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682	Simulation-Ready Graphene Oxide Structures with Hierarchical Complexity: A Modular Tiling Strategy.	O
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671	Physical Properties and Low-Frequency Polarizability Anisotropy and Dipole Responses of Phosphonium Bis(fluorosulfonyl)amide Ionic Liquids with Pentyl, Ethoxyethyl, or 2-(Ethylthio)ethyl Group.	O
670	Effects of the Jokela type of spinal muscular atrophy-related G66V mutation on the structural ensemble characteristics of CHCHD10.	0
669	Conformational Selection of a Tryptophan Side Chain Drives the Generalized Increase in Activity of PET Hydrolases through a Ser/Ile Double Mutation.	O
668	Specificity of Monoterpene Interactions with Insect Octopamine and Tyramine Receptors: Insights from in Silico Sequence and Structure Comparison.	O
667	Multi-ligand molecular docking, simulation, free energy calculations and wavelet analysis of the synergistic effects between natural compounds baicalein and cubebin for the inhibition of the main protease of SARS-CoV-2. <b>2023</b> , 121253	O
666	Ternary Synergy of Lys, Dopa, and Phe Results in Strong Cohesion of Peptide Films.	0
665	A structure-based virtual high-throughput screening, molecular docking, molecular dynamics and MM/PBSA study identified novel putative drug-like dual inhibitors of trypanosomal cruzain and rhodesain cysteine proteases.	0

664	An ensemble docking-based virtual screening according to different TRPV1 pore states toward identifying phytochemical activators.	0
663	Investigating the Solvent Effects on Binding Affinity of PAHsExBox4+ Complexes: An Alchemical Approach. <b>2023</b> , 127, 249-260	О
662	MoS2 laminate membranes with structural-phase-dependent permeation for molecular separation. <b>2023</b> , 101239	O
661	Direct detection of a single [4Fe-4S] cluster in a tungsten-containing enzyme: Electrochemical conversion of CO 2 into formate by formate dehydrogenase.	О
660	Graphene quantum dots harvest anti-trypanosomatid efficacy by disrupting antioxidant networks centered on trypanothione reductase.	О
659	Substrate selectivity and inhibition of histidine JmjC hydroxylases MINA53 and NO66.	O
658	Divide-and-Conquer Linear-Scaling Quantum Chemical Computations.	1
657	Dynamic conformational states of apo, ATP and cabozantinib bound TAM kinases to differentiate active-inactive kinetic models. 1-21	O
656	Design of a hydroxy channel based on the selectivity of water permeation via ions exclusion. <b>2023</b> , 6,	О
655	4-Cyanotryptophan as a Sensitive Fluorescence Probe of Local Electric Field of Proteins.	О
654	Identification of a Novel Dual Inhibitor of Acetylcholinesterase and Butyrylcholinesterase: In Vitro and In Silico Studies. <b>2023</b> , 16, 95	1
653	Discovery and Computational Studies of Potent Covalent Kinase Inhibitors with <b>Esubstituent</b> Electrophiles Targeting Cysteine.	О
652	Seleno-Analogs of Scaffolds Resembling Natural Products a Novel Warhead toward Dual Compounds. <b>2023</b> , 12, 139	1
651	On the Propensity of Excess Hydroxide Ions at the Alcohol MonolayerWater Interface.	О
650	Capturing charge and size effects of ions at the grapheneBlectrolyte interface using polarizable force field simulations.	0
649	Equivalence of charge imbalance and external electric fields during free energy calculations of membrane electroporation.	О
648	Anti-colorectal cancer of Ardisia gigantifolia Stapf. and targets prediction via network pharmacology and molecular docking study. <b>2023</b> , 23,	0
647	Fully Atomistic Molecular Dynamics Simulation of a TIPS-Pentacene:Polystyrene Mixed Film Obtained via the Solution Process. <b>2023</b> , 13, 312	1

646	ACES: Optimized Alchemically Enhanced Sampling.	Ο
645	Mechanisms by Which Small Molecules of Diverse Chemotypes Arrest Sec14 Lipid Transfer Activity. <b>2023</b> , 102861	O
644	Softening by charging: how collective modes of ionic association in concentrated redoxmer/electrolyte solutions define the structural and dynamic properties in different states of charge.	О
643	Computational protein design repurposed to explore enzyme vitality and help predict antibiotic resistance. 9,	О
642	Phosphorylation Regulation Mechanism of ₹ Integrin for the Binding of Filamin Revealed by Markov State Model.	0
641	Revealing the biotoxicity of phosphorene oxide nanosheets based on the villin headpiece.	Ο
640	Structural Analysis, Multi-Conformation Virtual Screening and Molecular Simulation to Identify Potential Inhibitors Targeting pS273R Proteases of African Swine Fever Virus. <b>2023</b> , 28, 570	Ο
639	Fructose-1,6-bisphosphatase 1 dephosphorylates IB and suppresses colorectal tumorigenesis.	Ο
638	Anionic Phospholipids Control Mechanisms of GPCR-G Protein Recognition.	0
637	Effect of Salts on the Conformational Dynamics of the Cytochrome P450 OleP. <b>2023</b> , 28, 832	O
636	Interaction of Chondroitin and Hyaluronan Glycosaminoglycans with Surfaces of Carboxylated Carbon Nanotubes Studied Using Molecular Dynamics Simulations. <b>2023</b> , 28, 826	Ο
635	Structural insights into ion conduction by novel cation channel, TMEM87A, in Golgi apparatus.	Ο
634	Molecular mechanism of binding between a therapeutic RNA aptamer and its protein target VEGF : A molecular dynamics study.	0
633	In Silico Mining of Natural Products Atlas (NPAtlas) Database for Identifying Effective Bcl-2 Inhibitors: Molecular Docking, Molecular Dynamics, and Pharmacokinetics Characteristics. <b>2023</b> , 28, 783	O
632	Discovery of Novel Chinese Medicine Compounds Targeting 3CL Protease by Virtual Screening and Molecular Dynamics Simulation. <b>2023</b> , 28, 937	0
631	An Imbalance in the Force: The Need for Standardized Benchmarks for Molecular Simulation.	O
630	Multiscale molecular dynamics simulations predict arachidonic acid binding sites in human ASIC1a and ASIC3 transmembrane domains. <b>2023</b> , 155,	1
629	Illuminating the mechanism and allosteric behavior of NanoLuc luciferase.	O

628	Conformational and mechanical stability of the isolated large subunit of membrane-bound [NiFe]-hydrogenase from Cupriavidus necator. 13,	О
627	Mechanistic Insights into the Reactive Uptake of Chlorine Nitrate at the AirWater Interface. <b>2023</b> , 145, 944-952	O
626	Ability of ionic liquids to inhibit the formation of methane hydrate: Insights from molecular dynamics simulations. <b>2023</b> , 204878	0
625	Interaction of gentamicin and gentamicin-AOT with poly-(lactide-co-glycolate) in a drug delivery system - density functional theory calculations and molecular dynamics simulation. <b>2023</b> , 106958	O
624	Fluorescent protein lifetimes report increased local densities and phases of nuclear condensates during embryonic stem cell differentiation.	0
623	Targeting RNA:protein interactions with an integrative approach leads to the identification of potent YBX1 inhibitors. 12,	O
622	Hydrophobic Hydration: A Theoretical Investigation of Structure and Dynamics. 2023, 135,	О
621	Silibinin chronic treatment in a rat model of Parkinson disease: A comprehensive in-vivo evaluation and in silico molecular modeling. <b>2023</b> , 175517	1
620	Mapping DNA Conformations Using Single-Molecule Conductance Measurements. <b>2023</b> , 13, 129	О
619	Computational Study of the Inhibition of RgpB Gingipain, a Promising Target for the Treatment of Alzheimer Disease.	o
618	Discovery of All-d-Peptide Inhibitors of SARS-CoV-2 3C-like Protease.	О
617	Antibiotic-sterol interactions provide insight into the selectivity of natural aromatic analogues of amphotericin B and their photoisomers. <b>2023</b> , 13,	O
616	Effective strategies toward imine-linked cationic covalent organic frameworks for rapid and selective removal of 99TcO4Ifrom water: insights from DFT and MD calculations.	О
615	Molecular Resolution Nanostructure and Dynamics of the Deep Eutectic Solvent©raphite Interface as a Function of Potential. 2204993	O
614	Multifunctional Electrolyte Additive Enables Highly Reversible Anodes and Enhanced Stable Cathodes for Aqueous Zinc-Ion Batteries.	0
613	Structural dynamics and susceptibility of isobutylamido thiazolyl resorcinol (ThiamidolTM) against human and mushroom tyrosinases. 1-8	O
612	Diffusion and dynamics of Noble Gases in Hydroquinone Clathrate channels.	0
611	Integrating microsecond timescale classical and biased molecular dynamics simulations to screen potential molecules for BRD4-BD1. <b>2023</b> , 167, 113061	1

610	Stretch-activated ionic currents through Ti3C2(OH)2 MXene nanopores. 2023, 147, 107434	O
609	New amidine-benzenesulfonamides as iNOS inhibitors for the therapy of the triple negative breast cancer. <b>2023</b> , 248, 115112	1
608	Molecular mechanisms of integrin 即 activation regulated by graphene, boron nitride and black phosphorus nanosheets. <b>2023</b> , 222, 113139	O
607	Metal-organic frameworks for high performance desalination through thickness control and structural fine-tuning. <b>2023</b> , 230, 119576	O
606	Discovery of inhibitors against SARS-CoV-2 main protease using fragment-based drug design. <b>2023</b> , 371, 110352	O
605	Employing an immunoinformatics approach revealed potent multi-epitope based subunit vaccine for lymphocytic choriomeningitis virus. <b>2023</b> , 16, 214-232	O
604	Atomistic study on thermo-mechanical behavior and structural anisotropy of montmorillonite under triaxial tension and compression. <b>2023</b> , 233, 106817	O
603	Insights into Lewis/Brfisted acidity of metal chlorides and solvent effect of alcohols for synthesis of Evalerolactone by combining molecular dynamics simulations and experiments. <b>2023</b> , 335, 126749	O
602	Surface-active ionic liquids near the electrode surface: Development and influence on molecular dynamics simulations. <b>2023</b> , 614, 156200	O
601	EGCG attenuates	O
600	Free energy landscape of wrapping of lipid nanocluster by polysaccharides. 2023, 294, 106956	O
599	Analysis of the structural dynamics of the mutations in the kinase domain of PINK1 protein associated with Parkinson disease. <b>2023</b> , 857, 147183	O
598	Electrophoretic coalescence behavior of oil droplets in oil-in-water emulsions containing SDS under DC electric field: A molecular dynamics study. <b>2023</b> , 338, 127258	O
597	Molecular interactions of resveratrol with A酙2 peptide and fibril during in-vitro A酙2 aggregation. <b>2023</b> , 7, 100060	O
596	Engineering gas separation property of metal®rganic framework membranes via polymer insertion. <b>2023</b> , 310, 123115	O
595	Ethanol-Induced Condensation and Decondensation in DNA-Linked Nanoparticles: A Nucleosome-like Model for the Condensed State. <b>2023</b> , 145, 706-716	O
594	High-Throughput Prediction of the Impact of Genetic Variability on Drug Sensitivity and Resistance Patterns for Clinically Relevant Epidermal Growth Factor Receptor Mutations from Atomistic Simulations. <b>2023</b> , 63, 321-334	0
593	Sequence Tendency for the Interaction between Low-Complexity Intrinsically Disordered Proteins.	O

