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#	Paper	IF	Citations
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2237	. **2016**,		11
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2232	Spatially resolved dielectric constant of confined water and its connection to the non-local nature of bulk water. **2016**, 145, 084901		29

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2228	Structure and dynamics of ionic liquids: Trimethylsilylpropyl-substituted cations and bis(sulfonyl)amide anions. **2016**, 145, 244506	20
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2202	Calculation of Enzyme Fluctuograms from All-Atom Molecular Dynamics Simulation. **2016**, 578, 327-42	1
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2200	Blind prediction of cyclohexane-water distribution coefficients from the SAMPL5 challenge. **2016**, 30, 927-944	80
2199	Structural and conformational insights into SOX2/OCT4-bound enhancer DNA: a computational perspective. **2016**, 6, 90138-90153	4
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2196	Polyethyleneimine loaded inverse SDS micelle in pentanol/toluene media. **2016**, 506, 402-408	3

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2194	Ensemble-based docking: From hit discovery to metabolism and toxicity predictions. **2016**, 24, 4928-4935	30
2193	Spontaneous Insertion, Helix Formation, and Hydration of Polyethylene Oxide in Carbon Nanotubes. **2016**, 117, 027801	19
2192	The effect of the environment on the methyl transfer reaction mechanism between trimethylsulfonium and phenolate. **2016**, 18, 24033-42	5
2191	Na+ coordination at the Na2 site of the Na+/I- symporter. **2016**, 113, E5379-88	17
2190	Membrane insertion of a Tc toxin in near-atomic detail. **2016**, 23, 884-890	67
2189	Discovery of 8-Trifluoromethyl-3-cyclopropylmethyl-7-[(4-(2,4-difluorophenyl)-1-piperazinyl)methyl]-1,2,4-triazolo[4,3-a]pyridine (JNJ-46356479), a Selective and Orally Bioavailable mGlu2 Receptor Positive Allosteric Modulator (PAM). **2016**, 59, 8495-507	24
2188	Predicting water-to-cyclohexane partitioning of the SAMPL5 molecules using dielectric balancing of force fields. **2016**, 30, 1059-1065	7
2187	The Ebola virus protein VP40 hexamer enhances the clustering of PI(4,5)P lipids in the plasma membrane. **2016**, 18, 28409-28417	34
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2184	Sampling Enhancement and Free Energy Prediction by the Flying Gaussian Method. **2016**, 12, 4644-50	7
2183	Lowered pH Leads to Fusion Peptide Release and a Highly Dynamic Intermediate of Influenza Hemagglutinin. **2016**, 120, 9654-60	13
2182	The structural basis of the dominant negative phenotype of the GH112 G203A/A326S heterotrimer. **2016**, 37, 1259-72	20
2181	Specific Binding of Cholesterol to C99 Domain of Amyloid Precursor Protein Depends Critically on Charge State of Protein. **2016**, 7, 3535-41	22
2180	Elucidating modes of activation and herbicide resistance by sequence assembly and molecular modelling of the Acetolactate synthase complex in sugarcane. **2016**, 407, 184-197	6
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2178	Appraisal of role of the polyanionic inducer length on amyloid formation by 412-residue 1N4R Tau protein: A comparative study. **2016**, 609, 1-19	18

2177	Graphics Processing Unit Acceleration and Parallelization of GENESIS for Large-Scale Molecular Dynamics Simulations. **2016**, 12, 4947-4958	20
2176	Adapting the semi-explicit assembly solvation model for estimating water-cyclohexane partitioning with the SAMPL5 molecules. **2016**, 30, 1067-1077	2
2175	Multiscale simulations on conformational dynamics and membrane interactions of the non-structural 2 (NS2) transmembrane domain. **2016**, 478, 193-198	4
2174	Ligand-induced Ordering of the C-terminal Tail Primes STING for Phosphorylation by TBK1. **2016**, 9, 87-96	26
2173	A molecular dynamics study of the effect of glycosidic linkage type in the hemicellulose backbone on the molecular chain flexibility. **2016**, 88, 56-70	39
2172	Calculating Partition Coefficients of Small Molecules in Octanol/Water and Cyclohexane/Water. **2016**, 12, 4015-24	104
2171	A molecular dynamics study of nanoparticle-formation from bioethanol-gasoline blend emissions. **2016**, 183, 55-63	7
2170	Water Dielectric Effects in Planar Confinement. **2016**, 117, 048001	137
2169	Comparison of systematic coarse-graining strategies for soluble conjugated polymers. **2016**, 225, 1441-1461	13
2168	Allosteric binding site in a Cys-loop receptor ligand-binding domain unveiled in the crystal structure of ELIC in complex with chlorpromazine. **2016**, 113, E6696-E6703	26
2167	Penicimenolides A-F, Resorcylic Acid Lactones from Penicillium sp., isolated from the Rhizosphere Soil of Panax notoginseng. **2016**, 6, 27396	16
2166	A quasi-liquid mediated continuum model of faceted ice dynamics. **2016**, 121, 14,035-14,055	6
2165	The C-terminal Domains of Apoptotic BH3-only Proteins Mediate Their Insertion into Distinct Biological Membranes. **2016**, 291, 25207-25216	8
2164	Imidazolium-Based Lipid Analogues and Their Interaction with Phosphatidylcholine Membranes. **2016**, 32, 12579-12592	35
2163	Molecular Mechanism and Energy Basis of Conformational Diversity of Antibody SPE7 Revealed by Molecular Dynamics Simulation and Principal Component Analysis. **2016**, 6, 36900	20
2162	Assessing the Quality of Solvents and Dispersants for Low-Dimensional Materials Using the Corresponding Distances Method. **2016**, 120, 11607-11617	2
2161	Acid activation mechanism of the influenza A M2 proton channel. **2016**, 113, E6955-E6964	51
2160	How Oliceridine (TRV-130) Binds and Stabilizes a □Opioid Receptor Conformational State That Selectively Triggers G Protein Signaling Pathways. **2016**, 55, 6456-6466	64

2159	Characterization of Mg Distributions around RNA in Solution. **2016**, 1, 680-688		24
2158	What Can We Learn about Cholesterol's Transmembrane Distribution Based on Cholesterol-Induced Changes in Membrane Dipole Potential?. **2016**, 7, 4585-4590		13
2157	Molecular Dynamics Study of the Morphology of Hydrated Perfluorosulfonic Acid Polymer Membranes. **2016**, 120, 25832-25842		48
2156	A Combined Experimental and Theoretical Study on the Extraction of Uranium by Amino-Derived Metal-Organic Frameworks through Post-Synthetic Strategy. **2016**, 8, 31032-31041		110
2155	Light-enhanced liquid-phase exfoliation and current photoswitching in graphene-azobenzene composites. **2016**, 7, 11090		85
2154	Self-Assembly of Catenanes from Lasso Peptides. **2016**, 138, 14214-14217		28
2153	Crystal Structure of the Human Cannabinoid Receptor CB. **2016**, 167, 750-762.e14		323
2152	Tautomeric Effect of Histidine on the Monomeric Structure of Amyloid Peptide(1-40). **2016**, 120, 11405-11411		24
2151	Computational insights into the protonation states of catalytic dyad in BACE1-acyl guanidine based inhibitor complex. **2016**, 70, 226-235		24
2150	Exploring Energy Efficiency for GPU-Accelerated POWER Servers. **2016**, 207-227		
2149	Energetics of side-chain snorkeling in transmembrane helices probed by nonproteinogenic amino acids. **2016**, 113, 10559-64		19
2148	Visualization of collective vortex-like motions in a computer model of liquid argon. **2016**, 57, 1660-1662		6
2147	Structure of the Bacterial Cytoskeleton Protein Bactofilin by NMR Chemical Shifts and Sequence Variation. **2016**, 110, 2342-2348		11
2146	C-language package for standalone embedded atom method molecular dynamics simulations of fcc structures. *SoftwareX*, **2016**, 5, 107-111	2.7	4
2145	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand-protein interactions. **2016**, 24, 4812-4825		95
2144	Improving the Efficiency and Activity of Electrocatalysts for the Reduction of CO2 through Supramolecular Assembly with Amino Acid-Modified Ligands. **2016**, 138, 8184-93		50
2143	Hybrid MPI/OpenMP Implementation of the ORAC Molecular Dynamics Program for Generalized Ensemble and Fast Switching Alchemical Simulations. **2016**, 56, 1117-21		34
2142	Crystal structure and dynamics of Spt16N-domain of FACT complex from Cicer arietinum. **2016**, 88, 36-43		6

2141	PEP-FOLD3: faster de novo structure prediction for linear peptides in solution and in complex. **2016**, 44, W449-54	399
2140	Structural Elements in the Gβ and Gγ C Termini That Mediate Selective G Protein-coupled Receptor (GPCR) Signaling. **2016**, 291, 17929-40	22
2139	Physico-chemical and in-silico analysis of a phytocystatin purified from Brassica juncea cultivar RoAgro 5444. **2016**, 94, 584-596	8
2138	Molecular Dynamics Simulation of Sulfobetaine-Type Zwitterionic Surfactants at the Decane/Water Interface: Structure, Interfacial Properties. **2016**, 37, 1710-1717	26
2137	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. **2016**, 12, 405-13	1303
2136	PARENT: A Parallel Software Suite for the Calculation of Configurational Entropy in Biomolecular Systems. **2016**, 12, 2055-65	21
2135	The good, the bad and the user in soft matter simulations. **2016**, 1858, 2529-2538	77
2134	Design, structure prediction and molecular dynamics simulation of a fusion construct containing malaria pre-erythrocytic vaccine candidate, PfCelTOS, and human interleukin 2 as adjuvant. **2016**, 17, 71	19
2133	Interaction of wine anthocyanin derivatives with lipid bilayer membranes. **2016**, 1077, 80-86	24
2132	Efficient preparation and analysis of membrane and membrane protein systems. **2016**, 1858, 2468-2482	23
2131	Exploration of Interfacial Hydration Networks of Target-Ligand Complexes. **2016**, 56, 148-58	17
2130	OpenGrowth: An Automated and Rational Algorithm for Finding New Protein Ligands. **2016**, 59, 4171-88	35
2129	AGGREGATES: Finding structures in simulation results of solutions. **2017**, 38, 753-765	28
2128	Structural basis of human PCNA sliding on DNA. **2017**, 8, 13935	45
2127	Molecular-Scale Biophysical Modulation of an Endothelial Membrane by Oxidized Phospholipids. **2017**, 112, 325-338	29
2126	Thermodynamics of Helix-Coil Transitions of Polyalanine in Open Carbon Nanotubes. **2017**, 8, 494-499	2
2125	Hampering Effect of Cholesterol on the Permeation of Reactive Oxygen Species through Phospholipids Bilayer: Possible Explanation for Plasma Cancer Selectivity. **2017**, 7, 39526	55
2124	Copernicus, a hybrid dataflow and peer-to-peer scientific computing platform for efficient large-scale ensemble sampling. **2017**, 71, 18-31	9

2123	The Multiple Roles of Waters in Protein Solvation. **2017**, 121, 3636-3643	13
2122	NMR investigation of the isolated second voltage-sensing domain of human Nav1.4 channel. **2017**, 1859, 493-506	9
2121	Impact of Turn Propensity on the Folding Rates of Z34C Protein: Implications for the Folding of Helix-Turn-Helix Motif. **2017**, 121, 1268-1283	1
2120	Sequence-, structure-, and dynamics-based comparisons of structurally homologous CheY-like proteins. **2017**, 114, 1578-1583	10
2119	Applications of Computational Methods to Simulations of Proteins Dynamics. **2017**, 1627-1669	1
2118	Identification of Inhibitors of CD36-Amyloid Beta Binding as Potential Agents for Alzheimer's Disease. **2017**, 8, 1232-1241	24
2117	C-Terminal residues in small potassium channel blockers OdK1 and OSK3 from scorpion venom fine-tune the selectivity. **2017**, 1865, 465-472	5
2116	The role of interfacial lipids in stabilizing membrane protein oligomers. **2017**, 541, 421-424	238
2115	Modeling Diversity in Structures of Bacterial Outer Membrane Lipids. **2017**, 13, 811-824	19
2114	Insights from molecular dynamics simulations for computational protein design. **2017**, 2, 9-33	98
2113	Enantioselective Catalysis by Using Short, Structurally Defined DNA Hairpins as Scaffold for Hybrid Catalysts. **2017**, 23, 6004-6008	15
2112	Determining energy barriers and selectivities of a multi-pathway system with infrequent metadynamics. **2017**, 146, 014108	11
2111	Identification of promising DNA GyrB inhibitors for Tuberculosis using pharmacophore-based virtual screening, molecular docking and molecular dynamics studies. **2017**, 90, 282-296	9
2110	A Temperature-Sensitive Lesion in the N-Terminal Domain of the Rotavirus Polymerase Affects Its Intracellular Localization and Enzymatic Activity. **2017**, 91,	10
2109	Electrostatic Stabilization Plays a Central Role in Autoinhibitory Regulation of the Na,K-ATPase. **2017**, 112, 288-299	16
2108	Structural insights into human microsomal epoxide hydrolase by combined homology modeling, molecular dynamics simulations, and molecular docking calculations. **2017**, 85, 720-730	8
2107	Synergistic effect of electric field and lipid oxidation on the permeability of cell membranes. **2017**, 1861, 839-847	83
2106	Membrane cholesterol access into a G-protein-coupled receptor. **2017**, 8, 14505	89

2105	Insights from molecular modeling into the selective inhibition of cathepsin S by its inhibitor. **2017**, 23, 92	8
2104	Structural dependence of MEH-PPV chromism in solution. **2017**, 23, 91	2
2103	Predicting Protein Dynamics and Allostery Using Multi-Protein Atomic Distance Constraints. **2017**, 25, 546-558	31
2102	Bulk Heterojunction Morphologies with Atomistic Resolution from Coarse-Grain Solvent Evaporation Simulations. **2017**, 139, 3697-3705	99
2101	Effect of conjugation on phase transitions in thermoresponsive polymers: an atomistic and coarse-grained simulation study. **2017**, 13, 2907-2918	33
2100	Mechanics of water pore formation in lipid membrane under electric field. **2017**, 33, 234-242	6
2099	Information-Driven, Ensemble Flexible Peptide Docking Using HADDOCK. **2017**, 1561, 109-138	20
2098	Mechanisms of Peptide Oxidation by Hydroxyl Radicals: Insight at the Molecular Scale. **2017**, 121, 5787-5799	11
2097	Molecular basis of interactions between SH3 domain-containing proteins and the proline-rich region of the ubiquitin ligase Itch. **2017**, 292, 6325-6338	11
2096	Long-Range Dispersion Effects on the Water/Vapor Interface Simulated Using the Most Common Models. **2017**, 121, 3798-3803	28
2095	Computational Prediction of the Heterodimeric and Higher-Order Structure of gpE1/gpE2 Envelope Glycoproteins Encoded by Hepatitis C Virus. **2017**, 91,	24
2094	Stabilization of peptides against proteolysis through disulfide-bridged conjugation with synthetic aromatics. **2017**, 15, 1921-1929	14
2093	New Insights on Signal Propagation by Sensory Rhodopsin II/Transducer Complex. **2017**, 7, 41811	18
2092	Calcium Assists Dopamine Release by Preventing Aggregation on the Inner Leaflet of Presynaptic Vesicles. **2017**, 8, 1242-1250	13
2091	Initial Substrate Binding of β-Secretase: The Role of Substrate Flexibility. **2017**, 8, 1279-1290	18
2090	A refined polarizable water model for the coarse-grained MARTINI force field with long-range electrostatic interactions. **2017**, 146, 054501	47
2089	The Startle Disease Mutation E103K Impairs Activation of Human Homomeric α1 Glycine Receptors by Disrupting an Intersubunit Salt Bridge across the Agonist Binding Site. **2017**, 292, 5031-5042	7
2088	Propagation of the Allosteric Modulation Induced by Sodium in the δ-Opioid Receptor. **2017**, 23, 4615-4624	13

2087	Assembly of photoactive orange carotenoid protein from its domains unravels a carotenoid shuttle mechanism. **2017**, 133, 327-341	36
2086	Prednisolone adsorption on lung surfactant models: insights on the formation of nanoaggregates, monolayer collapse and prednisolone spreading. **2017**, 7, 5272-5281	24
2085	Drastic Compensation of Electronic and Solvation Effects on ATP Hydrolysis Revealed through Large-Scale QM/MM Simulations Combined with a Theory of Solutions. **2017**, 121, 2279-2287	12
2084	Electron transfer pathways in a multiheme cytochrome MtrF. **2017**, 114, 2916-2921	32
2083	pmx Webserver: A User Friendly Interface for Alchemistry. **2017**, 57, 109-114	25
2082	Partitioning of caffeine in lipid bilayers reduces membrane fluidity and increases membrane thickness. **2017**, 19, 7101-7111	26
2081	Cellulose Nanopaper and Nanofoam for Patient-Tailored Drug Delivery. **2017**, 4, 1600655	27
2080	Solution behaviour of poly(N-isopropylacrylamide) stereoisomers in water: a molecular dynamics simulation study. **2017**, 19, 11892-11903	15
2079	Gating Charge Calculations by Computational Electrophysiology Simulations. **2017**, 112, 1396-1405	9
2078	Effect of methane-sugar interaction on the solubility of methane in an aqueous solution. **2017**, 500, 113-118	4
2077	Spectroscopic (FT-IR, FT-Raman, UV, NMR, NLO) investigation, molecular docking and molecular simulation dynamics on 1-Methyl-3-Phenylpiperazine. **2017**, 1143, 328-343	3
2076	Effect of an ionic liquid/air Interface on the structure and dynamics of amphiphilic peptides. **2017**, 236, 404-413	8
2075	Role of Hydrophobic/Aromatic Residues on the Stability of Double-Wall β-Sheet Structures Formed by a Triblock Peptide. **2017**, 121, 4115-4128	4
2074	Reverse Monte Carlo modeling of liquid water with the explicit use of the SPC/E interatomic potential. **2017**, 146, 064506	10
2073	Mapping the conformational free energy of aspartic acid in the gas phase and in aqueous solution. **2017**, 146, 145102	7
2072	Identification of a conserved 8 aa insert in the PIP5K protein in the Saccharomycetaceae family of fungi and the molecular dynamics simulations and structural analysis to investigate its potential functional role. **2017**, 85, 1454-1467	13
2071	ω-Conotoxin GeXIVA disulfide bond isomers exhibit differential sensitivity for various nicotinic acetylcholine receptors but retain potency and selectivity for the human α9α10 subtype. **2017**, 127, 243-252	20
2070	Design of electric field controlled molecular gates mounted on metal–organic frameworks. **2017**, 5, 8690-8696	41

2069	On the role of residue phosphorylation in 14-3-3 partners: AANAT as a case study. **2017**, 7, 46114	7
2068	Plasma membrane association facilitates conformational changes in the Marburg virus protein VP40 dimer. **2017**, 7, 22741-22748	9
2067	How a short pore forming peptide spans the lipid membrane. **2017**, 12, 02D405	3
2066	Analysis of Prepeak Structure of Concentrated Organic Lithium Electrolyte by Means of Neutron Diffraction with Isotopic Substitution and Molecular Dynamics Simulation. **2017**, 121, 5355-5362	14
2065	Transport Mechanism of Guest Methane in Water-Filled Nanopores. **2017**, 121, 15675-15686	50
2064	Molecular Explanation for the Abnormal Flux of Material into a Hot Spot in Ester Monolayers. **2017**, 121, 5621-5632	
2063	Structure of the MacAB-TolC ABC-type tripartite multidrug efflux pump. **2017**, 2, 17070	96
2062	Time-Resolved X-Ray Solution Scattering Reveals the Structural Photoactivation of a Light-Oxygen-Voltage Photoreceptor. **2017**, 25, 933-938.e3	27
2061	Perturbation-Response Scanning Reveals Key Residues for Allosteric Control in Hsp70. **2017**, 57, 1359-1374	43
2060	Developing and Validating a Set of All-Atom Potential Models for Sodium Dodecyl Sulfate. **2017**, 13, 2742-2750	16
2059	Viscoelastic relaxations of high alcohols and alkanes: Effects of heterogeneous structure and translation-orientation coupling. **2017**, 146, 094511	15
2058	Determining Atomistic SAXS Models of Tri-Ubiquitin Chains from Bayesian Analysis of Accelerated Molecular Dynamics Simulations. **2017**, 13, 2418-2429	10
2057	Markov modeling reveals novel intracellular modulation of the human TREK-2 selectivity filter. **2017**, 7, 632	10
2056	Competing Pathways and Multiple Folding Nuclei in a Large Multidomain Protein, Luciferase. **2017**, 112, 1829-1840	8
2055	Accurate Prediction of Complex Structure and Affinity for a Flexible Protein Receptor and Its Inhibitor. **2017**, 13, 2389-2399	32
2054	Elucidation and Comparison of the Effect of LiTFSI and LiNO Salts on Discharge Chemistry in Nonaqueous Li-O Batteries. **2017**, 9, 19319-19325	21
2053	Neural Network and Nearest Neighbor Algorithms for Enhancing Sampling of Molecular Dynamics. **2017**, 13, 2489-2500	37
2052	Conformational latitude - activity relationship of KPPR tetrapeptide analogues toward their ability to inhibit binding of vascular endothelial growth factor 165 to neuropilin-1. **2017**, 23, 445-454	12

2051	QM/MM Geometry Optimization on Extensive Free-Energy Surfaces for Examination of Enzymatic Reactions and Design of Novel Functional Properties of Proteins. **2017**, 68, 135-154	10
2050	Approaches for calculating solvation free energies and enthalpies demonstrated with an update of the FreeSolv database. **2017**, 62, 1559-1569	114
2049	Molecular Mechanism of Overhauser Dynamic Nuclear Polarization in Insulating Solids. **2017**, 8, 2137-2142	27
2048	LigParGen web server: an automatic OPLS-AA parameter generator for organic ligands. **2017**, 45, W331-W336	366
2047	Molecular insights into the inhibitory mechanism of rifamycin SV against ╫microglobulin aggregation: A molecular dynamics simulation study. **2017**, 102, 1025-1034	15
2046	Bioinformatics evaluation of novel ribosome display-selected single chain variable fragment (scFv) structure with factor H binding protein through docking. **2017**, 16, 1750021	4
2045	Rational Design of a Transferrin-Binding Peptide Sequence Tailored to Targeted Nanoparticle Internalization. **2017**, 28, 471-480	48
2044	Targeting Type 2 Diabetes with C-Glucosyl Dihydrochalcones as Selective Sodium Glucose Co-Transporter 2 (SGLT2) Inhibitors: Synthesis and Biological Evaluation. **2017**, 60, 568-579	35
2043	Alchemical determination of drug-receptor binding free energy: Where we stand and where we could move to. **2017**, 71, 233-241	15
2042	Martini Coarse-Grained Force Field: Extension to RNA. **2017**, 113, 246-256	74
2041	Structure-Activity Relationship in TLR4 Mutations: Atomistic Molecular Dynamics Simulations and Residue Interaction Network Analysis. **2017**, 7, 43807	25
2040	Modeling nanoscale ice adhesion. **2017**, 30, 224-226	8
2039	Hydrogen bond-Driven Self-Assembly between Amidinium Cations and Carboxylate Anions: A Combined Molecular Dynamics, NMR Spectroscopy, and Single Crystal X-ray Diffraction Study. **2017**, 12, 1587-1597	18
2038	Identification of a novel putative inhibitor of the Plasmodium falciparum purine nucleoside phosphorylase: exploring the purine salvage pathway to design new antimalarial drugs. **2017**, 21, 677-695	13
2037	Architecture of the paracellular channels formed by claudins of the blood-brain barrier tight junctions. **2017**, 1405, 131-146	36
2036	Structural Behavior of the Peptaibol Harzianin HK VI in a DMPC Bilayer: Insights from MD Simulations. **2017**, 112, 2602-2614	5
2035	Structure-activity relationship study of tetrapeptide inhibitors of the Vascular Endothelial Growth Factor A binding to Neuropilin-1. **2017**, 94, 25-32	14
2034	Intrinsic map dynamics exploration for uncharted effective free-energy landscapes. **2017**, 114, E5494-E5503	72

2033	Hidden electrostatic basis of dynamic allostery in a PDZ domain. **2017**, 114, E5825-E5834	58
2032	How proteins bind to DNA: target discrimination and dynamic sequence search by the telomeric protein TRF1. **2017**, 45, 7643-7654	16
2031	Oleuropein interactions with inner and outer surface of different types of carbon nanotubes: Insights from molecular dynamic simulation. **2017**, 241, 367-373	7
2030	Optimizing purification process of MIM-I-BAR domain by introducing atomic force microscope and dynamics simulations. **2017**, 157, 391-397	1
2029	Impact of Surface Ionization on Water Transport and Salt Leakage through Graphene Oxide Membranes. **2017**, 121, 13412-13420	27
2028	Docosahexaenoic acid preserves visual function by maintaining correct disc morphology in retinal photoreceptor cells. **2017**, 292, 12054-12064	75
2027	Energetic Analysis of Adsorption and Absorption of Small Molecule to Nanodroplet of Water. **2017**, 121, 5995-6001	4
2026	First-principle simulations of electronic structure in semicrystalline polyethylene. **2017**, 146, 204901	32
2025	Templating the 3D structure of conducting polymers with self-assembling peptides. **2017**, 5, 4690-4696	5
2024	Explicit Solvent Hydration Benchmark for Proteins with Application to the PBSA Method. **2017**, 13, 2762-2776	1
2023	Free Energy Landscape of Cellulose as a Driving Factor in the Mobility of Adsorbed Water. **2017**, 33, 5362-5370	6
2022	Evolutionary, computational, and biochemical studies of the salicylaldehyde dehydrogenases in the naphthalene degradation pathway. **2017**, 7, 43489	11
2021	Surface patterning of single-walled carbon nanotubes enhances their perturbation on a pulmonary surfactant monolayer: frustrated translocation and bilayer vesiculation. **2017**, 7, 20851-20864	9
2020	Herbicide targets and detoxification proteins in sugarcane: from gene assembly to structure modelling. **2017**, 60, 601-617	2
2019	Dynamic properties of the growth hormone releasing hormone receptor (GHRHR) and molecular determinants of GHRH binding. **2017**, 13, 1313-1322	6
2018	Structural insight into inhibition of REV7 protein interaction revealed by docking, molecular dynamics and MM/PBSA studies. **2017**, 7, 27780-27786	8
2017	OpenRBC: A Fast Simulator of Red Blood Cells at Protein Resolution. **2017**, 112, 2030-2037	34
2016	Curcumin Protects Membranes through a Carpet or Insertion Model Depending on Hydration. **2017**, 33, 8516-8524	19

2015	Effect of sampling on BACE-1 ligands binding free energy predictions via MM-PBSA calculations. **2017**, 38, 1941-1951	8
2014	YY1 Haploinsufficiency Causes an Intellectual Disability Syndrome Featuring Transcriptional and Chromatin Dysfunction. **2017**, 100, 907-925	77
2013	Inhibition of A Amyloid Growth and Toxicity by Silybins: The Crucial Role of Stereochemistry. **2017**, 8, 1767-1778	56
2012	The effect of water on the shape of aggregates in water-in-oil microemulsions according to data of computer simulation. **2017**, 79, 328-332	6
2011	Metadynamic metainference: Convergence towards force field independent structural ensembles of a disordered peptide. **2017**, 146, 165102	35
2010	Cantharidin inhibits competitively heme-Fe(III) binding to the FA1 site of human serum albumin. **2017**, 30, e2641	8
2009	Determining dominant driving forces affecting controlled protein release from polymeric nanoparticles. **2017**, 12, 02D412	4
2008	Structural analysis and insight into Zika virus NS5 mediated interferon inhibition. **2017**, 51, 143-152	11
2007	Simulative and Experimental Characterization of a pH-Dependent Clamp-like DNA Triple-Helix Nanoswitch. **2017**, 139, 5321-5329	19
2006	Structure and antagonism of the receptor complex mediated by human TSLP in allergy and asthma. **2017**, 8, 14937	76
2005	Bio-inspired CO reduction by a rhenium tricarbonyl bipyridine-based catalyst appended to amino acids and peptidic platforms: incorporating proton relays and hydrogen-bonding functional groups. **2017**, 198, 279-300	40
2004	Ionic tethering contributes to the conformational stability and function of complement C3b. **2017**, 85, 137-147	2
2003	Structure and dynamics of Type III periplasmic proteins VcFhuD and VcHutB reveal molecular basis of their distinctive ligand binding properties. **2017**, 7, 42812	5
2002	Exploring Fluorescent Dyes at Biomimetic Interfaces with Second Harmonic Generation and Molecular Dynamics. **2017**, 33, 3373-3383	7
2001	Structural basis for selectivity and diversity in angiotensin II receptors. **2017**, 544, 327-332	128
2000	The nanostructure of a lithium glyme solvate ionic liquid at electrified interfaces. **2017**, 19, 11004-11010	21
1999	Kinetics of CO diffusion in human carbonic anhydrase: a study using molecular dynamics simulations and the Markov-state model. **2017**, 19, 11690-11697	7
1998	Replica exchange molecular dynamics study of the amyloid beta (11 40) trimer penetrating a membrane. **2017**, 7, 7346-7357	30

1997	Critical Comparison of Biomembrane Force Fields: Protein-Lipid Interactions at the Membrane Interface. **2017**, 13, 2310-2321	42
1996	Membrane Phase-Dependent Occlusion of Intramolecular GLUT1 Cavities Demonstrated by Simulations. **2017**, 112, 1176-1184	11
1995	Structural insights into type I and type II of nsp4 porcine reproductive and respiratory syndrome virus (nsp4 PRRSV) by molecular dynamics simulations. **2017**, 74, 125-134	1
1994	Nanostructured solvation in mixtures of protic ionic liquids and long-chained alcohols. **2017**, 146, 124503	25
1993	Structures of closed and open states of a voltage-gated sodium channel. **2017**, 114, E3051-E3060	93
1992	Structural insights into ligand binding of PGRP1 splice variants in Chinese giant salamander (Andrias davidianus) from molecular dynamics and free energy calculations. **2017**, 23, 135	2
1991	PyCGTOOL: Automated Generation of Coarse-Grained Molecular Dynamics Models from Atomistic Trajectories. **2017**, 57, 650-656	34
1990	Role of Pore-Lining Residues in Defining the Rate of Water Conduction by Aquaporin-0. **2017**, 112, 953-965	11
1989	Lipid Nanodisc-Templated Self-Assembly of Gold Nanoparticles into Strings and Rings. **2017**, 11, 3651-3661	19
1988	Molecular simulation and experiments of water adsorption in a high surface area activated carbon: Hysteresis, scanning curves and spatial organization of water clusters. **2017**, 118, 127-138	31
1987	Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15. **2017**, 121, 4023-4039	147
1986	Coarse graining from variationally enhanced sampling applied to the Ginzburg-Landau model. **2017**, 114, 3370-3374	23
1985	Docking, molecular dynamics and free energy studies on aspartoacylase mutations involved in Canavan disease. **2017**, 74, 44-53	9
1984	Self-Assembly Nanostructures of Triglyceride-Water Interfaces Determine Functional Conformations of Candida antarctica Lipase B. **2017**, 33, 3151-3159	7
1983	Concentration gradient driven molecular dynamics: a new method for simulations of membrane permeation and separation. **2017**, 8, 3858-3865	43
1982	Fundamental issues on the influence of starch in amine adsorption by quartz. **2017**, 522, 642-651	28
1981	Identification of novel serotonin reuptake inhibitors targeting central and allosteric binding sites: A virtual screening and molecular dynamics simulations study. **2017**, 74, 193-202	5
1980	From Cooperative Self-Assembly to Water-Soluble Supramolecular Polymers Using Coarse-Grained Simulations. **2017**, 11, 1000-1011	56

1979	Predictions of Ligand Selectivity from Absolute Binding Free Energy Calculations. **2017**, 139, 946-957		94
1978	Novel flavonolignan hybrid antioxidants: From enzymatic preparation to molecular rationalization. **2017**, 127, 263-274		18
1977	On Atomistic Models for Molecular Oxygen. **2017**, 121, 518-528		10
1976	pysimm: A python package for simulation of molecular systems. *SoftwareX*, **2017**, 6, 7-12	2.7	35
1975	Shedding light on the puzzle of drug-membrane interactions: Experimental techniques and molecular dynamics simulations. **2017**, 65, 24-44		44
1974	Antiviral drug acyclovir exhibits antitumor activity via targeting TrCP1: Molecular docking and dynamics simulation study. **2017**, 72, 96-105		8
1973	Investigating the effect of charged amino acids on DNA conformation in EcoRI-DNA complex: a molecular dynamics simulation study. **2017**, 35, 3540-3554		2
1972	Drug-Excipient Interactions in the Solid State: The Role of Different Stress Factors. **2017**, 14, 4560-4571		10
1971	Structural Disruption of an Adenosine-Binding DNA Aptamer on Graphene: Implications for Aptasensor Design. **2017**, 2, 1602-1611		14
1970	Force field parametrization of hydrogenoxalate and oxalate anions with scaled charges. **2017**, 23, 327		14
1969	Combined x-ray crystallography and computational modeling approach to investigate the Hsp90 C-terminal peptide binding to FKBP51. **2017**, 7, 14288		15
1968	Phosphorylation versus O-GlcNAcylation: Computational Insights into the Differential Influences of the Two Competitive Post-Translational Modifications. **2017**, 121, 10618-10638		8
1967	Understanding of the Electrogenerated Bulk Electrolyte Species in Sodium-Containing Ionic Liquid Electrolytes During the Oxygen Reduction Reaction. **2017**, 121, 23307-23316		15
1966	Intrinsic structural variability in GNRA-like tetraloops: insight from molecular dynamics simulation. **2017**, 23, 300		
1965	Braun's Lipoprotein Facilitates OmpA Interaction with the Escherichia coli Cell Wall. **2017**, 113, 1496-1504		30
1964	Molecular Dynamics Simulation of the Adsorption and Aggregation of Ionic Surfactants at Liquid–Solid Interfaces. **2017**, 121, 25908-25920		27
1963	Insights on the Mechanism of Action of INH-C as an Antitubercular Prodrug. **2017**, 14, 4597-4605		10
1962	HtrA1 activation is driven by an allosteric mechanism of inter-monomer communication. **2017**, 7, 14804		13

1961	A glycerophospholipid-specific pocket in the RVFV class II fusion protein drives target membrane insertion. **2017**, 358, 663-667	35
1960	Molecular dynamics simulation of membrane in room temperature ionic liquids. **2017**,	2
1959	Teixobactin analogues reveal enduracididine to be non-essential for highly potent antibacterial activity and lipid II binding. **2017**, 8, 8183-8192	33
1958	Mechanistic principles underlying regulation of the actin cytoskeleton by phosphoinositides. **2017**, 114, E8977-E8986	60
1957	ATK-ForceField: a new generation molecular dynamics software package. **2017**, 25, 085007	50
1956	Stratified UWHAM and Its Stochastic Approximation for Multicanonical Simulations Which Are Far from Equilibrium. **2017**, 13, 4660-4674	5
1955	Enhancing Vaccine Efficacy by Engineering a Complex Synthetic Peptide To Become a Super Immunogen. **2017**, 199, 2794-2802	9
1954	Multiscale Methods for Fracture: A Review(^bigstar). **2017**, 97, 339-376	13
1953	Structure and Dynamics of Hydroxyl-Functionalized Protic Ammonium Carboxylate Ionic Liquids. **2017**, 121, 8097-8107	23
1952	Solvation of Carbon Nanoparticles in Water/Alcohol Mixtures: Using Molecular Simulation To Probe Energetics, Structure, and Dynamics. **2017**, 121, 22926-22938	8
1951	Surface Polarization Effects on Ion-Containing Emulsions. **2017**, 119, 138002	14
1950	Structural basis for maintenance of bacterial outer membrane lipid asymmetry. **2017**, 2, 1616-1623	73
1949	Freezing Temperatures, Ice Nanotubes Structures, and Proton Ordering of TIP4P/ICE Water inside Single Wall Carbon Nanotubes. **2017**, 121, 10371-10381	21
1948	Membrane Permeability of Fatty Acyl Compounds Studied via Molecular Simulation. **2017**, 121, 11311-11324	15
1947	Structural insights into the competitive inhibition of the ATP-gated P2X receptor channel. **2017**, 8, 876	49
1946	Molecular dynamics simulations of pyrrolidinium and imidazolium ionic liquids at graphene interfaces. **2017**, 19, 30010-30020	31
1945	Chromophore-Dependent Intramolecular Exciton-Vibrational Coupling in the FMO Complex: Quantification and Importance for Exciton Dynamics. **2017**, 121, 10026-10035	17
1944	Arginase Structure and Inhibition: Catalytic Site Plasticity Reveals New Modulation Possibilities. **2017**, 7, 13616	21

1943	QM/MM Study of the Nitrogenase MoFe Protein Resting State: Broken-Symmetry States, Protonation States, and QM Region Convergence in the FeMoco Active Site. **2017**, 56, 13417-13429	51
1942	GRadient Adaptive Decomposition (GRAD) Method: Optimized Refinement Along Macrostate Borders in Markov State Models. **2017**, 57, 2729-2740	2
1941	Molecular-Level Insight into the Interaction of Phospholipid Bilayers with Cellulose. **2017**, 33, 12793-12803	8
1940	The Multiple Origins of the Hydrophobicity of Fluorinated Apolar Amino Acids. **2017**, 3, 881-897	21
1939	Toward High-Throughput Computational Screening of Carbon Nanotube Solvents. **2017**, 33, 12267-12275	6
1938	Effect of oligonucleic acid (ONA) backbone features on assembly of ONA-star polymer conjugates: a coarse-grained molecular simulation study. **2017**, 13, 6770-6783	9
1937	Tracking Dehydration Mechanisms in Crystalline Hydrates with Molecular Dynamics Simulations. **2017**, 17, 5017-5022	17
1936	Probing Gas Adsorption in Metal□Organic Framework ZIF-8 by EPR of Embedded Nitroxides. **2017**, 121, 19880-19886	12
1935	The Effects of A21G Mutation on Transmembrane Amyloid Beta (11-40) Trimer: An In Silico Study. **2017**, 121, 8467-8474	20
1934	Making sense of the past: hyperstability of ancestral thioredoxins explained by free energy simulations. **2017**, 19, 23239-23246	4
1933	Interaction between 1-phenylethanone, 2-phenyl-2-propanol, and isopropenylbenzene with water molecules: A computational study. **2017**, 1117, 188-195	4
1932	Round Robin Study: Molecular Simulation of Thermodynamic Properties from Models with Internal Degrees of Freedom. **2017**, 13, 4270-4280	32
1931	Molecular simulation of caloric properties of fluids modelled by force fields with intramolecular contributions: Application to heat capacities. **2017**, 147, 034508	3
1930	Prion protein 2-2 loop conformational landscape. **2017**, 114, 9617-9622	16
1929	Atomistic simulations of cation hydration in sodium and calcium montmorillonite nanopores. **2017**, 147, 084705	17
1928	Molecular insights into A□protofibril destabilization with a fluorinated compound D744: A molecular dynamics simulation study. **2017**, 30, e2656	18
1927	Active site gate of M32 carboxypeptidases illuminated by crystal structure and molecular dynamics simulations. **2017**, 1865, 1406-1415	6
1926	Evaluation of the absolute affinity of neuraminidase inhibitor using steered molecular dynamics simulations. **2017**, 77, 137-142	9

