer mouse model: A preliminary study. **2023**, 636, 122784 ○
- 164 Adsorption of Biomimetic Amphiphilic Heteropolymers onto Graphene and Its Derivatives. **2023**, 56, 1798-1809 ○
- 163 In-silico natural product database mining for novel neuropilin-1 inhibitors: molecular docking, molecular dynamics and binding energy computations. **2023**, 17, ○
- 162 Metal-coordinated polybenzimidazole membranes with preferential K⁺ transport. **2023**, 14, ○
- 161 Heparan Sulfate and Enoxaparin Interact at the Interface of the Spike Protein of HCoV-229E but Not with HCoV-OC43. **2023**, 15, 663 ○

- 160 The Importance of Epigallocatechin as a Scaffold for Drug Development against Flaviviruses. **2023**, 15, 803
- 159 Singlet fission as a polarized spin generator for dynamic nuclear polarization. **2023**, 14,
- 158 Towards a Rational Design of Antibody-Recruiting Molecules through a Computational Microscopy View of their Interactions with the Target Antibody.
- 157 Molecular Insights into Cyclodextrin α -adamantane-Modified Copolymer Host α -Guest Interactions. **2023**, 39, 3619-3627
- 156 Systematic profiling of taxol and its analogues (taxalogues) binding to β -tubulin and molecular analysis of their effects on microtubule stabilization.
- 155 Formulation of inclusion complex of Abiraterone acetate with 2-Hydroxypropyl-Beta-Cyclodextrin: physiochemical characterization, molecular docking and bioavailability evaluation. **2023**, 82, 104321
- 154 Inhibition of microtubule affinity regulating kinase 4 by an acetylcholinesterase inhibitor, Huperzine A: Computational and experimental approaches. **2023**, 235, 123831
- 153 Additive energetic contributions of multiple peptide positions determine the relative promiscuity of viral and human sequences for PDZ domain targets. **2023**, 32,
- 152 Identification of Dietary Bioflavonoids as Potential Inhibitors against KRAS G12D Mutant α Level Insights from Computer-Aided Drug Discovery. **2023**, 45, 2136-2156
- 151 Catalytic cycle of formate dehydrogenase captured by single-molecule conductance. **2023**, 6, 266-275
- 150 Crosslinking Rapidly Cured Epoxy Resin Thermosets: Experimental and Computational Modeling and Simulation Study. **2023**, 15, 1325
- 149 Structural insight into the stabilization of microtubules by taxanes. 12,
- 148 Water clusters in liquid organic matrices of different polarity. **2023**, 378, 121580
- 147 Potential drug candidates as P-glycoprotein inhibitors to reverse multidrug resistance in cancer: an in silico drug discovery study. 1-16
- 146 A Multiple Proton Transfer Mechanism for the Charging Step of the Aminoacylation Reaction at the Active Site of Aspartyl tRNA Synthetase. **2023**, 63, 1819-1832
- 145 Evaluating performance of the approximate 3D-RISM-KH molecular solvation theory for solvation free energies in alkanes and alkane-water partition coefficients. **2023**, 378, 121597
- 144 Genetic algorithm-de novo, molecular dynamics and MMGBSA based modelling of a novel Benz-pyrazole based anticancer ligand to functionally revert mutant P53 into wild type P53. **2023**, 49, 678-689
- 143 Computational Methods for Molecular Understanding of the Antibiotic-Aminoacyl tRNA Synthetase Interaction. **2023**, 3,

- 142 Human sirtuin 2 inhibitors, their mechanisms and binding modes. **2023**, 15, 291-311 ○
- 141 Potential Energy Surfaces Sampled in Cremer-Pople Coordinates and Represented by Common Force Field Functionals for Small Cyclic Molecules. **2023**, 127, 2646-2663 ○
- 140 Antitumor activity of aumolertinib, a third-generation EGFR tyrosine kinase inhibitor, in non-small-cell lung cancer harboring uncommon EGFR mutations. **2023**, ○
- 139 Fluids and Electrolytes under Confinement in Single-Digit Nanopores. **2023**, 123, 2737-2831 ○
- 138 SAMPL9 blind predictions for toluene/water partition coefficients using nonequilibrium alchemical approaches. **2023**, 158, 124117 ○
- 137 Density of States Engineering of n-Doped Conjugated Polymers for High Charge Transport Performances. ○