592	Elucidation of pH-Induced Protein Structural Changes: A Combined 2D IR and Computational Approach. <b>2023</b> , 62, 451-461	0
591	A comprehensive computer simulation insight into inhibitory mechanisms of EGCG and NQTrp ligands on amyloid-beta assemblies as the Alzheimer disease insignia. 1-10	О
590	Insights into pralsetinib resistance to the non-gatekeeper RET kinase G810C mutation through molecular dynamics simulations. <b>2023</b> , 29,	0
589	CLIP-Seq Analysis Enables the Design of Ribosomal RNA Bait Oligonucleotides That Protect AgainstC9ORF72ALS/FTD-Associated Poly-GR Pathophysiology.	О
588	Embedding Dynamics in Intrinsic Physicochemical Profiles of Market-Stage Antibody-Based Biotherapeutics.	О
587	Deaza-modification of MR1 ligands modulates recognition by MR1-restricted T cells. <b>2022</b> , 12,	О
586	Computational and structural insights into the pre- and post-hydrolysis states of multidrug resistance associated protein 1 in lipid bilayer membranes.	0
585	Effect of Local Stress on Accurate Modeling of Bacterial Outer Membranes Using All-Atom Molecular Dynamics. <b>2023</b> , 19, 363-372	О
584	Interfacial dynamics and growth modes of -microglobulin dimers.	О
583	Cooperation of structural motifs controls drug selectivity in cyclin-dependent kinases: an advanced theoretical analysis. <b>2023</b> , 24,	О
582	An Efficient, Short Stimulus PANC-1 Cancer Cell Ablation and Electrothermal Therapy Driven by Hydrophobic Interactions. <b>2023</b> , 15, 106	O
581	An Open Source Graph-Based Weighted Cycle Closure Method for Relative Binding Free Energy Calculations.	О
580	Increasing the O2 Resistance of the [FeFe]-Hydrogenase CbA5H through Enhanced Protein Flexibility. <b>2023</b> , 13, 856-865	0
579	Citrus nutraceutical eriocitrin and its metabolites are partial agonists of peroxisome proliferator-activated receptor gamma (PPAR) a molecular docking and molecular dynamics study. 1-21	О
578	Direct Correlation between Short-Range Vibrational Spectral Diffusion and Localized Ion-Cage Dynamics of Water-in-Salt Electrolytes. <b>2023</b> , 127, 236-248	О
577	Exploring the possibility of drug repurposing for cancer therapy targeting human lactate dehydrogenase A: a computational approach. 1-10	О
576	Influence of polymer compatibility and layer thickness on the structural and thermophysical properties of polymer multilayer films.	О
575	Structural Factors That Determine the Activity of the Xenobiotic Reductase B Enzyme from Pseudomonas putida on Nitroaromatic Compounds. <b>2023</b> , 24, 400	O

574	Computer Simulation Techniques for Modelling Statics and Dynamics of Nanoscale Structures. <b>2014</b> , 230-299	О
573	Comparative Analysis of the Interfaces between Monomers in the Dimers of Bacterial Histone-Like HU Proteins by the MM-GBSA Method. <b>2022</b> , 67, 897-904	Ο
572	Comparison of force fields to study the zinc-finger containing protein NPL4, a target for Antabuse in cancer therapy.	Ο
571	Conformational preferences of inosine and its methyl derivatives: Comparison of the AMBER derived force field parameters and reparameterization of the glycosidic torsion parameters.	O
570	Nucleoside-Based Cross-Linkers for Hydrogels with Tunable Properties. 2023, 15, 7359-7370	О
569	Small Molecules Targeting the RNA-Binding Protein HuR Inhibit Tumor Growth in Xenografts. <b>2023</b> , 66, 2032-2053	Ο
568	Molecular Orientation of <b>P</b> O3H2 and <b>C</b> OOH Functionalized Dyes on TiO2, Al2O3, ZrO2, and ITO: A Comparative Study. <b>2023</b> , 127, 2705-2715	Ο
567	Computational investigation on the antioxidant activities and on the Mpro SARS-CoV-2 non-covalent inhibition of isorhamnetin. 11,	O
566	Displacement Characteristics of CO2 to CH4 in Heterogeneous Surface Slit Pores.	2
565	Azobenzene-Based Amino Acids for the Photocontrol of Coiled-Coil Peptides.	O
564	Sodium-Dependent Neutral Amino Acid Transporter 2 Can Serve as a Tertiary Carrier for l-Type Amino Acid Transporter 1-Utilizing Prodrugs. <b>2023</b> , 20, 1331-1346	0
563	Resistance to a tyrosine kinase inhibitor mediated by changes to the conformation space of the kinase.	O
562	In Silico Targeting of Fascin Protein for Cancer Therapy: Benchmarking, Virtual Screening and Molecular Dynamics Approaches. <b>2023</b> , 28, 1296	0
561	Structure, energetics and dynamics in crowded amino acid solutions: a molecular dynamics study.	Ο
560	Comparative Protein Structural Network Analysis Reveals C-Terminal Tail Phosphorylation Structural Communication Fingerprint in PTEN-Associated Mutations in Autism and Cancer. <b>2023</b> , 127, 634-647	1
559	Molecular dynamics simulations depict structural motions of the whole human aryl hydrocarbon receptor influencing its binding of ligands and HSP90. 1-16	Ο
558	Structural Investigation of CDCA3-Cdh1 Protein-Protein Interactions using in-vitro Studies and Molecular Dynamics Simulation.	0
557	Polypropylene carbonate-based electrolytes as model for a different approach towards improved ion transport properties for novel electrolytes. <b>2023</b> , 25, 4810-4823	O

556	Molecular Simulation of CO2 and H2 Encapsulation in a Nanoscale Porous Liquid. 2023, 13, 409	O
555	Loading and Co-Solvent-Triggered Release of Okanin, a C4 Plant Key Enzyme Inhibitor, into/from Functional Microgels. <b>2023</b> , 141631	O
554	In silico Identification of Triclosan Derivatives as Potential Inhibitors of Mutant Mycobacterium tuberculosis InhA.	0
553	Molecular Modeling Study of a Receptor Orthosteric Ligand Allosteric Modulator Signaling Complex. <b>2023</b> , 14, 418-434	O
552	Reconfigurable Peptide Analogs of Apolipoprotein A-I Reveal Tunable Features of Nanodisc Assembly.	O
551	Local Molecular Field Theory for Coulomb Interactions in Aqueous Solutions. <b>2023</b> , 127, 809-821	O
550	Molecular and Biological Investigation of Isolated Marine Fungal Metabolites as Anticancer Agents: A Multi-Target Approach. <b>2023</b> , 13, 162	O
549	Unveiling Growth and Dynamics of Liposomes by Graphene Liquid Cell-Transmission Electron Microscopy.	O
548	Effect of substrate charge density on the adsorption of intrinsically disordered protein amyloid 舉0: a molecular dynamics study.	O
547	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.	O
546	Molecular interaction of di-ester bonded cationic Gemini surfactants with pepsin: inlivitro and in silico perspectives. 1-16	O
545	Highlights in TMPRSS2 inhibition mechanism with guanidine derivatives approved drugs for COVID-19 treatment. 1-15	O
544	QDEIA Quantum Deep Potential Interaction Model for Drug Discovery.	2
543	Impact of an Ionic Liquid on Amino Acid Side Chains: A Perspective from Molecular Simulation Studies.	O
542	Residues E53, L55, H59, and G70 of the Cellular Receptor Protein Tva Mediate Cell Binding and Entry of Novel Subgroup K Avian Leukosis Virus. <b>2023</b> , 102962	O
541	Mapping the Three-Dimensional Nanostructure of the Ionic LiquidBolid Interface Using Atomic Force Microscopy and Molecular Dynamics Simulations. 2202110	O
540	A physicochemical cause of betaine lipid evolutionary loss in seed plants?.	О
539	In silico investigation of cytochrome bc1 molecular inhibition mechanism against Trypanosoma cruzi. <b>2023</b> , 17, e0010545	O

538	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. <b>2023</b> , 24, 2626	O
537	Molecular Dynamics and Experimental Study of the Effect of CeF3 and NdF3 Additives on the Physical Properties of FLiNaK. <b>2023</b> , 127, 1197-1208	O
536	Revisiting the Sweet Taste Receptor T1R2-T1R3 through Molecular Dynamics Simulations Coupled with a Noncovalent Interactions Analysis. <b>2023</b> , 127, 1110-1119	O
535	Effects of molecular size and orientation on the interfacial properties and wetting behavior of water/n-alkane systems: a molecular-dynamics study.	O
534	Plant Terpenoid Permeability through Biological Membranes Explored via Molecular Simulations. <b>2023</b> , 127, 1144-1157	0
533	Molecular Mechanics of Disordered Solids.	O
532	Effect of the QM Size, Basis Set, and Polarization on QM/MM Interaction Energy Decomposition Analysis.	1
531	Structure of alpha-synuclein fibrils derived from human Lewy body dementia tissue.	O
530	Elucidating the Sluggish Water Dynamics at the Ice-Binding Surface of the Hyperactive Tenebrio molitor Antifreeze Protein. <b>2023</b> , 127, 121-132	О
529	Control of Diblock Copolyelectrolyte Morphology through Electric Field Application.	1
528	Molecular dynamics investigation of the asphaltenellaolinite interactions in water, toluene, and waterfoluene mixtures.	0
527	Molecular dynamics study of Clipermeation through cystic fibrosis transmembrane conductance regulator (CFTR). <b>2023</b> , 80,	O
526	Coenzyme Engineering of Glucose-6-phosphate Dehydrogenase on a Nicotinamide-Based Biomimic and Its Application as a Glucose Biosensor. <b>2023</b> , 13, 1983-1998	О
525	Molecular Dynamics Simulations of Asphaltene Aggregation: Machine-Learning Identification of Representative Molecules, Molecular Polydispersity, and Inhibitor Performance. <b>2023</b> , 8, 4862-4877	O
524	Molecular Dynamics simulation based trinucleotide and tetranucleotide level structural and energy characterization of functional units of genomic DNA.	О
523	Structure of human NaV1.6 channel reveals Na+selectivity and pore blockade by 4,9-anhydro-tetrodotoxin.	O
522	Interactive computational and experimental approaches improve the sensitivity of periplasmic binding protein-based nicotine biosensors for measurements in biofluids.	О
521	Enhanced Grand Canonical Sampling of Occluded Water Sites Using Nonequilibrium Candidate Monte Carlo.	O