1925	Controlling Protein Surface Orientation by Strategic Placement of Oligo-Histidine Tags. **2017**, 11, 9068-9083	31
1924	A molecular dynamics study of conformations of beta-cyclodextrin and its eight derivatives in four different solvents. **2017**, 19, 24219-24229	22
1923	Stress Propagation through Biological Lipid Bilayers in Silico. **2017**, 139, 13588-13591	20
1922	Active subsite properties, subsite residues and targeting to lysosomes or midgut lumen of cathepsins L from the beetle Tenebrio molitor. **2017**, 89, 17-30	6
1921	Ionic interactions determine the morphology of dried alkali/liposome suspension droplets. **2017**, 160, 473-482	2
1920	Molecular Dynamics Study on the Mechanical Deformation of Hydrated Perfluorosulfonic Acid Polymer Membranes. **2017**, 121, 21374-21382	8
1919	Conformational Entropy as Collective Variable for Proteins. **2017**, 8, 4752-4756	11
1918	Engineered factor Xa variants retain procoagulant activity independent of direct factor Xa inhibitors. **2017**, 8, 528	18
1917	A nano-mechanical instability as primary contribution to rolling resistance. **2017**, 7, 11275	8
1916	Common behaviors associated with the glass transitions of water-like models. **2017**, 147, 034505	19
1915	The permeability enhancing mechanism of menthol on skin lipids: a molecular dynamics simulation study. **2017**, 23, 279	16
1914	Hydration Friction in Nanoconfinement: From Bulk via Interfacial to Dry Friction. **2017**, 17, 5969-5976	31
1913	Photoinduced Bimolecular Electron Transfer in Ionic Liquids. **2017**, 139, 14568-14585	25
1912	TPC2 polymorphisms associated with a hair pigmentation phenotype in humans result in gain of channel function by independent mechanisms. **2017**, 114, E8595-E8602	33
1911	Molecular dynamics simulations of ether- and ester-linked phospholipids. **2017**, 1859, 2297-2307	10
1910	New indole-based chalconoids as tubulin-targeting antiproliferative agents. **2017**, 75, 86-98	34
1909	Predicting Accurate Solvation Free Energy in n-Octanol Using 3D-RISM-KH Molecular Theory of Solvation: Making Right Choices. **2017**, 121, 9268-9273	18
1908	A Rising Star: Truxene as a Promising Hole Transport Material in Perovskite Solar Cells. **2017**, 121, 21729-21739	23

1907	In silico studies of solvated F19W amyloid β(11–40) trimer. **2017**, 7, 42379-42386	13
1906	Simulation of Reversible Protein-Protein Binding and Calculation of Binding Free Energies Using Perturbed Distance Restraints. **2017**, 13, 5697-5708	20
1905	Effects of Coarse Graining and Saturation of Hydrocarbon Chains on Structure and Dynamics of Simulated Lipid Molecules. **2017**, 7, 11476	11
1904	Fv-clasp: An Artificially Designed Small Antibody Fragment with Improved Production Compatibility, Stability, and Crystallizability. **2017**, 25, 1611-1622.e4	14
1903	Alamandine reverses hyperhomocysteinemia-induced vascular dysfunction via PKA-dependent mechanisms. **2017**, 35, e12306	20
1902	Crystal structure of a novel prolidase from Deinococcus radiodurans identifies new subfamily of bacterial prolidases. **2017**, 85, 2239-2251	2
1901	An iterative compound screening contest method for identifying target protein inhibitors using the tyrosine-protein kinase Yes. **2017**, 7, 12038	18
1900	Enhancing doping efficiency by improving host-dopant miscibility for fullerene-based n-type thermoelectrics. **2017**, 5, 21234-21241	56
1899	Brazilin inhibits fibrillogenesis of human islet amyloid polypeptide, disassembles mature fibrils, and alleviates cytotoxicity. **2017**, 7, 43491-43501	25
1898	Thermodynamics of camphor migration in cytochrome P450cam by atomistic simulations. **2017**, 7, 7736	9
1897	Genetic determinants restricting the reassortment of heterologous NSP2 genes into the simian rotavirus SA11 genome. **2017**, 7, 9301	8
1896	Dynamic and Kinetic Elements of μ-Opioid Receptor Functional Selectivity. **2017**, 7, 11255	29
1895	Pipelining Computation and Optimization Strategies for Scaling GROMACS on the Sunway Many-Core Processor. **2017**, 18-32	10
1894	Molecular Rationale behind the Differential Substrate Specificity of Bacterial RND Multi-Drug Transporters. **2017**, 7, 8075	43
1893	Sequential conformational transitions and α-helical supercoiling regulate a sensor histidine kinase. **2017**, 8, 284	39
1892	Wormlike Surfactant Micelles with Embedded Polymer Chains. **2017**, 50, 7299-7308	17
1891	On the Calculation of Acyl Chain Order Parameters from Lipid Simulations. **2017**, 13, 5683-5696	49
1890	The influence of solid scaffolds on flat and curved lipid membranes. **2017**, 7, 075007	3

1889	The correspondence between the conformational and chromophoric properties of amorphous conjugated polymers in mesoscale condensed systems. **2017**, 19, 20818-20828	5
1888	Character of Localization and Microenvironment of Solvatochromic Reichardt's Betaine Dye in Sodium n-Dodecyl Sulfate and Cetyltrimethylammonium Bromide Micelles: Molecular Dynamics Simulation Study. **2017**, 33, 8342-8352	14
1887	Molecular dynamics simulations of T-2410 and T-2429 HIV fusion inhibitors interacting with model membranes: Insight into peptide behavior, structure and dynamics. **2017**, 228, 69-80	2
1886	High-Throughput Automated Preparation and Simulation of Membrane Proteins with HTMD. **2017**, 13, 4003-4011	19
1885	Neutron total cross-section of hydrogenous and deuterated 1- and 2-propanol and n-butanol measured using the VESUVIO spectrometer. **2017**, 870, 84-89	17
1884	Role of Dispersive Fluorous Interaction in the Solvation Dynamics of the Perfluoro Group Containing Molecules. **2017**, 121, 7681-7688	7
1883	Membrane Binding of Recoverin: From Mechanistic Understanding to Biological Functionality. **2017** , 3, 868-874	12
1882	Role of the disulfide bond in stabilizing and folding of the fimbrial protein DraE from uropathogenic. **2017**, 292, 16136-16149	7
1881	Molecular Dynamics Simulation and Density Functional Theory Study of Chemisorption of Propranolol Optical Isomers on a Uracil-modified Carbon Paste Electrode. **2017**, 64, 1058-1064	3
1880	The properties of residual water molecules in ionic liquids: a comparison between direct and inverse Kirkwood-Buff approaches. **2017**, 19, 18924-18937	28
1879	Bacterial communication systems: A mathematical formulation of negative chemotaxis. **2017**, 30, e3365	1
1878	The impact of methylphenidate and its enantiomers on dopamine synthesis and metabolism in vitro. **2017**, 79, 281-288	9
1877	Solute Partitioning in Micelles: Combining Molecular Dynamics Simulations, COSMOmic, and Experiments. **2017**, 121, 5794-5809	24
1876	Insights into the Giardia intestinalis enolase and human plasminogen interaction. **2017**, 13, 2015-2023	4
1875	Homology model of the human tRNA splicing ligase RtcB. **2017**, 85, 1983-1993	9
1874	Characterization of SNPs in the dopamine-β-hydroxylase gene providing new insights into its structure-function relationship. **2017**, 18, 155-168	7
1873	An unusual cysteine V87 affects the antibody fragment conformations without interfering with the disulfide bond formation. **2017**, 90, 143-149	0
1872	PyRETIS: A well-done, medium-sized python library for rare events. **2017**, 38, 2439-2451	22

1871	A polar SxxS motif drives assembly of the transmembrane domains of Toll-like receptor 4. **2017**, 1859, 2086-2095	8
1870	Identification of Phosphorylation Codes for Arrestin Recruitment by G Protein-Coupled Receptors. **2017**, 170, 457-469.e13	225
1869	All-Atom MD Simulation of DNA Condensation Using Ab Initio Derived Force Field Parameters of Cobalt(III)-Hexammine. **2017**, 121, 7761-7770	10
1868	N-Terminal Acetylation Preserves Synuclein from Oligomerization by Blocking Intermolecular Hydrogen Bonds. **2017**, 8, 2145-2151	34
1867	Biomolecular conformational changes and ligand binding: from kinetics to thermodynamics. **2017**, 8, 6466-6473	36
1866	Simulation of Ligand Binding to Membrane Proteins. **2017**, 1635, 359-381	3
1865	One amino acid makes a difference-Characterization of a new TPMT allele and the influence of SAM on TPMT stability. **2017**, 7, 46428	12
1864	Connecting Structural and Transport Properties of Ionic Liquids with Cationic Oligoether Chains. **2017**, 164, H5247-H5262	17
1863	Atomistic insight into the role of amine groups in thermoresponsive poly(2-dialkylaminoethyl methacrylate)s. **2017**, 124, 219-225	7
1862	Theoretical Design of Highly Efficient CO2/N2 Separation Membranes Based on Electric Quadrupole Distinction. **2017**, 121, 17925-17931	14
1861	Calcium-Mediated Control of S100 Proteins: Allosteric Communication via an Agitator/Signal Blocking Mechanism. **2017**, 139, 11460-11470	10
1860	Site of Tagging Influences the Ochratoxin Recognition by Peptide NFO4: A Molecular Dynamics Study. **2017**, 57, 2035-2044	3
1859	Polarizable Embedding Approach for the Analytical Calculation of Raman and Raman Optical Activity Spectra of Solvated Systems. **2017**, 13, 4421-4435	32
1858	TFSI and TDI Anions: Probes for Solvate Ionic Liquid and Disproportionation-Based Lithium Battery Electrolytes. **2017**, 8, 3678-3682	16
1857	Into the Dynamics of a Supramolecular Polymer at Submolecular Resolution. **2017**, 8, 147	74
1856	Characterization of HIV-1 integrase interaction with human Ku70 protein and initial implications for drug targeting. **2017**, 7, 5649	10
1855	Interaction of hydrophobic polymers with model lipid bilayers. **2017**, 7, 6357	40
1854	Mean Activity Coefficients of NaCl in the Mixture of 2-Hydroxyethylammonium Butyrate + H2O at 298.15 K. **2017**, 62, 2384-2391	1

1853	Glutamate Water Gates in the Ion Binding Pocket of Na Bound Na, K-ATPase. **2017**, 7, 39829		7
1852	Interaction-component analysis of the effects of urea and its alkylated derivatives on the structure of T4-lysozyme. **2017**, 146, 225103		8
1851	Diblock copolymer bilayers as model for polymersomes: A coarse grain approach. **2017**, 146, 244904		9
1850	Effect of NaeI-L43K mutation on protein dynamics and DNA conformation: Insights from molecular dynamics simulations. **2017**, 76, 456-465		
1849	Molecular dynamics study of unfolding of lysozyme in water and its mixtures with dimethyl sulfoxide. **2017**, 76, 466-474		2
1848	A comparison of classical interatomic potentials applied to highly concentrated aqueous lithium chloride solutions. **2017**, 242, 845-858		19
1847	Particle-based and meshless methods with Aboria. *SoftwareX*, **2017**, 6, 172-178	2.7	9
1846	CHARMM-GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. **2017**, 38, 2354-2363		77
1845	Molecular Dynamics Simulations on Gas-Phase Proteins with Mobile Protons: Inclusion of All-Atom Charge Solvation. **2017**, 121, 8102-8112		20
1844	Structure of the Francisella response regulator QseB receiver domain, and characterization of QseB inhibition by antibiofilm 2-aminoimidazole-based compounds. **2017**, 106, 223-235		14
1843	Exciton Binding Energy in Molecular Triads. **2017**, 121, 17088-17095		31
1842	Identification of Key Interactions in the Initial Self-Assembly of Amylin in a Membrane Environment. **2017**, 56, 4884-4894		19
1841	Overcoming the Limitations of the MARTINI Force Field in Simulations of Polysaccharides. **2017**, 13, 5039-5053		47
1840	Coarse-Grained Directed Simulation. **2017**, 13, 4593-4603		10
1839	ms2: A molecular simulation tool for thermodynamic properties, release 3.0. **2017**, 221, 343-351		53
1838	Modeling of the Passive Permeation of Mercury and Methylmercury Complexes Through a Bacterial Cytoplasmic Membrane. **2017**, 51, 10595-10604		11
1837	Exploring Strategies for Labeling Viruses with Gold Nanoclusters through Non-equilibrium Molecular Dynamics Simulations. **2017**, 28, 2327-2339		6
1836	A comprehensive study of the complexation of alkali metal cations by lower rim calix[4]arene amide derivatives. **2017**, 19, 24316-24329		8

1835	Molecular Structuring and Phase Transition of Lipid-Based Formulations upon Water Dispersion: A Coarse-Grained Molecular Dynamics Simulation Approach. **2017**, 14, 4145-4153	13
1834	Structure, Dynamics, and Electron Transfer of Azurin Bound to a Gold Electrode. **2017**, 33, 9190-9200	5
1833	Modeling DMPC lipid membranes with SIRAH force-field. **2017**, 23, 259	17
1832	Message dissemination dynamics in biological communication systems: A reaction-diffusion approach. **2017**,	
1831	Statistical Analysis on the Performance of Molecular Mechanics Poisson-Boltzmann Surface Area versus Absolute Binding Free Energy Calculations: Bromodomains as a Case Study. **2017**, 57, 2203-2221	69
1830	Mapping Putative B-Cell Zika Virus NS1 Epitopes Provides Molecular Basis for Anti-NS1 Antibody Discrimination between Zika and Dengue Viruses. **2017**, 2, 3913-3920	24
1829	Glycan Reader is improved to recognize most sugar types and chemical modifications in the Protein Data Bank. **2017**, 33, 3051-3057	59
1828	Molecular Structure Inhibiting Synergism in Charged Surfactant Mixtures: An Atomistic Molecular Dynamics Simulation Study. **2017**, 33, 14093-14104	8
1827	Virtual screening for inhibitors of the human TSLP:TSLPR interaction. **2017**, 7, 17211	6
1826	Comprehensive computational design of ordered peptide macrocycles. **2017**, 358, 1461-1466	96
1825	Identification of Two New Cholesterol Interaction Sites on the A Adenosine Receptor. **2017**, 113, 2415-2424	49
1824	Modulation of the Neisseria gonorrhoeae drug efflux conduit MtrE. **2017**, 7, 17091	0
1823	Topologically frustrated ionisation in a water-ammonia ice mixture. **2017**, 8, 1065	13
1822	Prediction of New Stabilizing Mutations Based on Mechanistic Insights from Markov State Models. **2017**, 3, 1311-1321	36
1821	Focused conformational sampling in proteins. **2017**, 147, 195102	5
1820	Osmosensing by the bacterial PhoQ/PhoP two-component system. **2017**, 114, E10792-E10798	49
1819	Poly[]catenanes: Synthesis of molecular interlocked chains. **2017**, 358, 1434-1439	123
1818	Modeling Halogen Bonds in Ionic Liquids: A Force Field for Imidazolium and Halo-Imidazolium Derivatives. **2017**, 13, 6167-6176	7

1817	Improved Solution-State Properties of Monoclonal Antibodies by Targeted Mutations. **2017**, 121, 10818-10827	15
1816	Structure-function relationships in ABCG2: insights from molecular dynamics simulations and molecular docking studies. **2017**, 7, 15534	39
1815	Evaluating Force-Field London Dispersion Coefficients Using the Exchange-Hole Dipole Moment Model. **2017**, 13, 6146-6157	29
1814	HyRes: a coarse-grained model for multi-scale enhanced sampling of disordered protein conformations. **2017**, 19, 32421-32432	13
1813	Parameterization of Palmitoylated Cysteine, Farnesylated Cysteine, Geranylgeranylated Cysteine, and Myristoylated Glycine for the Martini Force Field. **2017**, 121, 11132-11143	13
1812	Mechanism of Competitive Inhibition and Destabilization of Acidothermus cellulolyticus Endoglucanase 1 by Ionic Liquids. **2017**, 121, 10793-10803	19
1811	Comparison of RESP and IPolQ-Mod Partial Charges for Solvation Free Energy Calculations of Various Solute/Solvent Pairs. **2017**, 13, 6266-6274	12
1810	Neural Network Based Prediction of Conformational Free Energies - A New Route toward Coarse-Grained Simulation Models. **2017**, 13, 6213-6221	21
1809	Large-scale and long-term correlations in collective motions of atoms of liquid argon. Computer simulation. **2017**, 106, 290-294	8
1808	Interaction between Water and Alkali Metal Ions and Its Temperature Dependence Revealed by Oxygen K-Edge X-ray Absorption Spectroscopy. **2017**, 121, 10957-10964	31
1807	Dynamic Stabilization of the Ligand-Metal Interface in Atomically Precise Gold Nanoclusters Au and Au Protected by meta-Mercaptobenzoic Acid. **2017**, 11, 11872-11879	29
1806	A coarse-grained polarizable force field for the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate. **2017**, 29, 504004	14
1805	Computational modeling and in-vitro/in-silico correlation of phospholipid-based prodrugs for targeted drug delivery in inflammatory bowel disease. **2017**, 31, 1021-1028	10
1804	Organosolv-Water Cosolvent Phase Separation on Cellulose and its Influence on the Physical Deconstruction of Cellulose: A Molecular Dynamics Analysis. **2017**, 7, 14494	23
1803	Dynamic changes in binding interaction networks of sex steroids establish their non-classical effects. **2017**, 7, 14847	2
1802	Transferable coarse-grained model for perfluorosulfonic acid polymer membranes. **2017**, 147, 094904	18
1801	Guest Controlled Nonmonotonic Deep Cavity Cavitand Assembly State Switching. **2017**, 121, 10717-10725	10
1800	Temperature-Dependent Implicit-Solvent Model of Polyethylene Glycol in Aqueous Solution. **2017**, 13, 6317-6327	17

1799	Similar Active Sites and Mechanisms Do Not Lead to Cross-Promiscuity in Organophosphate Hydrolysis: Implications for Biotherapeutic Engineering. **2017**, 139, 17533-17546	20
1798	Ionic liquids with anions based on fluorosulfonyl derivatives: from asymmetrical substitutions to a consistent force field model. **2017**, 19, 29617-29624	32
1797	Revisiting OPLS Force Field Parameters for Ionic Liquid Simulations. **2017**, 13, 6131-6145	159
1796	Photoisomerization of methylthiirane radical cations in freonic matrices at 77 K. **2017**, 27, 479-481	2
1795	Characterization of Solubilizing Nanoaggregates Present in Different Versions of Simulated Intestinal Fluid. **2017**, 121, 10869-10881	33
1794	Inhibition of Amyloid Channels with a Drug Candidate wgx-50 Revealed by Molecular Dynamics Simulations. **2017**, 57, 2811-2821	22
1793	Interactions between Chloramphenicol, Carrier Polymers, and Bacteria-Implications for Designing Electrospun Drug Delivery Systems Countering Wound Infection. **2017**, 14, 4417-4430	32
1792	EGCG inhibits the oligomerization of amyloid beta (16-22) hexamer: Theoretical studies. **2017**, 76, 1-10	30
1791	Molecular Switches of Allosteric Modulation of the Metabotropic Glutamate 2 Receptor. **2017**, 25, 1153-1162.e4	54
1790	Cation solvation with quantum chemical effects modeled by a size-consistent multi-partitioning quantum mechanics/molecular mechanics method. **2017**, 19, 17985-17997	8
1789	Exploiting heterogeneity of communication channels for efficient GPU selection on multi-GPU nodes. **2017**, 68, 3-16	1
1788	Frutapin, a lectin from (breadfruit): cloning, expression and molecular insights. **2017**, 37,	5
1787	Why human anti-Gal-4Gal-4Glc natural antibodies do not recognize the trisaccharide on erythrocyte membrane? Molecular dynamics and immunochemical investigation. **2017**, 90, 87-97	6
1786	Chemical space guided discovery of antimicrobial bridged bicyclic peptides against and its biofilms. **2017**, 8, 6784-6798	35
1785	Short-Time Dynamics Reveals Tg Suppression in Simulated Polystyrene Thin Films. **2017**, 50, 5599-5610	36
1784	The tyrosine Y250 in Frizzled 4 defines a conserved motif important for structural integrity of the receptor and recruitment of Dishevelled. **2017**, 38, 85-96	13
1783	Crystal structures of agonist-bound human cannabinoid receptor CB. **2017**, 547, 468-471	270
1782	Activation of the Unfolded Protein Response by Lipid Bilayer Stress. **2017**, 67, 673-684.e8	169

1781	Analysis of shear viscosity and viscoelastic relaxation of liquid methanol based on molecular dynamics simulation and mode-coupling theory. **2017**, 146, 244506	15
1780	Acceleration of Semiempirical QM/MM Methods through Message Passage Interface (MPI), Hybrid MPI/Open Multiprocessing, and Self-Consistent Field Accelerator Implementations. **2017**, 13, 3525-3536	11
1779	Complex Formations between Surfactants and Polyelectrolytes of the Same Charge on a Water Surface. **2017**, 33, 7940-7946	16
1778	Modelling parallel overhead from simple run-time records. **2017**, 73, 4390-4406	4
1777	Is the acid/base catalytic residue mutation in β-d-mannosidase DtMan from Dictyoglomus thermophilum sufficient enough to provide thioglycoligase activity?. **2017**, 137, 190-196	10
1776	Importance and Nature of Short-Range Excitonic Interactions in Light Harvesting Complexes and Organic Semiconductors. **2017**, 13, 3754-3763	19
1775	Orthogonal Electric Field Measurements near the Green Fluorescent Protein Fluorophore through Stark Effect Spectroscopy and pK Shifts Provide a Unique Benchmark for Electrostatics Models. **2017**, 121, 6799-6812	9
1774	Nonzero Ideal Gas Contribution to the Surface Tension of Water. **2017**, 8, 2608-2612	11
1773	Prediction of new Hsp90 inhibitors based on 3,4-isoxazolediamide scaffold using QSAR study, molecular docking and molecular dynamic simulation. **2017**, 25, 17	11
1772	Multiple molecular dynamics simulations of human LOX-1 and Trp150Ala mutant reveal the structural determinants causing the full deactivation of the receptor. **2017**, 85, 1902-1912	1
1771	Regulation of the Equilibrium between Closed and Open Conformations of Annexin A2 by N-Terminal Phosphorylation and S100A4-Binding. **2017**, 25, 1195-1207.e5	31
1770	Crowding in Cellular Environments at an Atomistic Level from Computer Simulations. **2017**, 121, 8009-8025	89
1769	Guest–host systems containing anthraquinone dyes with multiple visible transitions giving positive and negative dichroic order parameters: an assessment of principal molecular axes and computational methods. **2017**, 1-17	1
1768	Fick's Law Model Revisited: A New Approach to Modeling Multiple Sources Message Dissemination in Bacterial Communication Nanosystems. **2017**, 3, 89-105	4
1767	Temperature dependence of protein-water interactions in a gated yeast aquaporin. **2017**, 7, 4016	8
1766	Solvation of para-hydroxybenzoic acid and its esters (methylparaben, propylparaben) in supercritical carbon dioxide. Computer simulation. **2017**, 120, 59-64	6
1765	Exploring the structure and stability of cholesterol dimer formation in multicomponent lipid bilayers. **2017**, 38, 1479-1488	17
1764	Computational Chemistry Methods for Nanoporous Materials. **2017**, 29, 199-212	54

1763	Super RLuc8: A novel engineered Renilla luciferase with a red-shifted spectrum and stable light emission. **2017**, 96, 60-66	12
1762	Overview of the SAMPL5 host-guest challenge: Are we doing better?. **2017**, 31, 1-19	116
1761	Multiresolution molecular mechanics: Implementation and efficiency. **2017**, 328, 27-45	7
1760	Structure of the SLC4 transporter Bor1p in an inward-facing conformation. **2017**, 26, 130-145	26
1759	A coarse-grained model for PCL: conformation, self-assembly of MePEG-b-PCL amphiphilic diblock copolymers. **2017**, 43, 92-101	11
1758	Multiple program/multiple data molecular dynamics method with multiple time step integrator for large biological systems. **2017**, 38, 1410-1418	4
1757	Computational design of model scaffold for anion recognition based on the 'C NN' motif. **2017**, 108, e22921	5
1756	Force Field Parametrization of Colloidal CdSe Nanocrystals Using an Adaptive Rate Monte Carlo Optimization Algorithm. **2017**, 13, 297-308	7
1755	Understanding protein domain-swapping using structure-based models of protein folding. **2017**, 128, 113-120	32
1754	Structural dynamics of Casein Kinase I (CKI) from malarial parasite Plasmodium falciparum (Isolate 3D7): Insights from theoretical modelling and molecular simulations. **2017**, 71, 154-166	32
1753	Influence of specific intermolecular interactions on the thermal and dielectric properties of bulk polymers: atomistic molecular dynamics simulations of Nylon 6. **2017**, 13, 474-485	18
1752	CHARMM-GUI 10 years for biomolecular modeling and simulation. **2017**, 38, 1114-1124	119
1751	Quantitative Characterization of the Binding and Unbinding of Millimolar Drug Fragments with Molecular Dynamics Simulations. **2017**, 13, 3372-3377	70
1750	Rational design of cholesterol oxidase for efficient bioresolution of cholestane skeleton substrates. **2017**, 7, 16375	7
1749	External Potential Modifies Friction of Molecular Solutes in Water. **2017**, 7,	32
1748	Atomistic computer simulations on multi-loaded PAMAM dendrimers: a comparison of amine- and hydroxyl-terminated dendrimers. **2017**, 31, 1097-1111	12
1747	Atomistic Insights into Structural Differences between E3 and E4 Isoforms of Apolipoprotein E. **2017**, 113, 2682-2694	9
1746	Extending pressure-matching to inhomogeneous systems via local-density potentials. **2017**, 147, 134111	38

1745	Ligandbook: an online repository for small and drug-like molecule force field parameters. **2017**, 33, 1747-1749	11
1744	Origin of the blueshift of water molecules at interfaces of hydrophilic cyclic compounds. **2017**, 3, e1701400	16
1743	Protein conformational flexibility modulates kinetics and thermodynamics of drug binding. **2017**, 8, 2276	101
1742	Predicting Critical Micelle Concentrations with Molecular Dynamics Simulations and COSMOmic. **2017**, 89, 1288-1296	10
1741	Computer simulations of alkali-acetate solutions: Accuracy of the forcefields in difference concentrations. **2017**, 147, 194102	7
1740	Molecular Simulations of Thermodynamic Properties for the System Cyclodextrin/Alcohol in Aqueous Solution. **2017**, 89, 1306-1314	8
1739	Evaluation of Sox2 binding affinities for distinct DNA patterns using steered molecular dynamics simulation. **2017**, 7, 1750-1767	12
1738	Addressing the challenges of standalone multi-core simulations in molecular dynamics. **2017**, 2,	
1737	Localization and Ordering of Lipids Around Aquaporin-0: Protein and Lipid Mobility Effects. **2017**, 8, 124	17
1736	Integrative View of the Diversity and Evolution of SWEET and SemiSWEET Sugar Transporters. **2017**, 8, 2178	33
1735	Investigating Ebola virus pathogenicity using molecular dynamics. **2017**, 18, 566	7
1734	Molecular Dynamic Simulation of Space and Earth-Grown Crystal Structures of Thermostable T1 Lipase Geobacillus zalihae Revealed a Better Structure. **2017**, 22,	14
1733	Alcohol Interactions with Lipid Bilayers. **2017**, 22,	21
1732	Coupling Form and Function: How the Oligomerisation Symmetry of the SAS-6 Protein Contributes to the Architecture of Centriole Organelles. **2017**, 9, 74	
1731	Evaluation of Ochratoxin Recognition by Peptides Using Explicit Solvent Molecular Dynamics. **2017**, 9,	6
1730	Can Inhibitors of Snake Venom Phospholipases A Lead to New Insights into Anti-Inflammatory Therapy in Humans? A Theoretical Study. **2017**, 9,	13
1729	Tacticity-Dependent Interchain Interactions of Poly(N-Isopropylacrylamide) in Water: Toward the Molecular Dynamics Simulation of a Thermoresponsive Microgel. **2017**, 3,	8
1728	Designing the Sniper: Improving Targeted Human Cytolytic Fusion Proteins for Anti-Cancer Therapy via Molecular Simulation. **2017**, 5,	7

1727	Bladder-cancer-associated mutations in activate peroxisome proliferator-activated receptors to drive urothelial proliferation. **2017**, 6,	37
1726	The First Extracellular Linker Is Important for Several Aspects of the Gating Mechanism of Human TRPA1 Channel. **2017**, 10, 16	13
1725	Controversial Effects of D-Amino Acid Oxidase Activator (DAOA)/G72 on D-Amino Acid Oxidase (DAO) Activity in Human Neuronal, Astrocyte and Kidney Cell Lines: The N-methyl D-aspartate (NMDA) Receptor Hypofunction Point of View. **2017**, 10, 342	4
1724	Stabilization and structural analysis of a membrane-associated hIAPP aggregation intermediate. **2017**, 6,	47
1723	His-FLAG Tag as a Fusion Partner of Glycosylated Human Interferon-Gamma and Its Mutant: Gain or Loss?. **2017**, 2017, 3018608	2
1722	Biophysical and Computational Studies of the vCCI:vMIP-II Complex. **2017**, 18,	0
1721	Rational design of DKK3 structure-based small peptides as antagonists of Wnt signaling pathway and in silico evaluation of their efficiency. **2017**, 12, e0172217	11
1720	Waterdock 2.0: Water placement prediction for Holo-structures with a pymol plugin. **2017**, 12, e0172743	24
1719	Study of structural stability and damaging effect on membrane for four A▯2 dimers. **2017**, 12, e0179147	3
1718	Docking analysis and the possibility of prediction efficacy for an anti-IL-13 biopharmaceutical treatment with tralokinumab and lebrikizumab for bronchial asthma. **2017**, 12, e0188407	7
1717	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. **2017**, 13, e1005659	686
1716	Water permeation through the internal water pathway in activated GPCR rhodopsin. **2017**, 12, e0176876	10
1715	Sequence dependency of canonical base pair opening in the DNA double helix. **2017**, 13, e1005463	21
1714	Concerted regulation of npc2 binding to endosomal/lysosomal membranes by bis(monoacylglycero)phosphate and sphingomyelin. **2017**, 13, e1005831	23
1713	Systematic exploration of multiple drug binding sites. **2017**, 9, 65	9
1712	Transferability of Polymer Chain Properties between Coarse-Grained and Atomistic Models of Natural Rubber Molecule Validated by Molecular Dynamics Simulations. **2017**, 901, 012096	2
1711	Coding considerations for standalone molecular dynamics simulations of atomistic structures. **2017**, 905, 012018	
1710	Cholesterol binding to a conserved site modulates the conformation, pharmacology, and transport kinetics of the human serotonin transporter. **2018**, 293, 3510-3523	33

1709	Intermolecular Interactions of Pyridine in Liquid Phase and Aqueous Solution Studied by Soft X-ray Absorption Spectroscopy. **2018**, 232, 705-722	18
1708	Increasing Polypropylene High Temperature Stability by Blending Polypropylene-Bonded Hindered Phenol Antioxidant. **2018**, 51, 1927-1936	41
1707	Structural principles that enable oligomeric small heat-shock protein paralogs to evolve distinct functions. **2018**, 359, 930-935	29
1706	Poly(sodium 4-styrenesulfonate) Stabilized Janus Nanosheets in Brine with Retained Amphiphilicity. **2018**, 34, 3694-3700	13
1705	Temperature-dependent phase behaviour of tetrahydrofuran–water alters solubilization of xylan to improve co-production of furfurals from lignocellulosic biomass. **2018**, 20, 1612-1620	27
1704	Surface chemical heterogeneity modulates silica surface hydration. **2018**, 115, 2890-2895	57
1703	Interpretation of cytochrome P450 monooxygenase kinetics by modeling of thermodynamic activity. **2018**, 183, 172-178	6
1702	Effect of CO2 on the Interfacial and Transport Properties of Water/Binary and Asphaltenic Oils: Insights from Molecular Dynamics. **2018**, 32, 5409-5417	28
1701	Bending Lipid Bilayers: A Closed-Form Collective Variable for Effective Free-Energy Landscapes in Quantitative Biology. **2018**, 14, 2240-2245	11
1700	In Silico Investigations of Calcium Phosphate Mineralization in Extracellular Vesicles. **2018**, 122, 3782-3789	6
1699	Temperature-Dependent Lipid Extraction from Membranes by Boron Nitride Nanosheets. **2018**, 12, 2764-2772	32
1698	Blood Proteins and Their Interactions with Nanoparticles Investigated Using Molecular Dynamics Simulations. **2018**, 5-19	
1697	Permeability and ammonia selectivity in aquaporin TIP2;1: linking structure to function. **2018**, 8, 2995	17
1696	Development of a Coarse-Grained Model of Collagen-Like Peptide (CLP) for Studies of CLP Triple Helix Melting. **2018**, 122, 1929-1939	22
1695	Simulations of CYP51A from Aspergillus fumigatus in a model bilayer provide insights into triazole drug resistance. **2018**, 56, 361-373	6
1694	Exploring the Viral Channel Kcv Function via Computation. **2018**, 251, 419-430	5
1693	Virtual Site OPLS Force Field for Imidazolium-Based Ionic Liquids. **2018**, 122, 2962-2974	30
1692	Solvent-enabled control of reactivity for liquid-phase reactions of biomass-derived compounds. **2018**, 1, 199-207	147

1691	Modifications to a common phosphorylation network provide individualized control in caspases. **2018**, 293, 5447-5461	16
1690	Facilitated Water Transport through Graphene Oxide Membranes Functionalized with Aquaporin-Mimicking Peptides. **2018**, 30, e1705944	33
1689	Polychlorinated Diphenylsulfides Activate Aryl Hydrocarbon Receptor 2 in Zebrafish Embryos: Potential Mechanism of Developmental Toxicity. **2018**, 52, 4402-4412	13
1688	On the distinct binding modes of expansin and carbohydrate-binding module proteins on crystalline and nanofibrous cellulose: implications for cellulose degradation by designer cellulosomes. **2018**, 20, 8278-8293	6
1687	Visualization of the collective vortex-like motions in liquid argon and water: Molecular dynamics simulation. **2018**, 148, 094508	12
1686	In Silico Measurement of Elastic Moduli of Nematic Liquid Crystals. **2018**, 120, 107801	14
1685	A type III complement factor D deficiency: Structural insights for inhibition of the alternative pathway. **2018**, 142, 311-314.e6	7
1684	Local chemistry of the surfactant's head groups determines protein stability in reverse micelles. **2018**, 20, 8515-8522	15
1683	Crown Ether Effects on the Location of Charge Carriers in Electrospray Droplets: Implications for the Mechanism of Protein Charging and Supercharging. **2018**, 90, 4126-4134	14
1682	Perturbations of Native Membrane Protein Structure in Alkyl Phosphocholine Detergents: A Critical Assessment of NMR and Biophysical Studies. **2018**, 118, 3559-3607	101
1681	Binding Modes of Ligands Using Enhanced Sampling (BLUES): Rapid Decorrelation of Ligand Binding Modes via Nonequilibrium Candidate Monte Carlo. **2018**, 122, 5579-5598	38
1680	Further Insight into the Interactions of the Cytotoxic Macrolides Laulimalide and Peloruside A with Their Common Binding Site. **2018**, 3, 1770-1782	7
1679	A molecular dynamics study of lithium-containing aprotic heterocyclic ionic liquid electrolytes. **2018** , 148, 193834	26
1678	Aspirin locally disrupts the liquid-ordered phase. **2018**, 5, 171710	4
1677	Molecular Dynamics Study of the Solution Structure, Clustering, and Diffusion of Four Aqueous Alkanolamines. **2018**, 122, 2769-2778	11
1676	Computer simulations of the catalytic mechanism of wild-type and mutant ╫phosphoglucomutase. **2018**, 16, 2060-2073	9
1675	Phylogenetic spread of sequence data affects fitness of SOD1 consensus enzymes: Insights from sequence statistics and structural analyses. **2018**, 86, 609-620	6
1674	Intra-molecular Charge Transfer and Electron Delocalization in Non-fullerene Organic Solar Cells. **2018**, 10, 10043-10052	20

1673	Weaker N-Terminal Interactions for the Protective over the Causative A Peptide Dimer Mutants. **2018**, 9, 1247-1253	13
1672	Glucovanillin: A potent inhibitor of lipase from Acinetobacter radioresistens. **2018**, 10, 126-133	1
1671	Targeting a Subpocket in Trypanosoma brucei Phosphodiesterase B1 (TbrPDEB1) Enables the Structure-Based Discovery of Selective Inhibitors with Trypanocidal Activity. **2018**, 61, 3870-3888	23
1670	Force and time-dependent self-assembly, disruption and recovery of supramolecular peptide amphiphile nanofibers. **2018**, 29, 285701	3
1669	dbSWEET: An Integrated Resource for SWEET Superfamily to Understand, Analyze and Predict the Function of Sugar Transporters in Prokaryotes and Eukaryotes. **2018**, 430, 2203-2211	6
1668	Structural and thermodynamic insights into 1,2-glucooligosaccharide capture by a solute-binding protein in. **2018**, 293, 8812-8828	14
1667	Ligand-Triggered Structural Changes in the M Muscarinic Acetylcholine Receptor. **2018**, 58, 1074-1082	4
1666	An antimicrobial bicyclic peptide from chemical space against multidrug resistant Gram-negative bacteria. **2018**, 54, 5130-5133	18
1665	Electrostatic interactions in soft particle systems: mesoscale simulations of ionic liquids. **2018**, 14, 4252-4267	17
1664	Simulation Study for Wild-Type and C101F Mutant of LIM2 Domain in FHL1. **2018**,	
1663	Relevance of Local Flexibility Near the Active Site for Enzymatic Catalysis: Biochemical Characterization and Engineering of Cellulase Cel5A From Bacillus agaradherans. **2018**, 13, e1700669	14
1662	Accurate Methyl Group Dynamics in Protein Simulations with AMBER Force Fields. **2018**, 122, 5038-5048	22
1661	Amyloid-Peptide Interactions with Amphiphilic Surfactants: Electrostatic and Hydrophobic Effects. **2018**, 9, 1680-1692	22
1660	A Stereochemically Driven Supramolecular Polymerisation. **2018**, 24, 8195-8204	9
1659	Folding a viral peptide in different membrane environments: pathway and sampling analyses. **2018**, 44, 195-209	5
1658	Influence of various force fields in estimating the binding affinity of acetylcholinesterase inhibitors using fast pulling of ligand scheme. **2018**, 701, 65-71	9
1657	Molecular dynamics analysis of the influence of Coulomb and van der Waals interactions on the work of adhesion at the solid-liquid interface. **2018**, 148, 134707	20
1656	Computational Design of High-Block Oligomers for Accessing 1 nm Domains. **2018**, 12, 4351-4361	18