- 136 Allosteric inhibition of TEM-1 β -lactamase: Microsecond molecular dynamics simulations provide mechanistic insights. **2023**, 32, ○
- 135 Structural insight into TIPE1 functioning as a lipid transfer protein. 1-14 ○
- 134 Synergism for lowering interfacial tensions between betaines and extended surfactants: The role of self-regulating molecular size. **2023**, 378, 121605 ○
- 133 Deciphering Selectivity Mechanism of BRD9 and TAF1(2) toward Inhibitors Based on Multiple Short Molecular Dynamics Simulations and MM-GBSA Calculations. **2023**, 28, 2583 ○
- 132 HuR modulation counteracts lipopolysaccharide response in murine macrophages. **2023**, 16, ○
- 131 Molecular dynamics simulations reveal the impact of NUDT15 R139C and R139H variants in structural conformation and dynamics. 1-10 ○
- 130 Identification of host genomic biomarkers from multiple transcriptomics datasets for diagnosis and therapies of SARS-CoV-2 infections. **2023**, 18, e0281981 ○
- 129 Identification of Blood Transport Proteins to Carry Temoporfin: A Domino Approach from Virtual Screening to Synthesis and In Vitro PDT Testing. **2023**, 15, 919 ○
- 128 In silico study of interaction of (ZnO)₁₂ nanocluster to glucose oxidase-FAD in absence and presence of glucose. 1-9 ○
- 127 The T1150A cancer mutant of the protein lysine dimethyltransferase NSD2 can introduce H3K36 trimethylation. ○
- 126 Deep Learning Model for Efficient Protein-Ligand Docking with Implicit Side-Chain Flexibility. **2023**, 63, 1695-1707 ○
- 125 Quorum Quenchers from *Reynoutria japonica* in the Battle against Methicillin-Resistant *Staphylococcus aureus* (MRSA). **2023**, 28, 2635 ○

- 124 A hotspot for posttranslational modifications on the androgen receptor dimer interface drives pathology and anti-androgen resistance. **2023**, 9,
- 123 Influence of the Lennard-Jones Combination Rules on the Simulated Properties of Organic Liquids at Optimal Force-Field Parametrization. **2023**, 19, 2048-2063
- 122 Characterization of Two Novel Rumen-Derived Exo-Polygalacturonases: Catalysis and Molecular Simulations. **2023**, 11, 760
- 121 Insights into the binding mechanism between β -OH and CYP4F2: A homology modeling, molecular docking, and molecular dynamics simulation study. **2023**, 124, 573-585
- 120 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
- 119 Key Amino Acid Residues of Mitochondrial Transcription Factor A Synergize with Abasic (AP) Site Dynamics To Facilitate AP-Lyase Reactions.
- 118 Biomolecular glass with amino acid and peptide nanoarchitectonics. **2023**, 9,
- 117 The Bioactivity of Xylene, Pyridine, and Pyrazole Aza Macrocycles against Three Representative Leishmania Species. **2023**, 15, 992
- 116 Comprehensive Evaluation of End-Point Free Energy Techniques in Carboxylated-Pillar[6]arene Host-Guest Binding: III. Force-Field Comparison, Three-Trajectory Realization and Further Dielectric Augmentation. **2023**, 28, 2767
- 115 Deciphering the mechanistic basis for perfluoroalkyl-protein interactions.
- 114 Determining Lennard-Jones Parameters Using Multiscale Target Data through Presampling-Enhanced, Surrogate-Assisted Global Optimization. **2023**, 63, 1872-1881
- 113 Engineering of a P450-based Kemp eliminase with a new mechanism. **2023**, 47, 191-199
- 112 The Unusual Architecture of RNA-Dependent RNA Polymerase (RdRp)'s Catalytic Chamber Provides a Potential Strategy for Combination Therapy against COVID-19. **2023**, 28, 2806
- 111 How the Conformational Movement of the Substrate Drives the Regioselective C-N Bond Formation in P450 TleB: Insights from Molecular Dynamics Simulations and Quantum Mechanical/Molecular Mechanical Calculations. **2023**, 145, 7252-7267
- 110 Roles of Molecular Spatial Arrangement in Exciton Energy Transfer in Organic Light-Emitting Diodes: A Theoretical Study. **2023**, 127, 5950-5957
- 109 Accelerating Cryptic Pocket Discovery Using AlphaFold.