520	Can molecular dynamics simulations improve predictions of protein-ligand binding affinity with machine learning?.	1
519	Identifying Protein[ligand Interactions via a Novel Distance Self-Feedback Biomolecular Interaction Network. <b>2023</b> , 127, 899-911	O
518	Characterizing the Interactions of Cell Membrane-Disrupting Peptides with Lipid-Functionalized Single-Walled Carbon Nanotube Systems for Antimicrobial Screening.	0
517	Druggable sites identification in Streptococcus mutans VicRK system evaluated by catechols. 1-16	O
516	Release of nanodiscs from charged nano-droplets in the electrospray ionization revealed by molecular dynamics simulations. <b>2023</b> , 6,	О
515	Mechanistic Basis for Enhanced Strigolactone Sensitivity in KAI2 Triple Mutant.	O
514	Graph-based Quantum Response Theory and Shadow Born-Oppenheimer Molecular Dynamics.	1
513	Porous Electrospun Films with Reversible Photoresponsive Microenvironmental Humidity Regulation: A Controllable Hydrogen-Bonding Synergistic Effect Exhibited by Acrylic Acid Segments. <b>2023</b> , 15, 6187-6201	O
512	Aggregation of Asphaltene Subfractions A1 and A2 in Different Solvents from the Perspective of Molecular Dynamics Simulations.	О
511	FSHR activation through small molecule modulators: Mechanistic insights from MD simulations. <b>2023</b> , 154, 106588	O
510	Torque generation mechanism in Fo motor of ATP synthase elucidated by free-energy and Coulomb-energy landscapes along the c-ring rotation. <b>2023</b> ,	1
509	Mitochondrial Membranes: Model Lipid Compositions, Material Properties and the Changing Curvature of Cardiolipin.	O
508	Impact and structure of water in aqueous octanol mixtures: Hz-GHz dielectric relaxation measurements and computer simulations. <b>2023</b> , 439, 114600	O
507	Rational approaches to discover SARS-CoV-2/ACE2 interaction inhibitors: Pharmacophore-based virtual screening, molecular docking, molecular dynamics and binding free energy studies. <b>2023</b> , 375, 121345	0
506	Distinct roles of graphene and graphene oxide nanosheets in regulating phospholipid flip-flop. <b>2023</b> , 637, 112-122	O
505	Antiviral activity and molecular modeling studies on 1H-indole-2,3-diones carrying a naphthalene moiety. <b>2023</b> , 1281, 135100	O
504	Computational assessment of hexadecane freezing by equilibrium atomistic molecular dynamics simulations. <b>2023</b> , 638, 743-757	1
503	Carboxyl PEGylation of magnetic nanoparticles as antithrombotic and thrombolytic agents by calcium binding. <b>2023</b> , 638, 672-685	O

502	Distinct effects of zwitterionic molecules on ionic solvation in (ethylene oxide)10: a molecular dynamics simulation study. <b>2023</b> , 25, 8180-8189	Ο
501	The substrate specificity in the O-demethylation of 4-alkylguaiacols by cytochrome P450 AgcAP450. <b>2023</b> , 13, 2070-2079	Ο
500	Molecular dynamics study on evaporation of metal nitrate-containing nanodroplets in flame spray pyrolysis. <b>2023</b> , 15, 5877-5890	0
499	Identifying Mutational Hotspots using Differences in Atomic Fluctuations combined with Positional Variability.	Ο
498	Characterization of a TatA/TatB binding site on the TatC component of the Escherichia coli twin arginine translocase. <b>2023</b> , 169,	Ο
497	Scalable Inhibitors of the Nsp3Nsp4 Coupling in SARS-CoV-2. <b>2023</b> , 8, 5349-5360	Ο
496	Stability and structural evolution of double-stranded DNA molecules under high pressures: A molecular dynamics study. 11,	Ο
495	Accelerated Quantum Mechanics/Molecular Mechanics Simulations via Neural Networks Incorporated with Mechanical Embedding Scheme. <b>2023</b> , 19, 1157-1169	Ο
494	Gold Nanorods Inhibit Tumor Metastasis by Regulating MMP-9 Activity: Implications for Radiotherapy.	0
493	Evaluation of 6-OxP-CD, an Oxime-based cyclodextrin as a viable medical countermeasure against nerve agent poisoning: Experimental and molecular dynamic simulation studies on its inclusion complexes with cyclosarin, soman and VX. <b>2023</b> , 18, e0283181	Ο
492	Structural basis for bacterial energy extraction from atmospheric hydrogen. <b>2023</b> , 615, 541-547	Ο
491	DNA methylation of the promoter region at the CREB1 binding site is a mechanism for the epigenetic regulation of brain-specific PKM $\square$ 2023, 1866, 194909	Ο
490	Modeling the Infrared Spectroscopy of Oligonucleotides with 13C Isotope Labels. <b>2023</b> , 127, 2351-2361	Ο
489	Stabilization of Interdomain Interactions in G protein & Subunits Determines G & Subtype Signaling Specificity.	Ο
488	Evolutionary relevance of single hucleotide variants within the forebrain exclusive human accelerated enhancer regions. <b>2023</b> , 24,	0
487	Improving Properties of Podophyllic Aldehyde-Derived Cyclolignans: Design, Synthesis and Evaluation of Novel Lignohydroquinones, Dual-Selective Hybrids against Colorectal Cancer Cells. <b>2023</b> , 15, 886	Ο
486	Migration mediated by the oxysterol receptor GPR183 depends on arrestin coupling but not receptor internalization. <b>2023</b> , 16,	0
485	Partial Destabilization of Amyloid-Protofibril by Methionine Photo-Oxidation: A Molecular Dynamic Simulation Study. <b>2023</b> , 8, 10148-10159	Ο

484	Inner pore hydration free energy controls the activation of big potassium channels. 2023, 122, 1158-1167	O
483	Solidified Methane Storage Using an Efficient Class of Anionic Surfactants under Dynamic and Static Conditions: An Experimental and Computational Investigation.	O
482	Experimental and computational studies on the ion dissociation states of 1-butyl-3-methyimidazolium tetrafluoroborate in water and alcohols. <b>2023</b> , 375, 121370	0
481	Bias-force guided simulations combined with experimental validations towards GPR17 modulators identification. <b>2023</b> , 160, 114320	О
480	Contribution of air-water interface in removing PFAS from drinking water: adsorption, stability, interaction and machine learning studies. <b>2023</b> , 119947	О
479	The effects of adsorbed benzo(a)pyrene on dynamic behavior of polystyrene nanoplastics through phospholipid membrane: A molecular simulation study. <b>2023</b> , 224, 113211	O
478	Effect of temperature and salt addition on the structural properties of Triton X-100. 2023, 615, 128614	0
477	In-Depth Occlusion of Dentinal Tubules and Rapid Remineralization of Demineralized Dentin Induced by Polyelectrolyte-Calcium Complexes.	O
476	N?-Phenylacetohydrazide Derivatives as Potent Ebola Virus Entry Inhibitors with an Improved Pharmacokinetic Profile.	O
475	Highly (2 2 2)-oriented flexible hollow fiber-supported metal-organic framework membranes for ultra-permeable and selective H2/CO2 separation. <b>2023</b> , 461, 141976	О
474	Encapsulation of testosterone and dihydrotestosterone into chiral carbon nanotubes: A molecular dynamics study. <b>2023</b> , 376, 121426	O
473	Leveraging Advanced In Silico Techniques in Early Drug Discovery: A Study of Potent Small-Molecule YAP-TEAD PPI Disruptors.	O
472	Bridging Thermodynamics, Antimicrobial Activity, and pH Sensitivity of Cationic Membranolytic Heptapeptides Computational and Experimental Study.	O
471	Constrained catecholamines gain ZAR selectivity through allosteric effects on pocket dynamics. <b>2023</b> , 14,	O
470	The Impact of Pathogenic and Artificial Mutations on Claudin-5 Selectivity from Molecular Dynamics Simulations. <b>2023</b> ,	0
469	Oxidation of Dueling Cysteine Promotes Subunit Exchange in SOD1.	Ο
468	Embedding Beyond Electrostatics: The Extended Polarizable Density Embedding Model. <b>2023</b> , 127, 3248-325	
467	Simulating a flexible water model as rigid: Best practices and lessons learned. <b>2023</b> , 158, 134506	Ο

466	Structural evolution of the butylated hydroxytoluene/menthol hydrophobic eutectic solvent upon methanol and ethanol cosolvent addition. <b>2023</b> , 375, 121302	О
465	Finely tuning the microporosity in phosphoric acid doped triptycene-containing polybenzimidazole membranes for highly permselective helium and hydrogen recovery. <b>2023</b> , 672, 121474	O
464	Computer simulation study of ion-water and water-water hydrogen bonds in methanesulfonic acid solutions at room temperature. <b>2023</b> , 377, 121518	О
463	Inhibition effect of novel amphiphilic poly(amino acid)s on methane hydrate. <b>2023</b> , 113, 204971	O
462	In silico repurposing of CNS drugs for multiple sclerosis. <b>2023</b> , 73, 104622	О
461	Conformational stability of the deamidated and mutated human <b>B</b> 2-crystallin. <b>2023</b> , 296, 106986	O
460	Can sodium 1-alkylsulfonates participate in the sodium dodecyl sulfate micelle formation?. <b>2023</b> , 377, 121568	О
459	Atomic insights into the mechanism of trace water influence on lipase catalysis in organic media. <b>2023</b> , 464, 142610	O
458	Water-Mediated attraction between Like-charged species involved in calcium phosphate nucleation. <b>2023</b> , 378, 121585	О
457	Whether carbon nanotubes are suitable for delivering small drugs with aromatic rings through non-covalent adsorption?. <b>2023</b> , 378, 121595	O
456	New anticancer potential Pt complex with tertamyl dithiocarbamate ligand: Synthesis, DNA targeting behavior, molecular dynamic, and biological activity. <b>2023</b> , 379, 121651	О
455	Assessing the inhibition of glycation of Erystallin by thymoquinone: A mechanistic approach using experimental and computational methods. <b>2023</b> , 380, 121750	O
454	MgO/Molten salt interfacial thermal transport and its consequences on thermophysical property enhancement: A molecular dynamics study. <b>2023</b> , 207, 124022	О
453	Effect of water content on transport properties and interactions of amino-functionalized ionic liquids. <b>2023</b> , 569, 111852	O
452	Selective recovery of lithium from mother liquor of Li2CO3 by synergistic hydrophobic deep eutectic solvents: Performance and mechanistic insight. <b>2023</b> , 313, 123353	О
451	Discovery of the new alpha-glucosidase inhibitor with therapeutic potential in type 2 diabetes mellitus by a novel high-throughput virtual screening and free energy evaluation. <b>2023</b> , 121, 108447	О
450	Identification and structure-activity modeling of ACE inhibitory peptides demonstrating anti-inflammatory effects: Extracted from Antheraea assama and Philosomia ricnii pupae. <b>2023</b> , 53, 102625	О
449	Assessment of CO2-Oil swelling behavior using molecular dynamics simulation: CO2 utilization and storage implication. <b>2023</b> , 379, 121582	O