1655	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. **2018**, 58, 993-1004	27
1654	A Four-Site Molecular Model for Simulations of Liquid Methanol and Water-Methanol Mixtures: MeOH-4P. **2018**, 14, 2526-2537	9
1653	Tracking the NGS revolution: managing life science research on shared high-performance computing clusters. **2018**, 7,	8
1652	Functional role of the core gap in the middle part of tropomyosin. **2018**, 285, 871-886	14
1651	subunit stabilises sodium channel Nav1.7 against mechanical stress. **2018**, 596, 2433-2445	7
1650	How to run molecular dynamics simulations on electrospray droplets and gas phase proteins: Basic guidelines and selected applications. **2018**, 144, 104-112	23
1649	Atomistic Elucidation of Sorption Processes in Hydrogen Evolution Reaction on a van der Waals Heterostructure. **2018**, 122, 10034-10041	13
1648	Thermodynamic compatibility between cyclodextrin supramolecular complexes and surfactant. **2018**, 544, 203-212	3
1647	Absolute Alchemical Free Energy Calculations for Ligand Binding: A Beginner's Guide. **2018**, 1762, 199-232	23
1646	Macroion-Solvent Interactions in Charged Droplets. **2018**, 122, 5239-5250	8
1645	Exploring conformational states and helical packings in the P2X receptor transmembrane domain by molecular dynamics simulation. **2018**, 44, 331-344	1
1644	Probabilistic analysis for identifying the driving force of protein folding. **2018**, 148, 125101	8
1643	Flexible Versus Rigid G-Quadruplex DNA Ligands: Synthesis of Two Series of Bis-indole Derivatives and Comparison of Their Interactions with G-Quadruplex DNA. **2018**, 24, 7926-7938	11
1642	Pharmacokinetic interaction of diosmetin and silibinin with other drugs: Inhibition of CYP2C9-mediated biotransformation and displacement from serum albumin. **2018**, 102, 912-921	22
1641	Cell penetrating peptide modulation of membrane biomechanics by Molecular dynamics. **2018**, 73, 137-144	29
1640	On the molecular origin of the cooperative coil-to-globule transition of poly(N-isopropylacrylamide) in water. **2018**, 20, 9997-10010	66
1639	Salt effects in surfactant-free microemulsions. **2018**, 148, 222818	7
1638	The O-GlcNAc Transferase Intellectual Disability Mutation L254F Distorts the TPR Helix. **2018**, 25, 513-518.e4	18

1637	Combined Experimental, Theoretical, and Molecular Simulation Approach for the Description of the Fluid-Phase Behavior of Hydrocarbon Mixtures within Shale Rocks. **2018**, 32, 5750-5762	33
1636	Sharing of Na+ by Three □COO□ Groups at Deprotonated Carboxyl-Terminated Self-Assembled Monolayer-Charged Aqueous Interface. **2018**, 122, 9111-9116	3
1635	Tuning the Stereoselectivity and Solvation Selectivity at Interfacial and Bulk Environments by Changing Solvent Polarity: Isomerization of Glyoxal in Different Solvent Environments. **2018**, 140, 5535-5543	17
1634	Elucidating the key role of fluorine in improving the charge mobility of electron acceptors for non-fullerene organic solar cells by multiscale simulations. **2018**, 6, 4912-4918	25
1633	Single molecule FRET investigation of pressure-driven unfolding of cold shock protein A. **2018**, 148, 123336	2
1632	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. **2018**, 57, 5475-5485	4
1631	Computational design and experimental characterization of a novel □common receptor inhibitory peptide. **2018**, 104, 1-6	2
1630	Identification of cisplatin-binding sites on the large cytoplasmic loop of the Na/K-ATPase. **2018**, 33, 701-706	6
1629	Biomolecular Simulations under Realistic Macroscopic Salt Conditions. **2018**, 122, 5466-5486	28
1628	DNP-Enhanced MAS NMR: A Tool to Snapshot Conformational Ensembles of □Synuclein in Different States. **2018**, 114, 1614-1623	25
1627	Force Field Benchmark of Amino Acids: I. Hydration and Diffusion in Different Water Models. **2018**, 58, 1037-1052	56
1626	A comparative computational study of coarse-grained and all-atom water models in shock Hugoniot states. **2018**, 148, 144504	8
1625	Adaptive enhanced sampling by force-biasing using neural networks. **2018**, 148, 134108	26
1624	Propafenone effects on the stable structures of A□6-22 system. **2018**, 696, 55-60	4
1623	Theoretical Analysis of Carrier Ion Diffusion in Superconcentrated Electrolyte Solutions for Sodium-Ion Batteries. **2018**, 122, 2600-2609	46
1622	Density functional theory calculations and molecular dynamics simulations of the adsorption of ellipticine anticancer drug on graphene oxide surface in aqueous medium as well as under controlled pH conditions. **2018**, 255, 269-278	44
1621	Molecular polydispersity improves prediction of asphaltene aggregation. **2018**, 256, 382-394	32
1620	Ge-based bipolar small molecular host for highly efficient blue OLEDs: multiscale simulation of charge transport. **2018**, 6, 6146-6152	18

1619	Simulating the β-secretase enzyme: Recent advances and future directions. **2018**, 147, 130-135	11
1618	Dual Role for DsbA in Attacking and Targeted Bacterial Cells during Type VI Secretion System-Mediated Competition. **2018**, 22, 774-785	15
1617	Binding of alpha-synuclein to partially oxidized glyceraldehyde-3-phosphate dehydrogenase induces subsequent inactivation of the enzyme. **2018**, 642, 10-22	16
1616	Unique Features of Metformin: A Combined Experimental, Theoretical, and Simulation Study of Its Structure, Dynamics, and Interaction Energetics with DNA Grooves. **2018**, 122, 2227-2242	25
1615	Characterization of Interactions between Curcumin and Different Types of Lipid Bilayers by Molecular Dynamics Simulation. **2018**, 122, 2341-2354	27
1614	Rationale and design of an inhibitor of RecA protein as an inhibitor of Acinetobacter baumannii. **2018**, 71, 522-534	17
1613	Structural analysis of zwitterionic liquids vs. homologous ionic liquids. **2018**, 148, 193807	18
1612	Deep insights into the mode of ATP-binding mechanism in Zebrafish cyclin-dependent protein kinase-like 1 (zCDKL1): A molecular dynamics approach. **2018**, 81, 175-183	16
1611	Dynamics of the Interaction of RecG Protein with Stalled Replication Forks. **2018**, 57, 1967-1976	15
1610	Coupled regulation by the juxtamembrane and sterile α-motif (SAM) linker is a hallmark of ephrin tyrosine kinase evolution. **2018**, 293, 5102-5116	13
1609	Peptoid Backbone Flexibilility Dictates Its Interaction with Water and Surfaces: A Molecular Dynamics Investigation. **2018**, 19, 1006-1015	16
1608	Dual functional dinuclear platinum complex with selective reactivity towards c-myc G-quadruplex. **2018**, 8, 767	6
1607	The Water-Alkane Interface at Various NaCl Salt Concentrations: A Molecular Dynamics Study of the Readily Available Force Fields. **2018**, 8, 352	43
1606	Fully Anisotropic Rotational Diffusion Tensor from Molecular Dynamics Simulations. **2018**, 122, 5630-5639	16
1605	Antifreeze Glycoproteins Bind Reversibly to Ice via Hydrophobic Groups. **2018**, 140, 4803-4811	81
1604	Structural basis of the molecular ruler mechanism of a bacterial glycosyltransferase. **2018**, 9, 445	17
1603	Rare Variants in Tissue Inhibitor of Metalloproteinase 2 as a Risk Factor for Schizophrenia: Evidence From Familial and Cohort Analysis. **2019**, 45, 256-263	9
1602	Note: Second osmotic virial coefficients of short alkanes and their alcohol counterparts in water as a function of temperature. **2018**, 148, 016101	1

1601	Lipids Shape the Electron Acceptor-Binding Site of the Peripheral Membrane Protein Dihydroorotate Dehydrogenase. **2018**, 25, 309-317.e4	13
1600	The Role of Supercritical/Dense CO2 Gas in Altering Aqueous/Oil Interfacial Properties: A Molecular Dynamics Study. **2018**, 32, 2095-2103	27
1599	Reconstruction of Atomistic Structures from Coarse-Grained Models for Protein-DNA Complexes. **2018**, 14, 1682-1694	14
1598	A computational study for rational HIV-1 non-nucleoside reverse transcriptase inhibitor selection and the discovery of novel allosteric pockets for inhibitor design. **2018**, 38,	12
1597	Versatile Click Cyanine Amino Acid Conjugates Showing One-Atom-Influenced Recognition of DNA/RNA Secondary Structure and Mitochondrial Localisation in Living Cells. **2018**, 2018, 1682-1692	15
1596	Effect of Dimethyl Sulfoxide on the Binding of 1-Adamantane Carboxylic Acid to □and □Cyclodextrins. **2018**, 3, 1014-1021	8
1595	Communication between the leaflets of asymmetric membranes revealed from coarse-grain molecular dynamics simulations. **2018**, 8, 1805	21
1594	Spin-state dependence of the structural and vibrational properties of solvated iron(ii) polypyridyl complexes from AIMD simulations: aqueous [Fe(bpy)]Cl, a case study. **2018**, 20, 6236-6253	16
1593	Molecular mechanism for inhibition of twinfilin by phosphoinositides. **2018**, 293, 4818-4829	9
1592	Two microcephaly-associated novel missense mutations in CASK specifically disrupt the CASK-neurexin interaction. **2018**, 137, 231-246	16
1591	Molecular dynamic simulations reveal structural insights into substrate and inhibitor binding modes and functionality of Ecto-Nucleoside Triphosphate Diphosphohydrolases. **2018**, 8, 2581	13
1590	Molecular Dynamics Simulations of Glancing Angle Deposition of Polymer Nanoparticles. **2018**, 391-404	
1589	Probing biological activity through structural modelling of ligand-receptor interactions of 2,4-disubstituted thiazole retinoids. **2018**, 26, 1560-1572	9
1588	Dissecting the Forces that Dominate Dimerization of the Nucleotide Binding Domains of ABCB1. **2018**, 114, 331-342	19
1587	PyContact: Rapid, Customizable, and Visual Analysis of Noncovalent Interactions in MD Simulations. **2018**, 114, 577-583	39
1586	Metadynamics Enhanced Markov Modeling of Protein Dynamics. **2018**, 122, 5508-5514	31
1585	Molecular details of spontaneous insertion and interaction of HCV non-structure 3 protease protein domain with PIP2-containing membrane. **2018**, 86, 423-433	1
1584	Computing Curvature Sensitivity of Biomolecules in Membranes by Simulated Buckling. **2018**, 14, 1643-1655	7

1583	The fold preference and thermodynamic stability of -synuclein fibrils is encoded in the non-amyloid- component region. **2018**, 20, 4502-4512	11
1582	Polarizable Empirical Force Field for Halogen-Containing Compounds Based on the Classical Drude Oscillator. **2018**, 14, 1083-1098	30
1581	Design Rules for Graphene and Carbon Nanotube Solvents and Dispersants. **2018**, 12, 1043-1049	12
1580	A GPU-Accelerated Parameter Interpolation Thermodynamic Integration Free Energy Method. **2018**, 14, 1564-1582	26
1579	A domain specific language for performance portable molecular dynamics algorithms. **2018**, 224, 119-135	4
1578	Capillary condensation and capillary pressure of methane in carbon nanopores: Molecular Dynamics simulations of nanoconfinement effects. **2018**, 459, 196-207	16
1577	Enhanced dissolution of ibuprofen using ionic liquids as catanionic hydrotropes. **2018**, 20, 2094-2103	43
1576	Molecular dynamics simulations of asymmetric heterodimers of HER1/HER2 complexes. **2017**, 24, 30	1
1575	Predicting experimental results for polyethylene by computer simulation. **2018**, 99, 298-331	27
1574	The generation and characterisation of neutralising antibodies against the Theiler's murine encephalomyelitis virus (TMEV) GDVII capsid reveals the potential binding site of the host cell co-receptor, heparan sulfate. **2018**, 244, 153-163	4
1573	Hydration of copper(II) amino acids complexes. **2018**, 39, 821-826	6
1572	In Silico Study of Recognition between A and A Fibril Surfaces: An N-Terminal Helical Recognition Motif and Its Implications for Inhibitor Design. **2018**, 9, 935-944	10
1571	Determining the composition of the vacuum-liquid interface in ionic-liquid mixtures. **2018**, 206, 497-522	14
1570	Coarse-Grained Molecular Dynamics Force-Field for Polyacrylamide in Infinite Dilution Derived from Iterative Boltzmann Inversion and MARTINI Force-Field. **2018**, 122, 1516-1524	11
1569	Validation and Comparison of Force Fields for Native Cyclodextrins in Aqueous Solution. **2018**, 122, 1608-1626	25
1568	Structural insights into K48-linked ubiquitin chain formation by the Pex4p-Pex22p complex. **2018**, 496, 562-567	4
1567	Molecular dynamics simulations on interaction between bacterial proteins: Implication on pathogenic activities. **2018**, 86, 370-378	3
1566	A specific amino acid residue in the catalytic site of dandelion polyphenol oxidases acts as 'selector' for substrate specificity. **2018**, 96, 151-164	7

1565	Intracellular Transfer of Na in an Active-State G-Protein-Coupled Receptor. **2018**, 26, 171-180.e2	54
1564	FIH Is an Oxygen Sensor in Ovarian Cancer for G9a/GLP-Driven Epigenetic Regulation of Metastasis-Related Genes. **2018**, 78, 1184-1199	30
1563	Synthesis of a poly(ester) dendritic ‡cyclodextrin derivative by "click" chemistry: Combining the best of two worlds for complexation enhancement. **2018**, 184, 20-29	12
1562	GADDLE Maps: General Algorithm for Discrete Object Deformations Based on Local Exchange Maps. **2018**, 14, 466-478	5
1561	Structural Origin of Shear Viscosity of Liquid Water. **2018**, 122, 1255-1260	4
1560	Selectivity of Glycine for Facets on Gold Nanoparticles. **2018**, 122, 3491-3499	9
1559	Dynamics of OmpF Trimer Formation in the Bacterial Outer Membrane of Escherichia coli. **2018**, 34, 5623-5634	11
1558	Solvation of alcohols in ionic liquids - understanding the effect of the anion and cation. **2018**, 20, 2536-2548	14
1557	Coarse-grained A-graft-B model of poly(lactic acid) for molecular dynamics simulations. **2018**, 56, 604-612	4
1556	The Interplay between Salt Association and the Dielectric Properties of Low Permittivity Electrolytes: The Case of LiPF6 and LiAsF6 in Dimethyl Carbonate. **2018**, 122, 1990-1994	32
1555	Solution structure of an ultra-stable single-chain insulin analog connects protein dynamics to a novel mechanism of receptor binding. **2018**, 293, 69-88	8
1554	Investigation of Multiple Resistance Mechanisms in Voriconazole-Resistant Aspergillus flavus Clinical Isolates from a Chest Hospital Surveillance in Delhi, India. **2018**, 62,	25
1553	Interfacial Adsorption of Neutral and Ionic Solutes in a Water Droplet. **2018**, 122, 3447-3453	9
1552	Normal mode analysis of Zika virus. **2018**, 72, 53-61	6
1551	A Computational Assay of Estrogen Receptor ‡Antagonists Reveals the Key Common Structural Traits of Drugs Effectively Fighting Refractory Breast Cancers. **2018**, 8, 649	44
1550	Insights into the binding of agonist and antagonist to TAS2R16 receptor: a molecular simulation study. **2018**, 44, 322-329	9
1549	High-Strength, Durable All-Silk Fibroin Hydrogels with Versatile Processability toward Multifunctional Applications. **2018**, 28, 1704757	89
1548	The importance of nuclear quantum effects in spectral line broadening of optical spectra and electrostatic properties in aromatic chromophores. **2018**, 148, 102331	18

1547	TensorCalculator: exploring the evolution of mechanical stress in the CCMV capsid. **2018**, 30, 044006	3
1546	Mechanism and Determinants of Amphipathic Helix-Containing Protein Targeting to Lipid Droplets. **2018**, 44, 73-86.e4	98
1545	The Mechanism by Which Luteolin Disrupts the Cytoplasmic Membrane of Methicillin-Resistant Staphylococcus aureus. **2018**, 122, 1427-1438	9
1544	Effect of Ceramide Tail Length on the Structure of Model Stratum Corneum Lipid Bilayers. **2018**, 114, 113-125	27
1543	Identification of Factors Promoting HBV Capsid Self-Assembly by Assembly-Promoting Antivirals. **2018**, 58, 328-337	9
1542	Widom line, dynamical crossover, and percolation transition of supercritical oxygen via molecular dynamics simulations. **2018**, 148, 014502	11
1541	CO Diffusion in Various Carbonated Beverages: A Molecular Dynamics Study. **2018**, 122, 1655-1661	9
1540	Enhancing Molecular n-Type Doping of Donor-Acceptor Copolymers by Tailoring Side Chains. **2018**, 30, 1704630	157
1539	Identification of potential inhibitors against nuclear Dam1 complex subunit Ask1 of Candida albicans using virtual screening and MD simulations. **2018**, 72, 33-44	7
1538	Structural design of intrinsically fluorescent oxysterols. **2018**, 212, 26-34	8
1537	RNA Structural Dynamics As Captured by Molecular Simulations: A Comprehensive Overview. **2018**, 118, 4177-4338	235
1536	Ab Initio Prediction of NMR Spin Relaxation Parameters from Molecular Dynamics Simulations. **2018**, 14, 1009-1019	18
1535	System-Size Dependence of Electrolyte Activity Coefficients in Molecular Simulations. **2018**, 122, 3330-3338	12
1534	Robust Prediction of Resistance to Trimethoprim in Staphylococcus aureus. **2018**, 25, 339-349.e4	16
1533	Low-Density Lipoproteins and Human Serum Albumin as Carriers of Squalenoylated Drugs: Insights from Molecular Simulations. **2018**, 15, 585-591	18
1532	Towards predicting the power conversion efficiencies of organic solar cells from donor and acceptor molecule structures. **2018**, 6, 3276-3287	11
1531	Intrinsic Conformational Preferences and Interactions in □Synuclein Fibrils: Insights from Molecular Dynamics Simulations. **2018**, 14, 3298-3310	18
1530	Performance evaluation of the zero-multipole summation method in modern molecular dynamics software. **2018**, 39, 1551-1560	3

1529	Co-precipitation molecules hemopexin and transferrin may be key molecules for fibrillogenesis in TTR V30M amyloidogenesis. **2018**, 27, 15-23	5
1528	Lipid tempering simulation of model biological membranes on parallel platforms. **2018**, 1860, 1480-1488	3
1527	Conformational dynamics in crystals reveal the molecular bases for D76N beta-2 microglobulin aggregation propensity. **2018**, 9, 1658	35
1526	Homology modelling, molecular docking, and molecular dynamics simulations reveal the inhibition of Leishmania donovani dihydrofolate reductase-thymidylate synthase enzyme by Withaferin-A. **2018**, 11, 246	14
1525	Insight into the Molecular Mechanisms of AuNP-Based Aptasensor for Colorimetric Detection: A Molecular Dynamics Approach. **2018**, 34, 6161-6169	31
1524	Interactions of HP1 Bound to H3K9me3 Dinucleosome by Molecular Simulations and Biochemical Assays. **2018**, 114, 2336-2351	15
1523	Oil from the fruits of Pterodon emarginatus Vog.: A traditional anti-inflammatory. Study combining in vivo and in silico. **2018**, 222, 107-120	14
1522	Refining Collective Coordinates and Improving Free Energy Representation in Variational Enhanced Sampling. **2018**, 14, 2889-2894	13
1521	Molecular dynamics simulations using the drude polarizable force field on GPUs with OpenMM: Implementation, validation, and benchmarks. **2018**, 39, 1682-1689	53
1520	Phosphatidylinositol-3,5-bisphosphate lipid-binding-induced activation of the human two-pore channel 2. **2018**, 75, 3803-3815	18
1519	Bowl-in-bowl complex formation with mixed sized calixarenes: adaptivity towards guest binding. **2018**, 54, 7131-7134	5
1518	CHARMM Drude Polarizable Force Field for Glycosidic Linkages Involving Pyranoses and Furanoses. **2018**, 14, 3132-3143	17
1517	A Direct, Quantitative Connection between Molecular Dynamics Simulations and Vibrational Probe Line Shapes. **2018**, 9, 2560-2567	20
1516	Structural basis for the activation of acid ceramidase. **2018**, 9, 1621	48
1515	Erythromycin leads to differential protein expression through differences in electrostatic and dispersion interactions with nascent proteins. **2018**, 8, 6460	2
1514	Protein Partitioning into Ordered Membrane Domains: Insights from Simulations. **2018**, 114, 1936-1944	32
1513	Study of dual encapsulation possibility of hydrophobic and hydrophilic drugs into a nanocarrier based on bio-polymer coated graphene oxide using density functional theory, molecular dynamics simulation and experimental methods. **2018**, 262, 204-217	26
1512	Analysis of the influence of simulation parameters on biomolecule-linked water networks. **2018**, 82, 117-128	1

1511	Effect of PDGF-B aptamer on PDGFRβ/PDGF-B interaction: Molecular dynamics study. **2018**, 82, 145-156	17
1510	Human skin barrier structure and function analyzed by cryo-EM and molecular dynamics simulation. **2018**, 203, 149-161	40
1509	Enhanced Monte Carlo Methods for Modeling Proteins Including Computation of Absolute Free Energies of Binding. **2018**, 14, 3279-3288	20
1508	Electroporation of Skin Stratum Corneum Lipid Bilayer and Molecular Mechanism of Drug Transport: A Molecular Dynamics Study. **2018**, 34, 5860-5870	19
1507	Phosphoethanolamine induces caspase-independent cell death by reducing the expression of C-RAF and inhibits tumor growth in human melanoma model. **2018**, 103, 18-28	3
1506	The ionized graphene oxide membranes for water-ethanol separation. **2018**, 136, 262-269	30
1505	Penetration of antimicrobial peptides in a lung surfactant model. **2018**, 167, 345-353	17
1504	Toward Improved Understanding of the Interactions between Poorly Soluble Drugs and Cellulose Nanofibers. **2018**, 34, 5464-5473	22
1503	Free energy study of HO, NO, SO, and O gas sorption by water droplets/slabs. **2018**, 148, 164706	9
1502	Chemical potentials of alkaline earth metal halide aqueous electrolytes and solubility of their hydrates by molecular simulation: Application to CaCl, antarcticite, and sinjarite. **2018**, 148, 222832	13
1501	Saturation of charge-induced water alignment at model membrane surfaces. **2018**, 4, eaap7415	57
1500	Effects of Hydrophilic Residues and Hydrophobic Length on Flip-Flop Promotion by Transmembrane Peptides. **2018**, 122, 4318-4324	10
1499	Molecular dynamics characterization of the SAMHD1 Aicardi-Goutières Arg145Gln mutant: structural determinants for the impaired tetramerization. **2018**, 32, 623-632	1
1498	CONAN: A Tool to Decode Dynamical Information from Molecular Interaction Maps. **2018**, 114, 1267-1273	36
1497	Adsorption of human serum albumin on functionalized single-walled carbon nanotubes reduced cytotoxicity. **2018**, 295, 64-72	16
1496	Calculation of excess free energy of molecular solids comprised of flexible molecules using Einstein molecule method. **2018**, 44, 781-788	5
1495	A three-way inter-molecular network accounts for the Ca^{2+}-induced functional modulation of the pore-forming Ca1.2 subunit. **2018**, 293, 7176-7188	5
1494	Accurate Binding of Sodium and Calcium to a POPC Bilayer by Effective Inclusion of Electronic Polarization. **2018**, 122, 4546-4557	56

1493	Anomalous cation diffusion in salt-doped confined bilayer ice. **2018**, 10, 8962-8968	12
1492	Reinforced dynamics for enhanced sampling in large atomic and molecular systems. **2018**, 148, 124113	29
1491	Catching TFSI: A Computational-Experimental Approach to Cyclodextrin-Based Host-Guest Systems as electrolytes for Li-Ion Batteries. **2018**, 11, 1942-1949	2
1490	Structural Transitions in Ceramide Cubic Phases during Formation of the Human Skin Barrier. **2018**, 114, 1116-1127	8
1489	E7 oncoprotein of human papillomavirus: Structural dynamics and inhibitor screening study. **2018**, 658, 159-177	20
1488	On the Calculation of SAXS Profiles of Folded and Intrinsically Disordered Proteins from Computer Simulations. **2018**, 430, 2521-2539	41
1487	Mechanism of Mg-Accompanied Product Release in Sugar Nucleotidyltransferases. **2018**, 26, 459-466.e3	5
1486	How the Dynamics of a Supramolecular Polymer Determines Its Dynamic Adaptivity and Stimuli-Responsiveness: Structure-Dynamics-Property Relationships From Coarse-Grained Simulations. **2018**, 122, 4169-4178	18
1485	Calcium Sensing by Recoverin: Effect of Protein Conformation on Ion Affinity. **2018**, 9, 1613-1619	11
1484	Crystal structure of undecaprenyl-pyrophosphate phosphatase and its role in peptidoglycan biosynthesis. **2018**, 9, 1078	31
1483	Photoinduced transport in an H64Q neuroglobin antidote for carbon monoxide poisoning. **2018**, 148, 115101	1
1482	Early Performance Evaluation of the Hybrid Cluster with Torus Interconnect Aimed at Molecular-Dynamics Simulations. **2018**, 327-336	9
1481	Interaction of N-terminal peptide analogues of the Na,K-ATPase with membranes. **2018**, 1860, 1282-1291	22
1480	Molecular dynamics and ligand docking of a hinge region variant of South African HIV-1 subtype C protease. **2018**, 82, 1-11	10
1479	Water-mediated conformational preselection mechanism in substrate binding cooperativity to protein kinase A. **2018**, 115, 3852-3857	11
1478	Network and structure based inference of functional single nucleotide polymorphisms associated with the TGF gene and its role in colorectal cancer (CRC). **2018**, 11, 131-142	1
1477	Online Optimization of Total Acceptance in Hamiltonian Replica Exchange Simulations. **2018**, 122, 5448-5457	6
1476	Carbapenems and Lipid Bilayers: Localization, Partitioning, and Energetics. **2018**, 4, 926-935	12

1475	A local instantaneous surface method for extracting membrane elastic moduli from simulation: Comparison with other strategies. **2018**, 514, 31-43	11
1474	Computational science and HPC education for graduate students: Paving the way to exascale. **2018**, 118, 157-165	8
1473	Designing Highly Thermostable Lysozyme-Copolymer Conjugates: Focus on Effect of Polymer Concentration. **2018**, 19, 1175-1188	6
1472	Extension of the GROMOS 56a6 Force Field for Charged, Protonated, and Esterified Uronates. **2018**, 122, 3696-3710	14
1471	Molecular Mechanism of Uptake of Cationic Photoantimicrobial Phthalocyanine across Bacterial Membranes Revealed by Molecular Dynamics Simulations. **2018**, 122, 3711-3722	22
1470	Sequence-dependent response of DNA to torsional stress: a potential biological regulation mechanism. **2018**, 46, 1684-1694	21
1469	Direct evidences for the groove binding of the Clomifene to double stranded DNA. **2018**, 114, 40-53	25
1468	Understanding Ion Pairing in High-Salt Concentration Electrolytes Using Classical Molecular Dynamics Simulations and Its Implications for Nonaqueous Li□2 Batteries. **2018**, 122, 8094-8101	14
1467	A lithium-oxygen battery with a long cycle life in an air-like atmosphere. **2018**, 555, 502-506	303
1466	Structures of monomeric and oligomeric forms of the perforin-like protein 1. **2018**, 4, eaaq0762	20
1465	Implementation of replica-exchange umbrella sampling in GAMESS. **2018**, 228, 152-162	7
1464	Can the Dielectric Constant of Fullerene Derivatives Be Enhanced by Side-Chain Manipulation? A Predictive First-Principles Computational Study. **2018**, 122, 3919-3926	15
1463	Lipid composition dictates serum stability of reconstituted high-density lipoproteins: implications for in vivo applications. **2018**, 10, 7420-7430	7
1462	Metastable Prepores in Tension-Free Lipid Bilayers. **2018**, 120, 128103	23
1461	Human skin barrier formation takes place via a cubic to lamellar lipid phase transition as analyzed by cryo-electron microscopy and EM-simulation. **2018**, 366, 139-151	16
1460	Polarization Effects in Binary [BMIM][BF]/1,2-Dichloroethane, Acetone, Acetonitrile, and Water Electrolytes. **2018**, 122, 4345-4355	23
1459	Dynamic coarse-graining fills the gap between atomistic simulations and experimental investigations of mechanical unfolding. **2018**, 148, 044109	4
1458	Binding free energy analysis of protein-protein docking model structures by evERdock. **2018**, 148, 105101	14

1457	Impact of hydration and temperature history on the structure and dynamics of lignin. **2018**, 20, 1602-1611	19
1456	Atomistic Mechanism of Large-Scale Conformational Transition in a Heterodimeric ABC Exporter. **2018**, 140, 4543-4551	28
1455	On the thickness of the double layer in ionic liquids. **2018**, 20, 10275-10285	27
1454	Simple data and workflow management with the signac framework. **2018**, 146, 220-229	62
1453	Solvent scaling scheme for studying solvent restructuring thermodynamics in solvation processes. **2018**, 270, 114-127	1
1452	Update 0.2 to Pysimm: A python package for simulation of molecular systems *SoftwareX*, **2018**, 7, 70-732.7	7
1451	Design of Polyphosphate Inhibitors: A Molecular Dynamics Investigation on Polyethylene Glycol-Linked Cationic Binding Groups. **2018**, 19, 1358-1367	7
1450	Analysis of mutations in pncA reveals non-overlapping patterns among various lineages of Mycobacterium tuberculosis. **2018**, 8, 4628	4
1449	Picosecond Solvation Dynamics in Nanoconfinement: Role of Water and Host-Guest Complexation. **2018**, 122, 3996-4005	7
1448	Crystal structure of the human 5-HT serotonin receptor bound to an inverse agonist. **2018**, 4, 12	40
1447	In silico high-throughput virtual screening and molecular dynamics simulation study to identify inhibitor for AdeABC efflux pump of Acinetobacter baumannii. **2018**, 36, 1182-1194	47
1446	3D-QSAR, molecular docking, and molecular dynamic simulations for prediction of new Hsp90 inhibitors based on isoxazole scaffold. **2018**, 36, 1463-1478	16
1445	Dynamics of fluoroquinolones induced resistance in DNA gyrase of Mycobacterium tuberculosis. **2018**, 36, 362-375	21
1444	Insight into the intermolecular recognition mechanism involved in complement component 4 activation through serine protease-trypsin. **2018**, 36, 575-589	5
1443	Scrutiny of the mechanism of small molecule inhibitor preventing conformational transition of amyloid-β monomer: insights from molecular dynamics simulations. **2018**, 36, 663-678	26
1442	Evaluation of phase state and rotational viscosity of fast response liquid crystals using a fully atomistic molecular dynamics. **2018**, 45, 129-135	1
1441	Molecular dynamics recipes for genome research. **2018**, 19, 853-862	14
1440	Interfacial structure and structural forces in mixtures of ionic liquid with a polar solvent. **2018**, 206, 427-442	33

1439	In silico identification of potential drug compound against Peroxisome proliferator-activated receptor-gamma by virtual screening and toxicity studies for the treatment of Diabetic Nephropathy. **2018**, 36, 1776-1787	8
1438	A study of comparative modelling, simulation and molecular dynamics of CXCR3 receptor with lipid bilayer. **2018**, 36, 2361-2372	4
1437	Insights into channel dysfunction from modelling and molecular dynamics simulations. **2018**, 132, 20-30	9
1436	Evidence of anomalous behavior of intermolecular interactions at low concentration of methanol in ethanol-methanol binary system. **2018**, 188, 301-310	7
1435	Essential slow degrees of freedom in protein-surface simulations: A metadynamics investigation. **2018**, 498, 274-281	22
1434	Relative binding affinity prediction of farnesoid X receptor in the D3R Grand Challenge 2 using FEP. **2018**, 32, 265-272	9
1433	Wild-type catalase peroxidase vs G279D mutant type: Molecular basis of Isoniazid drug resistance in Mycobacterium tuberculosis. **2018**, 641, 226-234	13
1432	Investigating the Role of Phosphorylation in the Binding of Silaffin Peptide R5 to Silica with Molecular Dynamics Simulations. **2018**, 34, 1199-1207	23
1431	Unveiling the Role of Macrodipolar Interactions in the Properties of Self-Assembled Supramolecular Materials. **2018**, 24, 2609-2617	7
1430	Optical backbone-sidechain charge transfer transitions in proteins sensitive to secondary structure and modifications. **2018**, 207, 115-135	8
1429	In-silico screening and experimental validation reveal L-Adrenaline as anti-biofilm molecule against biofilm-associated protein (Bap) producing Acinetobacter baumannii. **2018**, 107, 1242-1252	26
1428	Identifying novel small molecule antagonists for mLST8 protein using computational approaches. **2018**, 38, 1-11	6
1427	Role of pncA gene mutations W68R and W68G in pyrazinamide resistance. **2018**, 119, 2567-2578	26
1426	Synthesis of graphene-based amphiphilic Janus nanosheets via manipulation of hydrogen bonding. **2018**, 126, 105-110	27
1425	Connections between the Anomalous Volumetric Properties of Alcohols in Aqueous Solution and the Volume of Hydrophobic Association. **2018**, 122, 3242-3250	7
1424	Atomistic Model for Nearly Quantitative Simulations of Langmuir Monolayers. **2018**, 34, 2565-2572	33
1423	Modeling of BACE-1 Inhibitors as Anti-Alzheimer's Agents. **2018**, 177-206	
1422	Biophysical and computational characterization of vandetanib-lysozyme interaction. **2018**, 189, 485-494	12

1421	Triazavirine supramolecular complexes as modifiers of the peptide oligomeric structure. **2018**, 36, 2694-2698	5
1420	Automated analysis and benchmarking of GCMC simulation programs in application to gas adsorption. **2018**, 44, 309-321	16
1419	In silico and empirical approaches toward understanding the structural adaptation of the alkaline-stable lipase KV1 from Acinetobacter haemolyticus. **2018**, 36, 3077-3093	15
1418	Efficient potential of mean force calculation from multiscale simulations: Solute insertion in a lipid membrane. **2018**, 498, 282-287	14
1417	Recruitment of the amyloid precursor protein by β-secretase at the synaptic plasma membrane. **2018**, 498, 334-341	10
1416	Unfolding dynamics of small peptides biased by constant mechanical forces. **2018**, 3, 204-213	2
1415	Testing the limits of model membrane simulations-bilayer composition and pressure scaling. **2018**, 39, 387-396	10
1414	The role of caveolin-1 in lipid droplets and their biogenesis. **2018**, 211, 93-99	11
1413	Interaction of photosynthetic pigments with single-walled carbon nanotube (15, 15): a molecular dynamics study. **2018**, 24, 43-51	3
1412	Solvatochromic betaine dyes of different hydrophobicity in ionic surfactant micelles: Molecular dynamics modeling of location character. **2018**, 538, 583-592	3
1411	Stereoselective and domain-specific effects of ibuprofen on the thermal stability of human serum albumin. **2018**, 112, 122-131	25
1410	Metastable State during Melting and Solid-Solid Phase Transition of [CMim][NO] (n = 4-12) Ionic Liquids by Molecular Dynamics Simulation. **2018**, 122, 229-239	15
1409	BOCS: Bottom-up Open-source Coarse-graining Software. **2018**, 122, 3363-3377	30
1408	Functional role of an unusual tyrosine residue in the electron transfer chain of a prokaryotic (6-4) photolyase. **2018**, 9, 1259-1272	10
1407	Molecular dynamics insights into the structure, function, and substrate binding mechanism of mucin desulfating sulfatase of gut microbe Bacteroides fragilis. **2018**, 119, 3618-3631	9
1406	Conformational dynamics of human protein kinase CK2α and its effect on function and inhibition. **2018**, 86, 344-353	8
1405	Can any "non-specific charge modification within microtubule binding domains of Tau" be a prerequisite of the protein amyloid aggregation? An in vitro study on the 1N4R isoform. **2018**, 109, 188-204	6
1404	Crystal Structure of Cleaved Serp-1, a Myxomavirus-Derived Immune Modulating Serpin: Structural Design of Serpin Reactive Center Loop Peptides with Improved Therapeutic Function. **2018**, 57, 1096-1107	17

1403	Exciton states and optical properties of the CP26 photosynthetic protein. **2018**, 72, 105-112	1
1402	Structural Insights into the Thermophilic Adaption Mechanism of Endo-1,4-β-Xylanase from Caldicellulosiruptor owensensis. **2018**, 66, 187-193	18
1401	Investigating Small-Molecule Ligand Binding to G Protein-Coupled Receptors with Biased or Unbiased Molecular Dynamics Simulations. **2018**, 1705, 351-364	10
1400	GPCRs: What Can We Learn from Molecular Dynamics Simulations?. **2018**, 1705, 133-158	9
1399	On-the-Fly Computation of Frontal Orbitals in Density Matrix Expansions. **2018**, 14, 139-153	2
1398	Structure and interaction of Corynebacterium pseudotuberculosis cold shock protein A with Y-box single-stranded DNA fragment. **2018**, 285, 372-390	6
1397	Molecular docking studies of bioactive compounds from Annona muricata Linn as potential inhibitors for Bcl-2, Bcl-w and Mcl-1 antiapoptotic proteins. **2018**, 23, 27-40	27
1396	Clustering and percolation theory for continuum systems: Clusters with nonspecific bonds and a residence time in their definition. **2018**, 270, 128-137	0
1395	Binding of 12-Crown-4 with Alzheimer's Aβ0 and Aβ2 Monomers and Its Effect on Their Conformation: Insight from Molecular Dynamics Simulations. **2018**, 15, 289-299	18
1394	Lipidated Peptide Dendrimers Killing Multidrug-Resistant Bacteria. **2018**, 140, 423-432	66
1393	Thermodynamic and first-principles biomolecular simulations applied to synthetic biology: promoter and aptamer designs. **2018**, 3, 19-37	8
1392	New semicarbazones as gorge-spanning ligands of acetylcholinesterase and potential new drugs against Alzheimer's disease: Synthesis, molecular modeling, NMR, and biological evaluation. **2018**, 36, 4099-4113	15
1391	Reverse mapping method for complex polymer systems. **2018**, 39, 648-664	10
1390	Ionic liquid structure, dynamics, and electrosorption in carbon electrodes with bimodal pores and heterogeneous surfaces. **2018**, 129, 104-118	30
1389	Conserved Lipid and Small-Molecule Modulation of COQ8 Reveals Regulation of the Ancient Kinase-like UbiB Family. **2018**, 25, 154-165.e11	40
1388	Probing nano-patterned peptide self-organisation at the aqueous graphene interface. **2017**, 10, 302-311	17
1387	Band-like Charge Photogeneration at a Crystalline Organic Donor/Acceptor Interface. **2018**, 8, 1701494	19
1386	Multiscale molecular dynamics simulations of rotary motor proteins. **2018**, 10, 605-615	11