- 108 Insights into receptor structure and dynamics at the surface of living cells. **2023**, 14,
- 107 Molecular recognition of tripeptides containing tryptophan by cucurbit[8]uril: A computational study. **2023**, 16, 104819

- 106 Path separation of dissipation-corrected targeted molecular dynamics simulations of protein-ligand unbinding. **2023**, 158, 124106 ○
- 105 Development of AMBER Parameters for Molecular Simulations of Selected Boron-Based Covalent Ligands. **2023**, 28, 2866 ○
- 104 Impact of Drug Repurposing on SARS-Cov-2 Main Protease. **2022**, 96, 3311-3330 ○
- 103 Finite-Temperature Mechanical Properties of Organic Molecular Crystals from Classical Molecular Simulation. **2023**, 23, 2155-2168 ○
- 102 Molecular simulations of SSTR2 dynamics and interaction with ligands. **2023**, 13, ○
- 101 Effect of temperature on the structure and drug-release behaviour of inclusion complex of β -cyclodextrin with cyclophosphamide: a molecular dynamics study. ○
- 100 Role of Non-Covalent Interactions in Carbonic Anhydrase II-topiramate Complex Based on QM/MM Approach. **2023**, 16, 479 ○
- 99 Hydroperoxidation of Docosahexaenoic Acid by Human ALOX12 and pigALOX15-mini-LOX. **2023**, 24, 6064 ○
- 98 Exploration of the binding of antifungal drugs to human P450 2C9 based on docking and molecular dynamics simulation. ○
- 97 Ca²⁺ ions facilitate the organization of the Annexin A2 / S100A10 heterotetramer. ○
- 96 Unraveling an Alternative Mechanism in Polymer Self-Assemblies: An Order-Order Transition with Unusual Molecular Interactions between Hydrophilic and Hydrophobic Polymer Blocks. **2023**, 17, 6932-6942 ○
- 95 Increased flexibility of the SARS-CoV-2 RNA-binding site causes resistance to remdesivir. **2023**, 19, e1011231 ○
- 94 Discrimination between cyclic nucleotides in a cyclic nucleotide-gated ion channel. **2023**, 30, 512-520 ○
- 93 Machine learning- and structure-based discovery of a novel chemotype as FXR agonists for potential treatment of nonalcoholic fatty liver disease. **2023**, 252, 115307 ○
- 92 Interplay Between Doping, Morphology, and Lattice Thermal Conductivity in PEDOT:PSS. ○
- 91 Discovery of Novel EGFR Inhibitor Targeting Wild-Type and Mutant Forms of EGFR: In Silico and In Vitro Study. **2023**, 28, 3014 ○
- 90 Riboflavin kinase and pyridoxine 5'-phosphate oxidase complex formation envisages transient interactions for FMN cofactor delivery. 10, ○
- 89 Design and Pharmacological Characterization of α 5 β 1 Integrin Cyclopeptide Agonists: Computational Investigation of Ligand Determinants for Agonism versus Antagonism. **2023**, 66, 5021-5040 ○

- 88 Molecular Modelling Study and Antibacterial Evaluation of Diphenylmethane Derivatives as Potential FabI Inhibitors. **2023**, 28, 3000 ○
- 87 Comprehensive Approach to Simulating Large Scale Conformational Changes in Biological Systems Utilizing a Path Collective Variable and New Barrier Restraint. ○
- 86 Repurposing FIASMAs against Acid Sphingomyelinase for COVID-19: A Computational Molecular Docking and Dynamic Simulation Approach. **2023**, 28, 2989 ○
- 85 Fluorescence enhancement of organic aggregates induced by bromine substituents: Heavy-atom effect and vibronic coupling. **2023**, 215, 111269 ○
- 84 Binding mechanism of andrographolide with intramolecular antiparallel G-quadruplexes of therapeutic importance: an in-silico analysis. **2023**, 49, 816-828 ○
- 83 Synthetic ERRα Agonist Induces an ERK2-Dependent Acute Aerobic Exercise Response and Enhances Exercise Capacity. **2023**, 18, 756-771 ○