448	GAP positions catalytic H-Ras residue Q61 for GTP hydrolysis in molecular dynamics simulations, complicating chemical rescue of Ras deactivation. <b>2023</b> , 104, 107835	O
447	A seminal perspective on the role of chondroitin sulfate in biomineralization. <b>2023</b> , 310, 120738	O
446	Revealing the confinement effects of graphitic carbon nitride nanochannels on the water desalination performance. <b>2023</b> , 314, 123553	0
445	Structure-based virtual screening for potent inhibitors of GH-20 ®N-acetylglucosaminidase: Classical and machine learning scoring functions, and molecular dynamics simulations. <b>2023</b> , 104, 107856	О
444	Insight into surfactant adsorption performance at asphaltene surface by in-situ DPI experiment and microscopic MD simulation. <b>2023</b> , 666, 131313	0
443	Molecular dynamics study of water rotational relaxation in saccharide solution for the development of bioprotective agent. <b>2023</b> , 380, 121707	O
442	Interaction of neutral and protonated Tamoxifen with the DPPC lipid bilayer using molecular dynamics simulation. <b>2023</b> , 194, 109225	0
441	Molecular dynamics simulation of ethanol electrohydrodynamic atomization: Microscopic mechanism of the operating parameter effects. <b>2023</b> , 379, 121602	O
440	Multicomponent Petasis reaction for the identification of pyrazine based multi-target directed anti-Alzheimer's agents: In-silico design, synthesis, and characterization. <b>2023</b> , 254, 115354	0
439	An exploration of efficiency of proposed drug delivery system including BNNT, C48N12, and TMZ in treating of glioblastoma through classical molecular dynamics. <b>2023</b> , 379, 121625	О
438	Comparing supercapacitors with graphene/graphyne electrodes and [Bmim][PF6], [Emim][BF4], [Ch][Gly] and [Pyr][Tfsi] ionic liquids using molecular dynamics. <b>2023</b> , 379, 121703	0
437	Bioinformatics and immunoinformatics approach to develop potent multi-peptide vaccine for coxsackievirus B3 capable of eliciting cellular and humoral immune response. <b>2023</b> , 239, 124320	О
436	Mechanism-driven moderate alkalinity release for efficient recovery of high-purity cobalt and nickel from spent lithium-ion batteries. <b>2023</b> , 315, 123645	0
435	Study on the structural characteristics and interaction mechanisms of ionic liquid mixtures with a common imidazolium cation. <b>2023</b> , 380, 121743	O
434	Elucidating the effects of emulsification on the thermal performances of palm oil-based phase change materials by molecular dynamics simulations. <b>2023</b> , 64, 107071	0
433	Aptamer affinity to P53 DBD: A molecular dynamics study. <b>2023</b> , 1284, 135355	O
432	Isothermal titration calorimetry and molecular modeling study of the complex formation of daclatasvir by Eyclodextrin and trimethyl-tyclodextrin. <b>2023</b> , 313, 120870	0
431	Identifying non-nucleoside inhibitors of RNA-dependent RNA-polymerase of SARS-CoV-2 through per-residue energy decomposition-based pharmacophore modeling, molecular docking, and molecular dynamics simulation. <b>2023</b> , 16, 501-519	O

430	Hierarchical Self-Assembly of OrganicIhorganic Hybrid Nanosheets to Construct Tubular Superstructures for Photocatalytic Degradation. <b>2023</b> , 6, 6270-6278	O
429	Influence of electronic polarization on the binding of anions to a chloride-pumping rhodopsin. <b>2023</b> , 122, 1548-1556	O
428	Steering phase-separated droplets to control fibrillar network evolution of supramolecular peptide hydrogels. <b>2023</b> ,	O
427	Miscibility of Phosphatidylcholines in Bilayers: Effect of Acyl Chain Unsaturation. 2023, 13, 411	O
426	Structural intrinsic disorder in a functionalized potyviral coat protein as a main viability determinant of its assembled nanoparticles. <b>2023</b> , 236, 123958	O
425	Photophysical and photochemical properties of 3-hydroxyflavone in ethanol solution: Implicit vs explicit solvent models. <b>2023</b> , 381, 121783	O
424	Ionizable lipids penetrate phospholipid bilayers with high phase transition temperatures: perspectives from free energy calculations. <b>2023</b> , 253, 105294	O
423	Specific ion effects on the aggregation of polysaccharide-based polyelectrolyte complex particles induced by monovalent ions within Hofmeister series. <b>2023</b> , 643, 305-317	O
422	The molecular basis of the antidepressant action of the magic mushroom extract, psilocin. <b>2023</b> , 1871, 140914	O
421	Effect of molecular dynamics water models on flux, diffusivity, and ion dynamics for polyamide membrane simulations. <b>2023</b> , 678, 121630	O
420	Molecular dynamics simulations of the calmodulin-induced thelix in the SK2 calcium-gated potassium ion channel. <b>2023</b> , 299, 102850	O
419	Pressure-driven flow behavior of small molecules through a carbon nanotube. <b>2023</b> , 374, 121276	O
418	Computer-aided affinity enhancement of a cross-reactive antibody against dengue virus envelope domain III.	O
417	Galantamine Based Novel Acetylcholinesterase Enzyme Inhibitors: A Molecular Modeling Design Approach. <b>2023</b> , 28, 1035	1
416	Asymmetry and Ion Selectivity Properties of Bacterial Channel NaK Mutants Derived from Ionotropic Glutamate Receptors. <b>2023</b> , 435, 167970	0
415	Hitto lead optimization and chemoinformatic studies for a new series of Autotaxin inhibitors. <b>2023</b> , 249, 115130	O
414	Atomistic insights on the adsorption of long-chain undecane molecules on carbon nanotubes: Roles of chirality and surface hydroxylation. <b>2023</b> , 133, 109706	O
413	Computational analysis of protein-ligand interaction by targeting a cell cycle restrainer. <b>2023</b> , 231, 107367	2

412	Molecular dynamics study of the effect of temperature on the flotation behavior of sodium oleate on the surface of diaspore. <b>2023</b> , 192, 108004	Ο
411	The role of conformational change and key glutamic acid residues in the ClC-ec1 antiporter. <b>2023</b> , 122, 1068-1085	O
410	On the Behavior of the Ethylene Glycol Components of Polydisperse Polyethylene Glycol PEG200. <b>2023</b> , 127, 1178-1196	Ο
409	Deciphering the mechanism of resistance by novel double mutations in pncA in Mycobacterium tuberculosis using protein structural graphs (PSG) and structural bioinformatic approaches. <b>2023</b> , 154, 106599	Ο
408	Novel Chimeric Amino Acid-Fatty Alcohol Ester Amphiphiles Self-Assemble into Stable Primitive Membranes in Diverse Geological Settings. <b>2023</b> , 23, 327-343	Ο
407	Structural analysis of water networks. <b>2022</b> , 11,	Ο
406	Effects of Water Deuteration on Thermodynamic and Structural Properties of Proteins and Biomembranes. <b>2023</b> , 127, 1138-1143	0
405	Investigation of the effects of N-Acetylglucosamine on the stability of the spike protein in SARS-CoV-2 by molecular dynamics simulations. <b>2023</b> , 1222, 114049	Ο
404	The Impact of Pathogenic and Artificial Mutations on Claudin-5 Selectivity from Molecular Dynamics Simulations.	0
403	Protein dynamics provide mechanistic insights about epistasis among common missense polymorphisms. <b>2023</b> ,	Ο
402	Elucidating the Molecular Origins of the Transference Number in Battery Electrolytes Using Computer Simulations. <b>2023</b> , 3, 306-315	0
401	Phosphate aggregation, diffusion, and adsorption on kaolinite in saline solutions by molecular dynamics simulation. <b>2023</b> , 233, 106844	Ο
400	Simulation of AOT reverse micelles with polyethylenimine in hexane. 2023, 301, 283-291	Ο
399	Construction of Fusion Protein with Carbohydrate-Binding Module and Leaf-Branch Compost Cutinase to Enhance the Degradation Efficiency of Polyethylene Terephthalate. <b>2023</b> , 24, 2780	Ο
398	Structural Basis for Agonistic Activity and Selectivity toward Melatonin Receptors hMT1 and hMT2. <b>2023</b> , 24, 2863	1
397	Rational Design of N-Methylcarbamoylguanidinyl Derivatives as Highly Potent Dual-Target Chitin Hydrolase Inhibitors for Retarding Growth of Pest Insects. <b>2023</b> , 71, 2817-2826	Ο
396	On the Sensitivity and Affinity of Gold, Silver, and Platinum Surfaces against the SARS-CoV-2 Virus: A Comparative Computational Study. <b>2023</b> , 63, 1276-1292	0
395	Substrate binding and lipid-mediated allostery in the human organic anion transporter 1 at the atomic-scale. <b>2023</b> , 160, 114342	Ο