1385	Novel 2-(2-arylmethylthio-4-chloro-5-methylbenzenesulfonyl)-1-(1,3,5-triazin-2-ylamino)guanidine derivatives: Inhibition of human carbonic anhydrase cytosolic isozymes I and II and the transmembrane tumor-associated isozymes IX and XII, anticancer activity, and molecular modeling studies. **2018**, 143, 1931-1941	21
1384	Inference of Calmodulin's Ca-Dependent Free Energy Landscapes via Gaussian Mixture Model Validation. **2018**, 14, 63-71	10
1383	Pyranose ring puckering in aldopentoses, ketohexoses and deoxyaldohexoses. A molecular dynamics study. **2018**, 455, 62-70	10
1382	Computational Optimization of Electric Fields for Improving Catalysis of a Designed Kemp Eliminase. **2018**, 8, 219-227	38
1381	Design, synthesis, anti-inflammatory antitumor activities, molecular modeling and molecular dynamics simulations of potential naprosyn analogs as COX-1 and/or COX-2 inhibitors. **2018**, 76, 188-201	10
1380	Characterization of the ligand binding of PGRP-L in half-smooth tongue sole (Cynoglossus semilaevis) by molecular dynamics and free energy calculation. **2018**, 31, 93-99	2
1379	Molecular Determinants for Substrate Interactions with the Glycine Transporter GlyT2. **2018**, 9, 603-614	19
1378	Structure-Property Relationships in Cu -Binding Tetramolecular G-Quadruplex DNA. **2018**, 24, 2117-2125	17
1377	Exploring the bulk-phase structure of ionic liquid mixtures using small-angle neutron scattering. **2018**, 206, 265-289	28
1376	New insights into the molecular characteristics behind the function of Renilla luciferase. **2018**, 119, 1780-1790	6
1375	Structural basis for Cullins and RING component inhibition: Targeting E3 ubiquitin pathway conductors for cancer therapeutics. **2018**, 106, 532-543	10
1374	Characterization of HIV-2 Protease Structure by Studying Its Asymmetry at the Different Levels of Protein Description. **2018**, 10, 644	4
1373	Molecular dynamics study of binary POPC bilayers: molecular condensing effects on membrane structure and dynamics. **2018**, 1136, 012022	7
1372	Stirring The Cauldron: Redefining Computational Archival Science (CAS) For The Big Data Domain. **2018**,	1
1371	. **2018**,	6
1370	Molecular dynamics simulation of the surface tension of aqueous sodium chloride: from dilute to highly supersaturated solutions and molten salt. **2018**, 18, 17077-17086	18
1369	Molecular dynamics simulation of the follicle-stimulating hormone receptor. Understanding the conformational dynamics of receptor variants at positions N680 and D408 from in silico analysis. **2018**, 13, e0207526	4
1368	Functional Status of Neuronal Calcium Sensor-1 Is Modulated by Zinc Binding. **2018**, 11, 459	8

1367	Ice-binding site of surface-bound type III antifreeze protein partially decoupled from water. **2018**, 20, 26926-26933	14
1366	Influence of membrane lipid composition on the structure and activity of □secretase. **2018**, 20, 27294-27304	14
1365	Dynamics changes of CRISPR-Cas9 systems induced by high fidelity mutations. **2018**, 20, 27439-27448	8
1364	Coarse-grained molecular dynamics simulation of the interface behaviour and self-assembly of CTAB cationic surfactants. **2018**, 20, 26422-26430	24
1363	Nanoparticles based on lipidyl-□cyclodextrins: synthesis, characterization, and experimental and computational biophysical studies for encapsulation of atazanavir. **2018**, 42, 20171-20179	5
1362	Theoretical analyses on water cluster structures in polymer electrolyte membrane by using dissipative particle dynamics simulations with fragment molecular orbital based effective parameters.. **2018**, 8, 34582-34595	20
1361	Atomistic investigation of an Iowa Amyloid-□trimer in aqueous solution.. **2018**, 8, 41705-41712	7
1360	Effects of lipid composition on membrane permeation. **2018**, 14, 8496-8508	16
1359	Single-stranded DNA oligomer brush structure is dominated by intramolecular interactions mediated by the ion environment. **2018**, 14, 9675-9680	2
1358	Quantifying the influence of the ion cloud on SAXS profiles of charged proteins. **2018**, 20, 26351-26361	7
1357	Aggregation response of triglyceride hydrolysis products in cyclohexane and triolein. **2018**, 20, 27192-27204	5
1356	Incorporation of transuranium elements: coordination of Cm(iii) to human serum transferrin. **2018**, 47, 14612-14620	3
1355	Fullerenemalonates inhibit amyloid beta aggregation, and evaluation.. **2018**, 8, 39667-39677	10
1354	Clustering algorithms to analyze molecular dynamics simulation trajectories for complex chemical and biological systems□ **2018**, 31, 404-420	14
1353	Flux: Overcoming Scheduling Challenges for Exascale Workflows. **2018**,	5
1352	Combining Virtual Screening, Molecular Docking and Simulation studies towards the discovery of □secretase (BACE) inhibitors. **2018**,	1
1351	Comprehensive efficiency analysis of supercomputer resource usage based on system monitoring data. **2018**, 973, 012068	
1350	Cholinium-based Good's buffers ionic liquids as remarkable stabilizers and recyclable preservation media for recombinant small RNAs. **2018**, 6, 16645-16656	18

1349	Design of metalloproteins and novel protein folds using variational autoencoders. **2018**, 8, 16189	50
1348	Relationships between Molecular Structure, Interfacial Structure, and Dynamics of Ionic Liquids near Neutral and Charged Surfaces. **2018**, 122, 27462-27468	10
1347	The Antibody Light-Chain Linker Regulates Domain Orientation and Amyloidogenicity. **2018**, 430, 4925-4940	15
1346	The architecture of EGFR's basal complexes reveals autoinhibition mechanisms in dimers and oligomers. **2018**, 9, 4325	37
1345	NaRIBaSA Scripting Framework for Computational Modeling of Nanomaterials and Room Temperature Ionic Liquids in Bulk and Slab. **2018**, 6, 57	5
1344	Determination of Structural Ensembles of Proteins: Restraining vs Reweighting. **2018**, 14, 6632-6641	31
1343	Analysis of interleukin 23 and 7G10 interactions for computational design of lead antibodies against immune-mediated inflammatory diseases. **2018**, 38, 327-334	2
1342	Molecular Basis of Aquaporin-7 Permeability Regulation by pH. **2018**, 7,	24
1341	Probing inhibition mechanisms of adenosine deaminase by using molecular dynamics simulations. **2018**, 13, e0207234	6
1340	Aromatic Motifs Dictate Nanohelix Handedness of Tripeptides. **2018**, 12, 12305-12314	30
1339	Folding a small protein using harmonic linear discriminant analysis. **2018**, 149, 194113	20
1338	Physicochemical and Tribological Performance of Bi-Component Supramolecular Gel Lubricants. **2018**, 6, 1801391	8
1337	Exploring the Ligand Efficacy of Cannabinoid Receptor 1 (CB1) using Molecular Dynamics Simulations. **2018**, 8, 13787	21
1336	Calcium interactions with Cx26 hemmichannel: Spatial association between MD simulations biding sites and variant pathogenicity. **2018**, 77, 331-342	6
1335	Differential Stabilization of the Metal Ligand Complexes between Organic and Aqueous Phases Drives the Selectivity of Phosphoric Acid Ligands toward Heavier Rare Earth Elements. **2018**, 57, 17209-17217	4
1334	Characterization of Hydroxyproline-Containing Hairpin-Like Antimicrobial Peptide EcAMP1-Hyp from Barnyard Grass (L.) Seeds: Structural Identification and Comparative Analysis of Antifungal Activity. **2018**, 19,	6
1333	Towards a molecular basis of ubiquitin signaling: A dual-scale simulation study of ubiquitin dimers. **2018**, 14, e1006589	15
1332	Using virtual reality for drug discovery: a promising new outlet for novel leads. **2018**, 13, 1103-1114	8

1331	Molecular simulation and in vitro evaluation of chitosan nanoparticles as drug delivery systems for the controlled release of anticancer drug cytarabine against solid tumours. **2018**, 8, 493	12
1330	Humidity Exposure Enhances Microscopic Mobility in a Room-Temperature Ionic Liquid in MXene. **2018**, 122, 27561-27566	11
1329	Structural Basis of Membrane Protein Chaperoning through the Mitochondrial Intermembrane Space. **2018**, 175, 1365-1379.e25	59
1328	BUMPy: A Model-Independent Tool for Constructing Lipid Bilayers of Varying Curvature and Composition. **2018**, 14, 6642-6652	13
1327	Molecular dynamics simulations of nucleotide release from the circadian clock protein KaiC reveal atomic-resolution functional insights. **2018**, 115, E11475-E11484	14
1326	Fabrication and Characterization of Recombinant Silk-Elastin-Like-Protein (SELP) Fiber. **2018**, 18, e1800265	18
1325	A TLR4-derived non-cytotoxic, self-assembling peptide functions as a vaccine adjuvant in mice. **2018**, 293, 19874-19885	13
1324	Unravelling the Role of O-glycans in Influenza A Virus Infection. **2018**, 8, 16382	15
1323	Domain rearrangement and denaturation in Ebola virus protein VP40. **2018**, 8, 125129	7
1322	A Molecular Dynamics Study to Assess the Positive Ion Distribution and the Effects of Protonation on the N-terminus Region of a Xylanase. **2018**, 1144, 012011	
1321	Atomistic molecular dynamics simulation of grapheneisoprene nanocomposites. **2018**, 1144, 012074	2
1320	Hybrid Methods for Modeling Protein Structures Using Molecular Dynamics Simulations and Small-Angle X-Ray Scattering Data. **2018**, 1105, 237-258	6
1319	Characterizing early drug resistance-related events using geometric ensembles from HIV protease dynamics. **2018**, 8, 17938	13
1318	Structural Model of the mIgM B-Cell Receptor Transmembrane Domain From Self-Association Molecular Dynamics Simulations. **2018**, 9, 2947	8
1317	Identification of Proteins Differentially Expressed in the Striatum by Melatonin in a Middle Cerebral Artery Occlusion Rat Model-a Proteomic and Approach. **2018**, 12, 888	36
1316	Multilevel Lattice Boltzmann-Particle Dynamics simulations at the Physics-Biology interface. **2018**, 1136, 012013	1
1315	The C Terminus of the Ribosomal-Associated Protein LrtA Is an Intrinsically Disordered Oligomer. **2018**, 19,	1
1314	An N-terminal heterozygous missense CASK mutation is associated with microcephaly and bilateral retinal dystrophy plus optic nerve atrophy. **2019**, 179, 94-103	7

1313	Updating RoNBio molecular modelling system to support in silico investigation of AMP activity on membrane models. **2018**,	
1312	Simulation of Capture and Release Processes of Hydrogen by Hydroquinone Clathrate. **2018**, 3, 18771-18782	8
1311	A generalised Landau-Lifshitz fluctuating hydrodynamics model for concurrent simulations of liquids at atomistic and continuum resolution. **2018**, 149, 244101	5
1310	Improved general-purpose five-point model for water: TIP5P/2018. **2018**, 149, 224507	14
1309	Adevonin, a novel synthetic antimicrobial peptide designed from the Adenanthera pavonina trypsin inhibitor (ApTI) sequence. **2018**, 112, 438-447	4
1308	Predictive Power of Biomolecular Simulations. **2018**, 1-26	
1307	Modeling Ligand Target Binding with Enhanced Sampling Simulations. **2018**, 43-66	
1306	An efficient strategy to estimate thermodynamics and kinetics of G protein-coupled receptor activation using metadynamics and maximum caliber. **2018**, 149, 224101	19
1305	Assessing the Charge Transfer at the Cytochrome c553/Graphene Interface: A Multiscale Investigation. **2018**, 122, 29405-29413	7
1304	3D structure of the electric double layer of ionic liquid-alcohol mixtures at the electrochemical interface. **2018**, 20, 30412-30427	16
1303	Triple-Helix Conformation of a Polysaccharide Determined with Light Scattering, AFM, and Molecular Dynamics Simulation. **2018**, 51, 10150-10159	27
1302	Structure-function-guided exploration of the antimicrobial peptide polybia-CP identifies activity determinants and generates synthetic therapeutic candidates. **2018**, 1, 221	61
1301	Inhibitor binding mode and allosteric regulation of Na-glucose symporters. **2018**, 9, 5245	19
1300	Tuning the collapse transition of weakly charged polymers by ion-specific screening and adsorption. **2018**, 14, 9631-9642	16
1299	Combined molecular dynamics and neural network method for predicting protein antifreeze activity. **2018**, 115, 13252-13257	25
1298	Spatially Resolving the Condensing Effect of Cholesterol in Lipid Bilayers. **2018**, 115, 2179-2188	26
1297	Encoding and selecting coarse-grain mapping operators with hierarchical graphs. **2018**, 149, 134106	19
1296	Extended coarse-grained dipole model for polar liquids: Application to bulk and confined water. **2018**, 98,	10

1295	Molecular Modeling and In Vitro Studies of a Neutral Oxime as a Potential Reactivator for Acetylcholinesterase Inhibited by Paraoxon. **2018**, 23,	12
1294	Dynamic Description of the Catalytic Cycle of Malate Enzyme: Stereoselective Recognition of Substrate, Chemical Reaction, and Ligand Release. **2018**, 122, 12241-12250	4
1293	DNA Base Pair Mismatches Induce Structural Changes and Alter the Free-Energy Landscape of Base Flip. **2018**, 122, 12251-12259	12
1292	Translation-orientation coupling and Cox-Merz rule of liquid hexane. **2018**, 149, 204502	2
1291	High and low density patches in simulated liquid water. **2018**, 149, 204507	22
1290	Aggregation of Influenza A Virus Nuclear Export Protein. **2018**, 83, 1411-1421	2
1289	Distribution of mechanical stress in the Escherichia coli cell envelope. **2018**, 1860, 2566-2575	48
1288	Reproducibility of Free Energy Calculations across Different Molecular Simulation Software Packages. **2018**, 14, 5567-5582	53
1287	Hypertrophic cardiomyopathy disease results from disparate impairments of cardiac myosin function and auto-inhibition. **2018**, 9, 4019	52
1286	Simulations of the regulatory ACT domain of human phenylalanine hydroxylase (PAH) unveil its mechanism of phenylalanine binding. **2018**, 293, 19532-19543	9
1285	Peptide-Templated Synthesis of TiO Nanofibers with Tunable Photocatalytic Activity. **2018**, 24, 18123-18129	7
1284	Norbornane-based cationic antimicrobial peptidomimetics targeting the bacterial membrane. **2018**, 160, 9-22	12
1283	Interactions between the Molecular Components of the Cowpea Chlorotic Mottle Virus Investigated by Molecular Dynamics Simulations. **2018**, 122, 9490-9498	5
1282	Mechanistic basis for the evolution of chalcone synthase catalytic cysteine reactivity in land plants. **2018**, 293, 18601-18612	15
1281	Structural evidence for the roles of divalent cations in actin polymerization and activation of ATP hydrolysis. **2018**, 115, 10345-10350	9
1280	Mechanism of Ostwald Ripening in 2D Physisorbed Assemblies at Molecular Time and Length Scale by Molecular Dynamics Simulations. **2018**, 122, 24380-24385	3
1279	Crucial role of fragmented and isolated defects in persistent relaxation of deeply supercooled water. **2018**, 149, 124504	40
1278	Interaction of PCL based self-assembled nano-polymeric micelles with model lipid bilayers using coarse-grained molecular dynamics simulations. **2018**, 712, 1-6	9

1277	Structural and functional characterization for interaction of silver nanoparticles with ergostrol in Trichoderma harzianum. **2018**, 125, 318-324	7
1276	Solid-State Rechargeable Zn//NiCo and Zn–Air Batteries with Ultralong Lifetime and High Capacity: The Role of a Sodium Polyacrylate Hydrogel Electrolyte. **2018**, 8, 1802288	146
1275	Choice of Adaptive Sampling Strategy Impacts State Discovery, Transition Probabilities, and the Apparent Mechanism of Conformational Changes. **2018**, 14, 5459-5475	32
1274	Polymorphism in Simvastatin: Twinning, Disorder, and Enantiotropic Phase Transitions. **2018**, 15, 5349-5360	12
1273	Structures, intermolecular interactions, and chemical hardness of binary water-organic solvents: a molecular dynamics study. **2018**, 24, 292	2
1272	Insights into Noncovalent Binding Obtained from Molecular Dynamics Simulations. **2018**, 90, 1864-1875	8
1271	Ab Initio Molecular Dynamics Simulations of Ionic Liquids. **2018**, 95-122	3
1270	Identification of (4-(9H-fluoren-9-yl) piperazin-1-yl) methanone derivatives as falcipain 2 inhibitors active against Plasmodium falciparum cultures. **2018**, 1862, 2911-2923	4
1269	Probing the effect of membrane contents on transmembrane protein-protein interaction using solution NMR and computer simulations. **2018**, 1860, 2486-2498	2
1268	Random Mutagenesis Analysis of the Influenza A M2 Proton Channel Reveals Novel Resistance Mutants. **2018**, 57, 5957-5968	9
1267	Template-Guided Protein Structure Prediction and Refinement Using Optimized Folding Landscape Force Fields. **2018**, 14, 6102-6116	10
1266	Using Polymer Hydrogels for Glyphosate Sequestration from Aqueous Solutions: Molecular Theory Study of Adsorption to Polyallylamine Films. **2018**, 34, 12560-12568	5
1265	Self-Constraint Gel Lubricants with High Phase Transition Temperature. **2018**, 6, 15801-15810	7
1264	The evolution of multiple active site configurations in a designed enzyme. **2018**, 9, 3900	50
1263	Tfo belongs to HmuY-like family of proteins but differs in heme-binding properties. **2018**, 38,	11
1262	Molecular Modeling Studies on the Interactions of Aflatoxin B1 and Its Metabolites with Human Acetylcholinesterase. Part II: Interactions with the Catalytic Anionic Site (CAS). **2018**, 10,	3
1261	Insights into the Folding of Disulfide-Rich δ-Conotoxins. **2018**, 3, 12330-12340	9
1260	Designed peptide with a flexible central motif from ranatuerins adapts its conformation to bacterial membranes. **2018**, 1860, 2655-2668	3

1259	Advanced simulation techniques for the thermodynamic and kinetic characterization of biological systems. **2018**, 3, 1477531	20
1258	K1.2 channel-specific blocker from Mesobuthus eupeus scorpion venom: Structural basis of selectivity. **2018**, 143, 228-238	14
1257	Driving Conformational Transitions in the Feature Space of Autoencoder Neural Network. **2018**, 122, 23224-23229	5
1256	Substrate binding allosterically relieves autoinhibition of the pseudokinase TRIB1. **2018**, 11,	28
1255	Capturing Phase Behavior of Ternary Lipid Mixtures with a Refined Martini Coarse-Grained Force Field. **2018**, 14, 6050-6062	42
1254	Exhaustive Exploration of the Conformational Landscape of Small Cyclic Peptides Using a Robotics Approach. **2018**, 58, 2355-2368	9
1253	Automated Topology Builder Version 3.0: Prediction of Solvation Free Enthalpies in Water and Hexane. **2018**, 14, 5834-5845	174
1252	Stability and Structural Analysis of A6R Polypeptide Nanosheets: A Theoretical Study Using the Classical Molecular Dynamics Simulation. **2018**, 122, 24445-24453	12
1251	A hybrid of mPEG-b-PCL and G1-PEA dendrimer for enhancing delivery of antibiotics. **2018**, 290, 112-128	24
1250	Escaping Atom Types in Force Fields Using Direct Chemical Perception. **2018**, 14, 6076-6092	62
1249	Structural insights into the interaction of helicase and primase in. **2018**, 475, 3493-3509	5
1248	Mycobacterium tuberculosis serine/threonine protein kinases: structural information for the design of their specific ATP-competitive inhibitors. **2018**, 32, 1315-1336	12
1247	Small Molecule Thermochemistry: A Tool for Empirical Force Field Development. **2018**, 122, 8982-8988	14
1246	Loop Motion in Triosephosphate Isomerase Is Not a Simple Open and Shut Case. **2018**, 140, 15889-15903	36
1245	Adaptive coupling of a deep neural network potential to a classical force field. **2018**, 149, 154107	5
1244	Biotite: a unifying open source computational biology framework in Python. **2018**, 19, 346	19
1243	The Impact of Using Single Atomistic Long-Range Cutoff Schemes with the GROMOS 54A7 Force Field. **2018**, 14, 5823-5833	16
1242	Novelty of Lithium Salt Solution in Sulfone and Dimethyl Carbonate-Based Electrolytes for Lithium-Ion Batteries: A Classical Molecular Dynamics Simulation Study of Optimal Ion Diffusion. **2018**, 122, 26315-26325	14

1241	Structural and dynamic basis of substrate permissiveness in hydroxycinnamoyltransferase (HCT). **2018**, 14, e1006511	15
1240	Exploring NS3/4A, NS5A and NS5B proteins to design conserved subunit multi-epitope vaccine against HCV utilizing immunoinformatics approaches. **2018**, 8, 16107	57
1239	Role of Computational Methods in Going beyond X-ray Crystallography to Explore Protein Structure and Dynamics. **2018**, 19,	33
1238	Uptake dynamics in the Lactose permease (LacY) membrane protein transporter. **2018**, 8, 14324	4
1237	Exploring the PXR ligand binding mechanism with advanced Molecular Dynamics methods. **2018**, 8, 16207	17
1236	Azidohomoalanine: A Minimally Invasive, Versatile, and Sensitive Infrared Label in Proteins To Study Ligand Binding. **2018**, 122, 10118-10125	14
1235	Total Description of Intrinsic Amphiphile Aggregation: Calorimetry Study and Molecular Probing. **2018**, 34, 14448-14457	8
1234	Structural basis of neurosteroid anesthetic action on GABA receptors. **2018**, 9, 3972	38
1233	Storing Energy in Biodegradable Electrochemical Supercapacitors. **2018**, 3, 13869-13875	29
1232	The Energetic Viability of Δ1-Piperideine Dimerization in Lysine-derived Alkaloid Biosynthesis. **2018**, 8,	7
1231	Discovery of Novel, Drug-Like Ferroptosis Inhibitors with in Vivo Efficacy. **2018**, 61, 10126-10140	33
1230	Shear Viscosity Computed from the Finite-Size Effects of Self-Diffusivity in Equilibrium Molecular Dynamics. **2018**, 14, 5959-5968	24
1229	Intermolecular Voids in Lipid Bilayers in the Presence of Glycyrrhizic Acid. **2018**, 122, 9938-9946	11
1228	Use of pH Gradients in Responsive Polymer Hydrogels for the Separation and Localization of Proteins from Binary Mixtures. **2018**, 51, 8205-8216	12
1227	Application of molecular dynamics simulations to design a dual-purpose oligopeptide linker sequence for fusion proteins. **2018**, 24, 313	11
1226	Phospholipid-Cellulose Interactions: Insight from Atomistic Computer Simulations for Understanding the Impact of Cellulose-Based Materials on Plasma Membranes. **2018**, 122, 9973-9981	6
1225	Allosteric potentiation of a ligand-gated ion channel is mediated by access to a deep membrane-facing cavity. **2018**, 115, 10672-10677	14
1224	Pharmacophore modeling, docking and molecular dynamics to identify Leishmania major farnesyl pyrophosphate synthase inhibitors. **2018**, 24, 314	3

1223	Deciphering ophthalmic adaptive inhibitors targeting RON4 of Toxoplasma gondii: An integrative in silico approach. **2018**, 213, 82-93	5
1222	Breakdown of Linear Dielectric Theory for the Interaction between Hydrated Ions and Graphene. **2018**, 9, 6463-6468	22
1221	Characterization of dynamics and mechanism in the self-assembly of AOT reverse micelles. **2018**, 149, 144901	6
1220	Calcium binding of the antifungal protein PAF: Structure, dynamics and function aspects by NMR and MD simulations. **2018**, 13, e0204825	5
1219	TTClust: A Versatile Molecular Simulation Trajectory Clustering Program with Graphical Summaries. **2018**, 58, 2178-2182	48
1218	Patchy Particle Model of the Hierarchical Self-Assembly of π-Conjugated Optoelectronic Peptides. **2018**, 122, 10219-10236	11
1217	Methionine 170 is an Environmentally Sensitive Membrane Anchor in the Disordered HVR of K-Ras4B. **2018**, 122, 10086-10096	10
1216	Engineering a responsive DNA triple helix into an octahedral DNA nanostructure for a reversible opening/closing switching mechanism: a computational and experimental integrated study. **2018**, 46, 9951-9959	12
1215	Does α-Tocopherol Flip-Flop Help to Protect Membranes Against Oxidation?. **2018**, 122, 10362-10370	16
1214	Confirmation of Bioinformatics Predictions of the Structural Domains in Honeybee Silk. **2018**, 10,	3
1213	Cryo-EM reveals two distinct serotonin-bound conformations of full-length 5-HT receptor. **2018**, 563, 270-274	64
1212	Role of the Interaction Motif in Maintaining the Open Gate of an Open Sodium Channel. **2018**, 115, 1920-1930	5
1211	On the Applicability of Force Fields To Study the Aggregation of Amyloidogenic Peptides Using Molecular Dynamics Simulations. **2018**, 14, 6063-6075	51
1210	Evidence for a Partially Stalled γ-Rotor in F-ATPase from Hydrogen-Deuterium Exchange Experiments and Molecular Dynamics Simulations. **2018**, 140, 14860-14869	6
1209	A hypothetical molecular mechanism for TRPV1 activation that invokes rotation of an S6 asparagine. **2018**, 150, 1554-1566	21
1208	Increasing Molecular Dynamics Simulations Throughput by Virtualizing Remote GPUs with rCUDA. **2018**,	2
1207	Quantitative Measurement of Intrinsic GTP Hydrolysis for Carcinogenic Glutamine 61 Mutants in H-Ras. **2018**, 57, 6356-6366	15
1206	Facilitated and Non-Gaussian Diffusion of Cholesterol in Liquid Ordered Phase Bilayers Depends on the Flip-Flop and Spatial Arrangement of Cholesterol. **2018**, 9, 6529-6535	11

1205	Lysophosphatidic acid produced by autotaxin acts as an allosteric modulator of its catalytic efficiency. **2018**, 293, 14312-14327	19
1204	Lipid Architectonics for Superior Oral Bioavailability of Nelfinavir Mesylate: Comparative in vitro and in vivo Assessment. **2018**, 19, 3584-3598	8
1203	Larger VH (Hole Distribution Volume)/VM (Molecular Volume) Induced Higher Charge Mobility of Group IVA Element-Based Host Materials for Potentially Highly Efficient Blue OLEDs. **2018**, 122, 22273-22279	7
1202	Structural and dynamic characterization of human Wnt2-Fzd7 complex using computational approaches. **2018**, 24, 274	7
1201	The Dimer-of-Trimers Assembly Prevents Catalysis at the Transferase Site of Prokaryotic FAD Synthase. **2018**, 115, 988-995	10
1200	Optimal Hydrophobicity and Reorientation of Amphiphilic Peptides Translocating through Membrane. **2018**, 115, 1045-1054	16
1199	Folding and Lipid Composition Determine Membrane Interaction of the Disordered Protein COR15A. **2018**, 115, 968-980	14
1198	Differential Capacitance and Energetics of the Electrical Double Layer of Graphene Oxide Supercapacitors: Impact of the Oxidation Degree. **2018**, 122, 21824-21832	22
1197	A novel p.(Glu111Val) missense mutation in GUCA1A associated with cone-rod dystrophy leads to impaired calcium sensing and perturbed second messenger homeostasis in photoreceptors. **2018**, 27, 4204-4217	18
1196	50 million atoms scale molecular dynamics modelling on a single consumer graphics card. **2018**, 124, 66-72	6
1195	Molecular Dynamics Study on Wettability of Poly(vinylidene fluoride) Crystalline and Amorphous Surfaces. **2018**, 34, 12214-12223	14
1194	Structure of the mechanosensitive OSCA channels. **2018**, 25, 850-858	68
1193	Enzyme-like Click Catalysis by a Copper-Containing Single-Chain Nanoparticle. **2018**, 140, 13695-13702	57
1192	Branched pentapeptides as potent inhibitors of the vascular endothelial growth factor 165 binding to Neuropilin-1: Design, synthesis and biological activity. **2018**, 158, 453-462	17
1191	Narrowing the gap between experimental and computational determination of methyl group dynamics in proteins. **2018**, 20, 24577-24590	21
1190	Interaction of 2'R-ochratoxin A with Serum Albumins: Binding Site, Effects of Site Markers, Thermodynamics, Species Differences of Albumin-binding, and Influence of Albumin on Its Toxicity in MDCK Cells. **2018**, 10,	7
1189	Effect of late endosomal DOBMP lipid and traditional model lipids of electrophysiology on the anthrax toxin channel activity. **2018**, 1860, 2192-2203	4
1188	FIH permits NAA10 to catalyze the oxygen-dependent lysyl-acetylation of HIF-1□**2018**, 19, 364-374	12

1187	A Robust Proton Flux (pHlux) Assay for Studying the Function and Inhibition of the Influenza A M2 Proton Channel. **2018**, 57, 5949-5956	11
1186	Dynamics and Microstructures of Nicotine/Water Binary Mixtures near the Lower Critical Solution Temperature. **2018**, 122, 9538-9548	7
1185	Kirkwood-Buff-Derived Alcohol Parameters for Aqueous Carbohydrates and Their Application to Preferential Interaction Coefficient Calculations of Proteins. **2018**, 122, 9350-9360	11
1184	Tc toxin activation requires unfolding and refolding of a β-propeller. **2018**, 563, 209-213	24
1183	Modeling structure and excitation of biliverdin-binding domains in infrared fluorescent proteins. **2018**, 710, 59-63	12
1182	Identification and analyses of natural compounds as potential inhibitors of TRAF6-Basigin interactions in melanoma using structure-based virtual screening and molecular dynamics simulations. **2018**, 85, 281-293	2
1181	Molecular Dynamics Simulation for All. **2018**, 99, 1129-1143	502
1180	Molecular Insights into Human Hereditary Apolipoprotein A-I Amyloidosis Caused by the Glu34Lys Mutation. **2018**, 57, 5738-5747	6
1179	Free Energy and Dynamics of Water Droplet Coalescence. **2018**, 122, 22975-22984	12
1178	Predicting polymorphism in molecular crystals using orientational entropy. **2018**, 115, 10251-10256	36
1177	Etersalate prevents the formations of 6Aβ16-22 oligomer: An in silico study. **2018**, 13, e0204026	10
1176	Mechanics and nanovoid nucleation dynamics: effects of polar functionality in glassy polymer networks. **2018**, 14, 8895-8911	12
1175	Testing for physical validity in molecular simulations. **2018**, 13, e0202764	22
1174	Monolayer Crystal Structure of the Organic Semiconductor 7-Decyl-2-phenyl[1]benzothieno[3,2-b][1]benzothiophene. **2018**, 122, 22225-22231	10
1173	Cholesterol Flip-Flop Impacts Domain Registration in Plasma Membrane Models. **2018**, 9, 5527-5533	28
1172	Riemann metric approach to optimal sampling of multidimensional free-energy landscapes. **2018**, 98, 023312	10
1171	5D Entanglement in Star Polymer Dynamics. **2018**, 1, 1800078	2
1170	Salt Bridge in Aqueous Solution: Strong Structural Motifs but Weak Enthalpic Effect. **2018**, 8, 13626	29

1169	Multiple binding modes of a moderate ice-binding protein from a polar microalga. **2018**, 20, 25295-25303	7
1168	Insights into the role of electrostatics in temperature adaptation: a comparative study of psychrophilic, mesophilic, and thermophilic subtilisin-like serine proteases.. **2018**, 8, 29698-29713	12
1167	Biomolecular Simulations of Halogen Bonds with a GROMOS Force Field. **2018**, 14, 5383-5392	14
1166	HUWE1 E3 ligase promotes PINK1/PARKIN-independent mitophagy by regulating AMBRA1 activation via IKK□**2018**, 9, 3755	115
1165	Engineering the affinity of a family 11 carbohydrate binding module to improve binding of branched over unbranched polysaccharides. **2018**, 120, 2509-2516	16
1164	On the Stability of Proteins Solvated in Imidazolium-Based Ionic Liquids Studied with Replica Exchange Molecular Dynamics. **2018**, 122, 9274-9288	9
1163	Molecular Dynamics Simulations of Kir2.2 Interactions with an Ensemble of Cholesterol Molecules. **2018**, 115, 1264-1280	32
1162	Engineering of 3-ketosteroid-□dehydrogenase based site-directed saturation mutagenesis for efficient biotransformation of steroidal substrates. **2018**, 17, 141	12
1161	Adaptive Resolution Molecular Dynamics Technique. **2018**, 1-15	2
1160	Disulfide bridge formation to increase thermostability of DFPase enzyme: A computational study. **2018**, 77, 272-278	6
1159	The Sodium Sialic Acid Symporter From Has Altered Substrate Specificity. **2018**, 6, 233	13
1158	Can Arginine Inhibit Insulin Aggregation? A Combined Protein Crystallography, Capillary Electrophoresis, and Molecular Simulation Study. **2018**, 122, 10069-10076	21
1157	Identification of small molecule inhibitors of ALK2: a virtual screening, density functional theory, and molecular dynamics simulations study. **2018**, 24, 262	8
1156	Molecular dynamics modeling of Pseudomonas aeruginosa outer membranes. **2018**, 20, 23635-23648	16
1155	Influence of pH and Salts on Partial Molar Volume of Lysozyme and Bovine Serum Albumin in Aqueous Solutions. **2018**, 41, 2337-2345	
1154	COBRAMM 2.0 - A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. **2018**, 24, 271	29
1153	Nanoscale cavitation in perforation of cellular membrane by shock-wave induced nanobubble collapse. **2018**, 149, 074902	7
1152	Assessment and optimization of collective variables for protein conformational landscape: GB1 -hairpin as a case study. **2018**, 149, 094101	16

1151	Role of glutamine synthetase in angiogenesis beyond glutamine synthesis. **2018**, 561, 63-69	68
1150	A Martini coarse-grained model of the calcein fluorescent dye. **2018**, 51, 384002	6
1149	Monolayer and Bilayer Structures of Mixtures of Ceramide IIIb and c16-Alkyl Glucosides. **2018**, 39, 982-987	
1148	Boron nitride nanotubes as a nanotransporter for anti-cancer docetaxel drug in water/ethanol solution. **2018**, 271, 151-156	30
1147	Presence and Role of Midplane Cholesterol in Lipid Bilayers Containing Registered or Antiregistered Phase Domains. **2018**, 122, 8193-8200	27
1146	RNA as a Complex Polymer with Coupled Dynamics of Ions and Water in the Outer Solvation Sphere. **2018**, 122, 11218-11227	5
1145	K binding and proton redistribution in the EP state of the H, K-ATPase. **2018**, 8, 12732	5
1144	In silico stress-strain measurements on self-assembled protein lattices. **2018**, 14, 8095-8104	1
1143	Molecular simulation study of CYP2B6 polymorphism with and without psoralen. **2018**, 44, 1402-1410	
1142	. **2018**,	12
1141	Unified Code Generation for the Parallel Computation of Pairwise Interactions Using Partial Evaluation. **2018**,	1
1140	Building and deploying a cyberinfrastructure for the data-driven design of chemical systems and the exploration of chemical space. **2018**, 44, 921-929	22
1139	Influence of fluorinated extractant aggregation in diluent on extraction of salicylic acid: Evidence from equilibrium, SAXS and molecular dynamics simulation. **2018**, 66, 168-175	2
1138	Estradiol dimer inhibits tubulin polymerization and microtubule dynamics. **2018**, 183, 68-79	12
1137	Rotational Dynamics of Proteins from Spin Relaxation Times and Molecular Dynamics Simulations. **2018**, 122, 6559-6569	15
1136	Mechanisms of Aggregation-Induced Emission and Photo/Thermal E/Z Isomerization of a Cyanostilbene Derivative: Theoretical Insights. **2018**, 122, 12434-12440	27
1135	Cholesterol suppresses membrane leakage by decreasing water penetrability. **2018**, 14, 5277-5282	8
1134	Fluctuating hydrogen-bond networks govern anomalous electron transfer kinetics in a blue copper protein. **2018**, 115, 6129-6134	27

1133	gRINN: a tool for calculation of residue interaction energies and protein energy network analysis of molecular dynamics simulations. **2018**, 46, W554-W562	47
1132	Optimizing Antimicrobial Peptide Dendrimers in Chemical Space. **2018**, 130, 8619-8623	1
1131	Structural Stability of Peptidic His-Containing Proton Wire in Solution and in the Adsorbed State. **2018**, 34, 6997-7005	4
1130	Coarse-Grained Molecular Dynamics Simulation of Sulerythrin and LARFH for Producing Protein Nanofibers. **2018**,	
1129	Structure-activity relationships of ╫hairpin mimics as modulators of amyloid ╫peptide aggregation. **2018**, 154, 280-293	9
1128	A Thermodynamic Funnel Drives Bacterial Lipopolysaccharide Transfer in the TLR4 Pathway. **2018**, 26, 1151-1161.e4	21
1127	Exploring Cryptic Pockets Formation in Targets of Pharmaceutical Interest with SWISH. **2018**, 14, 3321-3331	24
1126	Aqueous Hydrogen Sulfide in Slit-Shaped Silica Nanopores: Confinement Effects on Solubility, Structural, and Dynamical Properties. **2018**, 122, 14744-14755	16
1125	Oxidized Nanocarbons-Tripeptide Supramolecular Hydrogels: Shape Matters!. **2018**, 12, 5530-5538	44
1124	Static structure of sodium polystyrene sulfonate solutions obtained through a coarse-grained model. **2018**, 116, 2244-2253	1
1123	Structural and enzymatic characterization of acetolactate decarboxylase from Bacillus subtilis. **2018**, 102, 6479-6491	9
1122	Effect of surfactants on the interaction of phenol with laccase: Molecular docking and molecular dynamics simulation studies. **2018**, 357, 10-18	44
1121	Effect of Salt on Antiagglomerant Surface Adsorption in Natural Gas Hydrates. **2018**, 122, 12839-12849	24
1120	Integrin ⍺4⍵7 switches its ligand specificity via distinct conformer-specific activation. **2018**, 217, 2799-2812	19
1119	Copper-redox cycling by coumarin-di(2-picolyl)amine hybrid molecule leads to ROS-mediated DNA damage and apoptosis: A mechanism for cancer chemoprevention. **2018**, 290, 64-76	14
1118	On the mechanism of spontaneous thiol-disulfide exchange in proteins. **2018**, 20, 16222-16230	12
1117	Redox-dependent control of i-Motif DNA structure using copper cations. **2018**, 46, 5886-5893	31
1116	Discovery of Highly Potent Pinanamine-Based Inhibitors against Amantadine- and Oseltamivir-Resistant Influenza A Viruses. **2018**, 61, 5187-5198	15