- 82 Correlation of Emulsion Chemistry, Film Morphology, and Device Performance in Polyfluorene LEDs Deposited by RIR-MAPLE. **2023**, 15, 18153-18165 ○
- 81 Mechanism exploration and prognosis study of Astragali Radix-Spreading hedyotis herb for the treatment of lung adenocarcinoma based on bioinformatics approaches and molecular dynamics simulation. 11, ○
- 80 Critical Analysis of Association Constants between Calixarenes and Nitroaromatic Compounds Obtained by Fluorescence. Implications for Explosives Sensing. **2023**, 28, 3052 ○
- 79 Spectroscopy, docking and molecular dynamics studies on the interaction between cis and trans palladium-alanine complexes with calf-thymus DNA and antitumor activities. 1-24 ○
- 78 Controllably Adjusting the Hydrophobicity of Collagen Fibers for Enhancing the Adsorption Rate, Retention Capacity, and Separation Performance of Flavonoid Aglycones. **2023**, 15, 18516-18527 ○
- 77 Developing a comprehensive solution aimed to disrupt LARS1/RagD protein-protein interaction. 1-12 ○
- 76 Evaluation of autophagy inhibition to combat cancer: (vanadium complex) protein interactions, parameterization, and validation of a new force field. **2023**, 29, ○
- 75 Structural investigation of Keap1/Nrf2 protein-protein interaction (PPI) inhibitors for treating myocarditis through molecular simulations. ○
- 74 A General Picture of Cucurbit[8]uril Host-Guest Binding: Recalibrating Bonded Interactions. **2023**, 28, 3124 ○
- 73 AmberMDrun: A Scripting Tool for Running Amber MD in an Easy Way. **2023**, 13, 635 ○
- 72 Mechanistic Insights into the Binding of Different Positron Emission Tomography Tracers to Chronic Traumatic Encephalopathy Tau Protofibrils. ○
- 71 Structure and mechanism of oxalate transporter OxIT in an oxalate-degrading bacterium in the gut microbiota. **2023**, 14, ○

- 70 Insight into Tyrosine-Containing Pharmaceuticals as Potential Inhibitors of SARS-CoV-2 3CLpro and NSP16: Structural Analysis, Docking Studies, Molecular Dynamics Simulations, and Density Functional Theory Investigations. **2023**, 5, 762-777 ○
- 69 In silico study of HASDI (high-affinity selective DNA intercalator) as a new agent capable of highly selective recognition of the DNA sequence. **2023**, 13, ○
- 68 Expanding the Paradigm of Structure-Based Drug Design: Molecular Dynamics Simulations Support the Development of New Pyridine-Based Protein Kinase C-Targeted Agonists. **2023**, 66, 4588-4602 ○
- 67 Prediction of dynamic allostery for the transmembrane domain of the sweet taste receptor subunit, TAS1R3. **2023**, 6, ○
- 66 Computational Investigations into Two-Photon Fibril Imaging Using the DANIR-2c Probe. **2023**, 127, 3119-3125○
- 65 Influence of Core Topologies on Poly-l-lysine Dendrimer Structures. **2023**, 127, 3364-3371 ○
- 64 Thermal-triggered loading and GSH-responsive releasing property of HBc particles for drug delivery. **2023**, ○
- 63 Identifying novel selective PPO inhibitors through structure-based virtual screening and bio-evaluation. **2023**, 13, 10873-10883 ○
- 62 Proton Transport in Perfluorinated Ionomer Simulated by Machine-Learned Interatomic Potential. **2023**, 14, 3581-3588 ○
- 61 X-ray Structure Characterization of the Selective Recognition of AT Base Pair Sequences. ○
- 60 A Benzohydrazide-Based Artificial Ion Channel that Modulates Chloride Ion Concentration in Cancer Cells and Induces Apoptosis by Disruption of Autophagy. ○
- 59 Selectivity and Ranking of Tight-Binding JAK-STAT Inhibitors Using Markovian Milestoning with Voronoi Tessellations. ○
- 58 Extraordinary Control of Photosensitized Singlet Oxygen Generation by Acyclic Cucurbituril-like Containers. **2023**, 127, 3443-3451 ○