394	Analogue and structure based approaches for modelling HIV-1 integrase inhibitors. 1-11	O
393	How Can Static and Oscillating Electric Fields Serve in Decomposing Alzheimer and Other Senile Plaques?. <b>2023</b> , 145, 3543-3553	O
392	Multi-Hydration Induced Zwitterionic Hydrogel with Open Environment Stability for Chemical Sensing. 2200061	О
391	On the interplay between lipids and asymmetric dynamics of an NBS degenerate ABC transporter. <b>2023</b> , 6,	O
390	Development of a Syrian hamster anti-PD-L1 monoclonal antibody enables oncolytic adenoviral immunotherapy modelling in an immunocompetent virus replication permissive setting. 14,	1
389	Coulombic Organization in Membrane-Embedded Rotary Motor of ATP Synthase. <b>2023</b> , 127, 1552-1562	1
388	Structure of Geobacter cytochrome OmcZ identifies mechanism of nanowire assembly and conductivity. <b>2023</b> , 8, 284-298	О
387	Thermodynamic regulation over nano-heterogeneous structure of electrolyte solution to improve stability of flow batteries. <b>2023</b> , 270, 118534	O
386	Mechanistic Insights into Substrate Positioning That Distinguish Non-heme Fe(II)/Eketoglutarate-Dependent Halogenases and Hydroxylases. <b>2023</b> , 13, 2489-2501	O
385	High-throughput single-molecule quantification of individual base stacking energies in nucleic acids. <b>2023</b> , 14,	O
384	Critical Role of Position 10 Residue in the Polymyxin Antimicrobial Activity. 2023, 66, 2865-2876	0
383	Entropically-Driven Co-assembly of l-Histidine and l-Phenylalanine to Form Supramolecular Materials. <b>2023</b> , 17, 3506-3517	O
382	Antiplasmodial activity of coumarins isolated from Polygala boliviensis: in⊡itro and in silico studies. 1-21	O
381	Computer-Aided Virtual Screening and In Vitro Validation of Biomimetic Tyrosinase Inhibitory Peptides from Abalone Peptidome. <b>2023</b> , 24, 3154	O
380	Computational modeling of cyanobacterial phytoconstituents against toll-like receptors of skin cancer. 1-13	O
379	Thermal site energy fluctuations in photosystem I: new insights from MD/QM/MM calculations. <b>2023</b> , 14, 3117-3131	O
378	Insightful Improvement in the Design of Potent Uropathogenic E. coli FimH Antagonists. 2023, 15, 527	О
377	Addressing the Structural Organization of Silicone Alternatives in Formulations by Molecular Dynamics Simulations and a Novel Equilibration Protocol. <b>2023</b> , 15, 796	Ο

376	In silico drug discovery of SIRT2 inhibitors from natural source as anticancer agents. <b>2023</b> , 13,	0
375	Molecular Mechanism in the Disruption of Chronic Traumatic Encephalopathy-Related R3 <b>R</b> 4 Tau Protofibril by Quercetin and Gallic Acid: Similarities and Differences. <b>2023</b> , 14, 897-908	O
374	Structural Insights into ATP-Sensitive Potassium Channel Mechanics: A Role of Intrinsically Disordered Regions. <b>2023</b> , 63, 1806-1818	0
373	Dynamic molecular ordering in multiphasic nanoconfined ionic liquids detected with time-resolved diffusion NMR. <b>2023</b> , 4,	1
372	Ensemble-based virtual screening of human PI4KIII⊞nhibitors toward the Hepatitis C virus. <b>2023</b> , 815, 140354	0
371	Discovery of New Quinoline-Based Diarylamides as Potent B-RAFV600E/C-RAF Kinase Inhibitors Endowed with Promising In Vitro Anticancer Activity. <b>2023</b> , 24, 3216	O
370	Dynamic Electric Field Alignment Determines the Water Rotational Motion around Protein. <b>2023</b> , 127, 1376-1384	0
369	Systematically testing human HMBS missense variants to reveal mechanism and pathogenic variation.	O
368	Can Resveratrol Influence the Activity of 11旪ydroxysteroid Dehydrogenase Type 1? A Combined In Silico and In Vivo Study. <b>2023</b> , 16, 251	0
367	Identification of potential ATP-competitive cyclin-dependent kinase 1 inhibitors: De novo drug generation, molecular docking, and molecular dynamics simulation. <b>2023</b> , 155, 106645	O
366	Molecular basis of RNA recognition by TBP of HIV -1 from multiple molecular dynamics simulations and energy predictions. <b>2023</b> , 44, 1291-1299	0
365	May the force be with you: The role of hyper-mechanostability of the bone sialoprotein binding protein during early stages of Staphylococci infections. 11,	O
364	Investigating the validity of the Bosanquet equation for predicting the self-diffusivities of fluids inside nanotubes using equilibrium molecular dynamics simulations. <b>2023</b> , 13, 025338	0
363	The Mechanism of Channel Opening of Anion Channelrhodopsin GtACR1: A Molecular Dynamics Simulation. <b>2023</b> , 11, 510	Ο
362	RNA G-quadruplex folding is a multi-pathway process with a variety of short-lived intermediates.	0
361	Molecular Dynamics Refinement of Open State Serotonin 5-HT3A Receptor Structures. <b>2023</b> , 63, 1196-1207	O
360	An Adaptive Local Iterative Method for Fast Calculation of Electrostatic Interactions between Charged Polymers in Dielectric Inhomogeneous System. <b>2023</b> , 6,	0
359	Coupled binding and folding of disordered SPIN N-terminal region in myeloperoxidase inhibition. 10,	O

358	Lipidation Alters the Structure and Hydration of Myristoylated Intrinsically Disordered Proteins. <b>2023</b> , 24, 1244-1257	0
357	Local Hydration Control and Functional Implications Through S-Nitrosylation of Proteins: Kirsten Rat Sarcoma Virus (K-RAS) and Hemoglobin (Hb). <b>2023</b> , 127, 1526-1539	Ο
356	Molecular docking and molecular simulation studies for N-degron selectivity of chloroplastic ClpS from Chlamydomonas reinhardtii. <b>2023</b> , 103, 107825	0
355	Design of a multi-epitope vaccine against six Nocardia species based on reverse vaccinology combined with immunoinformatics. 14,	0
354	Benchmarking Molecular Dynamics Force Fields for All-Atom Simulations of Biological Condensates.	0
353	Discovery of potential FGFR3 inhibitors via QSAR, pharmacophore modeling, virtual screening and molecular docking studies against bladder cancer. <b>2023</b> , 21,	O
352	Rationalizing the Design of PluronicsBurfactant Mixed Micelles through Molecular Simulations and Experiments. <b>2023</b> , 39, 2692-2709	O
351	Exploring the potential and identifying Withania somnifera alkaloids as novel dihydrofolate reductase (DHFR) inhibitors by the AlteQ method. 1-14	0
350	Investigating the binding affinity of andrographolide against human SARS-CoV-2 spike receptor-binding domain through docking and molecular dynamics simulations. 1-16	O
349	An Efficient Multilayer Approach to Model DNA-Based Nanobiosensors. <b>2023</b> , 127, 1513-1525	O
348	Selective 日本 Nicotinic Acetylcholine Receptor Ligand as a Potential Tracer for Drug Addiction. <b>2023</b> , 24, 3614	O
347	Structures of NF- <b>B</b> p52 homodimer-DNA complexes rationalize binding mechanisms and transcription activation. 12,	O
346	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
345	Integration of immunoinformatics and cheminformatics to design and evaluate a multitope vaccine against Klebsiella pneumoniae and Pseudomonas aeruginosa coinfection. 10,	O
344	Anionic phospholipids control mechanisms of GPCR-G protein recognition. 2023, 14,	O
343	Hexamethylenetetramine additive with zincophilic head and hydrophobic tail for realizing ultra-stable Zn anode. <b>2023</b> , 460, 141902	O
342	The impact of SARS-CoV-2 3CL protease mutations on nirmatrelvir inhibitory efficiency. Computational insights into potential resistance mechanisms. <b>2023</b> , 14, 2686-2697	0
341	Catalytic site mutations confer multiple states of G protein activation. 2023, 16,	O

340	The Conformational Dynamics of the Ligands Determines the Electronic Circular Dichroism of the Chiral Au38(SC2H4Ph)24 Cluster. <b>2023</b> , 14, 1941-1948	О
339	Using High-Throughput Molecular Dynamics Simulation to Enhance the Computational Design of Kemp Elimination Enzymes. <b>2023</b> , 63, 1323-1337	O
338	Therapeutic phosphorodiamidate morpholino oligonucleotides: Physical properties, solution structures, and folding thermodynamics. <b>2023</b> , 31, 631-647	О
337	Novel Inhibitory Role of Fenofibric Acid by Targeting Cryptic Site on the RBD of SARS-CoV-2. <b>2023</b> , 13, 359	O
336	Phosphorylation at Ser289 Enhances the Oligomerization of Tau Repeat R2. 2023, 63, 1351-1361	О
335	Insights into the Degradation of Polymer <b>D</b> rug Conjugates by an Overexpressed Enzyme in Cancer Cells. <b>2023</b> , 66, 2761-2772	O
334	Self-inhibited State of Venezuelan Equine Encephalitis Virus (VEEV) nsP2 Cysteine Protease: A Crystallographic and Molecular Dynamics Analysis. <b>2023</b> , 435, 168012	О
333	Cytocompatibility of Ti3C2Tx MXene with Red Blood Cells and Human Umbilical Vein Endothelial Cells and the Underlying Mechanisms. <b>2023</b> , 36, 347-359	O
332	Efficient production of salvianic acid A from L-dihydroxyphenylalanine through a tri-enzyme cascade.	О
331	Engineered Glycosidase for Significantly Improved Production of Naturally Rare Vina-Ginsenoside R7. <b>2023</b> , 71, 3852-3861	O
330	Conformational ensemble of the NSP1 CTD in SARS-CoV-2: Perspectives from the free energy landscape. <b>2023</b> ,	О
329	Influence of gelation temperature on physicochemical properties of cellulose hydrogels prepared from ionic liquid/DMSO solution. <b>2023</b> , 376, 121465	O
328	Study on host-guest interaction of aroma compounds/Etyclodextrin inclusion complexes. <b>2023</b> , 178, 114589	О
327	Re-Balancing Replica Exchange with Solute Tempering for Sampling Dynamic Protein Conformations. <b>2023</b> , 19, 1602-1614	O
326	Unravelling the destabilization potential of ellagic acid on ⊞ynuclein fibrils using molecular dynamics simulations. <b>2023</b> , 25, 8128-8143	0
325	Fabrication of doxorubicin loaded aptamer-functionalized cationic <code>Hactoglobulin</code> nanocomplex: A biocompatible multifunctional nanoplatform for encapsulation and controlled release of anticancer drugs. <b>2023</b> , 81, 104254	Ο
324	Relaxation dynamics measure the aggregation propensity of amyloid-hand its mutants. 2023, 158, 105101	0
323	Assessments of Variational Autoencoder in Protein Conformation Exploration. 1-13	O