1115	Membrane potential and dynamics in a ternary lipid mixture: insights from molecular dynamics simulations. **2018**, 20, 15841-15851	6
1114	Molecular details of dimerization kinetics reveal negligible populations of transient μ-opioid receptor homodimers at physiological concentrations. **2018**, 8, 7705	26
1113	Consistent Prediction of Mutation Effect on Drug Binding in HIV-1 Protease Using Alchemical Calculations. **2018**, 14, 3397-3408	13
1112	Understanding the Role of Hydrophobic Terminal in the Hydrogen Bond Network of the Aqueous Mixture of 2,2,2-Trifluoroethanol: IR, Molecular Dynamics, Quantum Chemical as Well as Atoms in Molecules Studies. **2018**, 122, 6616-6626	4
1111	Contrasting Modes of Self-Assembly and Hydrogen-Bonding Heterogeneity in Chlorosomes of. **2018**, 122, 14877-14888	15
1110	Salvianolic acids from antithrombotic Traditional Chinese Medicine Danshen are antagonists of human P2Y and P2Y receptors. **2018**, 8, 8084	13
1109	Interactive structural analysis of TrCP1 and PER2 phosphoswitch binding through dynamics simulation assay. **2018**, 651, 34-42	5
1108	Comparative structural analysis of fruit and stem bromelain from Ananas comosus. **2018**, 266, 183-191	22
1107	Competitive Microstructures Versus Cooperative Dynamics of Hydrogen Bonding and Type Stacking Interactions in Imidazolium Bis(oxalato)borate Ionic Liquids. **2018**, 122, 6570-6585	17
1106	Using Intrinsic Surfaces To Calculate the Free-Energy Change When Nanoparticles Adsorb on Membranes. **2018**, 122, 6417-6422	6
1105	Morphology and ion diffusion in PEDOT:Tos. A coarse grained molecular dynamics simulation. **2018**, 20, 17188-17198	43
1104	Generalized Markov State Modeling Method for Nonequilibrium Biomolecular Dynamics: Exemplified on Amyloid Conformational Dynamics Driven by an Oscillating Electric Field. **2018**, 14, 3579-3594	10
1103	Optothermophoretic Manipulation of Colloidal Particles in Nonionic Liquids. **2018**, 122, 24226-24234	18
1102	Fast Approximate Evaluation of Parallel Overhead from a Minimal Set of Measured Execution Times. **2018**, 28, 1850003	0
1101	Impact of the ceramide subspecies on the nanostructure of stratum corneum lipids using neutron scattering and molecular dynamics simulations. Part I: impact of CER[NS]. **2018**, 214, 58-68	14
1100	Profilin Negatively Regulates Formin-Mediated Actin Assembly to Modulate PAMP-Triggered Plant Immunity. **2018**, 28, 1882-1895.e7	25
1099	The structure of aqueous lithium chloride solutions at high concentrations as revealed by a comparison of classical interatomic potential models. **2018**, 264, 179-197	19
1098	Faster Simulations with a 5 fs Time Step for Lipids in the CHARMM Force Field. **2018**, 14, 3342-3350	24

1097	Structural basis of actin monomer re-charging by cyclase-associated protein. **2018**, 9, 1892	37
1096	Optimizing Antimicrobial Peptide Dendrimers in Chemical Space. **2018**, 57, 8483-8487	32
1095	BET bromodomain ligands: Probing the WPF shelf to improve BRD4 bromodomain affinity and metabolic stability. **2018**, 26, 2937-2957	12
1094	Nitrobenzoxadiazole-Appended Cell Membrane Modifiers for Efficient Optoporation with Noncoherent Light. **2018**, 29, 2068-2073	4
1093	Prediction of Binding Energy of Keap1 Interaction Motifs in the Nrf2 Antioxidant Pathway and Design of Potential High-Affinity Peptides. **2018**, 122, 5851-5859	15
1092	Average and Local Tg Shifts of Plasticized PVC from Simulations. **2018**, 51, 3865-3873	12
1091	Insights into Magneto-Optics of Helical Conjugated Polymers. **2018**, 140, 6501-6508	53
1090	Elucidating the role of surface chemistry on cationic phosphorus dendrimer-siRNA complexation. **2018**, 10, 10952-10962	17
1089	The glycolipid GM1 reshapes asymmetric biomembranes and giant vesicles by curvature generation. **2018**, 115, 5756-5761	53
1088	Polymorphism in disease-related apolipoprotein C-II amyloid fibrils: a structural model for rod-like fibrils. **2018**, 285, 2799-2812	3
1087	Partial Intrinsic Disorder Governs the Dengue Capsid Protein Conformational Ensemble. **2018**, 13, 1621-1630	13
1086	Refined Alkali Metal Ion Parameters for the OPC Water Model. **2018**, 39, 931-935	
1085	The Role of Water in the Stability of Wild-type and Mutant Insulin Dimers. **2018**, 122, 7038-7048	15
1084	Transferable MARTINI Model of Poly(ethylene Oxide). **2018**, 122, 7436-7449	62
1083	Re-designing the □synuclein tetramer. **2018**, 54, 8080-8083	16
1082	Probing the early stages of prion protein (PrP) aggregation with atomistic molecular dynamics simulations. **2018**, 54, 8007-8010	9
1081	Coupled-perturbed DFTB-QM/MM metadynamics: Application to proton-coupled electron transfer. **2018**, 149, 072328	8
1080	A simulation method for the phase diagram of complex fluid mixtures. **2018**, 148, 244903	6

1079	RNA Environment Is Responsible for Decreased Photostability of Uracil. **2018**, 140, 8714-8720	15
1078	Unexpected Composition Dependence of the First Sharp Diffraction Peak in an Alcohol–Aldehyde Liquid Mixture: n-Pentanol and Pentanal. **2018**, 255, 1800130	2
1077	Investigation of the interaction of allergens of Glycine max with IgE-antibody for designing of peptidomimetics based anti-allergen. **2018**, 61, 394-404	4
1076	Differences in substrate specificity of V. cholerae FabH enzymes suggest new approaches for the development of novel antibiotics and biofuels. **2018**, 285, 2900-2921	1
1075	Structural basis for terminal loop recognition and stimulation of pri-miRNA-18a processing by hnRNP A1. **2018**, 9, 2479	41
1074	Effect of Ca2+ on the promiscuous target-protein binding of calmodulin. **2018**, 14, e1006072	23
1073	Crystal Growth in Polyethylene by Molecular Dynamics: The Crystal Edge and Lamellar Thickness. **2018**, 51, 4865-4873	21
1072	Formulation and Molecular Dynamics Simulations of a Fusidic Acid Nanosuspension for Simultaneously Enhancing Solubility and Antibacterial Activity. **2018**, 15, 3512-3526	33
1071	Conglomeration of novel Culex quinquefasciatus salivary proteins to contrive multi-epitope subunit vaccine against infections caused by blood imbibing transmitter. **2018**, 118, 834-843	9
1070	Targeting Myeloid Differentiation Using Potent 2-Hydroxypyrazolo[1,5- a]pyridine Scaffold-Based Human Dihydroorotate Dehydrogenase Inhibitors. **2018**, 61, 6034-6055	38
1069	Transient antibody-antigen interactions mediate the strain-specific recognition of a conserved malaria epitope. **2018**, 1, 58	5
1068	Stress-structure coupling and nonlinear rheology of Lennard-Jones liquid. **2018**, 148, 234507	8
1067	A description of hydroquinone clathrates using molecular dynamics: Molecular model and crystalline structures for CH and CO guests. **2018**, 148, 244502	7
1066	The molecular recognition of phosphatidic acid by an amphipathic helix in Opi1. **2018**, 217, 3109-3126	30
1065	Partition coefficients of methylated DNA bases obtained from free energy calculations with molecular electron density derived atomic charges. **2018**, 39, 1728-1737	3
1064	HIV-1 Env gp41 Transmembrane Domain Dynamics Are Modulated by Lipid, Water, and Ion Interactions. **2018**, 115, 84-94	9
1063	Local low dose curcumin treatment improves functional recovery and remyelination in a rat model of sciatic nerve crush through inhibition of oxidative stress. **2018**, 139, 98-116	28
1062	Unfolding Hidden Barriers by Active Enhanced Sampling. **2018**, 121, 010601	21

1061	Colloidal suspension by SRDPMD simulation on GPU. **2018**, 232, 35-45	2
1060	Bridging the Microscopic and Macroscopic in Thermodynamics with Molecular Dynamics Simulations: Lab Exercises for Undergraduate Physical Chemistry. **2018**, 33-48	1
1059	Solvation of Al cations in bulk and confined protic ionic liquids: a computational study. **2018**, 20, 19071-19081	11
1058	Enabling rootless Linux Containers in multi-user environments: The udocker tool. **2018**, 232, 84-97	26
1057	Mechanical transduction of cytoplasmic-to-transmembrane-domain movements in a hyperpolarization-activated cyclic nucleotide-gated cation channel. **2018**, 293, 12908-12918	14
1056	Targeting Outer Membrane Protein Component AdeC for the Discovery of Efflux Pump Inhibitor against AdeABC Efflux Pump of Multidrug Resistant Acinetobacter baumannii. **2018**, 76, 391-400	14
1055	Pharmacological characterization of the neurotrophic sesquiterpene jiadifenolide reveals a non-convulsant signature and potential for progression in neurodegenerative disease studies. **2018**, 155, 61-70	12
1054	Molecular Mechanism of Lipid Nanodisk Formation by Styrene-Maleic Acid Copolymers. **2018**, 115, 494-502	45
1053	Molecular recognition of RAS/RAF complex at the membrane: Role of RAF cysteine-rich domain. **2018**, 8, 8461	53
1052	Cellulose crystals plastify by localized shear. **2018**, 115, 7260-7265	25
1051	Chain Ejection Model for Electrospray Ionization of Unfolded Proteins: Evidence from Atomistic Simulations and Ion Mobility Spectrometry. **2018**, 90, 10069-10077	18
1050	Force Field Benchmark of Amino Acids. 2. Partition Coefficients between Water and Organic Solvents. **2018**, 58, 1669-1681	28
1049	QM/MM Description of Newly Selected Catalytic Bioscavengers Against Organophosphorus Compounds Revealed Reactivation Stimulus Mediated by Histidine Residue in the Acyl-Binding Loop. **2018**, 9, 834	6
1048	Modeling Soft Supramolecular Nanostructures by Molecular Simulations. **2018**,	
1047	Computational Spectroscopy of Ionic Liquids for Bulk Structure Elucidation. **2018**, 1, 1800084	13
1046	Insights into the Mechanism of Antimicrobial Activity of Seven-Residue Peptides. **2018**, 61, 7614-7629	11
1045	A geometrical criterion for glass transition in soft-sphere fluids. **2018**, 14, 7075-7082	5
1044	HTMoL: full-stack solution for remote access, visualization, and analysis of molecular dynamics trajectory data. **2018**, 32, 869-876	13

1043	Molecular insights into the effect L17A/F19A double mutation on the structure and dynamics of A : A molecular dynamics simulation study. **2018**, 119, 8949-8961	7
1042	Dynamics with Explicit Solvation Reveals Formation of the Prereactive Dimer as Sole Determining Factor for the Efficiency of Ru(bda)L2 Catalysts. **2018**, 8, 8642-8648	24
1041	Aromatic Rings Commonly Used in Medicinal Chemistry: Force Fields Comparison and Interactions With Water Toward the Design of New Chemical Entities. **2018**, 9, 395	23
1040	Novel Tubulin Mutations Conferring Resistance to Dinitroaniline Herbicides in. **2018**, 9, 97	31
1039	Interactions of zearalenone and its reduced metabolites zearalenol and zearalenol with serum albumins: species differences, binding sites, and thermodynamics. **2018**, 34, 269-278	23
1038	How Meaningful Is the Halogen Bonding in 1-Ethyl-3-methyl Imidazolium-Based Ionic Liquids for CO Capture?. **2018**, 122, 7907-7914	6
1037	How do hydrogen bonds break in supercooled water?: Detecting pathways not going through saddle point of two-dimensional potential of mean force. **2018**, 148, 244501	5
1036	Computational discovery of chemically patterned surfaces that effect unique hydration water dynamics. **2018**, 115, 8093-8098	30
1035	Protein-Ligand Interaction Energy-Based Entropy Calculations: Fundamental Challenges For Flexible Systems. **2018**, 122, 7821-7827	10
1034	PackMem: A Versatile Tool to Compute and Visualize Interfacial Packing Defects in Lipid Bilayers. **2018**, 115, 436-444	27
1033	Novel fluorescent antifolates that target folate receptors and Molecular dynamics and density functional theory study. **2018**, 85, 40-47	6
1032	Antibacterial Activity of Teixobactin Derivatives on Clinically Relevant Bacterial Isolates. **2018**, 9, 1535	19
1031	Thermostability and Specific-Activity Enhancement of an Arginine Deiminase from Enterococcus faecalis SK23.001 via Semirational Design for l-Citrulline Production. **2018**, 66, 8841-8850	3
1030	A molecular dynamics framework to explore the structure and dynamics of layered double hydroxides. **2018**, 163, 164-177	18
1029	A polarizable MARTINI model for monovalent ions in aqueous solution. **2018**, 149, 163319	17
1028	Application of Multiscale Simulation Tools on GPCRs. An Example with Angiotensin II Type 1 Receptor. **2018**, 1824, 431-448	
1027	Disorder guides domain rearrangement in elongation factor Tu. **2018**, 86, 1037-1046	10
1026	A coarse-grained approach to studying the interactions of the antimicrobial peptides aurein 1.2 and maculatin 1.1 with POPG/POPE lipid mixtures. **2018**, 24, 208	7

1025	Biophysical experiments and biomolecular simulations: A perfect match?. **2018**, 361, 355-360	110
1024	Physicochemical properties and formation mechanism of electrostatic complexes based on ε-polylysine and whey protein: Experimental and molecular dynamics simulations study. **2018**, 118, 2208-2215	13
1023	Generating conformational transition paths with low potential-energy barriers for proteins. **2018**, 32, 853-867	3
1022	The influence of hydrophilicity on the orientational dynamics and structures of imidazolium-based ionic liquid/water binary mixtures. **2018**, 149, 044501	16
1021	Substrate-Dependent Morphology and Its Effect on Electrical Mobility of Doped Poly(3,4-ethylenedioxythiophene) (PEDOT) Thin Films. **2018**, 10, 29115-29126	29
1020	Insight into Phosphatidylinositol-Dependent Membrane Localization of the Innate Immune Adaptor Protein Toll/Interleukin 1 Receptor Domain-Containing Adaptor Protein. **2018**, 9, 75	7
1019	Computational Insight Into the Structural Organization of Full-Length Toll-Like Receptor 4 Dimer in a Model Phospholipid Bilayer. **2018**, 9, 489	13
1018	Molecular Determinants of the Promiscuity of MexB and MexY Multidrug Transporters of. **2018**, 9, 1144	24
1017	Interfacing Graphene-Based Materials With Neural Cells. **2018**, 12, 12	61
1016	Detailed Analysis of 17β-Estradiol-Aptamer Interactions: A Molecular Dynamics Simulation Study. **2018**, 23,	12
1015	Crosslinked Poly(tetrahydrofuran) as a Loosely Coordinating Polymer Electrolyte. **2018**, 8, 1800703	95
1014	Anti-quorum sensing and antibiofilm potential of Alternaria alternata, a foliar endophyte of Carica papaya, evidenced by QS assays and in-silico analysis. **2018**, 122, 998-1012	17
1013	Computer Simulation of Luminophore Solubilization in Reverse Micelles. **2018**, 80, 266-271	2
1012	In Silico evaluation and identification of fungi capable of producing endo-inulinase enzyme. **2018**, 13, e0200607	3
1011	Differential Enzymatic Activity of Rat ADAR2 Splicing Variants Is Due to Altered Capability to Interact with RNA in the Deaminase Domain. **2018**, 9,	7
1010	Electrolyte cation length influences electrosorption and dynamics in porous carbon supercapacitors. **2018**, 283, 882-893	15
1009	Demystifying the pH dependent conformational changes of human heparanase pertaining to structure-function relationships: an in silico approach. **2018**, 32, 821-840	7
1008	Computational modelling approaches as a potential platform to understand the molecular genetics association between Parkinson's and Gaucher diseases. **2018**, 33, 1835-1847	26

1007	The potential impact of carboxylic-functionalized multi-walled carbon nanotubes on trypsin: A Comprehensive spectroscopic and molecular dynamics simulation study. **2018**, 13, e0198519	10
1006	Synthesis and Self-Assembly of Amphiphilic Star/Linear-Dendritic Polymers: Effect of Core versus Peripheral Branching on Reverse Micelle Aggregation. **2018**, 19, 3177-3189	9
1005	Glyphosate Resistance in Tridax procumbens via a Novel EPSPS Thr-102-Ser Substitution. **2018**, 66, 7880-7888	34
1004	Graphene quantum dots prevent □synucleinopathy in Parkinson's disease. **2018**, 13, 812-818	207
1003	Structural and functional characterization of suramin-bound MjTX-I from Bothrops moojeni suggests a particular myotoxic mechanism. **2018**, 8, 10317	17
1002	Poly-N-Acetyllactosamine Neo-Glycoproteins as Nanomolar Ligands of Human Galectin-3: Binding Kinetics and Modeling. **2018**, 19,	30
1001	Conformational Dynamics and Stability of U-Shaped and S-Shaped Amyloid □Assemblies. **2018**, 19,	27
1000	The Cyanobacterial Ribosomal-Associated Protein LrtA from sp. PCC 6803 Is an Oligomeric Protein in Solution with Chameleonic Sequence Properties. **2018**, 19,	4
999	Design, Synthesis, and Docking Studies of New Torin2 Analogs as Potential ATR/mTOR Kinase Inhibitors. **2018**, 23,	8
998	Computational Insight into the Effect of Natural Compounds on the Destabilization of Preformed Amyloid-□1?40) Fibrils. **2018**, 23,	21
997	Screening of Isocitrate Lyase for Novel Anti-Buruli Ulcer Natural Products Originating from Africa. **2018**, 23,	12
996	In Silico Study, Synthesis, and Cytotoxic Activities of Porphyrin Derivatives. **2018**, 11,	7
995	Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size. **2018**, 7,	51
994	In´vitro and in silico studies of naphthoquinones and peptidomimetics toward Plasmodium falciparum plasmepsin V. **2018**, 152, 159-173	5
993	Catalytic, Computational, and Evolutionary Analysis of the d-Lactate Dehydrogenases Responsible for d-Lactic Acid Production in Lactic Acid Bacteria. **2018**, 66, 8371-8381	15
992	Role of MDH2 pathogenic variant in pheochromocytoma and paraganglioma patients. **2018**, 20, 1652-1662	33
991	Structural and functional studies of the metalloregulator Fur identify a promoter-binding mechanism and its´role in virulence. **2018**, 1, 93	12
990	Computational insights about the dynamic behavior for the inclusion process of deprotonated and neutral aspirin in □cyclodextrin. **2018**, 92, 115-127	4

989	Mechanically inferior constituents in spider silk result in mechanically superior fibres by adaptation to harsh hydration conditions: a molecular dynamics study. **2018**, 15,	5
988	Oligomer Formation Propensities of Dimeric Bundle Peptides Correlate with Cell Penetration Abilities. **2018**, 4, 885-893	10
987	Leveraging Cloud Computing for In-Silico Drug Design Using the Quantum Molecular Design (QMD) Framework. **2018**, 20, 66-73	8
986	ColDock: Concentrated Ligand Docking with All-Atom Molecular Dynamics Simulation. **2018**, 122, 7191-7200	8
985	Roles of PIP2 in the membrane binding of MIM I-BAR: insights from molecular dynamics simulations. **2018**, 592, 2533-2542	8
984	Continuous Uptake or Saturation-Investigation of Concentration and Surface-Packing-Specific Hemin Interaction with Lipid Membranes. **2018**, 122, 7547-7554	8
983	Molecular Dynamics Simulation of Water-Based Fracturing Fluids in Kaolinite Slit Pores. **2018**, 122, 17170-17183	39
982	Butane dihedral angle dynamics in water is dominated by internal friction. **2018**, 115, 5169-5174	36
981	Design, selection and optimization of an anti-TRAIL-R2/anti-CD3 bispecific antibody able to educate T cells to recognize and destroy cancer cells. **2018**, 10, 1084-1097	8
980	Dynamics of Dof domain-DNA interaction in wheat: Insights from atomistic simulations and free energy landscape. **2018**, 119, 8818-8829	2
979	Dynamics of Dystrophin's Actin-Binding Domain. **2018**, 115, 445-454	6
978	Dynamic States of the Ligand-Free Class A G Protein-Coupled Receptor Extracellular Side. **2018**, 57, 4767-4775	2
977	Supercharged Polyplexes: Full-Atom Molecular Dynamics Simulations and Experimental Study. **2018** , 51, 5450-5459	8
976	Crystalline Cyclophane-Protein Cage Frameworks. **2018**, 12, 8029-8036	27
975	Antagonistic role of Klotho-derived peptides dynamics in the pancreatic cancer treatment through obstructing WNT-1 and Frizzled binding. **2018**, 240, 107-117	12
974	Molecular and in silico analyses validates pathogenicity of homozygous mutations in the NPR2 gene underlying variable phenotypes of Acromesomelic dysplasia, type Maroteaux. **2018**, 102, 76-86	9
973	Electrospray Ionization of Polypropylene Glycol: Rayleigh-Charged Droplets, Competing Pathways, and Charge State-Dependent Conformations. **2018**, 90, 9912-9920	15
972	Structural Behavior of Isolated Asphaltene Molecules at the Oil–Water Interface. **2018**, 32, 8259-8267	11

971	Conformational Free Energy Changes via an Alchemical Path without Reaction Coordinates. **2018**, 9, 4428-4435	6
970	Direct knock-on of desolvated ions governs strict ion selectivity in K channels. **2018**, 10, 813-820	88
969	Free-energy analysis of physisorption on solid-liquid interface with the solution theory in the energy representation. **2018**, 149, 014504	4
968	Adaptive resolution molecular dynamics technique: Down to the essential. **2018**, 149, 024104	25
967	Both reentrant loops of the sodium-coupled glutamate transporters contain molecular determinants of cation selectivity. **2018**, 293, 14200-14209	3
966	How to minimize dye-induced perturbations while studying biomembrane structure and dynamics: PEG linkers as a rational alternative. **2018**, 1860, 2436-2445	21
965	Stoichiometry dependent inhibition of rat □□ nicotinic acetylcholine receptor by the ribbon isomer of □conotoxin AuIB. **2018**, 155, 288-297	7
964	Structure of monomeric full-length ARC sheds light on molecular flexibility, protein interactions, and functional modalities. **2018**, 147, 323-343	16
963	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. **2018**, 9, 956-972	122
962	Electrostatic lock in the transport cycle of the multidrug resistance transporter EmrE. **2018**, 115, E7502-E7511	21
961	Incorporating uracil and 5-halouracils into short peptide nucleic acids for enhanced recognition of A-U pairs in dsRNAs. **2018**, 46, 7506-7521	18
960	Discovery of Novel Bovine Viral Diarrhea Inhibitors Using Structure-Based Virtual Screening on the Envelope Protein E2. **2018**, 6, 79	10
959	Molecular dynamics simulations revealed structural differences among WRKY domain-DNA interaction in barley (Hordeum vulgare). **2018**, 19, 132	38
958	Molecular Dynamics Analysis of Cardiolipin and Monolysocardiolipin on Bilayer Properties. **2018**, 114, 2116-2127	17
957	Glycerol Solvates DPPC Headgroups and Localizes in the Interfacial Regions of Model Pulmonary Interfaces Altering Bilayer Structure. **2018**, 34, 6941-6954	13
956	Computational analysis of the receptor binding specificity of novel influenza A/H7N9 viruses. **2018**, 19, 88	7
955	A polarizable embedding approach to second harmonic generation (SHG) of molecular systems in aqueous solutions. **2018**, 137, 1	23
954	A molecular simulation approach to the computation of mutual solubility of water and organic liquids: Application to fatty acids. **2018**, 472, 48-55	6

953	Unraveling the Molecular Mechanisms of Thermo-responsive Properties of Silk-Elastin-Like Proteins by Integrating Multiscale Modeling and Experiment. **2018**, 6, 3727-3734	14
952	Asymmetric nucleophilic fluorination under hydrogen bonding phase-transfer catalysis. **2018**, 360, 638-642	92
951	MD-modeling of the intermediate scattering function for argon-like liquids and water. **2018**, 263, 200-208	1
950	p.R180C mutation of glycosyltransferase B leads to B subgroup, an in vitro and in silico study. **2018**, 113, 476	3
949	Rotational Diffusion Depends on Box Size in Molecular Dynamics Simulations. **2018**, 9, 2874-2878	22
948	Dimer Interface of the Human Serotonin Transporter and Effect of the Membrane Composition. **2018**, 8, 5080	22
947	Investigation of immunogenic properties of Hemolin from silkworm, Bombyx mori as carrier protein: an immunoinformatic approach. **2018**, 8, 6957	13
946	How to simulate patchy particles. **2018**, 41, 59	22
945	The Dipole Moment of Reverse Micelles according to Computer Simulation Data. **2018**, 80, 184-188	2
944	A molecular dynamics simulation study on the conformational stability of amylose-linoleic acid complex in water. **2018**, 196, 56-65	38
943	Crowding Stabilizes DMSO-Water Hydrogen-Bonding Interactions. **2018**, 122, 5984-5990	16
942	Growth of wormlike micelles of surfactant induced by embedded polymer: role of polymer chain length. **2018**, 14, 4792-4804	16
941	Optimizing Protein-Polymer Interactions in a Poly(ethylene glycol) Coarse-Grained Model. **2018**, 122, 7997-8005	15
940	A Novel Polar Core and Weakly Fixed C-Tail in Squid Arrestin Provide New Insight into Interaction with Rhodopsin. **2018**, 430, 4102-4118	4
939	Effective Removal of Phenylamine, Quinoline, and Indole from Light Oil by ‖Cyclodextrin Aqueous Solution through Molecular Inclusion. **2018**, 32, 9280-9288	3
938	How Reactive are Druggable Cysteines in Protein Kinases?. **2018**, 58, 1935-1946	27
937	Rational Design of Thermostable Carbonic Anhydrase Mutants Using Molecular Dynamics Simulations. **2018**, 122, 8526-8536	18
936	Effect of Surfactants on Surface-Induced Denaturation of Proteins: Evidence of an Orientation-Dependent Mechanism. **2018**, 122, 11390-11399	20

935	Engineering E. coli cell surface in order to develop a one-step purification method for recombinant proteins. **2018**, 8, 107	5
934	Impact of Dispersion Coefficient on Simulations of Proteins and Organic Liquids. **2018**, 122, 8018-8027	12
933	A molecular dynamics simulation study on the mechanism of loading of gemcitabine and camptothecin in poly lactic-co-glycolic acid as a nano drug delivery system. **2018**, 269, 110-118	27
932	X-Ray Diffraction and Computer Simulation Studies of the Structure of Liquid Aliphatic Aldehydes: From Propanal to Nonanal. **2018**, 255, 1800127	2
931	Emergent Properties of Antiagglomerant Films Control Methane Transport: Implications for Hydrate Management. **2018**, 34, 9701-9710	18
930	Engineering a Single-Agent Cytokine/Antibody Fusion That Selectively Expands Regulatory T Cells for Autoimmune Disease Therapy. **2018**, 201, 2094-2106	25
929	Membrane-Modulating Drugs can Affect the Size of Amyloid-β Aggregates in Anionic Membranes. **2018**, 8, 12367	5
928	Distinct Differences in Peptide Adsorption on Palladium and Gold: Introducing a Polarizable Model for Pd(111). **2018**, 122, 19625-19638	5
927	Specific Ion Effects on Zwitterionic Micelles Are Independent of Interfacial Hydration Changes. **2018**, 34, 11049-11057	7
926	Homology modeling, molecular docking, and dynamics of two α-methyl-D-mannoside-specific lectins from Arachis genus. **2018**, 24, 251	3
925	Hydrophobic gating in BK channels. **2018**, 9, 3408	35
924	Distinct but overlapping binding sites of agonist and antagonist at the relaxin family peptide 3 (RXFP3) receptor. **2018**, 293, 15777-15789	9
923	Improvement of Performance, Stability and Continuity by Modified Size-Consistent Multipartitioning Quantum Mechanical/Molecular Mechanical Method. **2018**, 23,	11
922	Atomistic dewetting mechanics of Wenzel and monostable Cassie-Baxter states. **2018**, 20, 24759-24767	17
921	Molecular Dynamics Simulations of the Silica–Cell Membrane Interaction: Insights on Biomineralization and Nanotoxicity. **2018**, 122, 21330-21343	15
920	Towards a coarse-grained model of the peptoid backbone: the case of N,N-dimethylacetamide. **2018**, 20, 23386-23396	6
919	. **2018**,	2
918	Determining the molecular basis of voltage sensitivity in membrane proteins. **2018**, 150, 1444-1458	10

917	Altered conformational landscape and dimerization dependency underpins the activation of EGFR by C-4 loop insertion mutations. **2018**, 115, E8162-E8171	32
916	Atomistic-Level Investigation of a LL37-Conjugated Gold Nanoparticle By Well-Tempered Metadynamics. **2018**, 122, 8359-8366	10
915	Computational design of new protein kinase 2 inhibitors for the treatment of inflammatory diseases using QSAR, pharmacophore-structure-based virtual screening, and molecular dynamics. **2018**, 24, 225	15
914	Semantics for an Integrative and Immersive Pipeline Combining Visualization and Analysis of Molecular Data. **2018**, 15,	15
913	Folding Mechanism of the SH3 Domain from Grb2. **2018**, 122, 11166-11173	6
912	Structural Properties of Span 80/Tween 80 Reverse Micelles by Molecular Dynamics Simulations. **2018**, 122, 8047-8055	8
911	Understanding three-body contributions to coarse-grained force fields. **2018**, 20, 22387-22394	20
910	OPLS Force Field for Choline Chloride-Based Deep Eutectic Solvents. **2018**, 122, 9982-9993	78
909	p15PAF binding to PCNA modulates the DNA sliding surface. **2018**, 46, 9816-9828	10
908	A Hotspot for Disease-Associated Variants of Human PGM1 Is Associated with Impaired Ligand Binding and Loop Dynamics. **2018**, 26, 1337-1345.e3	13
907	Hydration Free Energies in the FreeSolv Database Calculated with Polarized Iterative Hirshfeld Charges. **2018**, 58, 1779-1797	20
906	Licochalcone C induced apoptosis in human oral squamous cell carcinoma cells by regulation of the JAK2/STAT3 signaling pathway. **2018**, 119, 10118-10130	15
905	A Hierarchical Model To Understand the Processing of Polysaccharides/Protein-Based Films in Ionic Liquids. **2018**, 19, 3970-3982	19
904	The structure of the ubiquitin-like modifier FAT10 reveals an alternative targeting mechanism for proteasomal degradation. **2018**, 9, 3321	14
903	Crystal structure of the Frizzled 4 receptor in a ligand-free state. **2018**, 560, 666-670	51
902	Molecular clustering and percolation characteristics near the glass transition in aqueous trehalose and choline dihydrogen phosphate solutions. **2018**, 20, 20899-20909	
901	Negatively Charged Gangliosides Promote Membrane Association of Amphipathic Neurotransmitters. **2018**, 384, 214-223	10
900	Agronomic evaluation and molecular characterisation of the acetolactate synthase gene in imazapyr tolerant sugarcane (Saccharum hybrid) genotypes. **2018**, 37, 1201-1213	2

899	Self-Consistent Framework Connecting Experimental Proxies of Protein Dynamics with Configurational Entropy. **2018**, 14, 3796-3810	1
898	Validating Molecular Dynamics Simulations against Experimental Observables in Light of Underlying Conformational Ensembles. **2018**, 122, 6673-6689	41
897	Structural transitions of F-actin upon ATP hydrolysis at near-atomic resolution revealed by cryo-EM. **2018**, 25, 528-537	90
896	Interfacial behaviour of substituted dibenzothiophenes for their extraction in biphasic dodecane-ionic liquid systems. **2018**, 511, 54-62	3
895	Predicting drug permeability through skin using molecular dynamics simulation. **2018**, 283, 269-279	60
894	Quantitative Assessment of Methods Used To Obtain Rate Constants from Molecular Dynamics Simulations-Translocation of Cholesterol across Lipid Bilayers. **2018**, 14, 3840-3848	10
893	Self-Assembly Simulations of Classic Claudins-Insights into the Pore Structure, Selectivity, and Higher Order Complexes. **2018**, 122, 7463-7474	20
892	Insights into Membrane Translocation of Protegrin Antimicrobial Peptides by Multistep Molecular Dynamics Simulations. **2018**, 3, 6056-6065	19
891	Modulation of phase transition of thermosensitive liposomes with leucine zipper-structured lipopeptides. **2018**, 20, 15916-15925	2
890	Quantifying the Effects of Hydrogen Bonding on Nitrile Frequencies in GFP: Beyond Solvent Exposure. **2018**, 122, 6733-6743	16
889	In silico identification of AChE and PARP-1 dual-targeted inhibitors of Alzheimer's disease. **2018**, 24, 151	10
888	Biophysical studies and modelling indicate the binding preference of TAZ WW domain for LATS1 PPxY motif. **2018**, 502, 307-312	1
887	ELF: An Extended-Lagrangian Free Energy Calculation Module for Multiple Molecular Dynamics Engines. **2018**, 58, 1315-1318	8
886	Coupling between the mesoscopic dynamics and shear stress of a room-temperature ionic liquid. **2018**, 20, 17809-17817	17
885	How fine-tuned for energy transfer is the environmental noise produced by proteins around biological chromophores?. **2018**, 20, 17279-17288	6
884	Molecular transport through membranes: Accurate permeability coefficients from multidimensional potentials of mean force and local diffusion constants. **2018**, 149, 072310	26
883	Biochemical characterization and molecular mechanism of acid denaturation of a novel □-amylase from Aspergillus niger. **2018**, 137, 222-231	7
882	The Intracellular Loop of the Na/Ca Exchanger Contains an "Awareness Ribbon"-Shaped Two-Helix Bundle Domain. **2018**, 57, 5096-5104	6

881	Stability of Biological Membranes upon Mechanical Indentation. **2018**, 122, 7073-7079	3
880	Computational Design To Reduce Conformational Flexibility and Aggregation Rates of an Antibody Fab Fragment. **2018**, 15, 3079-3092	15
879	Opioid receptor signaling, analgesic and side effects induced by a computationally designed pH-dependent agonist. **2018**, 8, 8965	37
878	Continuous version of a square-well potential of variable range and its application in molecular dynamics simulations. **2018**, 116, 3355-3365	4
877	Computational study of HIV gp120 as a target for polyanionic entry inhibitors: Exploiting the V3 loop region. **2018**, 13, e0190658	6
876	The influences of E22Q mutant on solvated 3Aβpeptide: A REMD study. **2018**, 83, 122-128	4
875	βHelix or βTurn? An Investigation into N-Terminally Constrained Analogues of Glucagon-like Peptide 1 (GLP-1) and Exendin-4. **2018**, 57, 4148-4154	8
874	The impact of tensorial temperature on equilibrium thermodynamics. **2018**, 20, 16910-16912	0
873	Molecular Insights into Variable Electron Transfer in Amphibian Cryptochrome. **2018**, 114, 2563-2572	12
872	Comparison of Structures and Energies of Metal Complexes Coordinated with Hydroxyoxime and Carboxylic Acid Extractants by Using Molecular Simulations. **2018**, 25, 59-69	3
871	Coarse-grained molecular dynamics simulations of polymerization with forward and backward reactions. **2018**, 39, 1764-1778	7
870	Gradual Crossover from Subdiffusion to Normal Diffusion: A Many-Body Effect in Protein Surface Water. **2018**, 120, 248101	45
869	Different footprints of the Zika and dengue surface proteins on viral membranes. **2018**, 14, 5615-5621	4
868	Mechanical properties of drug loaded diblock copolymer bilayers: A molecular dynamics study. **2018**, 148, 214901	4
867	Ligand-induced perturbation of the HIF-2αARNT dimer dynamics. **2018**, 14, e1006021	14
866	A direct interaction of cholesterol with the dopamine transporter prevents its out-to-inward transition. **2018**, 14, e1005907	51
865	Computer simulations reveal changes in the conformational space of the transcriptional regulator MosR upon the formation of a disulphide bond and in the collective motions that regulate its DNA-binding affinity. **2018**, 13, e0192826	3
864	Universal Implementation of a Residue-Specific Force Field Based on CMAP Potentials and Free Energy Decomposition. **2018**, 14, 4474-4486	18

863	An efficient hybrid adsorbent based on silica-supported amino penta-carboxylic acid for water purification. **2018**, 6, 13096-13109	22
862	The chromatin nuclear protein NUPR1L is intrinsically disordered and binds to the same proteins as its paralogue. **2018**, 475, 2271-2291	8
861	Search for the Source of an Apparent Interfacial Resistance To Mass Transfer of CnEm Surfactants To the Water/Oil Interface. **2019**, 35, 2898-2908	5
860	Folding thermodynamics of PET-hydrolyzing enzyme Cut190 depending on Ca2+ concentration. **2019**, 135, 2655-2663	21
859	A double-edged sword: supramolecular complexes of triazavirine display multicenter binding effects which influence aggregate formation. **2019**, 37, 3041-3047	3
858	Licochalcone D directly targets JAK2 to induced apoptosis in human oral squamous cell carcinoma. **2019**, 234, 1780-1793	8
857	Influence of dendrimer surface chemistry and pH on the binding and release pattern of chalcone studied by molecular dynamics simulations. **2019**, 32, e2757	16
856	Simulating vertical excitation energies of solvated dyes: From continuum to polarizable discrete modeling. **2019**, 119, e25684	26
855	Insights into the DNA binding induced thermal stabilization of transcription factor FOXP3. **2019**, 37, 2219-2229	6
854	The effects of oxidised phospholipids and cholesterol on the biophysical properties of POPC bilayers. **2019**, 1861, 210-219	14
853	Delineating the active site architecture of G9a lysine methyltransferase through substrate and inhibitor binding mode analysis: a molecular dynamics study. **2019**, 37, 2581-2592	6
852	In silico site-directed mutagenesis of neutralizing mAb 4C4 and analysis of its interaction with G-H loop of VP1 to explore its therapeutic applications against FMD. **2019**, 37, 2641-2651	
851	Molecular Dynamics and Simulation. **2019**, 550-566	8
850	Protein-Protein Interactions: An Overview. **2019**, 821-833	
849	A non-functional galanin receptor-2 in a multiple sclerosis patient. **2019**, 19, 72-82	4
848	Molecular dynamics simulations of CO2 permeation through ionic liquids confined in □alumina nanopores. **2019**, 206, 301-317	3
847	Molecular modeling studies on the interactions of aflatoxin B1 and its metabolites with the peripheral anionic site of human acetylcholinesterase. **2019**, 37, 2041-2048	14
846	Thermodynamics of Helix formation in small peptides of varying lengthin vacuo, implicit solvent and explicit solvent: Comparison between AMBER force fields. **2019**, 18, 1950015	6