- 57 Influence of hydrostatic pressure during gelation on physicochemical properties of cellulose hydrogels prepared from ionic liquid/DMSO solution. **2023**, 381, 121810 ○
- 56 Role of the Polar Proportion of Compound Collectors in Low-Rank Coal Flotation Upgrading: Insights from the Molecular Scale. **2023**, 13, 524 ○
- 55 Chemical Promoter Performance for CO₂ Hydrate Growth: A Molecular Perspective. **2023**, 37, 6002-6011 ○
- 54 Molecular Recognition of Methacryllsine and Crotonyllysine by the AF9 YEATS Domain. **2023**, 24, 7002 ○
- 53 Substituted Oligosaccharides as Protein Mimics: Deep Learning Free Energy Landscapes. ○

- 52 Water-Soluble Cellulose As a New Class of Green CH₄ Hydrate Inhibitors: Insights from Experiments and Molecular Dynamics Simulations. ○
- 51 Hierarchical biopolymer-based materials and composites. ○
- 50 Magnetic Polaron States in Photoluminescent Carbon Dots Enable Hydrogen Peroxide Photoproduction. ○
- 49 Nucleobase Specific Understanding about the Interaction of Antimalarial Drug Chloroquine with Duplex DNA. **2023**, 127, 3341-3351 ○
- 48 Clinical side-effects based drug repositioning for anti-epileptic activity. 1-12 ○
- 47 Engineering C_α Bond Cleavage Activity into a P450 Monooxygenase Enzyme. ○
- 46 Targeting the I7L Protease: A Rational Design for Anti-Monkeypox Drugs?. **2023**, 24, 7119 ○
- 45 Interactions between curcumin and human salt-induced kinase 3 elucidated from computational tools and experimental methods. 14, ○
- 44 An Expedited Route to Optical and Electronic Properties at Finite Temperature via Unsupervised Learning. **2023**, 28, 3411 ○
- 43 Exploitation of Dimeric Cyclic Cysteine as Helix Inducer in Ultra-Short Peptides for Cu(II)-Catalysed Asymmetric Michael Addition on Chalcones. ○
- 42 Geometric Deep Learning for Molecular Crystal Structure Prediction. ○
- 41 Peroxo-Diiron(III/III) as the Reactive Intermediate for N-Hydroxylation Reactions in the Multidomain Metalloenzyme SznF: Evidence from Molecular Dynamics and Quantum Mechanical/Molecular Mechanical Calculations. 5808-5818 ○
- 40 Cytotoxicity Profiles and Neuroprotective Properties of the Novel Ifenprodil Analogues as Sigma Ligands. **2023**, 28, 3431 ○
- 39 Autochthonous Peruvian Natural Plants as Potential SARS-CoV-2 Mpro Main Protease Inhibitors. **2023**, 16, 585 ○
- 38 Towards Computational Modeling of Ligand Binding to the ILPR G-Quadruplex. **2023**, 28, 3447 ○
- 37 Computational Insights into Prostaglandin E₂ Ligand Binding and Activation of G-Protein-Coupled Receptors. ○
- 36 Computer-aided de novo design and optimization of novel potential inhibitors of HIV-1 Nef protein. **2023**, 104, 107871 ○
- 35 Computational insights into ligand-induced G protein and β arrestin signaling of the dopamine D₁ receptor. ○

- 34 Does a Machine-Learned Potential Perform Better Than an Optimally Tuned Traditional Force Field? A Case Study on Fluorohydrins. ○
- 33 Computational Characterization of the Inhibition Mechanism of Xanthine Oxidoreductase by Topiroxostat. 6023-6043 ○
- 32 Origin of the kinetic HDAC2 -selectivity of an HDAC inhibitor. ○
- 31 Bayesian Optimization for Ternary Complex Prediction (BOTCP). 2023, 100072 ○
- 30 Molecular Simulation Strategies for Understanding the Degradation Mechanisms of Acrylic Polymers. ○
- 29 Barley HvNIP2;1 aquaporin permeates water, metalloids, saccharides, and ion pairs due to structural plasticity and diversification. ○
- 28 Bioisosteric Design Identifies Inhibitors of Mycobacterium tuberculosis DNA Gyrase ATPase Activity. ○