322	Effect of histidine covalent modification on strigolactone receptor activation and selectivity. <b>2023</b> , 1219-1228	О
321	How ractopamine binds to bovine serum albumin at the drug site 1. <b>2023</b> , 49, 599-607	О
320	i-Motif folding intermediates with zero-nucleotide loops are trapped by 2?-fluoroarabinocytidine via FIIIH and OIIIH hydrogen bonds. <b>2023</b> , 6,	1
319	Inhibition of 3-Hydroxykynurenine Transaminase from Aedes aegypti and Anopheles gambiae: A Mosquito-Specific Target to Combat the Transmission of Arboviruses. <b>2023</b> , 3, 211-222	o
318	NanoModeler CG: A Tool for Modeling and Engineering Functional Nanoparticles at a Coarse-Grained Resolution. <b>2023</b> , 19, 1582-1591	O
317	Molecular Dynamic Simulation Analysis of a Novel Missense Variant in CYB5R3 Gene in Patients with Methemoglobinemia. <b>2023</b> , 59, 379	2
316	Molecular dynamics simulations reveal the importance of amyloid-beta oligomer 點heet edge conformations in membrane permeabilization. <b>2023</b> , 299, 103034	0
315	In Silico Analysis of the Structural Dynamics and Substrate Recognition Determinants of the Human Mitochondrial Carnitine/Acylcarnitine SLC25A20 Transporter. <b>2023</b> , 24, 3946	О
314	Discovery of potent inhibitors targeting Glutathione S-transferase of Wuchereria bancrofti: a step toward the development of effective anti-filariasis drugs.	0
313	Impact of Hydrogen Bonds on CO2 Binding in Eutectic Solvents: An Experimental and Computational Study toward Sorbent Design for CO2 Capture. <b>2023</b> , 11, 3740-3749	o
312	Cholesterol esters form supercooled lipid droplets whose nucleation is facilitated by triacylglycerols. <b>2023</b> , 14,	0
311	Dynamic Heterogeneity of Solvent Motion and Ion Transport in Concentrated Electrolytes. <b>2023</b> , 127, 1803-1810	O
310	Molecular dynamics simulation of infrared absorption spectra of one-dimensional ordered single-file water. <b>2023</b> , 72, 084207	0
309	Preparation, identification, computational analysis of antioxidative peptides derived from Lumbricus protein and prevention of UV-B radiation-induced skin damaged. <b>2023</b> , 52, 102492	0
308	Unraveling topoisomerase IA gate dynamics in presence of PPEF and its preclinical evaluation against multidrug-resistant pathogens. <b>2023</b> , 6,	O
307	Conformational changes in the human Cx43/GJA1 gap junction channel visualized using cryo-EM. <b>2023</b> , 14,	0
306	Structural basis of the activation of PPARIby the plasticizer metabolites MEHP and MINCH. <b>2023</b> , 173, 107822	0
305	Influence of Mutations of Conserved Arginines on Neuropeptide Binding in the DPP III Active Site. <b>2023</b> , 28, 1976	О

304	Self-Organization of Mobile, Polyelectrolytic Dendrons on Stable, Amphiphile-Based Spherical Surfaces. <b>2023</b> , 39, 3439-3449	Ο
303	Conformational landscapes of artificial peptides predicted by various force fields: are we ready to simulate 曲mino acids?. <b>2023</b> , 25, 7466-7476	О
302	Study on molecular mechanisms of CD4 dependency and independency of HIV-1 gp120. <b>2023</b> , 13, 6274-6286	О
301	Atomistic molecular insight on Angiotensin-(1-7) interpeptide interactions.	O
300	Evaluation of polyanionic cyclodextrins as high affinity binding scaffolds for fentanyl. 2023, 13,	O
299	Identification of and Mechanistic Insights into SARS-CoV-2 Main Protease Non-Covalent Inhibitors: An In-Silico Study. <b>2023</b> , 24, 4237	O
298	Understanding Drug Resistance of Wild-Type and L38HL Insertion Mutant of HIV-1 C Protease to Saquinavir. <b>2023</b> , 14, 533	О
297	AI-Accelerated Design of Targeted Covalent Inhibitors for SARS-CoV-2. <b>2023</b> , 63, 1438-1453	1
296	Mechanism of external K+ sensitivity of KCNQ1 channels. <b>2023</b> , 155,	1
295	Experimental and Simulation Study for the Dissociation Behavior of Gas Hydrates-Part II: sII Mixed Gas Hydrates. <b>2023</b> , 37, 4497-4514	О
294	Allosteric regulation of ₩eaction stage I in tryptophan synthase upon the 且igand binding. <b>2023</b> , 158, 115101	0
293	Coumarin linked thiazole derivatives as potential Ælucosidase inhibitors to treat Diabetes Mellitus.	О
292	Recognition and Cleavage of Human tRNA Methyltransferase TRMT1 by the SARS-CoV-2 Main Protease.	О
291	Characterization of the coupling mechanism of scorpion the urotoxins on the voltage-gated sodium channel hNav1.6. 1-9	О
290	Predicting mechanical properties of silk from its amino acid sequences via machine learning. <b>2023</b> , 140, 105739	О
289	Concentration-Dependent Inhibition of Mesophilic PETases on Poly(ethylene terephthalate) Can Be Eliminated by Enzyme Engineering. <b>2023</b> , 16,	О
288	Probing the Mechanisms of Inhibitors Binding to Presenilin Homologue Using Molecular Dynamics Simulations. <b>2023</b> , 28, 2076	О
287	Co-Assembly of Carbon Nanotube Porins into Biomimetic Peptoid Membranes. 2206810	О

286	Hierarchical Aggregation in a Complex Fluid-The Role of Isomeric Interconversion. <b>2023</b> , 127, 2052-2065	0
285	Solid phase extraction with rotating cigarette filter for determination of bisphenol A in source and drinking water: computational and analytical studies. <b>2023</b> , 39, 607-617	O
284	Venetoclax analogs as promising anticancer therapeutics via targeting Bcl-2 protein: in-silico drug discovery study. 1-17	0
283	Structural basis of lysophosphatidylserine receptor GPR174 ligand recognition and activation. <b>2023</b> , 14,	O
282	Structural Basis of the Binding Mode of the Antineoplastic Compound Motixafortide (BL-8040) in the CXCR4 Chemokine Receptor. <b>2023</b> , 24, 4393	0
281	Phenotypic Discovery of Thiocarbohydrazone with Anticancer Properties and Catalytic Inhibition of Human DNA Topoisomerase II <b>-2023</b> , 16, 341	O
280	In silico prediction of potential inhibitors for SARS-CoV-2 Omicron variant using molecular docking and dynamics simulation-based drug repurposing. <b>2023</b> , 29,	0
279	Deformation constraints of graphene oxide nanochannels under reverse osmosis. 2023, 14,	O
278	Structure of human NaV1.6 channel reveals Na+ selectivity and pore blockade by 4,9-anhydro-tetrodotoxin. <b>2023</b> , 14,	0
277	Structural Elucidation of Ivermectin Binding to ∄nAChR and the Induced Channel Desensitization. <b>2023</b> , 14, 1156-1165	O
276	Experimental and Simulation Study for the Dissociation Behavior of Gas Hydrates Part I: CH4 Hydrates. <b>2023</b> , 37, 4484-4496	1
275	Uncovering the Interaction Interface Between Harpin (Hpa1) and Rice Aquaporin (OsPIP1;3) Through Protein Protein Docking: An In Silico Approach.	O
274	Energy Coupling and Stoichiometry of Zn2+/H+Antiport by the Cation Diffusion Facilitator YiiP.	0
273	HilE represses the activity of HilD via a mechanism distinct from that of intestinal long-chain fatty acids.	O
272	Molecular effects of site-specific phosphate-methylated primer on the structure and motions of Taq DNA polymerase. <b>2023</b> , 21, 1820-1827	0
271	Phosphorylation motif dictates GPCR C-terminal domain conformation and arrestin interaction.	O
270	Tween-80 on Water/Oil Interface: Structure and Interfacial Tension by Molecular Dynamics Simulations. <b>2023</b> , 39, 3255-3265	О
269	What is the Optimal Dipole Moment for Nonpolarizable Models of Liquids?. <b>2023</b> , 19, 1790-1804	O

268	In silico target specific design of potential quinazoline-based anti-NSCLC agents. 1-12	О
267	Influence of ALS -linked M337V mutation on the conformational ensembles of TDP-43 321B40 peptide monomer and dimer.	1
266	Cyclodextrin-Based Displacement Strategy of Sterigmatocystin from Serum Albumin as a Novel Approach for Acute Poisoning Detoxification. <b>2023</b> , 24, 4485	Ο
265	Modelling Complex Bimolecular Reactions in a Condensed Phase: The Case of Phosphodiester Hydrolysis. <b>2023</b> , 28, 2152	Ο
264	Noncanonical electromechanical coupling paths in cardiac hERG potassium channel. 2023, 14,	O
263	Design-Rules for Stapled Alpha-Helical Peptides with On-Target In Vivo Activity: Application to Mdm2/X dual antagonists.	Ο
262	Water⊠ motions in x-y and z directions of 2D nanochannels: Entirely different but tightly coupled.	О
261	An in silico approach to determine inter-subunit affinities in human septin complexes.	O
260	Reversible Zinc Electrodeposition at 🛭 0 🖒 Using a Deep Eutectic Electrolyte for Low-Temperature Zinc Metal Batteries. <b>2023</b> , 14, 2378-2386	O
259	2D MoS2 and BN Nanosheets Damage Mitochondria through Membrane Penetration. <b>2023</b> , 17, 4716-4728	O
258	Dual photoisomerization mechanism of azobenzene embedded in a lipid membrane. <b>2023</b> , 11, 2518-2529	О
257	Simulated Tempering-Enhanced Umbrella Sampling Improves Convergence of Free Energy Calculations of Drug Membrane Permeation. <b>2023</b> , 19, 1898-1907	Ο
256	In-silico natural product database mining for novel neuropilin-1 inhibitors: molecular docking, molecular dynamics and binding energy computations. <b>2023</b> , 17,	О
255	Investigation of the Impact of Lipid Acyl Chain Saturation on Fusion Peptide Interactions with Lipid Bilayers. <b>2023</b> , 3, 121-138	O
254	Predicting locations of cryptic pockets from single protein structures using the PocketMiner graph neural network. <b>2023</b> , 14,	1
253	Computational design of a cyclic peptide that inhibits the CTLA4 immune checkpoint.	O
252	Structural basis for DARC binding in reticulocyte invasion byPlasmodium vivax.	О
251	The interactions of monomeric acridines and unsymmetrical bisacridines (UAs) with DNA duplexes: an insight provided by NMR and MD studies. <b>2023</b> , 13,	O