845	Molecular dynamics study of solubilization of cyclohexane, benzene, and phenol into mixed micelles composed of sodium dodecyl sulfate and octaethylene glycol monododecyl ether. **2019**, 40, 2722-2729	3
844	Ligand-Binding Calculations with Metadynamics. **2019**, 2022, 233-253	1
843	Targeting multiple G-quadruplex-forming DNA sequences: Design, biophysical and biological evaluations of indolo-naphthyridine scaffold derivatives. **2019**, 182, 111627	10
842	A two-component protease in with high activity toward the peptide precursor of the redox cofactor pyrroloquinoline quinone. **2019**, 294, 15025-15036	9
841	Hydrogen Permeation in Hydrated Perfluorosulfonic Acid Polymer Membranes: Effect of Polymer Crystallinity and Equivalent Weight. **2019**, 123, 20628-20638	16
840	Membrane-Disrupting Nanofibrous Peptide Hydrogels. **2019**, 5, 4657-4670	23
839	Highly sensitive and selective detection of single-nucleotide polymorphisms using gold nanoparticle MutS enzymes and a micro cantilever resonator. **2019**, 205, 120154	10
838	Quick temperature-sweep pure-shift NMR: the case of solvent effects in atorvastatin. **2019**, 21, 19209-19215	4
837	Generalized Markov modeling of nonreversible molecular kinetics. **2019**, 150, 174103	7
836	Two distinct anionic phospholipid-dependent events involved in SecA-mediated protein translocation. **2019**, 1861, 183035	8
835	Past-future information bottleneck for sampling molecular reaction coordinate simultaneously with thermodynamics and kinetics. **2019**, 10, 3573	41
834	Molecular cloning, gene expression analysis, and in silico characterization of UDP-N-acetylglucosamine pyrophosphorylase from Bombyx mori. **2019**, 66, 880-899	2
833	Hydantoin and Its Derivatives Reduce the Viscosity of Concentrated Antibody Formulations by Inhibiting Associations via Hydrophobic Amino Acid Residues. **2019**, 58, 16296-16306	4
832	Identification of lysine methylation in the core GTPase domain by GoMADScan. **2019**, 14, e0219436	3
831	Enhancing the activity and thermostability of Streptomyces mobaraensis transglutaminase by directed evolution and molecular dynamics simulation. **2019**, 151, 107333	9
830	Stereoselective pH Responsive Peptide Dendrimers for siRNA Transfection. **2019**, 30, 2165-2182	13
829	Rationalizing the Phase Behavior of Triblock Copolymers through Experiments and Molecular Simulations. **2019**, 123, 21224-21236	19
828	Structure and Dynamics of an Ionic Liquid Mixture Film Confined by Mica. **2019**, 123, 20971-20979	3

827	Interaction of carbohydrate binding module 20 with starch substrates.. **2019**, 9, 24833-24842	5
826	SESCA: Predicting Circular Dichroism Spectra from Protein Molecular Structures. **2019**, 15, 5087-5102	22
825	The conduction pathway of potassium channels is water free under physiological conditions. **2019**, 5, eaaw6756	32
824	Vibrational spectroscopy combined with molecular dynamics simulations as a tool for studying behavior of reactive aldehydes inserted in phospholipid bilayers. **2019**, 225, 104793	2
823	Stationary-Phase Contributions to Surface Diffusion in Reversed-Phase Liquid Chromatography: Chain Length versus Ligand Density. **2019**, 123, 21617-21628	11
822	Electrolytes under Inhomogeneous Nanoconfinement: Water Structuring-Mediated Local Ion Accumulation. **2019**, 10, 4895-4902	4
821	Predicting Kinase Inhibitor Resistance: Physics-Based and Data-Driven Approaches. **2019**, 5, 1468-1474	15
820	Prediction of Partition Coefficients of Environmental Toxins Using Computational Chemistry Methods. **2019**, 4, 13772-13781	15
819	Histone chaperone exploits intrinsic disorder to switch acetylation specificity. **2019**, 10, 3435	16
818	Are Gaming-Enabled Graphic Processing Unit Cards Convenient for Molecular Dynamics Simulation?. **2019**, 15, 1176934319850144	9
817	Towards the competent conformation for catalysis in the ferredoxin-NADP reductase from the Brucella ovis pathogen. **2019**, 1860, 148058	4
816	Photophysics of BODIPY-Based Photosensitizer for Photodynamic Therapy: Surface Hopping and Classical Molecular Dynamics. **2019**, 15, 5046-5057	8
815	Thyroid Peroxidase Activity is Inhibited by Phenolic Compounds-Impact of Interaction. **2019**, 24,	8
814	The effect of CO loading on alkanolamine absorbents in aqueous solutions. **2019**, 21, 18386-18392	6
813	Enabling sequential rupture for lowering atomistic ice adhesion. **2019**, 11, 16262-16269	13
812	If You Cannot Win Them, Join Them: Understanding New Ways to Target STAT3 by Small Molecules. **2019**, 4, 13913-13921	3
811	The ghrelin -acyltransferase structure reveals a catalytic channel for transmembrane hormone acylation. **2019**, 294, 14166-14174	14
810	Immunoinformatics-Aided Design and Evaluation of a Potential Multi-Epitope Vaccine against. **2019**, 7,	50

809	Synergistic Sorption of Mixed Solvents in Wood Cell Walls: Experimental and Theoretical Approach. **2019**, 386, 1900022	5
808	Defining and detecting links in chromosomes. **2019**, 9, 11753	4
807	Teaching High Performance Computing through Parallel Programming Marathons. **2019**,	0
806	PepVis: An integrated peptide virtual screening pipeline for ensemble and flexible docking protocols. **2019**, 94, 2041-2050	10
805	Molecular Dynamics Study of Triazole Derivative Binding to the Active Site of Imidazole Glycerol Phosphate Dehydratase from Mycobacterium tuberculosis. **2019**, 64, 608-610	2
804	X-Ray Crystal Structure of a Second-Generation Peptide Dendrimer in Complex with Pseudomonas aeruginosa Lectin LecB. **2019**, 102, e1900178	3
803	Fat SIRAH: Coarse-Grained Phospholipids To Explore Membrane-Protein Dynamics. **2019**, 15, 5674-5688	19
802	Lipid Head Group Parameterization for GROMOS 54A8: A Consistent Approach with Protein Force Field Description. **2019**, 15, 5175-5193	7
801	The key to the yellow-to-cyan tuning in the green fluorescent protein family is polarisation. **2019**, 21, 18988-18998	14
800	The Marriage of Protein and Lanthanide: Unveiling a Time-Resolved Fluorescence Sensor Array Regulated by pH toward High-Throughput Assay of Metal Ions in Biofluids. **2019**, 91, 11170-11177	40
799	Importance of the β5-β6 Loop for the Structure, Catalytic Efficiency, and Stability of Carbapenem-Hydrolyzing Class D βLactamase Subfamily OXA-143. **2019**, 58, 3604-3616	0
798	Prediction of Noncompetitive Inhibitor Binding Mode Reveals Promising Site for Allosteric Modulation of Falcipain-2. **2019**, 123, 7327-7342	5
797	Fick diffusion coefficients of binary fluid mixtures consisting of methane, carbon dioxide, and propane via molecular dynamics simulations based on simplified pair-specific ab initio-derived force fields. **2019**, 502, 112257	6
796	The synergic effect of water and biomolecules in intracellular phase separation. **2019**, 3, 552-561	34
795	Double-Stranded RNA Synthesis by Rotavirus Polymerase Mutants with Lesions at Core Shell Contact Sites. **2019**, 93,	4
794	AHR and GPER mediate the stimulatory effects induced by 3-methylcholanthrene in breast cancer cells and cancer-associated fibroblasts (CAFs). **2019**, 38, 335	19
793	Phase Behaviors of Ionic Liquids Heating from Different Crystal Polymorphs toward the Same Smectic-A Ionic Liquid Crystal by Molecular Dynamics Simulation. **2019**, 9, 26	6
792	Peptide-Based Subunit Vaccine Design of T- and B-Cells Multi-Epitopes against Zika Virus Using Immunoinformatics Approaches. **2019**, 7,	16

791	Effects of the Q80K Polymorphism on the Physicochemical Properties of Hepatitis C Virus Subtype 1a NS3 Protease. **2019**, 11,	1
790	Atomistic Simulation Tools to Study Protein Self-Aggregation. **2019**, 2039, 243-262	1
789	The H channel is not a proton transfer path in yeast cytochrome c oxidase. **2019**, 1860, 717-723	6
788	Molecular Energetics of Doxorubicin Pumping by Human P-Glycoprotein. **2019**, 59, 3889-3898	5
787	Computational Characterization of a Cholesterol-Based Molecular Rotor in Lipid Membranes. **2019**, 123, 7313-7326	4
786	Dynamic Protonation Dramatically Affects the Membrane Permeability of Drug-like Molecules. **2019**, 141, 13421-13433	22
785	Promoting transparency and reproducibility in enhanced molecular simulations. **2019**, 16, 670-673	271
784	Catalytically Competent Non-transforming H-RAS Mutant Provides Insight into Molecular Switch Function and GAP-independent GTPase Activity of RAS. **2019**, 9, 10967	3
783	Identification of evolutionary and kinetic drivers of NAD-dependent signaling. **2019**, 116, 15957-15966	27
782	BOOTABLE: Bioinformatics Benchmark Tool Suite. **2019**,	
781	Simulation-based protein engineering of FMN oxidoreductase (DszD). **2019**, 5, e02193	2
780	Toward Understanding the Impact of Dimerization Interfaces in Angiotensin II Type 1 Receptor. **2019**, 59, 4314-4327	6
779	Steering the Lipid Transfer To Unravel the Mechanism of Cholesteryl Ester Transfer Protein Inhibition. **2019**, 58, 3789-3801	1
778	Energy Transport Pathways in Proteins: A Non-equilibrium Molecular Dynamics Simulation Study. **2019**, 15, 5750-5757	12
777	How membrane lipids influence plasma delivery of reactive oxygen species into cells and subsequent DNA damage: an experimental and computational study. **2019**, 21, 19327-19341	19
776	Physics-based oligomeric models of the yeast mitofusin Fzo1 at the molecular scale in the context of membrane docking. **2019**, 49, 234-244	8
775	In Silico Reoptimization of Binding Affinity and Drug-Resistance Circumvention Ability in Kinase Inhibitors: A Case Study with RL-45 and Src Kinase. **2019**, 123, 6664-6672	6
774	Testing the Robustness of Solution Force Fields for MD Simulations on Gaseous Protein Ions. **2019**, 123, 6705-6715	6

773	Uptake of Common Atmospheric Gases by Organic-Coated Water Droplets. **2019**, 123, 18924-18931	6
772	Conformation space of a heterodimeric ABC exporter under turnover conditions. **2019**, 571, 580-583	94
771	Biological relevance of charge transfer branching pathways in photolyases. **2019**, 21, 17072-17081	2
770	A novel peptide-based sensor platform for detection of anti-Toxoplasma gondii immunoglobulins. **2019**, 175, 112778	5
769	Effects of N-Glycosylation on the Structure, Function, and Stability of a Plant-Made Fc-Fusion Anthrax Decoy Protein. **2019**, 10, 768	16
768	A comparative multivariate analysis of nitrilase enzymes: An ensemble based computational approach. **2019**, 83, 107095	7
767	Magnesium interactions with a CX26 connexon in lipid bilayers. **2019**, 25, 232	2
766	A multi-lock inhibitory mechanism for fine-tuning enzyme activities of the HECT family E3 ligases. **2019**, 10, 3162	14
765	Using Small-Angle Scattering Data and Parametric Machine Learning to Optimize Force Field Parameters for Intrinsically Disordered Proteins. **2019**, 6, 64	11
764	Multi-Target ╫Protease Inhibitors from : In Silico and In Vitro Studies. **2019**, 8,	14
763	Structure, function and dynamics in acyl carrier proteins. **2019**, 14, e0219435	12
762	Multiple C2 domains and transmembrane region proteins (MCTPs) tether membranes at plasmodesmata. **2019**, 20, e47182	46
761	TacoxDNA: A user-friendly web server for simulations of complex DNA structures, from single strands to origami. **2019**, 40, 2586-2595	27
760	Molecular basis of egg coat cross-linking sheds light on ZP1-associated female infertility. **2019**, 10, 3086	25
759	Solvation in ionic liquid-water mixtures: A computational study. **2019**, 292, 111273	7
758	Molecular docking studies of chloroquine and its derivatives against P23 domain of chikungunya virus: Implication in designing of novel therapeutic strategies. **2019**, 120, 18298-18308	5
757	Molecular Dynamics Simulation of Paracetamol Drug Adsorption on Boron Nitride Nanotube: Effects of Temperature, Nanotube Length, Diameter, and Chirality. **2019**, 4, 7866-7873	5
756	Structural basis of microcystinase activity for biodegrading microcystin-LR. **2019**, 236, 124281	9

755	In Silico Analysis of the Effect of Alkyl Tail Length on Antiagglomerant Adsorption to Natural Gas Hydrates in Brine. **2019**, 123, 17239-17248	9
754	Identification of a distal allosteric ligand binding pocket in HtrA3. **2019**, 516, 1130-1136	2
753	Shear Thinning and Nonlinear Structural Deformation of Ionic Liquids with Long Alkyl Chains Studied by Molecular Dynamics Simulation. **2019**, 123, 6260-6265	3
752	Resurrection of efficient Precambrian endoglucanases for lignocellulosic biomass hydrolysis. **2019**, 2,	11
751	Mutations in a conserved loop in the PSST subunit of respiratory complex I affect ubiquinone binding and dynamics. **2019**, 1860, 573-581	19
750	Affinity-Triggered Assemblies Based on a Designed Peptide-Peptide Affinity Pair. **2019**, 14, e1800559	2
749	Effect of external and internal plasticization on the glass transition temperature of (Meth)acrylate polymers studied with molecular dynamics simulations and calorimetry. **2019**, 179, 121635	14
748	Assessment of Enzyme Functionality at Metal□Organic Framework Interfaces Developed through Molecular Simulations. **2023**, 39, 1750-1763	0
747	Single Copper Atom Photocatalyst Powers an Integrated Catalytic Cascade for Drug-Resistant Bacteria Elimination.	1
746	What Drives Chorismate Mutase to Top Performance? Insights from a Combined In Silico and In Vitro Study. **2023**, 62, 782-796	0
745	Efficient polyethylene terephthalate degradation at moderate temperature: a protein engineering study of LC -cutinase highlights the key role of residue 243.	1
744	pH modulates the role of SP6 RNA polymerase in transcription process: an in silico study. 1-18	0
743	Robust anti-inflammatory activity of genistein against neutrophil elastase: a microsecond molecular dynamics simulation study. 1-17	1
742	Comparative Protein Structural Network Analysis Reveals C-Terminal Tail Phosphorylation Structural Communication Fingerprint in PTEN-Associated Mutations in Autism and Cancer. **2023**, 127, 634-647	1
741	NE-RDFE : A protocol and toolkit for computing relative dissociation free energies with GROMACS between dissimilar molecules using bidirectional nonequilibrium dual topology schemes.	0
740	Capillary force exerted by water bridge on cellulose nanocrystals: Effect of an external electric field..	0
739	Polypropylene carbonate-based electrolytes as model for a different approach towards improved ion transport properties for novel electrolytes. **2023**, 25, 4810-4823	0
738	Molecular Simulation of CO2 and H2 Encapsulation in a Nanoscale Porous Liquid. **2023**, 13, 409	0

737	Water model determines thermosensitive and physicochemical properties of poly(N-isopropylacrylamide) in molecular simulations. 10,	0
736	In silico profiling of nonsynonymous SNPs of fat mass and obesity-associated gene: possible impacts on the treatment of non-alcoholic fatty liver disease. **2023**, 22,	0
735	Identification of potential inhibitor molecule against MabA protein of Mycobacterium leprae by integrated in silico approach. 1-16	0
734	HuR modulation with tanshinone mimics impairs LPS response in murine macrophages.	0
733	Molecular Simulation of Pervaporation on Polyurethane Membranes. **2023**, 13, 128	0
732	Site-Specific Antibody Assembly on Nanoparticles via a Versatile Coating Method for Improved Cell Targeting. 2206546	0
731	Genomics, metagenomics, and pan-genomics approaches in COVID-19. **2023**, 23-39	0
730	Elucidating Collective Translocation of Nanoparticles Across the Skin Lipid Matrix: A Molecular Dynamics Study.	0
729	Reconfigurable Peptide Analogs of Apolipoprotein A-I Reveal Tunable Features of Nanodisc Assembly.	0
728	Allosteric communication induced by GTP binding sets off a closed-to-open transition in a bacterial dynamin-like protein.	0
727	Estimation of Nanoparticle□ Surface Electrostatic Potential in Solution Using Acid□Base Molecular Probes I: In Silico Implementation for Surfactant Micelles. **2023**, 127, 1022-1030	1
726	Local Molecular Field Theory for Coulomb Interactions in Aqueous Solutions. **2023**, 127, 809-821	0
725	Assessment of Different Parameters on the Accuracy of Computational Alanine Scanning of Protein□Protein Complexes with the Molecular Mechanics/Generalized Born Surface Area Method. **2023**, 127, 944-954	0
724	Effect of substrate charge density on the adsorption of intrinsically disordered protein amyloid □40: a molecular dynamics study.	0
723	Physical properties of phospholipids at low temperatures through Slipid force field. **2023**, 2436, 012025	1
722	Study on the solubilization effect of 7-ethyl-10-hydroxycamptothecin based on molecular docking and molecular dynamics simulation. **2023**, 29,	0
721	Upstream of N-Ras C-terminal cold shock domains mediate poly(A) specificity in a novel RNA recognition mode and bind poly(A) binding protein.	0
720	Complexity of Guanine Quadruplex Unfolding Pathways Revealed by Atomistic Pulling Simulations.	0

719	Influencing Molecular Dynamics Simulations of Ion-Exchange Membranes by Considering Comonomer Propagation.	0
718	Rigid Base Biasing in Molecular Dynamics Enables Enhanced Sampling of DNA Conformations.	0
717	Lateral membrane organization as target of an antimicrobial peptidomimetic compound.	0
716	Discovery of differentially expressed novel miRNAs in breast normal cells and their putative targets.	0
715	Interaction of Tryptophan- and Arginine-Rich Antimicrobial Peptide with E. coli Outer Membrane: A Molecular Simulation Approach. **2023**, 24, 2005	1
714	Impact of an Ionic Liquid on Amino Acid Side Chains: A Perspective from Molecular Simulation Studies.	0
713	Mapping the Three-Dimensional Nanostructure of the Ionic Liquid–Solid Interface Using Atomic Force Microscopy and Molecular Dynamics Simulations. 2202110	0
712	A physicochemical cause of betaine lipid evolutionary loss in seed plants?.	0
711	Molecular Simulation on Hydrate Nucleation in the Presence of Initial Ih Ice and Nanobubble.	0
710	In silico investigation of cytochrome bc1 molecular inhibition mechanism against Trypanosoma cruzi. **2023**, 17, e0010545	0
709	A Computational Inter-Species Study on Safrole Phase I Metabolism-Dependent Bioactivation: A Mechanistic Insight into the Study of Possible Differences among Species. **2023**, 15, 94	0
708	Roles of Tryptophan and Charged Residues on the Polymorphisms of Amyloids Formed by K-Peptides of Hen Egg White Lysozyme Investigated through Molecular Dynamics Simulations. **2023**, 24, 2626	0
707	In silico Identification of Potential Human Acetylcholinesterase Inhibitors from the Nigella sativa Phytochemicals. **2023**, 13, 112-117	0
706	Molecular Modeling and In Vitro Antiproliferative Activity Studies of Some Imidazole and Isoxazole Derivatives. **2023**, 135066	1
705	Surface Properties of N,N-Dimethylformamide–Water Mixtures, As Seen from Computer Simulations. **2023**, 127, 1050-1062	0
704	Manifestation of Hydrogen Bonding and Exciton Delocalization on the Absorption and Two-Dimensional Electronic Spectra of Chlorosomes. **2023**, 127, 1097-1109	0
703	Revisiting the Sweet Taste Receptor T1R2-T1R3 through Molecular Dynamics Simulations Coupled with a Noncovalent Interactions Analysis. **2023**, 127, 1110-1119	0
702	Effects of molecular size and orientation on the interfacial properties and wetting behavior of water/n-alkane systems: a molecular-dynamics study.	0

701	GPU-Enhanced DFTB Metadynamics for Efficiently Predicting Free Energies of Biochemical Systems. **2023**, 28, 1277	0
700	Effect of Charge State on the Equilibrium and Kinetic Properties of Mechanically Interlocked [5]Rotaxane: A Molecular Dynamics Study. **2023**, 127, 1254-1263	0
699	Tackling hysteresis in conformational sampling how to be forgetful with MEMENTO.	0
698	Conformational Dynamics and Stability of Bilayers Formed by Mycolic Acids from the Mycobacterium tuberculosis Outer Membrane. **2023**, 28, 1347	0
697	Inhibited complete folding of consecutive human telomeric G-quadruplexes.	0
696	Dimerization mechanism of an inverted-topology ion channel in membranes.	0
695	Molecular engineering of a minimal E-cadherin inhibitor protein derived from Clostridium botulinum hemagglutinin. **2023**, 102944	0
694	In vitro contraceptive activities, molecular docking, molecular dynamics, MM-PBSA, non-covalent interaction and DFT studies of bioactive compounds from Aegle marmelos. Linn., leaves. 11,	0
693	Molecular dynamics study of Cl permeation through cystic fibrosis transmembrane conductance regulator (CFTR). **2023**, 80,	0
692	Density functional modeling, and molecular docking with SARS-CoV-2 spike protein (Wuhan) and omicron S protein (variant) studies of new heterocyclic compounds including a pyrazoline nucleus. 1-15	0
691	In silico approach to identify novel allosteric intracellular antagonist for blocking the interleukin-8/CXCR2 receptor signaling pathway. 1-14	0
690	Anillin Related Mid1 as an Adaptive and Multimodal Contractile Ring Anchoring Protein: A Simulation Study.	0
689	Study of the Rv1417 and Rv2617c Membrane Proteins and Their Interactions with Nicotine Derivatives as Potential Inhibitors of Erp Virulence-Associated Factor in Mycobacterium tuberculosis: An In Silico Approach. **2023**, 13, 248	0
688	Extraction of Cerium (III) by a Solvent Extraction Technique Using Diaminododecylphosphonic Acid (DADTMTPA): Experimental, Density Functional Theory and Molecular Dynamic Studies. **2023**, 8,	0
687	Molecular interaction modeling of carbon nanotubes and fullerene toward prioritized targets of SARS-CoV-2 by computer-aided screening and docking studies. **2023**, 157-179	0
686	Molecular Dynamics Simulations of Asphaltene Aggregation: Machine-Learning Identification of Representative Molecules, Molecular Polydispersity, and Inhibitor Performance. **2023**, 8, 4862-4877	0
685	Identification of Novel CB2 Ligands through Virtual Screening and In Vitro Evaluation.	0
684	The molecular mechanism of selective and active transport in a Na+/Ca2+exchanger.	1

683	Membrane cholesterol regulates inhibition and substrate transport by the glycine transporter, GlyT2. **2023**, 6, e202201708	0
682	Toward an understanding of the conformational plasticity of S100A8 and S100A9 Ca2+-binding proteins. **2023**, 102952	0
681	Druggable sites identification in Streptococcus mutans VicRK system evaluated by catechols. 1-16	0
680	Impact of structural sampling, coupling scheme and state of interest on the energy transfer in CP29.	0
679	MetaDOCK: A Combinatorial Molecular Docking Approach.	0
678	Human Amylin in the Presence of SARS-COV-2 Protein Fragments.	0
677	Japanese evaluated nuclear data library version 5: JENDL-5. **2023**, 60, 1-60	3
676	Porous Electrospun Films with Reversible Photoresponsive Microenvironmental Humidity Regulation: A Controllable Hydrogen-Bonding Synergistic Effect Exhibited by Acrylic Acid Segments. **2023**, 15, 6187-6201	0
675	Theoretical and Experimental Study of Molecular Interactions of Fluralaner with Lipid Membranes. **2023**, 71, 2134-2142	0
674	Structural Insights into Plasticity and Discovery of Flavonoid Allosteric Inhibitors of Flavivirus NS2B□NS3 Protease. **2023**, 3, 71-92	0
673	High-density liquid (HDL) adsorption at the supercooled water/vapor interface and its possible relation to the second surface tension inflection point. **2023**, 158, 054503	2
672	FSHR activation through small molecule modulators: Mechanistic insights from MD simulations. **2023**, 154, 106588	0
671	Distinct roles of graphene and graphene oxide nanosheets in regulating phospholipid flip-flop. **2023**, 637, 112-122	0
670	Interaction mechanisms of the binding of polychlorinated biphenyls to thyroid hormone transporters revealed based on quantum chemistry and spectroscopy. **2023**, 1281, 135104	0
669	Carboxyl PEGylation of magnetic nanoparticles as antithrombotic and thrombolytic agents by calcium binding. **2023**, 638, 672-685	0
668	A molecular dynamics study on nanobubble formation and dynamics via methane hydrate dissociation. **2023**, 341, 127650	0
667	Assessment of alteration in antiviral plasma concentration across dialysis days: computational and analytical study. **2022**, 14, 1563-1581	0
666	Screening of Secondary Metabolite Compounds of Gorontalo Traditional Medicinal Plants Using the In Silico Method as a Candidate for SARS-CoV-2 Antiviral. **2023**, 25, 382-393	0

665	MISA-MD: A New Design of Molecular Dynamics Software for GPU Architecture *. **2022**,	0
664	State-of-the-art experimental and computational approaches to investigate structure, substrate recognition, and catalytic mechanism of enzymes. **2023**, 75-107	0
663	Distinct effects of zwitterionic molecules on ionic solvation in (ethylene oxide)10: a molecular dynamics simulation study. **2023**, 25, 8180-8189	0
662	The Effect of Cholesterol in SOPC Lipid Bilayers at Low Temperatures. **2023**, 13, 275	0
661	Theoretical Study on Thermal Structural Fluctuation Effects of Intermolecular Configurations on Singlet Fission in Pentacene Crystal Models. **2023**, 127, 1883-1893	0
660	Influence of the Chemical Structure on the Mechanical Relaxation of Dendrimers. **2023**, 15, 833	0
659	Computational analysis of structural and functional evaluation of the deleterious missense variants in the human CTLA4 gene. 1-18	0
658	Molecular Dynamics Simulation of Adsorption and Absorption Behavior of Shale Oil in Realistic Kerogen Slits. **2023**, 37, 3654-3671	0
657	Identification and Molecular Mechanism of Novel Immunomodulatory Peptides from Gelatin Hydrolysates: Molecular Docking, Dynamic Simulation, and Cell Experiments. **2023**, 71, 2924-2934	0
656	Effect of Newly Synthesized Structures of Peptides on the Stability of the Monolayers Formed. **2023**, 24, 4318	0
655	Ambipolar charge transport in a non-fullerene acceptor. **2023**, 11, 021105	0
654	The effect of rhamnolipids on fungal membrane models as described by their interactions with phospholipids and sterols: An in silico study. 11,	0
653	Bottom-Up Informed and Iteratively Optimized Coarse-Grained Non-Markovian Water Models with Accurate Dynamics. **2023**, 19, 1099-1110	0
652	Stability and structural evolution of double-stranded DNA molecules under high pressures: A molecular dynamics study. 11,	0
651	Gold Nanorods Inhibit Tumor Metastasis by Regulating MMP-9 Activity: Implications for Radiotherapy.	0
650	Physics-based generative model of curvature sensing peptides; distinguishing sensors from binders. **2023**, 9,	0
649	Exploring the structural basis to develop efficient multi-epitope vaccines displaying interaction with HLA and TAP and TLR3 molecules to prevent NIPAH infection, a global threat to human health. **2023**, 18, e0282580	0
648	Machine learning based charge mobility prediction for organic semiconductors. **2023**, 158, 094102	0

647	OneOPES, a combined enhanced sampling method to rule them all.	0
646	Insight to the Local Structure of Mixtures of Imidazolium-Based Ionic Liquids and Molecular Solvents from Molecular Dynamics Simulations and Voronoi Analysis. **2023**, 127, 2534-2545	0
645	Cage Dynamics-Mediated High Ionic Transport in Li-O2 Batteries with a Hybrid Aprotic Electrolyte: LiTFSI, Sulfolane, and N,N-Dimethylacetamide. **2023**, 127, 2991-3000	0
644	Discovering highly potent antimicrobial peptides with deep generative model HydrAMP. **2023**, 14,	1
643	Toward overcoming pyrethroid resistance in mosquito control: the role of sodium channel blocker insecticides.	0
642	Partial Destabilization of Amyloid-Protofibril by Methionine Photo-Oxidation: A Molecular Dynamic Simulation Study. **2023**, 8, 10148-10159	0
641	Label-Free Digital Holotomography Reveals Ibuprofen-Induced Morphological Changes to Red Blood Cells.	0
640	AB-Gen: Antibody Library Design with Generative Pre-trained Transformer and Deep Reinforcement Learning.	0
639	Inner pore hydration free energy controls the´activation of big potassium channels. **2023**, 122, 1158-1167	0
638	Experimental and computational studies on the ion dissociation states of 1-butyl-3-methyimidazolium tetrafluoroborate in water and alcohols. **2023**, 375, 121370	0
637	Memorable full-color circularly polarized luminescence from chiral co-assembled polymer films enabled by multipath transfer. **2023**, 66, 1169-1178	1
636	In silico design of photoresponsive peptide-based hydrogel with controllable structural and rheological properties. **2023**, 663, 131020	1
635	Bias-force guided simulations combined with experimental validations towards GPR17 modulators identification. **2023**, 160, 114320	0
634	Contribution of air-water interface in removing PFAS from drinking water: adsorption, stability, interaction and machine learning studies. **2023**, 119947	0
633	P1 Push-Pull Dye as a Case Study in QM/MM Theoretical Characterization for Dye-sensitized Solar Cell Organic Chromophores**. **2023**, 8,	0
632	The effects of adsorbed benzo(a)pyrene on dynamic behavior of polystyrene nanoplastics through phospholipid membrane: A molecular simulation study. **2023**, 224, 113211	0
631	High-efficiency stretchable light-emitting polymers from thermally activated delayed fluorescence.	0
630	Unique structure of ozoralizumab, a trivalent anti-TNFNANOBODY compound, offers the potential advantage of mitigating the risk of immune complex-induced inflammation. 14,	0

629	Leveraging Advanced In Silico Techniques in Early Drug Discovery: A Study of Potent Small-Molecule YAP-TEAD PPI Disruptors.	0
628	Bioinformatics and computational chemistry approaches to explore the mechanism of the anti-depressive effect of ligustilide. **2023**, 13,	0
627	Bridging Thermodynamics, Antimicrobial Activity, and pH Sensitivity of Cationic Membranolytic Heptapeptides: A Computational and Experimental Study.	0
626	Designing of multi-epitope peptide vaccine against Acinetobacter baumannii through combined immunoinformatics and protein interaction based approaches.	0
625	Triazole based Schiff bases and their oxovanadium(IV) complexes: Synthesis, characterization, antibacterial assay, and computational assessments. **2023**, 9, e15239	0
624	Sub-millisecond conformational dynamics of the A2A adenosine receptor revealed by single-molecule FRET. **2023**, 6,	0
623	Embedding Beyond Electrostatics: The Extended Polarizable Density Embedding Model. **2023**, 127, 3248-3256	0
622	Compartmentalization of the SUMO/RNF4 pathway by SLX4 drives DNA repair. **2023**,	0
621	Gamma-Hemolysin Components: Computational Strategies for LukF-Hlg2 Dimer Reconstruction on a Model Membrane. **2023**, 24, 7113	0
620	Molecular dynamics investigation on the vapor–liquid interface behavior of long-chain alkanes, alcohols, and their mixtures. **2023**, 375, 121283	0
619	Structural evolution of the butylated hydroxytoluene/menthol hydrophobic eutectic solvent upon methanol and ethanol cosolvent addition. **2023**, 375, 121302	0
618	Exploring the deagglomerating behaviors of selected additives on oxidized asphaltenes using the steered molecular dynamics approach. **2023**, 375, 121327	0
617	Finely tuning the microporosity in phosphoric acid doped triptycene-containing polybenzimidazole membranes for highly permselective helium and hydrogen recovery. **2023**, 672, 121474	0
616	Phosphatidylcholine in the tear film of the eye: Enhanced topical delivery of fluorometholone to the eye. **2023**, 150, 110506	0
615	Network pharmacology-integrated molecular docking analysis of phytocompounds of Caesalpinia pulcherrima (peacock flower) as potential anti-metastatic agents. 1-17	0
614	Inhibition effect of novel amphiphilic poly(amino acid)s on methane hydrate. **2023**, 113, 204971	0
613	Free volume in physical absorption of carbon dioxide in ionic liquids: Molecular dynamics supported modeling. **2023**, 313, 123464	0
612	Multiscale modeling of molecule transport through skin: deeper layers. **2023**, 26, 100267	0

611 Influence of BAKs on tear film lipid layer: In vitro and in silico models. **2023**, 186, 65-73 0

610 Room for improvement in the initial martini 3 parameterization of peptide interactions. **2023**, 819, 140436 0

609 Ethanol effects on L-type voltage-gated calcium channel performance. **2023**, 378, 121634 0

608 Conformational stability of the deamidated and mutated human β2-crystallin. **2023**, 296, 106986 0

607 Bioinformatics approaches to discovering food-derived bioactive peptides: Reviews and perspectives. **2023**, 162, 117051 0

606 Computational design of cyclic peptides to inhibit protein-peptide interactions. **2023**, 296, 106987 0

605 Novel NQO1 substrates bearing two nitrogen redox centers: Design, synthesis, molecular dynamics simulations, and antitumor evaluation. **2023**, 134, 106480 0

604 Identification of alkaloid compounds as potent inhibitors of Mycobacterium tuberculosis NadD using computational strategies **2023**, 158, 106863 0

603 In silico evaluation of geroprotective phytochemicals as potential sirtuin 1 interactors. **2023**, 161, 114425 0

602 2?,4?-Dihydroxy-6?-methoxy-3?,5?-dimethylchalcone and its amino acid-conjugated derivatives induce G0/G1 cell cycle arrest and apoptosis via BAX/BCL2 ratio upregulation and in silico insight in SiHa cell lines. **2023**, 184, 106390 0

601 Molecular modelling of ionic liquids: Perfluorinated anionic species with enlarged halogen substitutions. **2023**, 378, 121599 0

600 Aqueous solutions of chiral ionic liquids based on (l)-menthol: An experimental and computational study of volumetric and transport properties. **2023**, 378, 121591 0

599 The state of art in the prediction of efficiency and modeling of the processes of benzene removal from water environment. **2023**, 378, 121553 0

598 Synthesis of benzylidene-indandione derivatives as quantification of amyloid fibrils. **2023**, 296, 106982 0

597 Effect of water content on transport properties and interactions of amino-functionalized ionic liquids. **2023**, 569, 111852 0

596 Selective recovery of lithium from mother liquor of Li2CO3 by synergistic hydrophobic deep eutectic solvents: Performance and mechanistic insight. **2023**, 313, 123353 0

595 Towards understanding the interaction of quercetin with chitosan-phytate complex: An experimental and computational investigation. **2023**, 380, 121673 0

594 Assessment of CO2-Oil swelling behavior using molecular dynamics simulation: CO2 utilization and storage implication. **2023**, 379, 121582 0

593	Selective vitamins as potential options for dietary therapeutic interventions: In silico and In vitro insights from mutant C terminal fragment of FGA. **2023**, 230, 106290	0
592	GAP positions catalytic H-Ras residue Q61 for GTP hydrolysis in molecular dynamics simulations, complicating chemical rescue of Ras deactivation. **2023**, 104, 107835	0
591	Experimental and computational approaches to characterize a novel amidase that initiates the biodegradation of the herbicide propanil in Bosea sp. P5. **2023**, 451, 131155	0
590	A seminal perspective on the role of chondroitin sulfate in biomineralization. **2023**, 310, 120738	0
589	Computational identification of drug-like marine natural products as potential RNA polymerase inhibitors against Nipah virus. **2023**, 104, 107850	0
588	Molecular dynamics simulation study on interfacial behaviors of betaines and extended surfactants. **2023**, 666, 131323	0
587	Molecular insight into the effect of the number of introduced ethoxy groups on the calcium resistance of anionic-nonionic surfactants at the oil/water interface. **2023**, 667, 131382	0
586	The crystal structure of Mycobacterium thermoresistibile MurE ligase reveals the binding mode of the substrate m-diaminopimelate. **2023**, 215, 107957	0
585	Solvation structure and dynamics of a small ion in an organic electrolyte. **2023**, 440, 114666	0
584	A computational study of cellulose regeneration: All-atom molecular dynamics simulations. **2023**, 311, 120768	0
583	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	0
582	The state of art in the prediction of mechanism and modeling of the processes of surface functionalized carbon nanotubes into the membrane cell. **2023**, 623, 157039	0
581	Comparing supercapacitors with graphene/graphyne electrodes and [Bmim][PF6], [Emim][BF4], [Ch][Gly] and [Pyr][Tfsi] ionic liquids using molecular dynamics. **2023**, 379, 121703	0
580	The effects of functionalization of imidazolium-based ionic liquid electrolytes on the lithium-ion transport. **2023**, 64, 107197	0
579	Effects of nanobubbles on methane hydrate dissociation: A molecular simulation study. **2023**, 345, 128230	0
578	Theoretical study on the mechanism of aggregation-induced emission in red thermally activated delayed fluorescence molecules: trans/cis-arrangement effect. **2023**, 119, 106811	0
577	Elucidating the effects of emulsification on the thermal performances of palm oil-based phase change materials by molecular dynamics simulations. **2023**, 64, 107071	0
576	5-Oxohexahydroquinolines bearing 4-pyridyl methyl carboxylate as P-glycoprotein inhibitors and multidrug resistance reversal agents in cancer cells. **2023**, 1285, 135427	0

575	A molecular dynamics study on polybenzimidazole based proton exchange membrane with dual proton conductors. **2023**, 677, 121618	0
574	Non-aqueous organic redox active materials for a bicontinuous microemulsion-based redox flow battery. **2023**, 34, 101286	0
573	Hierarchical Self-Assembly of Organic–Inorganic Hybrid Nanosheets to Construct Tubular Superstructures for Photocatalytic Degradation. **2023**, 6, 6270-6278	0
572	Influence of electronic polarization on the binding of anions to a chloride-pumping rhodopsin. **2023**, 122, 1548-1556	0
571	Miscibility of Phosphatidylcholines in Bilayers: Effect of Acyl Chain Unsaturation. **2023**, 13, 411	0
570	Resolving Protein Conformational Plasticity and Substrate Binding via Machine Learning.	0
569	Numerical simulation of peristalsis to study co-localization and intestinal distribution of a macromolecular drug and permeation enhancer. **2023**, 240, 124388	0
568	Specific ion effects on the aggregation of polysaccharide-based polyelectrolyte complex particles induced by monovalent ions within Hofmeister series. **2023**, 643, 305-317	0
567	The molecular basis of the antidepressant action of the magic mushroom extract, psilocin. **2023**, 1871, 140914	0
566	Study on the zinc ions binding to human lactoferrin. **2023**, 1282, 135149	0
565	Composition effects on thermodynamic properties and interfacial structure in styrene-butadiene rubber: A combined experimental and simulation study. **2023**, 275, 118750	0
564	Synthesis and evaluation of the antioxidant and anti-tyrosinase activities of thiazolyl hydrazone derivatives and their application in the anti-browning of fresh-cut potato. **2023**, 414, 135745	0
563	Uncovering the mechanisms of cyclic peptide self-assembly in membranes with the chirality-aware MA(R/S)TINI forcefield. **2023**, 642, 84-99	0
562	Molecular dynamics simulations of the calmodulin-induced α-helix in the SK2 calcium-gated potassium ion channel. **2023**, 299, 102850	0
561	Structure restoration and aggregate inhibition of V30M mutant transthyretin protein by potential quinoline molecules. **2023**, 231, 123318	2
560	Interphase chromosomes of the Aedes aegypti mosquito are liquid crystalline and can sense mechanical cues. **2023**, 14,	0
559	Omicron mutations increase interdomain interactions and reduce epitope exposure in the SARS-CoV-2 spike. **2023**, 26, 105981	0
558	Photosensitizers Dispersed on Nanosized Triterpenoid Matrix with Deaggregation-Enhanced Singlet Oxygen Production. **2023**, 15, 4973-4983	0