- 27 Structure and dynamics of a glucose-based cryoprotectant mixture: a computer simulation study. 2023, 142, ○
- 26 Effect of double chain anionic surfactant on the dynamic interfacial tensions of betaine solutions. 2023, 121866 ○
- 25 Quantum mechanics/fluctuating charge calculations for absorption spectra of aqueous green fluorescent protein chromophore. ○
- 24 Morphology prediction for organic molecular crystals using various force fields in ADDICT. ○
- 23 Solving Chemical Absorption Equilibria using Free Energy and Quantum Chemistry Calculations: Methodology, Limitations, and New Open-Source Software. ○
- 22 Discovery of Selective P2Y6R Antagonists with High Affinity and In Vivo Efficacy for Inflammatory Disease Therapy. ○
- 21 Insight into the structural and transport properties of methyl and benzyl triphenyl phosphonium based deep eutectic solvents using molecular dynamics simulations. 2023, 100998 ○
- 20 Exploiting nonaqueous self-stratified electrolyte systems toward large-scale energy storage. 2023, 14, ○
- 19 Enzyme-responsive biomimetic solid lipid nanoparticles for antibiotic delivery against hyaluronidase-secreting bacteria. 2023, 122967 ○
- 18 Lenalidomide Stabilizes Protein-Protein Complexes by Turning Labile Intermolecular H-Bonds into Robust Interactions. ○
- 17 Characterizing Soft Matter Self-Assembly and Material Properties with Advanced Molecular Dynamics and Data-Driven Methods. 2023, 1197-1220 ○

- 16 Theories and radial distribution function of MD and MC simulations. **2023**, 271-290 ○
- 15 Molecular Dynamics Study of Cured ED-20 Epoxy Resin for Predicting the Glass Transition Temperature and Relationship with Structure Features. ○
- 14 A quantitative analysis on the rheological characteristics of polyurea thickeners with the geometry of helical fiber and nanotube. **2023**, ○
- 13 The geometry of calix[3]pyrrole and the formation of the calix[3]pyrrole- π complex in solution. **2023**, 142, ○
- 12 Inhibitory effect of baicalein against glycation in HSA: an *in vitro* approach. 1-13 ○
- 11 Phenanthridine- β cyrene conjugates as fluorescent probes for DNA/RNA and an inactive mutant of dipeptidyl peptidase enzyme. 19, 550-565 ○
- 10 Investigating structural features of dimeric SARS-CoV-2 Mpro catalytic site with bound covalent ligands at physiological temperature. **2023**, 2485, 012006 ○
- 9 Quantum evaluation and therapeutic activity of (E)-N-(4-methoxyphenyl)-2-(4-(3-oxo-3-phenylprop-1-en-1-yl) phenoxy)acetamide and its modified derivatives against EGFR and VEGFR-2 in the treatment of triple-negative cancer via *in silico* approach. **2023**, 23, ○
- 8 Theoretical study on counter anion- and solvent-dependent fluorescence quenching mechanism of 2-phenylbenzo[b]phospholium salts. **2023**, 382, 121934 ○
- 7 Semi-Rational Design of L-Isoleucine Dioxygenase Generated Its Activity for Aromatic Amino Acid Hydroxylation. **2023**, 28, 3750 ○
- 6 Polymers of intrinsic microporosity containing aryl-phthalimide moieties: synthesis, modeling, and membrane gas transport properties. **2023**, 14, 2363-2373 ○
- 5 Mechanisms for mechanical responses of asphalt under uniaxial tension with computational simulation. **2023**, 385, 131497 ○
- 4 Molecular Dynamics Simulations as a Tool to Understand Drug Solubilization in Pharmaceutical Systems. **2023**, ○
- 3 Molecular Dynamics Simulations of Ionic Liquid Crystals. **2023**, ○
- 2 Design and Identification of Inhibitors for the Spike-ACE2 Target of SARS-CoV-2. **2023**, 24, 8814 ○
- 1 Catalytic Reaction Mechanism of Glyoxalase II: A Quantum Mechanics/Molecular Mechanics Study. ○