250	Vibrational spectroscopy simulation of solvation effects on a G-quadruplex. 1-11	O
249	The Importance of Epigallocatechin as a Scaffold for Drug Development against Flaviviruses. <b>2023</b> , 15, 803	O
248	Singlet fission as a polarized spin generator for dynamic nuclear polarization. 2023, 14,	O
247	Phenothiazine-Based LSD1 Inhibitor Promotes T-Cell Killing Response of Gastric Cancer Cells. <b>2023</b> , 66, 3896-3916	O
246	Long-range communication between transmembrane- and nucleotide-binding domains does not depend on drug binding to mutant P-glycoprotein. 1-10	О
245	Mechanistic Insight into the Amyloid Fibrillation Inhibition of Hen Egg White Lysozyme by Three Different Bile Acids. <b>2023</b> , 127, 2198-2213	O
244	In silico investigation of binding propensity of hematoxylin derivative and damnacanthal for their potential inhibitory effect on HIV-1 Vpr from different subtypes. 1-12	O
243	Computational design of fusion proteins against ErbB2-amplified tumors inspired by ricin toxin. 10,	O
242	Effects of representative point mutations on dynamic behavior of the DISC1Ndel1 complex: a molecular dynamics study. 1-7	0
241	Molecular Insights into CyclodextrinAdamantane-Modified Copolymer HostQuest Interactions. <b>2023</b> , 39, 3619-3627	O
240	Modulated protein-sterol interactions drive oxysterol-induced impaired CXCR4 signalling.	O
239	Atomistic origins of biomass recalcitrance in organosolv pretreatment. <b>2023</b> , 272, 118587	O
238	Solvation free energy arithmetic for small organic molecules. 2023, 44, 1263-1277	O
237	Systematic profiling of taxol and its analogues (taxalogues) binding to 胜ubulin and molecular analysis of their effects on microtubule stabilization.	O
236	Insights at the atomistic resolution of lantibiotics using multiscale simulations. 2023, 241-253	O
235	Microscopic Understanding of the Conformational Stability of the Aggregated Nonamyloid   Components of   Synuclein. <b>2023</b> , 63, 1542-1555	O
234	The thermodynamics of enhanced dope stability of cellulose solution in NaOH solution by urea. <b>2023</b> , 311, 120744	O
233	Structural and Dynamical Properties of Elastin-Like Peptides near Their Lower Critical Solution Temperature. <b>2023</b> , 24, 1912-1923	O

232	Molecular dynamics simulations of water-ethanol droplet on silicon surface. 2022,	O
231	Modern semiempirical electronic structure methods and machine learning potentials for drug discovery: Conformers, tautomers, and protonation states. <b>2023</b> , 158, 124110	О
230	ProteinVAE: Variational AutoEncoder for Translational Protein Design.	O
229	Coarse-Grained Force Field for Polyethylene Oxide and Polyethylene Glycol Aqueous Solutions Based on a Polarizable Water Model. <b>2023</b> , 19, 1864-1874	O
228	Identification of novel inhibitors for SARS-CoV-2 as therapeutic options using machine learning-based virtual screening, molecular docking and MD simulation. 10,	O
227	Activation mechanism of the human Smoothened receptor. <b>2023</b> , 122, 1400-1413	O
226	Unraveling the Interactions between Human DPP4 Receptor, SARS-CoV-2 Variants, and MERS-CoV, converged for Pulmonary Disorders Integrating through Immunoinformatics and Molecular Dynamics.	О
225	Expanding the molecular language of protein liquid-liquid phase separation.	O
224	Identifying and overcoming the sampling challenges in relative binding free energy calculations of a model protein:protein complex.	О
223	Uracil-DNA glycosylase efficiency is modulated by substrate rigidity. <b>2023</b> , 13,	O
222	On the Use of Water and Methanol with Zeolites for Heat Transfer. <b>2023</b> , 11, 4317-4328	O
221	Autoregulation of GPCR signalling through the third intracellular loop. <b>2023</b> , 615, 734-741	O
220	IDP Force Fields Applied to Model PPII-Rich 33-mer Gliadin Peptides. 2023, 127, 2407-2417	O
219	Growth Reaction of Gold Nanorods in the Presence of Mutated Peptides and Amine-Modified Single-Stranded Nucleic Acids. <b>2023</b> , 18,	O
218	Mechanism of Chiral-Selective Aminoacylation of an RNA Minihelix Explored by QM/MM Free-Energy Simulations. <b>2023</b> , 13, 722	О
217	Exploration of potent antiviral phytomedicines from Lauraceae family plants against SARS-CoV-2 RNA-dependent RNA polymerase. 1-21	O
216	Antimicrobial cellulose paper tuned with chitosan fibers for high-flux oil/water separation. <b>2023</b> , 312, 120794	O
215	Unsupervised Data-Driven Reconstruction of Molecular Motifs in Simple to Complex Dynamic Micelles. <b>2023</b> , 127, 2595-2608	O

214	Hepatic COX1 loss leads to impaired autophagic flux and exacerbates nonalcoholic steatohepatitis. <b>2023</b> ,	Ο
213	Lipid Bicelles in the Study of Biomembrane Characteristics. <b>2023</b> , 19, 1908-1921	O
212	Intermediate-state-trapped mutants pinpoint G protein-coupled receptor conformational allostery. <b>2023</b> , 14,	0
211	Alternatively spliced exon regulates context-dependent MEF2D higher-order assembly during myogenesis. <b>2023</b> , 14,	O
210	Cryo-EM structures of human Cx36/GJD2 neuronal gap junction channel. <b>2023</b> , 14,	Ο
209	QSAR via multisite Edynamics in the orphaned TSSK1B kinase. <b>2023</b> , 32,	O
208	Impact of Phosphorylation on alpha-Synuclein Structural Determinants.	О
207	Electronic Excitation Response of DNA to High-Energy Proton Radiation in Water. 2023, 130,	O
206	Theoretical Study on the Gas-Phase and Aqueous Interface Reaction Mechanism of Criegee Intermediates with 2-Methylglyceric Acid and the Nucleation of Products. <b>2023</b> , 24, 5400	0
205	Deciphering Selectivity Mechanism of BRD9 and TAF1(2) toward Inhibitors Based on Multiple Short Molecular Dynamics Simulations and MM-GBSA Calculations. <b>2023</b> , 28, 2583	O
204	Development of multi-epitope vaccines against the monkeypox virus based on envelope proteins using immunoinformatics approaches. 14,	0
203	Polarity-dependence of the nonlinear dielectric response in interfacial water. <b>2023</b> , 158, 134716	O
202	Trypanosoma cruzi Sirtuin 2 as a Relevant Druggable Target: New Inhibitors Developed by Computer-Aided Drug Design. <b>2023</b> , 16, 428	0
201	Structural Analysis of Interactions between Epidermal Growth Factor Receptor (EGFR) Mutants and Their Inhibitors. <b>2023</b> , 3, 203-213	O
200	The T1150A cancer mutant of the protein lysine dimethyltransferase NSD2 can introduce H3K36 trimethylation.	0
199	Extended-sampling QM/MM simulation of biochemical reactions involving PN bonds. 2023, 25, 9824-9836	O
198	Bubble wall confinement driven molecular assembly toward sub 12 nm and beyond precision patterning. <b>2023</b> , 9,	О
197	Slow spectral diffusion of the NO stretching mode of [RuCl5(NO)]2[In D2O studied by 2D-IR spectroscopy and molecular dynamics simulations. <b>2023</b> , 158, 134510	Ο

196	Molecular dynamics study of collective water vibrations in a DNA hydration shell. 2023, 52, 69-79	O
195	A hotspot for posttranslational modifications on the androgen receptor dimer interface drives pathology and anti-androgen resistance. <b>2023</b> , 9,	o
194	Stable LiF-Rich Electrode <b>E</b> lectrolyte Interface toward High-Voltage and High-Energy-Density Lithium Metal Solid Batteries. 2300494	O
193	Structural basis of odorant recognition by a human odorant receptor. <b>2023</b> , 615, 742-749	O
192	Unveiling the Mechanistic Singularities of Caspases: A Computational Analysis of the Reaction Mechanism in Human Caspase-1. <b>2023</b> , 13, 4348-4361	0
191	Direct Calculation of the Interfacial Free Energy between NaCl Crystal and Its Aqueous Solution at the Solubility Limit. <b>2023</b> , 130,	o
190	Molecular Basis of RNA-Driven ATP Hydrolysis in DExH-Box Helicases. 2023, 145, 6691-6701	0
189	Theoretical Spectroscopy Aided Validation of the Hydration Structure of Trimethylamine N-Oxide (TMAO). <b>2023</b> , 127, 2774-2783	0
188	Insights into substrate transport and water permeation in the mycobacterial transporter MmpL3. <b>2023</b> ,	O
187	Aggregation of chlorophylls on plant thylakoid membranes using coarse-grained simulations.	o
186	Conformational Behavior of SARS-Cov-2 Spike Protein Variants: Evolutionary Jumps in Sequence Reverberate in Structural Dynamic Differences. <b>2023</b> , 19, 2120-2134	0
185	Structure-based small inhibitors search combined with molecular dynamics driven energies for human programmed cell death-1 (PD-1) protein. 1-15	1
184	Molecular analyses of the C-terminal CRAF variants associated with cardiomyopathy reveal their opposing impacts on the active conformation of the kinase domain. 1-11	0
183	Free Energy Differences from Molecular Simulations: Exact Confidence Intervals from Transition Counts. <b>2023</b> , 19, 2102-2108	o
182	Insights into the binding mechanism between ⊞OH and CYP4F2: A homology modeling, molecular docking, and molecular dynamics simulation study. <b>2023</b> , 124, 573-585	0
181	In Silico Prediction of Stratum Corneum Partition Coefficients via COSMOmic and Molecular Dynamics Simulations. <b>2023</b> , 127, 2719-2728	o
180	Decoding the Conformational Selective Mechanism of FGFR Isoforms: A Comparative Molecular Dynamics Simulation. <b>2023</b> , 28, 2709	0
179	Unraveling Binding Mechanism and Stability of Urease Inhibitors: A QM/MM MD Study. <b>2023</b> , 28, 2697	O