557	The heptapeptide somatostatin analogue TT-232 exerts analgesic and anti-inflammatory actions via SST4 receptor activation: In silico, in vitro and in vivo evidence in mice. **2023**, 209, 115419	0
556	Exposure to the electric field: A potential way to block the aggregation of histidine tautomeric isomers of β-amyloid. **2023**, 232, 123385	0
555	Deciphering the interactions of genistein with β-cyclodextrin derivatives through experimental and microsecond timescale umbrella sampling simulations. **2023**, 374, 121295	0
554	Simulation of two-dimensional infrared Raman spectroscopy with application to proteins. **2023**, 158, 064106	0
553	Epigallocatechin gallate inhibits Francisella tularensis growth and suppresses the function of DNA-binding protein HU. **2023**, 176, 105999	0
552	Molecular dynamics study of the effect of temperature on the flotation behavior of sodium oleate on the surface of diaspore. **2023**, 192, 108004	0
551	Unexpected Behavior of Chloride and Sulfate Ions upon Surface Solvation of Martian Salt Analogue. **2023**, 7, 350-359	0
550	The role of conformational change and key glutamic acid residues in the ClC-ec1 antiporter. **2023**, 122, 1068-1085	0
549	Structural basis for triacylglyceride extraction from mycobacterial inner membrane by MFS transporter Rv1410.	0
548	Integrated computational and experimental approach for novel anti-leishmanial molecules by targeting Dephospho-coenzyme A kinase. **2023**, 232, 123441	0
547	Insights into sorption and molecular transport of atrazine, testosterone, and progesterone onto polyamide microplastics in different aquatic matrices. **2023**, 318, 137949	0
546	On the Behavior of the Ethylene Glycol Components of Polydisperse Polyethylene Glycol PEG200. **2023**, 127, 1178-1196	0
545	Biochemical Properties of Naturally Occurring Human Bloom Helicase Variants.	0
544	Crystal Structure of the Extracellular Domains of GPR110. **2023**, 435, 167979	0
543	Molecular dynamics study of the exchange processes of heavy metals into montmorillonite: Characterization of hydrated edge surfaces and dynamic exchange mechanism. **2023**, 150, 105587	0
542	Computational analysis of water dynamics in AOT reverse micelles. **2023**, 375, 121340	0
541	A high-resolution α-glucosidase inhibition profiling for targeted identification of natural antidiabetic products from Lycopodiella cernua (L.) Pic. Serm and their inhibitory mechanism study. 1-13	0
540	Molecular Dynamics Simulation& X-Ray Scattering Show κ-Carrageenan Disorder-Order Transition to Be Double-Helix Formation.	0

539	Theoretical and experimental studies of chitin nanocrystals treated with ionic liquid or deep eutectic solvent to afford nanochitosan sheets. **2023**, 375, 121350	0
538	The molecular mechanisms of plasticizers in rejuvenating oxidized asphalt: A preliminary study. **2023**, 226, 111677	0
537	Structural analysis of water networks. **2022**, 11,	0
536	Long-time-step molecular dynamics can retard simulation of protein-ligand recognition process. **2023**, 122, 802-816	0
535	Identification of peptide binding sequence of TRIM25 on 14-3-3□by bioinformatics and biophysical techniques. 1-11	0
534	Mutated axon guidance gene PLXNB2 sustains growth and invasiveness of stem cells isolated from cancers of unknown primary. **2023**, 15,	1
533	Unique effect of clozapine on adenosine A2A-dopamine D2 receptor heteromerization. **2023**, 160, 114327	2
532	Exploring staphylococcal superantigens to design a potential multi-epitope vaccine against Staphylococcus aureus: an in-silico reverse vaccinology approach. 1-15	0
531	Elucidating the Molecular Origins of the Transference Number in Battery Electrolytes Using Computer Simulations. **2023**, 3, 306-315	0
530	Investigation of biological activities of two cultivars of Cicer arietinum proteins mass associated with A lzheimer's disease.	0
529	Phosphate aggregation, diffusion, and adsorption on kaolinite in saline solutions by molecular dynamics simulation. **2023**, 233, 106844	0
528	Simulation of AOT reverse micelles with polyethylenimine in hexane. **2023**, 301, 283-291	0
527	Functional analysis of metalloenzymes from human gut microbiota and their role in ulcerative colitis. **2023**, 134,	0
526	Structural Basis for Agonistic Activity and Selectivity toward Melatonin Receptors hMT1 and hMT2. **2023**, 24, 2863	1
525	Toxicological impacts and likely protein targets of bisphenol a in Paramecium caudatum. **2023**, 88, 125958	0
524	Unveiling New Druggable Pockets in Influenza Non-Structural Protein 1: NS1□Host Interactions as Antiviral Targets for Flu. **2023**, 24, 2977	0
523	Topological dual and extended relations between networks of clathrate hydrates and Frank-Kasper phases. **2023**, 14,	0
522	Design, Synthesis, and Biological Evaluation of 2-Aminothiazole Derivatives as Novel Checkpoint Kinase 1 (CHK1) Inhibitors. **2023**, 18,	0

521	Multi-Hydration Induced Zwitterionic Hydrogel with Open Environment Stability for Chemical Sensing. 2200061	0
520	Interaction of guanidinium and ammonium cations with phosphatidylcholine and phosphatidylserine lipid bilayers Calorimetric, spectroscopic and molecular dynamics simulations study. **2023**, 1865, 184122	0
519	Fostering discoveries in the era of exascale computing: How the next generation of supercomputers empowers computational and experimental biophysics alike. **2023**,	0
518	Development of a Syrian hamster anti-PD-L1 monoclonal antibody enables oncolytic adenoviral immunotherapy modelling in an immunocompetent virus replication permissive setting. 14,	1
517	Three-Dimensional-QSAR and Relative Binding Affinity Estimation of Focal Adhesion Kinase Inhibitors. **2023**, 28, 1464	0
516	In silico identification of a promising inhibitor of Fusarium oxysporum f. sp. Lycopersici, Secreted in Xylem 1 protein.	0
515	Understanding the Free Energy Landscape of Phase Separation in Lipid Bilayers using Molecular Dynamics.	0
514	Thermodynamic regulation over nano-heterogeneous structure of electrolyte solution to improve stability of flow batteries. **2023**, 270, 118534	0
513	The effects of size and surface functionalization of polystyrene nanoplastics on stratum corneum model membranes: An experimental and computational study. **2023**, 638, 778-787	0
512	High-throughput single-molecule quantification of individual base stacking energies in nucleic acids. **2023**, 14,	0
511	Alternative Strategy for Spectral Tuning of Flavin-Binding Fluorescent Proteins. **2023**, 127, 1301-1311	0
510	HPV and molecular mimicry in systemic lupus erythematosus and an impact of compiling B-cell epitopes and MHC-class II binding profiles with in silico evidence. 1-9	0
509	Terahertz Waves Enhance the Permeability of Sodium Channels. **2023**, 15, 427	0
508	Monitoring Conformational Changes of Lysozyme Polyelectrolyte Complexes Using Trapped Ion Mobility-Mass Spectrometry (IM-MS). **2023**, 56, 1377-1398	0
507	Secreted Aspartyl Proteinases Targeted Multi-Epitope Vaccine Design for Candida dubliniensis Using Immunoinformatics. **2023**, 11, 364	0
506	Ubiquitylation of BBSome is required for ciliary assembly and signaling. **2023**, 24,	0
505	Atomistic Details of Peptide Reversed-Phase Liquid Chromatography from Molecular Dynamics Simulations. **2023**, 95, 3892-3900	0
504	Computer-Aided Virtual Screening and In Vitro Validation of Biomimetic Tyrosinase Inhibitory Peptides from Abalone Peptidome. **2023**, 24, 3154	0

503	Integrated use of ligand and structure-based virtual screening, molecular dynamics, free energy calculation and ADME prediction for the identification of potential PTP1B inhibitors.	0
502	Computational modeling of cyanobacterial phytoconstituents against toll-like receptors of skin cancer. 1-13	0
501	Thermal site energy fluctuations in photosystem I: new insights from MD/QM/MM calculations. **2023**, 14, 3117-3131	0
500	Deciphering the therapeutic role of Kigelia africana fruit in erectile dysfunction through metabolite profiling and molecular modelling. **2023**, 37, 101190	0
499	Addressing the Structural Organization of Silicone Alternatives in Formulations by Molecular Dynamics Simulations and a Novel Equilibration Protocol. **2023**, 15, 796	0
498	New 1,11-dimethyl-3,6,9-triazatricyclo[7.3.1.13,11]tetradecane-4,8,12-trione derivative as an allosteric modulator of the glutamatergic system. **2023**, 33, 70-72	0
497	APL@voro□nteractive visualization and analysis of cell membrane simulations. **2023**, 39,	0
496	Libfabric-based Injection Solutions for Portable Containerized MPI Applications. **2022**,	0
495	Comprehensive Automated Routine Implementation, Validation, and Benchmark of the Anisotropic Force Field (AUA4) Using Python and GROMACS. **2023**, 127, 1555-1563	0
494	Molecular interaction of ethylene glycol to hurt Myoglobin: Insights from spectroscopic and molecular modeling studies. **2023**, 376, 121399	0
493	Exploring anticancer potential of nintedanib conjugated magnetic nanoparticles: In-vitro and in-silico studies. **2023**, 81, 104213	0
492	Instigating the in vitro antidiabetic activity of new tridentate Schiff base ligand appended M(II) complexes: From synthesis, structural characterization, quantum computational calculations to molecular docking, and molecular dynamics simulation studies. **2023**, 37,	0
491	Structural Insights into ATP-Sensitive Potassium Channel Mechanics: A Role of Intrinsically Disordered Regions. **2023**, 63, 1806-1818	0
490	Flexibility of the Rotavirus NSP2 C-Terminal Region Supports Factory Formation via Liquid-Liquid Phase Separation. **2023**, 97,	0
489	Mechanistic Insight into the Inhibition of Choline Acetyltransferase by Proton Pump Inhibitors. **2023**, 14, 749-765	0
488	Evaluation of free radical quenching, anti-inflammatory activity together with anticancer potential of Lychnis coronaria and characterization of novel molecules from its extract through high resolution-liquid chromatography mass spectrometry coupled to structural biochemistry approach. 1-15	0
487	A variational formulation of the Harris functional as a correction to approximate Kohn□ham density functional theory. **2023**, 158, 054111	0
486	Quality assessment of VHH models. 1-15	0

485	May the force be with you: The role of hyper-mechanostability of the bone sialoprotein binding protein during early stages of Staphylococci infections. 11,	0
484	Structure-based virtual screening of novel natural products as chalcone derivatives against SARS-CoV-2 Mpro. 1-15	0
483	Papaverinol-N-Oxide: A Microbial Biotransformation Product of Papaverine with Potential Antidiabetic and Antiobesity Activity Unveiled with In Silico Screening. **2023**, 28, 1583	0
482	Vanillin-Based Indolin-2-one Derivative Bearing a Pyridyl Moiety as a Promising Anti-Breast Cancer Agent via Anti-Estrogenic Activity. **2023**, 8, 6968-6981	0
481	In Silico Discovery of Small Molecule Modulators Targeting the Achilles□Heel of SARS-CoV-2 Spike Protein.	0
480	Alizarin as a potential protector of proteins against damage caused by hydroperoxyl radical. **2023**, 373, 110395	0
479	Sodium/Iodide Symporter Metastable Intermediates Provide Insights into Conformational Transition between Principal Thermodynamic States. **2023**, 127, 1540-1551	0
478	Coupled binding and folding of disordered SPIN N-terminal region in myeloperoxidase inhibition. 10,	0
477	Does the SARS-CoV-2 Spike Receptor-Binding Domain Hamper the Amyloid Transformation of Alpha-Synuclein after All?. **2023**, 11, 498	0
476	Bringing Quantum Mechanics to Coarse-Grained Soft Materials Modeling. **2023**, 35, 1470-1486	0
475	Lipidation Alters the Structure and Hydration of Myristoylated Intrinsically Disordered Proteins. **2023**, 24, 1244-1257	0
474	Predicting binding affinity changes from long-distance mutations using molecular dynamics simulations and Rosetta.	0
473	Mechanism of Calcium Permeation in a Glutamate Receptor Ion Channel. **2023**, 63, 1293-1300	1
472	Structural Insights into the Antiparallel G-Quadruplex in the Presence of K+ and Mg2+ Ions. **2023**, 127, 1499-1512	0
471	New benzimidazole-oxadiazole derivatives: Synthesis, □glucosidase, □amylase activity, and molecular modeling studies as potential antidiabetic agents.	0
470	Computational multi-target approach to target essential enzymes of Leishmania donovani using comparative molecular dynamic simulations and MMPBSA analysis.	0
469	Engineering solvation in initiated chemical vapour deposition for control over polymerization kinetics and material properties. **2023**, 2, 373-383	0
468	Discovery of potential FGFR3 inhibitors via QSAR, pharmacophore modeling, virtual screening and molecular docking studies against bladder cancer. **2023**, 21,	0

467	Insights into the substrate specificity, structure, and dynamics of plant histidinol-phosphate aminotransferase (HISN6). **2023**, 196, 759-773	0
466	Caffeic Acid Has Antiviral Activity against Ilh□s Virus In Vitro. **2023**, 15, 494	0
465	Machine learning facilitated structural activity relationship approach for the discovery of novel inhibitors targeting EGFR. 1-19	0
464	Discovery of AcrAB-TolC pump inhibitors: Virtual screening and molecular dynamics simulation approach. 1-18	0
463	Identification of metal ion-binding sites in RNA structures using deep learning method. **2023**, 24,	0
462	Effect of carbonaceous ultrafine particles on the structure and oligomerization of A□2 peptide. **2023**, 323, 121273	0
461	Histone variant H2A.Z modulates nucleosome dynamics to promote DNA accessibility. **2023**, 14,	0
460	Investigating the binding affinity of andrographolide against human SARS-CoV-2 spike receptor-binding domain through docking and molecular dynamics simulations. 1-16	0
459	Unique Amphipathic□helix Drives Membrane Insertion and Enzymatic Activity of ATG3.	0
458	The Evolution of Hydrogen Bond Network in Nafion via Molecular Dynamics Simulation. **2023**, 56, 1688-1703	0
457	Molecular Thermodynamic Origin of Substrate Promiscuity in the Enzyme Laccase: Toward a Broad-Spectrum Degrader of Dye Effluents. **2023**, 14, 1892-1898	0
456	NS1 from Two Zika Virus Strains Differently Interact with a Membrane: Insights to Understand Their Differential Virulence. **2023**, 63, 1386-1400	0
455	Design of multi-epitope based vaccine against Mycobacterium tuberculosis: a subtractive proteomics and reverse vaccinology based immunoinformatics approach. 1-19	0
454	Illumination of a progressive allosteric mechanism mediating the glycine receptor activation. **2023**, 14,	0
453	Structures of NF-□ p52 homodimer-DNA complexes rationalize binding mechanisms and transcription activation. 12,	0
452	Rheological Performance of High-Temperature-Resistant, Salt-Resistant Fracturing Fluid Gel Based on Organic-Zirconium-Crosslinked HPAM. **2023**, 9, 151	0
451	Molecular dynamics simulations reveal the effect of mutations in the RING domains of BRCA1-BARD1 complex and its relevance to the prognosis of breast cancer. 1-19	0
450	Temperature dependence of DNA elasticity: An all-atom molecular dynamics simulation study. **2023** , 158, 094902	0

449	Sensory input-dependent gain modulation of the optokinetic nystagmus by mid-infrared stimulation in pigeons. 12,	0
448	Structure-modified polymeric carbon-dots with lowered retention and enhanced colloidal stability in porous media for tracer application at extreme reservoir condition. **2023**, 32, 101014	0
447	The combination of polyphenols and phospholipids as an efficient platform for delivery of natural products. **2023**, 13,	0
446	Understanding hydrogen adsorption performance of lithium-doped MIL-101(Cr) by molecular simulations: Effects of lithium distribution. **2023**,	0
445	A localized high concentration carboxylic ester-based electrolyte for high-voltage and low temperature lithium batteries. **2023**, 461, 141904	0
444	Determination of protein conformation and orientation at buried solid/liquid interfaces. **2023**, 14, 2999-3009	1
443	Hexamethylenetetramine additive with zincophilic head and hydrophobic tail for realizing ultra-stable Zn anode. **2023**, 460, 141902	0
442	Investigating the self-assembling of nicotinic hydrazide-based amphiphile into nano-range vesicles and its amphotericin B loading applications. **2023**, 30,	0
441	Evaluation of the affinity of asphaltene molecular models A1 and A2 by the water/oil interfaces based on a novel concept of solubility parameter profiles obtained from MD simulations. **2023**, 376, 121430	0
440	Inviting C5-Trifluoromethylated Pseudoprolines into Collagen Mimetic Peptides. **2023**, 24, 1555-1562	0
439	Using High-Throughput Molecular Dynamics Simulation to Enhance the Computational Design of Kemp Elimination Enzymes. **2023**, 63, 1323-1337	0
438	Novel Inhibitory Role of Fenofibric Acid by Targeting Cryptic Site on the RBD of SARS-CoV-2. **2023**, 13, 359	0
437	Discovery of DNA aptamers targeting SARS-CoV-2 nucleocapsid protein and protein-binding epitopes for label-free COVID-19 diagnostics. **2023**, 31, 731-743	0
436	Bestatin analogs-4-quinolinone hybrids as antileishmanial hits: Design, repurposing rational, synthesis, in vitro and in silico studies. **2023**, 250, 115211	0
435	SNP based analysis depicts phenotypic variability in heme oxygenase-1 protein. **2023**,	0
434	A computational investigation on Rho-related GTP-binding protein RhoB through molecular modeling and molecular dynamics simulation study.	0
433	Computational and Experimental Evaluation of Linker Peptides and Thioredoxin Fusion Tag in CD20-rituximab Specific Interactions. **2023**, 21,	0
432	MoSDeF-GOMC: Python Software for the Creation of Scientific Workflows for the Monte Carlo Simulation Engine GOMC. **2023**, 63, 1218-1228	1

431	Re-Balancing Replica Exchange with Solute Tempering for Sampling Dynamic Protein Conformations. **2023**, 19, 1602-1614	0
430	Unravelling the destabilization potential of ellagic acid on □synuclein fibrils using molecular dynamics simulations. **2023**, 25, 8128-8143	0
429	Structure□Thermodynamic Relationship of a Polysaccharide Gel (Alginate) as a Function of Water Content and Counterion Type (Na vs Ca). **2023**, 127, 1828-1841	0
428	Permethrin as a Potential Furin Inhibitor through a Novel Non-Competitive Allosteric Inhibition. **2023**, 28, 1883	0
427	The influence of pH on the structure and stability of the Grb2 dimer reveals changes in the inter-domain and molecular interaction: Could it be a modulation mechanism?. **2023**, 295, 106973	0
426	NanoModeler CG: A Tool for Modeling and Engineering Functional Nanoparticles at a Coarse-Grained Resolution. **2023**, 19, 1582-1591	0
425	Molecular dynamics simulations reveal the importance of amyloid-beta oligomer □sheet edge conformations in membrane permeabilization. **2023**, 299, 103034	0
424	Designing and In Silico Evaluation of Some Non-Nucleoside MbtA Inhibitors: On Track to Tackle Tuberculosis.	0
423	Structural basis for membrane attack complex inhibition by CD59. **2023**, 14,	0
422	In Silico Analysis of the Structural Dynamics and Substrate Recognition Determinants of the Human Mitochondrial Carnitine/Acylcarnitine SLC25A20 Transporter. **2023**, 24, 3946	0
421	Discovery of potent inhibitors targeting Glutathione S-transferase of Wuchereria bancrofti: a step toward the development of effective anti-filariasis drugs.	0
420	2,5-Pyridinedicarboxylic acid is a bioactive and highly selective inhibitor of D-dopachrome tautomerase. **2023**, 31, 355-367.e4	1
419	Ligand- and structure-based identification of GPER-binding small molecules. **2023**, 49, 489-496	0
418	Optimal Bond Constraint Topology for Molecular Dynamics Simulations of Cholesterol. **2023**, 19, 1592-1601	0
417	Cholesterol esters form supercooled lipid droplets whose nucleation is facilitated by triacylglycerols. **2023**, 14,	0
416	Dynamic Heterogeneity of Solvent Motion and Ion Transport in Concentrated Electrolytes. **2023**, 127, 1803-1810	0
415	Conformational changes in the human Cx43/GJA1 gap junction channel visualized using cryo-EM. **2023**, 14,	0
414	Insights into the Formation of Intermolecular Complexes of Fluorescent Probe 10-N-Nonyl Acridine Orange with Cardiolipin and Phosphatidylglycerol in Bacterial Plasma Membrane by Molecular Modeling. **2023**, 28, 1929	0

413	Structural Characterization of Nanobodies during Germline Maturation. **2023**, 13, 380	0
412	Utilizing Machine Learning to Greatly Expand the Range and Accuracy of Bottom-Up Coarse-Grained Models through Virtual Particles.	1
411	Structural and dynamic insights into □synuclein dimer conformations. **2023**, 31, 411-423.e6	0
410	Conformational Control of Fast Asparagine Deamidation in a Norovirus Capsid Protein. **2023**, 62, 1032-1043	0
409	Free energy change in the complete transport of all water molecules through a carbon nanotube. **2023**, 25, 7032-7046	0
408	Understanding the formation of surface relief gratings in azopolymers: A combined molecular dynamics and experimental study. **2023**, 158, 104905	0
407	All-Atom Molecular Dynamics Simulations Indicated the Involvement of a Conserved Polar Signaling Channel in the Activation Mechanism of the Type I Cannabinoid Receptor. **2023**, 24, 4232	0
406	Preparation of extracellular matrix of fish swim bladders by decellularization with supercritical carbon dioxide. **2023**, 10,	0
405	Study on molecular mechanisms of CD4 dependency and independency of HIV-1 gp120. **2023**, 13, 6274-6286	0
404	Quantifying Magnetic Resonance Effects Due to Solid□luid Interactions on Confined Water within Quartz-Lined Nanopores via Molecular Dynamics Simulations. **2023**, 127, 4283-4294	0
403	Determination of elastic parameters of lipid membranes from simulation under varied external pressure. **2023**, 107,	0
402	Field-Induced Hydration Shell Reorganization Enables Electro-osmotic Flow in Nanochannels. **2023**, 130,	0
401	Identification of and Mechanistic Insights into SARS-CoV-2 Main Protease Non-Covalent Inhibitors: An In-Silico Study. **2023**, 24, 4237	0
400	An in silico investigation of 1,2,4-triazole derivatives as potential antioxidant agents using molecular docking, MD simulations, MM-PBSA free energy calculations and ADME predictions. **2023**, 70, 139-153	0
399	Intrinsically disordered region of talin□ FERM domain functions as an initial PIP2 recognition site. **2023**, 122, 1277-1286	0
398	Molecular dynamics simulations and bioinformatics□analysis of deleterious missense single nucleotide polymorphisms in Glyoxalase-1 gene. 1-11	0
397	Allosteric regulation of □reaction stage I in tryptophan synthase upon the □igand binding. **2023**, 158, 115101	0
396	Molecular rotations trigger a glass-to-plastic fcc heterogeneous crystallization in high-pressure water. **2023**, 158, 114501	0

395	Molecular Dynamic Simulations Unravel the Underlying Impact of Missense Mutation in Autoimmunity Gene PTPN22 on Predisposition to Rheumatoid Arthritis. **2023**, 43, 121-132	0
394	Perylene Diimide-Containing Dynamic Hyper-crosslinked Ionic Porous Organic Polymers: Modulation of Assembly and Gas Storage. **2023**, 5, 2097-2104	0
393	MiMiCPy: An Efficient Toolkit for MiMiC-Based QM/MM Simulations. **2023**, 63, 1406-1412	0
392	Human Glucosylceramide Synthase at Work as Provided by In Silico Molecular Docking, Molecular Dynamics, and Metadynamics. **2023**, 8, 8755-8765	0
391	Influence of Cholesterol on the Membrane Binding and Conformation of Synuclein. **2023**, 127, 1956-1964	0
390	Does variation in composition affect dynamics when approaching the eutectic composition?. **2023**, 158, 114203	0
389	Characterization of the coupling mechanism of scorpion neurotoxins on the voltage-gated sodium channel hNav1.6. 1-9	0
388	Predicting mechanical properties of silk from its amino acid sequences via machine learning. **2023**, 140, 105739	0
387	Inhibiting Leishmania donovani Sterol Methyltransferase to Identify Lead Compounds Using Molecular Modelling. **2023**, 16, 330	1
386	Discovery of 4-(1,2,4-Oxadiazol-5-yl)azepan-2-one Derivatives as a New Class of Cannabinoid Type 2 Receptor Agonists for the Treatment of Inflammatory Pain. **2023**, 66, 3460-3483	0
385	Molecular Dynamics Simulation of CO2 Hydrate Growth in NaCl Aqueous Solution. **2023**, 1-7	0
384	Hierarchical Aggregation in a Complex Fluid-The Role of Isomeric Interconversion. **2023**, 127, 2052-2065	0
383	Solid phase extraction with rotating cigarette filter for determination of bisphenol A in source and drinking water: computational and analytical studies. **2023**, 39, 607-617	0
382	In-silico structural characterization and phylogenetic analysis of Nucleoside diphosphate kinase: A novel antiapoptotic protein of Porphyromonas gingivalis. **2023**, 124, 545-556	0
381	Analysis of Protein Folding Simulation with Moving Root Mean Square Deviation. **2023**, 63, 1529-1541	0
380	Common framework mutations impact antibody interfacial dynamics and flexibility. 14,	0
379	Anastrozole-mediated modulation of mitochondrial activity by inhibition of mitochondrial permeability transition pore opening: an initial perspective. 1-17	0
378	Microphysics of liquid water in sub-10 nm ultrafine aerosol particles. **2023**, 23, 2525-2556	0

377	Dissecting Phenotype from Genotype with Clinical Isolates of SARS-CoV-2 First Wave Variants. **2023**, 15, 611	1
376	Structural Elucidation of a Polypeptoid Chain in a Crystalline Lattice Reveals Key Morphology-Directing Role of the N-Terminus. **2023**, 17, 4958-4970	0
375	Machine Learning-based Modeling of Olfactory Receptors in their Inactive State: Human OR51E2 as a Case Study.	0
374	Computational predictions on Brønsted acidic ionic liquid-catalyzed carbon dioxide conversion to five-membered heterocyclic carbonyl derivatives. **2023**, 25, 8624-8630	0
373	Scaling Protein–Water Interactions in the Martini 3 Coarse-Grained Force Field to Simulate Transmembrane Helix Dimers in Different Lipid Environments. **2023**, 19, 2109-2119	1
372	Uncovering the Interaction Interface Between Harpin (Hpa1) and Rice Aquaporin (OsPIP1;3) Through Protein–Protein Docking: An In Silico Approach.	0
371	Repurposing of phyto-ligand molecules from the honey bee products for Alzheimer's disease as novel inhibitors of BACE-1: small molecule bioinformatics strategies as amyloid-based therapy. **2023**, 30, 51143-51169	0
370	Energy Coupling and Stoichiometry of Zn2+/H+Antiport by the Cation Diffusion Facilitator YiiP.	0
369	Light-Driven Conversion of Silicon Nitride Nanopore to Nanonet for Single-Protein Trapping Analysis. **2023**, 35,	0
368	The Nanostructure of Alkyl-Sulfonate Ionic Liquids: Two 1-Alkyl-3-methylimidazolium Alkyl-Sulfonate Homologous Series. **2023**, 28, 2094	0
367	Nanoscale and Real-Time Nuclear–Electronic Dynamics Simulation Study of Charge Transfer at the Donor–Acceptor Interface in Organic Photovoltaics. **2023**, 14, 2292-2300	0
366	Designing multi-epitope vaccine against important colorectal cancer (CRC) associated pathogens based on immunoinformatics approach. **2023**, 24,	0
365	Targeting 'Immunogenic hotspots' in Dengue and Zika virus: an in silico approach to a common vaccine candidate. **2023**, 18, 87-106	0
364	On the Role of Molecular Conformation of the 8-Oxoguanine Lesion in Damaged DNA Processing by Polymerases. **2023**, 63, 1521-1528	0
363	Simultaneously optimizing multiple properties of β-glucosidase Bgl6 using combined (semi-)rational design strategies and investigation of the underlying mechanisms. **2023**, 374, 128792	1
362	Tween-80 on Water/Oil Interface: Structure and Interfacial Tension by Molecular Dynamics Simulations. **2023**, 39, 3255-3265	0
361	Cation–Interactions Contribute to Hydrophobic Humic Acid Removal for the Control of Hydraulically Irreversible Membrane Fouling. **2023**, 57, 3853-3863	0
360	What is the Optimal Dipole Moment for Nonpolarizable Models of Liquids?. **2023**, 19, 1790-1804	0

359	Machine learning combines atomistic simulations to predict SARS-CoV-2 Mpro inhibitors from natural compounds.	0
358	Investigating a Library of Flavonoids as Potential Inhibitors of a Cancer Therapeutic Target MEK2 Using in Silico Methods. **2023**, 24, 4446	0
357	Structural-based design of HD-TAC7 PROteolysis TArgeting chimeras (PROTACs) candidate transformations to abrogate SARS-CoV-2 infection. 1-16	0
356	Control of boundary slip by interfacial nanobubbles: A perspective from molecular dynamics simulations. **2023**, 35, 032108	0
355	Influence of ALS -linked M337V mutation on the conformational ensembles of TDP-43 321□340 peptide monomer and dimer.	1
354	Insights into the binding mechanism of ascorbic acid and violaxanthin with violaxanthin de-epoxidase (VDE) and chlorophycean violaxanthin de-epoxidase (CVDE) enzymes.	0
353	Recent Advances in Molecular Dynamics Simulations of Tau Fibrils and Oligomers. **2023**, 13, 277	0
352	The Mechanism of Action of SAAP-148 Antimicrobial Peptide as Studied with NMR and Molecular Dynamics Simulations. **2023**, 15, 761	0
351	Effect of macrocyclization and tetramethylrhodamine labeling on chemokine binding peptides.	0
350	Modelling Complex Bimolecular Reactions in a Condensed Phase: The Case of Phosphodiester Hydrolysis. **2023**, 28, 2152	0
349	Novel in-frame duplication variant characterization in late infantile metachromatic leukodystrophy using whole-exome sequencing and molecular dynamics simulation. **2023**, 18, e0282304	0
348	Effects of flexibility in coarse-grained models for bovine serum albumin and immunoglobulin G. **2023**, 158, 084112	0
347	The Atomistic Understanding of the Ice Recrystallization Inhibition Activity of Antifreeze Glycoproteins. **2023**, 13, 405	0
346	Revealing the Key Packing Features Determining the Stability of Peptide Bilayer Membrane.	0
345	Water□ motions in x-y and z directions of 2D nanochannels: Entirely different but tightly coupled.	0
344	ATP binding by an F1Fo ATP synthase □ subunit is pH dependent, suggesting a diversity of □ subunit functional regulation in bacteria. 10,	0
343	An in silico approach to determine inter-subunit affinities in human septin complexes.	0
342	Reversible Zinc Electrodeposition at □0 °C Using a Deep Eutectic Electrolyte for Low-Temperature Zinc Metal Batteries. **2023**, 14, 2378-2386	0

341	Dipole Cooperativity and Polarization Frustration Determine the Secondary Structure Distribution of Short Alanine Peptides in Water. **2023**, 127, 3126-3138	0
340	2D MoS2 and BN Nanosheets Damage Mitochondria through Membrane Penetration. **2023**, 17, 4716-4728	0
339	Neurotherapeutic Effects of Quercetin and Its Metabolite Compounds on Cognitive Impairment and Parkinson's Disease: An In Silico Study. **2023**, 48, 151-169	0
338	Thermodynamics of the self-assembly of N-annulated perylene bisimides in water. Disentangling the enthalpic and entropic contributions. **2023**, 10, 1959-1967	0
337	Sorption–Deformation–Percolation Model for Diffusion in Nanoporous Media. **2023**, 17, 4507-4514	0
336	Effect of Glycone Diversity on the Interaction of Triterpenoid Saponins and Lipid Bilayers.	0
335	A computational study on the biotransformation of alkenylbenzenes by a selection of CYPs: Reflections on their possible bioactivation. **2023**, 488, 153471	0
334	In-vitro antigout potential of Alstonia scholaris flower, characterization and prospective ligand-receptor interaction of bioactive lead compound. **2023**, 9, e14093	0
333	Conserved folding landscape of monomeric initiator caspases. **2023**, 299, 103075	0
332	Novel Mixed Matrix Membranes Based on Poly(vinylidene fluoride): Development, Characterization, Modeling. **2023**, 15, 1222	0
331	Bimodal 1/f Noise and Anticorrelation between DNA-Water and DNA-Ion Energy Fluctuations. **2023**, 127, 1965-1975	0
330	Investigation of the Impact of Lipid Acyl Chain Saturation on Fusion Peptide Interactions with Lipid Bilayers. **2023**, 3, 121-138	0
329	Predicting locations of cryptic pockets from single protein structures using the PocketMiner graph neural network. **2023**, 14,	1
328	In silico analysis of marine natural product for protein arginine methyltransferase 5(PRMT5) inhibitors based on pharmacophore and molecular docking. 1-18	0
327	The interactions of monomeric acridines and unsymmetrical bisacridines (UAs) with DNA duplexes: an insight provided by NMR and MD studies. **2023**, 13,	0
326	Sonochemical Formation of Fluorouracil Nanoparticles: Toward Controlled Drug Delivery from Polymeric Surfaces. **2023**, 6, 4271-4278	0
325	Insights into the Substrate Uptake Mechanism of Mycobacterium Tuberculosis Ribose 5-Phosphate Isomerase and Perspectives on Drug Development. **2023**, 3, 139-157	0
324	Molecular recognition of bio-active triterpenoids from Swertia chirayita towards hepatitis Delta antigen: a mechanism through docking, dynamics simulation, Gibbs free energy landscape. 1-14	2

323	Conformational and oligomeric states of SPOP from small-angle X-ray scattering and molecular dynamics simulations. 12,	0
322	Design, synthesis and evaluation of 5-chloro-6-methylaurone derivatives as potential anti-cancer agents. 1-22	0
321	Long-range communication between transmembrane- and nucleotide-binding domains does not depend on drug binding to mutant P-glycoprotein. 1-10	0
320	Highly-Selective Harvesting of (6,4) SWCNTs Using the Aqueous Two-Phase Extraction Method and Nonionic Surfactants. 2207218	0
319	Structural details of a Class B GPCR-arrestin complex revealed by genetically encoded crosslinkers in living cells. **2023**, 14,	2
318	Chain Sliding versus ‖Sheet Formation upon Shearing Single ⍈Helical Coiled Coils. 2200563	0
317	Mechanistic Insight into the Amyloid Fibrillation Inhibition of Hen Egg White Lysozyme by Three Different Bile Acids. **2023**, 127, 2198-2213	0
316	Molecular dynamics simulation of membrane systems in the context of traumatic brain injury. **2023**, 27, 100453	0
315	Molecular Dynamics Assessment of Mechanical Properties of the Thin Filaments in Cardiac Muscle. **2023**, 24, 4792	0
314	GB1 Dimerization in Crowders: A Multiple Resolution Approach. **2023**, 63, 1570-1577	0
313	Probing Redox Properties of Extreme Concentrations Relevant for Nonaqueous Redox-Flow Batteries. **2023**, 6, 2819-2831	0
312	The structure of pathogenic huntingtin exon 1 defines the bases of its aggregation propensity. **2023**, 30, 309-320	0
311	Mechanism of proton-coupled electron transfer described with QM/MM implementation of coupled-perturbed density-functional tight-binding. **2023**, 158, 124107	0
310	Atomistic origins of biomass recalcitrance in organosolv pretreatment. **2023**, 272, 118587	0
309	Rational Computational Approaches in Drug Discovery: Potential Inhibitors for Allosteric Regulation of Mutant Isocitrate Dehydrogenase-1 Enzyme in Cancers. **2023**, 28, 2315	0
308	Discovery of novel acetylcholinesterase inhibitors through integration of machine learning with genetic algorithm based in silico screening approaches. 16,	0
307	Insights at the atomistic resolution of lantibiotics using multiscale simulations. **2023**, 241-253	0
306	Microscopic Understanding of the Conformational Stability of the Aggregated Nonamyloid ‖ Components of ⍈ynuclein. **2023**, 63, 1542-1555	0

305	Chemical, biological and in silico assessment of date (P. dactylifera L.) fruits grown in Ha□l region. 11,	0
304	Antimicrobial Hybrid Amphiphile via Dynamic Covalent Bonds Enables Bacterial Biofilm Dispersal and Bacteria Eradication. 2214299	1
303	Additive energetic contributions of multiple peptide positions determine the relative promiscuity of viral and human sequences for PDZ domain targets. **2023**, 32,	0
302	Photoallosteric Polymersomes toward On-Demand Drug Delivery and Multimodal Cancer Immunotherapy.	0
301	SARS-CoV-2-related bat virus behavior in human-relevant models sheds light on the origin of COVID-19. **2023**, 24,	1
300	Discovery of novel inhibitor of 11 beta-hydroxysteroid dehydrogenase type 1 using in silico structure-based screening approach for the treatment of type 2 diabetes.	0
299	Novel Variant of the SLC4A1 Gene Associated with Hereditary Spherocytosis. **2023**, 11, 784	0
298	Anti-quorum sensing effects of batatasin III: in ́vitro and in silico studies. 1-12	0
297	Understanding Passive Membrane Permeation of Peptides: Physical Models and Sampling Methods Compared. **2023**, 24, 5021	1
296	Stereo-complementary epoxidation of 4-vinyl-2,3-dihydrobenzofuran using mutants of SeStyA with enhanced stability and enantioselectivity. **2023**, 540, 113055	0
295	ALS-Linked A315T and A315E Mutations Enhance □Barrel Formation of the TDP-43307□319 Hexamer: A REST2 Simulation Study. **2023**, 14, 1310-1320	0
294	In silico screening of inhibitors against human dihydrofolate reductase to identify potential anticancer compounds. 1-13	0
293	Odorant-Binding Protein 6 Contributes High Binding Affinity to Insecticides in a Parasitic Wasp Meteorus pulchricornis (Hymenoptera: Braconidae). **2023**, 71, 4498-4509	0
292	Combining experiments and simulations to examine the temperature-dependent behaviour of a disordered protein.	0
291	Efficient Purification of Cowpea Chlorotic Mottle Virus by a Novel Peptide Aptamer. **2023**, 15, 697	0
290	Predicting the feasibility of targeting a conserved region on the S2 domain of the SARS-CoV-2 spike protein.	0
289	Growth Reaction of Gold Nanorods in the Presence of Mutated Peptides and Amine-Modified Single-Stranded Nucleic Acids. **2023**, 18,	0
288	Bsc2 is a novel regulator of triglyceride lipolysis that demarcates a lipid droplet subpopulation.	0

287	In vitro and in silico evaluations of actinomycin X2and actinomycin D as potent anti-tuberculosis agents. 11, e14502	0
286	Investigating the antibacterial mechanism of Ampelopsis cantoniensis extracts against methicillin-resistant Staphylococcus aureus via in ́vitro and in silico analysis. 1-12	0
285	Human sirtuin 2 inhibitors, their mechanisms and binding modes. **2023**, 15, 291-311	0
284	Immunoglobulin adsorption and film formation on mechanically wrinkled and crumpled surfaces at submonolayer coverage. **2023**, 5, 2085-2095	0
283	How NaFTA salt affects the structural landscape and transport properties of Pyrr1,3FTA ionic liquid. **2023**, 158, 104502	0
282	Lipid Bicelles in the Study of Biomembrane Characteristics. **2023**, 19, 1908-1921	0
281	Intermediate-state-trapped mutants pinpoint G protein-coupled receptor conformational allostery. **2023**, 14,	0
280	Selecting High-Dimensional Representations of Physical Systems by Reweighted Diffusion Maps. **2023**, 14, 2778-2783	0
279	Density of States Engineering of n-Doped Conjugated Polymers for High Charge Transport Performances.	0
278	Cryo-EM structures of human Cx36/GJD2 neuronal gap junction channel. **2023**, 14,	0
277	Computational insight into structural basis of human ELOVL1 inhibition. **2023**, 157, 106786	0
276	Electronic Excitation Response of DNA to High-Energy Proton Radiation in Water. **2023**, 130,	0
275	Solvation Shell Structures of Ammonia in Reline and Ethaline Deep Eutectic Solvents. **2023**, 127, 2499-2510	0
274	In silico modelling of the function of disease-related CAZymes. **2023**, 67, 355-372	1
273	Biophysical Interpretation of Evolutionary Consequences on the SARS-CoV2 Main Protease through Molecular Dynamics Simulations and Network Topology Analysis. **2023**, 127, 2331-2343	0
272	HuR modulation counteracts lipopolysaccharide response in murine macrophages. **2023**, 16,	0
271	TMAO: Protecting proteins from feeling the heat. **2023**, 122, 1414-1422	0
270	Atomistic MD Simulations of n -Alkanes in a Phospholipid Bilayer: CHARMM36 versus Slipids. 2200078	0

269	Structural basis of GAIN domain autoproteolysis and cleavage-resistance in the adhesion G-protein coupled receptors.	0
268	Single Amino Acid Modifications for Controlling the Helicity of Peptide-Based Chiral Gold Nanoparticle Superstructures. **2023**, 145, 6546-6553	0
267	Improving the on-target activity of high-fidelity Cas9 editors by combining rational design and random mutagenesis. **2023**, 107, 2385-2401	0
266	Design, Synthesis, In Silico and POM Studies for the Identification of the Pharmacophore Sites of Benzylidene Derivatives. **2023**, 28, 2613	0
265	Extended-sampling QM/MM simulation of biochemical reactions involving PN bonds. **2023**, 25, 9824-9836	0
264	Identification of a Thermostable Levansucrase from Pseudomonas orientalis That Allows Unique Product Specificity at Different Temperatures. **2023**, 15, 1435	0
263	Surfactant Proteins SP-B and SP-C in Pulmonary Surfactant Monolayers: Physical Properties Controlled by Specific Protein Lipid Interactions. **2023**, 39, 4338-4350	0
262	Structural Optimization of an Hairpinin Blocking Potassium Channels KV1.3. **2023**, 59, 192-199	0
261	Predicting residue cooperativity during protein folding: A combined, molecular dynamics and unsupervised learning approach. **2023**, 158, 134108	0
260	The Impact of Antimicrobial Peptides on the Acinetobacter baumannii Inner Membrane Is Modulated by Lipid Polyunsaturation. **2023**, 9, 815-826	0
259	Engineering Nanomolar Potent Protein-based Inhibitors for Papain-like Protease Guided by Residue Correlation Network.	0
258	Stable LiF-Rich Electrode Electrolyte Interface toward High-Voltage and High-Energy-Density Lithium Metal Solid Batteries. 2300494	0
257	Cristae formation is a mechanical buckling event controlled by the inner membrane lipidome.	0
256	Ensemble-based molecular docking and spectrofluorometric analysis of interaction between cytotoxin and tumor necrosis factor receptor 1. 1-15	0
255	Investigations on molecular interactions of memantine hydrochloride in aqueous solutions by thermophysical methods and molecular dynamics simulations at different temperatures. **2023**, 100, 100967	0
254	Aggregation of chlorophylls on plant thylakoid membranes using coarse-grained simulations.	0
253	Identification of novel inhibitors of tetranectin plasminogen interaction to suppress breast cancer invasion: an integrated computational and cell-based investigation. 1-10	0
252	Creatinase: Using Increased Entropy to Improve the Activity and Thermostability. **2023**, 127, 2671-2682	0

251	Waste to drugs: identification of pyrolysis by-products as antifungal agents against Cryptococcus neoformans. 1-14	0
250	Predicted structure and cell signaling of TAS2R14 reveal receptor hyper-flexibility for detecting diverse bitter tastes. **2023**, 26, 106422	0
249	Diclofenac and other non-steroidal anti-inflammatory drugs (NSAIDs) are competitive antagonists of the human P2X3 receptor. 14,	0
248	The architecture of transmembrane and cytoplasmic juxtamembrane regions of Toll-like receptors. **2023**, 14,	0
247	Identifying promising druggable binding sites and their flexibility to target the receptor-binding domain of SARS-CoV-2 spike protein. **2023**, 21, 2339-2351	0
246	Investigation of the dual role of acyl phloroglucinols as a new hope for antibacterial and anti-SARS-CoV-2 agents employing integrated in ́vitro and multi-phase in silico approaches. 1-18	0
245	Unraveling the connection between calreticulin and myeloproliferative neoplasms via calcium signaling.	0
244	Computational screening of FDA-approved drugs to identify potential aromatase receptor inhibitors for polycystic ovary syndrome. 1-13	0
243	Auranofin Targeting the NDM-1 Beta-Lactamase: Computational Insights into the Electronic Configuration and Quasi-Tetrahedral Coordination of Gold Ions. **2023**, 15, 985	0
242	Molecular docking and dynamics simulation study of quinones and pyrones from Alternaria solani and Alternaria alternata with HSP90: an important therapeutic target of cancer. 1-13	0
241	Insights on the interaction of SARS-CoV-2 variant B.1.617.2 with antibody CR3022 and analysis of antibody resistance. **2023**, 21,	0
240	Solution Structures of Europium Terpyridyl Complexes with Nitrate and Triflate Counterions in Acetonitrile. **2023**, 62, 5207-5218	0
239	Methane Gas Bubbles Affecting the Formation and Distribution of Hydrates in Kaolinite Slit Pores: A Molecular Dynamics Study. **2023**, 37, 5102-5113	0
238	Highly stable lithium-ion wide-temperature storage performance achieved via anion-dominated solvation structure and electric double-layer engineering. **2023**, 567, 232975	0
237	Structural Dynamics of Lys11-Selective Deubiquitinylase Cezanne-1 during the Catalytic Cycle. **2023** , 63, 2084-2094	0
236	Time-resolved cryo-EM of G protein activation by a GPCR.	0
235	Insights Into Targeting the SARS-CoV-2: Design, Synthesis, In Silico Studies and Antiviral Evaluation of New Dimethylxanthine Derivatives.	0
234	Looking for chiral recognition in photoinduced bimolecular electron transfer using ultrafast spectroscopy.	0

233	On quantum computing and geometry optimization.	0
232	A cooperative knock-on mechanism underpins Ca2+-selective cation permeation in TRPV channels. **2023**, 155,	0
231	Designing Hybrid Lanthanum Stannate/Functionalized Halloysite Nanotubes as Electrode Material for Electrochemical Detection of 4-(Methylamino)phenol (Metol) in Environmental Samples. **2023**, 11, 5072-5081	0
230	The ATP-bound State of the Uncoupling Protein 1 (UCP1) from Molecular Simulations.	0
229	Determination of Antioxidant Activities of Viscum album L.: First Report on Interaction of Phenolics with Survivin Protein using in silico Analysis. **2023**, 8,	1
228	Mitigation of membrane morphology defects explain stability and orientational specificity of CLC dimers.	0
227	Delineating the impact of pathogenic mutations on the conformational dynamics of HDL□ vital protein ApoA1: a combined computational and molecular dynamic simulation approach. 1-21	0
226	Chemical Feedback in the Self-Assembly and Function of Air□iquid Interfaces: Insight into the Bottlenecks of CO2 Direct Air Capture. **2023**, 15, 19634-19645	0
225	Human Pol□Natural Polymorphic Variants G118V and R149I Affects Substate Binding and Catalysis. **2023**, 24, 5892	0
224	Accelerating Cryptic Pocket Discovery Using AlphaFold.	0
223	Detection of natural compounds by virtual screening, molecular docking and dynamics studies and evaluation of their effects on tau level in ́vitro Alzheimer□ model. 1-9	0
222	Exploring the volatile metabolites of three Chorisia species: Comparative headspace GC□MS, multivariate chemometrics, chemotaxonomic significance, and anti-SARS-CoV-2 potential. **2023**,	0
221	Regularized Bennett and Zwanzig free energy estimators. **2023**, 158, 124101	0
220	Structure and Dynamics of Three Escherichia coli NfsB Nitro-Reductase Mutants Selected for Enhanced Activity with the Cancer Prodrug CB1954. **2023**, 24, 5987	0
219	Path separation of dissipation-corrected targeted molecular dynamics simulations of protein□gand unbinding. **2023**, 158, 124106	0
218	Structural basis of mitochondrial membrane bending by the I□□I2□V2 supercomplex. **2023**, 615, 934-938	0
217	Structural and functional characterization of novel F7 mutations identified in Chinese factor VII -deficient patients.	0
216	Finite-Temperature Mechanical Properties of Organic Molecular Crystals from Classical Molecular Simulation. **2023**, 23, 2155-2168	0

215	Synthesis, molecular docking and dynamics studies of pyridazino[4,5-b]quinoxalin-1(2H)-ones as targeting main protease of COVID-19. 1-13	0
214	Distinct structure and gating mechanism in diverse NMDA receptors with GluN2C and GluN2D subunits.	0
213	Human Amylin in the Presence of SARS-COV-2 Protein Fragments. **2023**, 8, 12501-12511	0
212	Discovery of a cryptic pocket in the AI-predicted structure of PPM1D phosphatase explains the binding site and potency of its allosteric inhibitors.	0
211	Study on Interactions of the SARS-CoV-2 Spike Proteins with the Human Toll-like Receptor 4 using Molecular Dynamic Simulations. **2023**, 4, 34-46	0
210	Calculations of the binding free energies of the Comprehensive <i>in vitro</i> Proarrhythmia Assay (CiPA) reference drugs to cardiac ion channels. **2023**, 20, n/a	0
209	Effective Molecular Dynamics from Neural Network-Based Structure Prediction Models. **2023**, 19, 1965-1975	0
208	Interaction of Uperin Peptides with Model Membranes: Molecular Dynamics Study. **2023**, 13, 370	0
207	In silico characterization of cysteine-stabilized ß-defensins from neglected unicellular microeukaryotes. **2023**, 23,	0
206	Atomistic molecular simulations of A$Zn conformational ensembles.	0
205	Multiscale Computational Framework to Investigate Integrin Mechanosensing and Cell Adhesion.	0
204	Physicochemical Properties and Route of Systemic Delivery Control the In Vivo Dynamics and Breakdown of Radiolabeled Gold Nanostars.	0
203	Conformational transitions and allosteric modulation in a heteromeric glycine receptor. **2023**, 14,	0
202	Structural mechanism of Fab domain dissociation as a measure of interface stability. **2023**, 37, 201-215	0
201	EphrinA5 regulates cell motility by modulating the targeting of DNMT1 to theNcam1promoter via lncRNA/DNA triplex formation.	0
200	Design of new reversible and selective inhibitors of monoamine oxidase A and a comparison with drugs already approved. **2023**, 47,	0
199	The Mechanism Underlying the Amylose-Zein Complexation Process and the Stability of the Molecular Conformation of Amylose-Zein Complexes in Water Based on Molecular Dynamics Simulation. **2023**, 12, 1418	0
198	Internal Normal Mode Analysis Applied to RNA Flexibility and Conformational Changes.	0

197	Computational Design of Peptides for Biomaterials Applications.	0
196	Vaccinomics Approach for Multi-Epitope Vaccine Design against Group A Rotavirus Using VP4 and VP7 Proteins. **2023**, 11, 726	0
195	Interplay of lipid head group and packing defects in driving amyloid-beta-mediated myelin-like model membrane deformation. **2023**, 299, 104653	0
194	Discrimination between cyclic nucleotides in a cyclic nucleotide-gated ion channel. **2023**, 30, 512-520	0
193	Machine learning- and structure-based discovery of a novel chemotype as FXR agonists for potential treatment of nonalcoholic fatty liver disease. **2023**, 252, 115307	0
192	Folding and modulation of the helical conformation of Glycophorin A by point mutations. **2023**, 25, 10885-10893	3
191	2D-QSAR, molecular docking and MD simulation based virtual screening of the herbal molecules against Alzheimer's disorder: an approach to predict CNS activity. 1-15	0
190	Effect of Electric Field on α-Synuclein Fibrils: Revealed by Molecular Dynamics Simulations. **2023**, 24, 6312	0
189	Bovine serum albumin prevents human hemoglobin aggregation and retains its chaperone-like activity. 1-16	0
188	Soft Matter under Pressure: Pushing Particle-Field Molecular Dynamics to the Isobaric Ensemble. **2023**, 63, 2207-2217	0
187	Riboflavin kinase and pyridoxine 5?-phosphate oxidase complex formation envisages transient interactions for FMN cofactor delivery. 10,	0
186	Underpinning Endogeneous Damp EDA-Fibronectin in the Activation of Molecular Targets of Rheumatoid Arthritis and Identifcation of its Effective Inhibitors by Computational Methods.	0
185	Statistical learning of protein elastic network from positional covariance matrix. **2023**, 21, 2524-2535	0
184	Kaurane-Type Diterpenoids as Potential Inhibitors of Dihydrofolate Reductase-Thymidylate Synthase in New World Leishmania Species. **2023**, 12, 663	0
183	The influence of single-point mutation D614G on the binding process between human angiotensin-converting enzyme 2 and the SARS-CoV-2 spike protein-an atomistic simulation study. **2023**, 13, 9800-9810	0
182	Next Generation of Ovarian Cancer Detection Using Aptamers. **2023**, 24, 6315	0
181	Retinoic acid shows direct parasiticidal activity by targeting ergosterol pathway in Leishmania donovani: a potential therapeutic advancement. 1-11	0
180	Docking and Molecular Dynamics Identify Leads against 5 Alpha Reductase 2 for Benign Prostate Hyperplasia Treatment. **2023**, 2023, 1-20	0

179	How Single Amino Acid Substitutions Can Disrupt a Protein Hetero-Dimer Interface: Computational and Experimental Studies of the LigAB Dioxygenase from Sphingobium sp. Strain SYK-6. **2023**, 24, 6319	0
178	Identification of Novel Tau-Tubulin Kinase 2 Inhibitors Using Computational Approaches. **2023**, 8, 13026-13037	0
177	Converging PMF calculations of antibiotic permeation across an outer membrane porin with sub-kilocalorie per mole accuracy.	0
176	Cheminformatics-Based Study Identifies Potential Ebola VP40 Inhibitors. **2023**, 24, 6298	1
175	Discovery and Binding Mechanism of Pyrazoloisoquinoline-Based Novel β-Arrestin Inverse Agonists of the Kappa-Opioid Receptor. **2023**, 66, 5154-5170	0
174	KIFKey Interactions Finder: A program to identify the key molecular interactions that regulate protein conformational changes. **2023**, 158, 144114	0
173	Rare deleterious mutations in Bruton's tyrosine kinase as biomarkers for ibrutinib-based therapy: an in silico insight. **2023**, 29,	0
172	Characterization of the role of Kunitz-type protease inhibitor domain in dimerization of amyloid precursor protein.	0
171	An improved analytical model of protein dynamics at the sub-nanosecond timescale.	0
170	Crystal Structure of Bright Fluorescent Protein BrUSLEE with Subnanosecond Fluorescence Lifetime; Electric and Dynamic Properties. **2023**, 24, 6403	0
169	Effect of temperature on hepatitis a virus and exploration of binding mode mechanism of phytochemicals from tinospora cordifolia: an insight into molecular docking, MM/GBSA, and molecular dynamics simulation study. 1-17	0
168	Computational analysis and molecular dynamics simulation of high-risk single nucleotide polymorphisms of the ADAM10 gene. 1-13	0
167	Molecular simulation of confined ethaline-based deep eutectic solvents for separations of carbon dioxide from methane.	0
166	In-depth molecular profiling of an intronic GNAO1 mutant as the basis for personalized high-throughput drug screening. **2023**,	0
165	Benchmarking In Silico Tools for Cysteine pKa Prediction. **2023**, 63, 2170-2180	0
164	A General Picture of Cucurbit[8]uril Host–Guest Binding: Recalibrating Bonded Interactions. **2023**, 28, 3124	0
163	Rational strategies for enhancing mAb binding to SARS-CoV-2 variants through CDR diversification and antibody-escape prediction. 14,	0
162	Mechanistic Insights into the Binding of Different Positron Emission Tomography Tracers to Chronic Traumatic Encephalopathy Tau Protofibrils.	0

161	Metadynamics simulations for the investigation of drug loading on functionalized inorganic nanoparticles.	0
160	Molecular insights into the stereospecificity of arginine in RNA tetraloop folding.	0
159	Efficient seawater desalination in lamellar nanochannel-based boridene filtration membrane.	0
158	IFITM3 blocks influenza virus entry by sorting lipids and stabilizing hemifusion. **2023**, 31, 616-633.e20	0
157	Oncogene-mediated nuclear accumulation of lactate promotes epigenetic alterations to induce cancer cell proliferation. **2023**, 124, 495-519	0
156	Celastrol suppresses humoral immune responses and autoimmunity by targeting the COMMD3/8 complex. **2023**, 8,	0
155	Insight into intermolecular binding mechanism of apatinib mesylate and human alpha-1-acid glycoprotein: combined multi-spectroscopic approaches with in silico. 1-12	0
154	In silico screening of phytochemicals from Dissotis rotundifolia against Plasmodium falciparum Dihydrofolate Reductase. **2023**, 3, 100447	0
153	How SGLT2 inhibitors interact with metformin? A molecular dynamics study. 1-10	0
152	Computational screening of FDA-approved drugs to identify potential TgDHFR, TgPRS, and TgCDPK1 proteins inhibitors against Toxoplasma gondii. **2023**, 13,	0
151	The structural integrity of the membrane-embedded bacterial division complex FtsQBL studied with molecular dynamics simulations. **2023**, 21, 2602-2612	0
150	In silico and in vitro Identification of Compounds with Dual Pharmacological Activity against Metionyl-tRNA Synthetase and Isoleucyl-tRNA Synthetase of Staphylococcus aureus. **2023**, 8,	0
149	Large piezoelectric response in a Jahn-Teller distorted molecular metal halide. **2023**, 14,	0
148	The targeted next-generation sequence revealed SMAD4, AKT1, and TP53 mutations from circulating cell-free DNA of breast cancer and its effect on protein structure □A computational approach. 1-14	0
147	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,	0
146	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	0
145	Structural and molecular insights into tacrine-benzofuran hybrid induced inhibition of amyloid-╫ peptide aggregation and BACE1 activity. 1-17	0
144	pH-Sensitive Liposomes with Embedded 3-(isobutylamino)cholan-24-oic Acid: What Is the Possible Mechanism of Fast Cargo Release?. **2023**, 13, 407	0

143	Effect of Force Field Resolution on Membrane Mechanical Response and Mechanoporation Damage under Deformation Simulations.	0
142	Molecular contacts in the Cren7-DNA complex: A quantitative investigation for electrostatic interaction. **2023**,	0
141	1-Benzyl-5-bromo-3-hydrazonoindolin-2-ones as Novel Anticancer Agents: Synthesis, Biological Evaluation and Molecular Modeling Insights. **2023**, 28, 3203	0
140	Single-molecule fingerprinting of protein-drug interaction using a funneled biological nanopore. **2023**, 14,	0
139	Constant chemical potential quantum mechanical molecular dynamics simulations of the graphene electrolyte double layer. **2023**, 158, 134714	0
138	An Affordable Topography-Based Protocol for Assigning a Residue Character on a Hydropathy (PARCH) Scale.	0
137	Influence of Core Topologies on Poly-l-lysine Dendrimer Structures. **2023**, 127, 3364-3371	0
136	Coating of favipiravir (FVP) on silver nanoparticles: First principle study. **2023**,	0
135	Evaluation of Antimalarial Activity of Ethanolic Extract of Annona muricata L.: An in vivo and an in silico Approach. **2023**, 28, 2515690X2311651	0
134	Deep Eutectic Solvents for the Enzymatic Synthesis of Sugar Esters: A Generalizable Strategy?. **2023**, 11, 5926-5936	0
133	Molecular dynamics of the ERR ligand-binding domain bound with agonist and inverse agonist. **2023**, 18, e0283364	0
132	In Silico Structural and Functional Analysis of the Mitochondrial Malate Transporters in Oleaginous Fungus Mucor circinelloides WJ11. **2023**, 13, 705	0
131	New azole-derived hemiaminal ethers as promising acetylcholinesterase inhibitors: synthesis, X-ray structures, in vitro and in silico studies. 1-14	0
130	Carbon nanotube recognition by human Siglec-14 provokes inflammation.	0
129	Repurposing immune boosting and anti-viral efficacy of Parkia bioactive entities as multi-target directed therapeutic approach for SARS-CoV-2: exploration of lead drugs by drug likeness, molecular docking and molecular dynamics simulation methods. 1-39	0
128	Molecular dynamics simulation of pyruvate kinase to investigate improved thermostability of artificially selected strain in Enterococcus faecium.	0
127	Sodium is a negative allosteric regulator of the ghrelin receptor. **2023**, 42, 112320	0
126	Continuous millisecond conformational cycle of a DEAH box helicase reveals control of domain motions by atomic-scale transitions. **2023**, 6,	0

125	Circuit Topology Approach for the Comparative Analysis of Intrinsically Disordered Proteins.	0
124	Coarse-Grained MD Simulations of Opioid Interactions with the Opioid Receptor and the Surrounding Lipid Membrane. **2023**, 3, 263-275	0
123	Synthesis, Biological Activity Evaluation, Docking and Molecular Dynamics Studies of New Triazole-Tetrahydropyrimidinone(thione) Hybrid Scaffolds as Urease Inhibitors.	0
122	G slow conformational transition upon GTP binding and a novel G regulator. **2023**, 26, 106603	0
121	Developmental and epileptic encephalopathy 89: A novel bi-allelic variant, molecular dynamics simulation, and a comprehensive clinical and molecular profile.	0
120	Conformational cycle of human polyamine transporter ATP13A2. **2023**, 14,	0
119	Molecular origin of the two-step mechanism of gellan aggregation. **2023**, 9,	0
118	In silico investigation of the structural stability as the origin of the pathogenicity of synuclein protofibrils. 1-13	0
117	Role of the Polar Proportion of Compound Collectors in Low-Rank Coal Flotation Upgrading: Insights from the Molecular Scale. **2023**, 13, 524	0
116	Function and dynamics of the intrinsically disordered carboxyl terminus of adrenergic receptor. **2023**, 14,	0
115	Chemical Promoter Performance for CO2 Hydrate Growth: A Molecular Perspective. **2023**, 37, 6002-6011	0
114	Interfacial properties of protein nanofibrils with different morphology prepared using aqueous solvent with ethanol: Part I. preparation and characterization. **2023**, 142, 108754	0
113	Comparative molecular dynamics simulations of pathogenic and non-pathogenic huntingtin protein monomers and dimers. 10,	0
112	Ceramide-1-phosphate transfer protein enhances lipid transport by disrupting hydrophobic lipid embrane contacts. **2023**, 19, e1010992	0
111	Inhibitory Potential of the Ocimum sanctum Phytochemicals on Bruton Tyrosine Kinase, a Well-Known Drug Target for Treatment of Chronic Lymphocytic Leukemia: An In Silico Investigation. **2023**, 28, 3287	0
110	Mapping Protein Targets of Carnosol, a Molecule Identified in Rosmarinus officinalis: In Silico Docking Studies and Network Pharmacology. **2023**, 91, 19	0
109	Ion Conduction Mechanisms in Potassium Channels Revealed by Permeation Cycles.	0
108	Improving the activity of horseradish peroxidase in betaine-based natural deep eutectic systems.	0

107	Structural insights into angiotensin receptor signaling modulation by balanced and biased agonists.	0
106	SPEADI: Accelerated Analysis of IDP-Ion Interactions from MD-Trajectories. **2023**, 12, 581	0
105	Substituted Oligosaccharides as Protein Mimics: Deep Learning Free Energy Landscapes.	0
104	Molecular Rotations, Multiscale Order, Hyperuniformity, and Signatures of Metastability during the Compression/Decompression Cycles of Amorphous Ices.	0
103	Enhanced Thermostability and Catalytic Activity of Streptomyces mobaraenesis Transglutaminase by Rationally Engineering Its Flexible Regions.	0
102	Triazole□Peptide Conjugate as a Modulator of A□Aggregation, Metal-Mediated A□Aggregation, and Cytotoxicity.	0
101	Tool and Techniques on Computer-Aided Drug Design for Targeted Cancer Therapy. **2023**, 781-829	0
100	Direct monitoring of the thermodynamics and kinetics of DNA and RNA dinucleotide dehybridization from gaps and overhangs.	0
99	Clinical side-effects based drug repositioning for anti-epileptic activity. 1-12	0
98	Structure based High-Throughput Virtual Screening, Molecular Docking and Molecular Dynamics Study of anticancer natural compounds against fimbriae (FimA) protein of Porphyromonas gingivalis in oral squamous cell carcinoma.	0
97	Engineering C□ Bond Cleavage Activity into a P450 Monooxygenase Enzyme.	0
96	Optimizing the Martini 3 Force Field Reveals the Effects of the Intricate Balance between Protein□Water Interaction Strength and Salt Concentration on Biomolecular Condensate Formation.	0
95	Lysine Deacetylase Substrate Selectivity: Distinct Interaction Surfaces Drive Positive and Negative Selection for Residues Following Acetyllysine.	0
94	Prediction of zwitterion hydration and ion association properties using machine learning.	0
93	Collagen breaks at weak sacrificial bonds taming its mechanoradicals. **2023**, 14,	0
92	Binding kinetics study of SARS-CoV-2 main protease and potential inhibitors via molecular dynamics simulations.	0
91	Disulfide bridge-dependent dimerization triggers FGF2 membrane translocation into the extracellular space.	0
90	The role of ETFS amino acids on the stability and inhibition of p53-MDM2 complex of anticancer p53-derivatives peptides: Density functional theory and molecular docking studies. **2023**, 122, 108472	0

89	Molecular Insights of Cellobiose Dehydrogenase Adsorption on Self-Assembled Monolayers.	0
88	Identification and mechanistic exploration of structural and conformational dynamics of NF-kB inhibitors: rationale insights from in silico and in´vitro studies. 1-21	0
87	Vitamin D analog calcitriol for breast cancer therapy; an integrated drug discovery approach. 1-27	0
86	A soft co-crystalline solid electrolyte for lithium-ion batteries.	0
85	Equivalence of Charge Imbalance and External Electric Fields during Free Energy Calculations of Membrane Electroporation.	0
84	Identification of a novel drug molecule for Neurodegenerative Disease from marine algae through In-silico analysis.	0
83	Identification of common candidate genes and pathways for Spina Bifida and Wilm Tumor using an integrative bioinformatics analysis. 1-16	0
82	The Interaction Mechanism of Intramuscular Gene Delivery Materials with Cell Membranes. **2023**, 14, 219	0
81	IDH3 functions as a redox switch regulating mitochondrial energy metabolism and contractility in the heart. **2023**, 14,	0
80	Computer-aided de novo design and optimization of novel potential inhibitors of HIV-1 Nef protein. **2023**, 104, 107871	0
79	Ligand-based 3D pharmacophore modeling, virtual screening, and molecular dynamic simulation of potential smoothened inhibitors. **2023**, 29,	0
78	Central cavity dehydration as a gating mechanism of potassium channels. **2023**, 14,	0
77	Molecular Dynamics Simulations Suggest SARS-CoV-2 3CLpro Mutations in Beta and Omicron Variants Do Not Alter Binding Affinities for Cleavage Sites of Non-Structural Proteins. **2023**, 3, 622-636	0
76	Influence of Ethanol Parametrization on Diffusion Coefficients Using OPLS-AA Force Field. **2023**, 24, 7316	0
75	Chemically routed interpore molecular diffusion in metal-organic framework thin films. **2023**, 14,	0
74	Genetic Analysis of Patients with Congenital Hypogonadotropic Hypogonadism: A Case Series. **2023**, 24, 7428	0
73	Interactions between carbon nanotubes and external structures of SARS-CoV-2 using molecular docking and molecular dynamics. **2023**, 1286, 135604	0
72	Targeting the PEDV 3CL protease for identification of small molecule inhibitors: an insight from virtual screening, ADMET prediction, molecular dynamics, free energy landscape, and binding energy calculations. **2023**, 17,	0

71	Protein Crowding and Cholesterol Increase Cell Membrane Viscosity in a Temperature Dependent Manner.	0
70	Synthesis, anticancer activity, molecular docking and molecular dynamics studies of some pyrazole□halcone hybrids. 1-11	0
69	Design of Potent Inhibitors Targeting the Main Protease of SARS-CoV-2 Using QSAR Modeling, Molecular Docking, and Molecular Dynamics Simulations. **2023**, 16, 608	0
68	Cryo-EM structure of the folded-back state of human □cardiac myosin*.	0
67	Selectivity filter mutations shift ion permeation mechanism in potassium channels.	0
66	Hofmeister Effects Influence Bulk Nanostructure in a Protic Ionic Liquid. **2023**,	0
65	Discovery of a cryptic pocket in the AI-predicted structure of PPM1D phosphatase explains the binding site and potency of its allosteric inhibitors. 10,	0
64	Transmembrane dimers of type 1 receptors sample alternate configurations: MD simulations using coarse grain Martini 3 versus AlphaFold2 Multimer. **2023**,	0
63	Mechanisms of Electronic and Ionic Transport during Mg Intercalation in Mg□ Cathode Materials and Their Decomposition Products.	0
62	Micro- and Nanoplastics Breach the Blood□Brain Barrier (BBB): Biomolecular Corona□ Role Revealed. **2023**, 13, 1404	0
61	Molecular Simulation Strategies for Understanding the Degradation Mechanisms of Acrylic Polymers.	0
60	Phase Transition and Phase Separation in Realistic Thylakoid Lipid Membrane of Marine Algae in All-Atom Simulations.	0
59	Discovery of seven-membered ring berberine analogues as highly potent and specific hCES2A inhibitors. **2023**, 378, 110501	0
58	Machine Learning-Driven Multiscale Modeling: Bridging the Scales with a Next-Generation Simulation Infrastructure.	0
57	Biophysical and in-silico studies on the structure-function relationship of Brugia malayi protein disulfide isomerase. 1-11	0
56	Identification of FDA-approved drugs with triple targeting mode of action for the treatment of monkeypox: a high throughput virtual screening study.	0
55	Cholesterol and melatonin regulated membrane fluidity does not affect the membrane breakage triggered by amyloid-beta peptide. **2023**, 107023	0
54	Structure based virtual screening, molecular dynamic simulation to identify the oxadiazole derivatives as inhibitors of Enterococcus D-Ala-D-Ser ligase for combating vancomycin resistance. **2023**, 106965	0

53	Study of the binding interaction of salmon sperm DNA with nintedanib, a tyrosine kinase inhibitor using multi-spectroscopic, thermodynamic, and in silico approaches. 1-11	0
52	Cellular uptake of rose bengal is mediated by OATP1B1/1B3 transporters. **2023**, 108449	0
51	Discovery of a novel dual functional phenylpyrazole-styryl hybrid that induces apoptotic and autophagic cell death in bladder cancer cells. **2023**, 115335	0
50	O-GlcNAcylation promotes the cytosolic localization of the m6A reader YTHDF1 and colorectal cancer tumorigenesis. **2023**, 104738	0
49	Conformational and Interface Variability in Multivalent SIM–SUMO Interaction.	0
48	Molecular mechanism underlying the increased risk of colorectal cancer metastasis caused by single nucleotide polymorphisms in LI-cadherin gene. **2023**, 13,	0
47	Biological evaluation and in silico studies of novel compounds as potent TAAR1 agonists that could be used in schizophrenia treatment. 14,	0
46	Molecular Origin of High Cation Transference in Mixtures of Poly(pentyl malonate) and Lithium Salt. 612-618	0
45	Radial distribution and hydrogen bonded network graphs of alcohol-aniline binary mixture. **2023**, 29,	0
44	Development of a Data-Driven Integrative Model of a Bacterial Chromosome.	0
43	Experimental and Simulation Studies on Hematite Interaction with Na-Metasilicate Pentahydrate. **2023**, 28, 3629	0
42	The Ebola virus VP40 matrix layer undergoes endosomal disassembly essential for membrane fusion.	0
41	Covalent Adduct Formation as a Strategy for Efficient CO2 Fixation in Crotonyl-CoA Carboxylases/Reductases. 6230-6241	0
40	Effect of maleylation and denaturation of human serum albumin on its interaction with scavenger receptors.	0
39	Identification of core therapeutic targets for Monkeypox virus and repurposing potential of drugs against them: An in silico approach. **2023**, 106971	0
38	Influence of the substrate on the density and infrared spectra of the adsorbed methanol ice of different thicknesses using molecular dynamics simulation.	0
37	De Novo Evolution of an Antibody-Mimicking Multivalent Aptamer via a DNA Framework.	0
36	Computational design and molecular dynamics simulations suggest the mode of substrate binding in ceramide synthases. **2023**, 14,	0

35	Mutation detection of urinary cell-free DNA via catch-and-release isolation on nanowires for liquid biopsy. **2023**, 115318	0
34	On a mechanistic impact of transmembrane tetramerization in the pathological activation of RTKs. **2023**,	0
33	Seipin concentrates distinct neutral lipids via interactions with their acyl chain carboxyl esters. **2022**, 221,	0
32	Discovery of sulfonamide-tethered isatin derivatives as novel anticancer agents and VEGFR-2 inhibitors. **2023**, 38,	0
31	Purification and identification of xanthine oxidase inhibitory peptides from enzymatic hydrolysate of α-lactalbumin and bovine colostrum casein. **2023**, 169, 112882	0
30	Insights into the self-assembly of fampridine hydrochloride: how the choice of the solvent affects the crystallization of a simple salt. **2023**,	0
29	AI-Predicted mTOR Inhibitor Reduces Cancer Cell Proliferation and Extends the Lifespan of C. elegans. **2023**, 24, 7850	0
28	Visualizing the Residue Interaction Landscape of Proteins by Temporal Network Embedding.	0
27	Visualizing the disordered nuclear transport machinery in situ. **2023**, 617, 162-169	0
26	Modern Approaches to Protein Engineering to Create Enzymes with New Catalytic Properties. **2023**, 57, 204-213	0
25	Wolbachia Ferrochelatase as a potential drug target against filarial infections. **2023**, 122, 108490	0
24	Structural insights into SARS-CoV-2 main protease conformational plasticity.	0
23	Determination of self and cross contributions to the dipole–dipole correlations function from analysis of dielectric measurements. **2023**, 382, 121907	0
22	Multi-scale modeling of natural organic matter–heavy metal cations interactions: Aggregation and stabilization mechanisms. **2023**, 238, 120007	0
21	Non-equilibrium virus particle dynamics: Microsecond MD simulations of the complete Flock House virus capsid under different conditions. **2023**, 215, 107964	0
20	Propyl-cyanide isomer formation on interstellar ices from radical association: a quantum theoretical study. **2023**, 522, 5254-5266	0
19	Discovering potential inhibitors of Raf proto-oncogene serine/threonine kinase 1: a virtual screening approach towards anticancer drug development. 1-12	0
18	The Dramatic Effect of Water Structure on Hydration Forces and the Electrical Double Layer. **2023**, 127, 8429-8447	0

17	Measuring pico-Newton Forces with Lipid Anchors as Force Sensors in Molecular Dynamics Simulations. **2023**, 127, 4081-4089	0
16	On the allosteric puzzle and pocket crosstalk through computational means. **2023**, 158,	0
15	Paradoxical effect of A‖bn protein levels of ABCA1 in astrocytes, microglia, and neurons isolated from C57BL/6 mice: an in´vitro and in silico study to elucidate the effect of A‖bn ABCA1 in the brain cells. 1-14	0
14	Exploration of natural compounds against the human mpox virus DNA-dependent RNA polymerase in silico. **2023**, 16, 996-1003	0
13	Atomic Models of All Major Trans-Envelope Complexes Involved in Lipid Trafficking inEscherichia ColiConstructed Using a Combination of AlphaFold2, AF2Complex, and Membrane Morphing Simulations.	0
12	Multi-pathogen based chimeric vaccine to fight against COVID-19 and concomitant coinfections.	0
11	Exploring the structure of halomethanes with xenon: An NMR and MD investigation. **2023**, 382, 122011	0
10	Discovery and analysis of a novel antimicrobial peptide B1AW from the skin secretion of Amolops wuyiensis and improving the membrane-binding affinity through the construction of the lysine-introduced analogue. **2023**, 21, 2960-2972	0
9	Pathogenic HER3 dimerization domain mutations create a structural bias towards un-conventional EGFR-HER3 signalling axis in breast cancer. **2023**, 242, 124765	0
8	Molecular Dynamics Simulations of Ionic Liquid Crystals. **2023**,	0
7	Isatin-pyrimidine hybrid derivatives as enoyl acyl carrier protein reductase (InhA) inhibitors against Mycobacterium tuberculosis. **2023**, 138, 106591	0
6	Structure of aqueous solutions of lignin treated by sub- and supercritical water: Experiment and simulation. **2023**, 383, 122030	0
5	N-Acetylation of Biodegradable Supramolecular Peptide Nanofilaments Selectively Enhances Their Proteolytic Stability for Targeted Delivery of Gold-Based Anticancer Agents.	0
4	Markov State Models Reconcile Conformational Plasticity of GTPase with Its Substrate Binding Event.	0
3	Curvature Matters: Modeling Calcium Binding to Neutral and Anionic Phospholipid Bilayers.	0
2	Dissociation Rate Calculation via Constant-Force Steered Molecular Dynamics Simulation.	0
1	Peganum harmala active compounds as potent inhibitors of Pseudomonas syringae virulent effectors. In silico study. 1-27	0