178	Discovery of a Novel 3site State as the Multi-Substrate Bound State of P450cam.	O
177	Comparison of Empirical Zn2+ Models in ProteinDNA Complexes. 2023, 3, 214-230	O
176	Investigation of dynamic solution interactions between NET-1 and UNC-5B by multi-wavelength analytical ultracentrifugation.	O
175	Binding of berberine derivates to G-quadruplex: insight from a computational study. <b>2023</b> , 25, 10741-10748	O
174	Structural insights into a cooperative switch between one and two FimH bacterial adhesins binding pauci- and high-mannose type N-glycan receptors. <b>2023</b> , 299, 104627	O
173	Methane Gas Bubbles Affecting the Formation and Distribution of Hydrates in Kaolinite Slit Pores: A Molecular Dynamics Study. <b>2023</b> , 37, 5102-5113	O
172	Structural Dynamics of Lys11-Selective Deubiquitinylase Cezanne-1 during the Catalytic Cycle. <b>2023</b> , 63, 2084-2094	О
171	Inhibitory mechanism of n-MTAB AuNPs for Bynuclein aggregation. <b>2023</b> , 29,	O
170	Effects of chain length and anions on ion transport in PEO-lithium salt systems. 2023, 49, 720-728	O
169	Time-resolved cryo-EM of G protein activation by a GPCR.	O
169 168	Time-resolved cryo-EM of G protein activation by a GPCR.  Binding to nucleosome poises SIRT6 for histone H3 de-acetylation.	0
168	Binding to nucleosome poises SIRT6 for histone H3 de-acetylation.  A cooperative knock-on mechanism underpins Ca2+-selective cation permeation in TRPV channels.	0
168 167	Binding to nucleosome poises SIRT6 for histone H3 de-acetylation.  A cooperative knock-on mechanism underpins Ca2+-selective cation permeation in TRPV channels.  2023, 155,	0
168 167 166	Binding to nucleosome poises SIRT6 for histone H3 de-acetylation.  A cooperative knock-on mechanism underpins Ca2+-selective cation permeation in TRPV channels.  2023, 155,  The ATP-bound State of the Uncoupling Protein 1 (UCP1) from Molecular Simulations.	o o o
168 167 166	Binding to nucleosome poises SIRT6 for histone H3 de-acetylation.  A cooperative knock-on mechanism underpins Ca2+-selective cation permeation in TRPV channels.  2023, 155,  The ATP-bound State of the Uncoupling Protein 1 (UCP1) from Molecular Simulations.  Binding order and apparent binding affinity in the bisubstrate activity of strictosidine synthase. 1-13  How the Conformational Movement of the Substrate Drives the Regioselective CN Bond Formation in P450 TleB: Insights from Molecular Dynamics Simulations and Quantum	o o o
168 167 166 165	Binding to nucleosome poises SIRT6 for histone H3 de-acetylation.  A cooperative knock-on mechanism underpins Ca2+-selective cation permeation in TRPV channels. 2023, 155,  The ATP-bound State of the Uncoupling Protein 1 (UCP1) from Molecular Simulations.  Binding order and apparent binding affinity in the bisubstrate activity of strictosidine synthase. 1-13  How the Conformational Movement of the Substrate Drives the Regioselective CN Bond Formation in P450 TleB: Insights from Molecular Dynamics Simulations and Quantum Mechanical/Molecular Mechanical Calculations. 2023, 145, 7252-7267  The intramembrane COOH-terminal domain of PRRT2 regulates voltage-dependent Na+ channels.	<ul><li>O</li><li>O</li><li>O</li><li>O</li><li>O</li></ul>

160	Mechanistic insights into the inhibition of amyloid-軸ggregation by chitosan. <b>2023</b> , 25, 10113-10120	О
159	Uncovering the folding mechanism of pertactin: A comparative study of isolated and vectorial folding. <b>2023</b> ,	O
158	An Interaction Network Driven Approach for Identifying Cervical, Endometrial, Vulvar Carcinomic Biomarkers and Their Multi-targeted Inhibitory Agents from Few Widely Available Medicinal Plants.	О
157	FTD-tau S320F mutation stabilizes local structure and allosterically promotes amyloid motif-dependent aggregation. <b>2023</b> , 14,	Ο
156	A Multi-Enzyme Cascade for Efficient Production of Pyrrolidone from l- Glutamate.	Ο
155	Finite-Temperature Mechanical Properties of Organic Molecular Crystals from Classical Molecular Simulation. <b>2023</b> , 23, 2155-2168	O
154	Molecular simulations of SSTR2 dynamics and interaction with ligands. <b>2023</b> , 13,	0
153	Effect of temperature on the structure and drug-release behaviour of inclusion complex of Ecyclodextrin with cyclophosphamide: a molecular dynamics study.	O
152	Structure of interpolymer complex between poly(acrylic acid) and poly(ethylene oxide) in aqueous salt solution: a molecular dynamics simulation study. <b>2023</b> , 49, 743-757	0
151	Experimental study combined with density functional theory and molecular dynamics simulation on the mechanism of glucose alcoholysis reaction.	0
150	Unveil the role of structural vacancy in Mn-based Prussian blue for energy storage application.	0
149	Electric-field induced entropic effects in liquid water.	O
148	Conformational dynamics of A30G Bynuclein that causes familial Parkinson disease. 1-13	0
147	Molecular modeling and simulations of some antiviral drugs, benzylisoquinoline alkaloid, and coumarin molecules to investigate the effects on Mpro main viral protease inhibition. <b>2023</b> , 34, 101459	O
146	Optimizing the binding of OGT and a peptidic substrate towards pseudo-substrate inhibitors via molecular dynamic simulations.	0
145	Calculations of the binding free energies of the Comprehensive <i>in vitro</i> Proarrhythmia Assay (CiPA) reference drugs to cardiac ion channels. <b>2023</b> , 20, n/a	O
144	Decarboxylation and Protonation Enigma in the H85Q Mutant of Cytochrome P450OleT. <b>2023</b> , 127, 2927-2	<b>933</b> 0
143	In silico characterization of cysteine-stabilized <b>粗</b> efensins from neglected unicellular microeukaryotes. <b>2023</b> , 23,	O

142	Identification of non-histone substrates of the lysine methyltransferase PRDM9. 2023, 104651	0
141	Internal Normal Mode Analysis Applied to RNA Flexibility and Conformational Changes.	O
140	Efficient helium separation through SIFSIX-3-Cu membrane: A molecular dynamics study. <b>2023</b> , 223, 112143	O
139	Effects of pH and NaCl on the Spatial Structure and Conformation of Myofibrillar Proteins and the Emulsion Gel SystemIhsights from Computational Molecular Dynamics on Myosin of Golden Pompano. <b>2023</b> , 9, 270	O
138	Mechanism of antibody-specific deglycosylation and immune evasion by Streptococcal IgG-specific endoglycosidases. <b>2023</b> , 14,	0
137	Discrimination between cyclic nucleotides in a cyclic nucleotide-gated ion channel. <b>2023</b> , 30, 512-520	O
136	Folding and modulation of the helical conformation of Glycophorin A by point mutations. <b>2023</b> , 25, 10885-108	393
135	Synthetic Curcumin Analogues Present Antiflavivirus Activity In Vitro with Potential Multiflavivirus Activity from a Thiazolylhydrazone Moiety. <b>2023</b> , 3, 364-378	O
134	2D-QSAR, molecular docking and MD simulation based virtual screening of the herbal molecules against Alzheimer disorder: an approach to predict CNS activity. 1-15	0
133	A theoretical survey to find potential natural compound for inhibition of binding the RBD domain to ACE2 receptor based on plant antivirals. 1-26	O
132	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. <b>2023</b> , 13, 9800-9810	0
131	Investigation of the Entry Pathway and Molecular Nature of 🛭 Receptor Ligands. 2023, 24, 6367	O
130	The path towards type V deep eutectic solvents: inductive effects and steric hindrance in the system tert-butanol + perfluoro tert-butanol.	O
129	Unraveling the molecular mechanism of novel leukemia mutations on NTRK2 (A203T & 2008) and NTRK3 (E176D & 2008) genes using molecular dynamics simulations approach. 12, 345	O
128	Converging PMF calculations of antibiotic permeation across an outer membrane porin with sub-kilocalorie per mole accuracy.	0
127	Binding mechanism of andrographolide with intramolecular antiparallel G-quadruplexes of therapeutic importance: an in-silico analysis. <b>2023</b> , 49, 816-828	O
126	Correlation of Emulsion Chemistry, Film Morphology, and Device Performance in Polyfluorene LEDs Deposited by RIR-MAPLE. <b>2023</b> , 15, 18153-18165	О
125	Energetics and kinetics of membrane permeation of photoresists for bioprinting.	O

124	Conserved Conformational Dynamics Reveal a Key Dynamic Residue in the Gatekeeper Loop of Human Cyclophilins. <b>2023</b> , 127, 3139-3150	0
123	Enhanced Interfacial H-Bond Networks Promote Glycan©lycan Recognition and Interaction. <b>2023</b> , 15, 17592-17600	Ο
122	Effect of Single-Residue Mutations on CTCF Binding to DNA: Insights from Molecular Dynamics Simulations. <b>2023</b> , 24, 6395	0
121	In Silico Analyses of a Promising Drug Candidate for the Treatment of Amyotrophic Lateral Sclerosis Targeting Superoxide Dismutase I Protein. <b>2023</b> , 15, 1095	O
120	Release of frustration drives corneal amyloid disaggregation by brain chaperone. 2023, 6,	0
119	Impact of wettability on storage and recovery of hydrogen gas in the lesueur sandstone formation (Southwest hub project, Western Australia). <b>2023</b> ,	O
118	Evaluation of autophagy inhibition to combat cancer: (vanadium complex)protein interactions, parameterization, and validation of a new force field. <b>2023</b> , 29,	О
117	Connecting Diffraction Experiments and Network Analysis Tools for the Study of Hydrogen-Bonded Networks. <b>2023</b> , 127, 3109-3118	0
116	Orphan receptor GPR158 serves as a metabotropic glycine receptor: mGlyR. <b>2023</b> , 379, 1352-1358	0
115	Mechanistic Insights into the Binding of Different Positron Emission Tomography Tracers to Chronic Traumatic Encephalopathy Tau Protofibrils.	O
114	Autocatalytic effect boosts the production of medium-chain hydrocarbons by fatty acid photodecarboxylase. <b>2023</b> , 9,	0
113	Aggregation Interface and Rigid Spots Sustain the Stable Framework of a Thermophilic N-Demethylase. <b>2023</b> , 71, 5614-5629	O
112	Molecular insights into the stereospecificity of arginine in RNA tetraloop folding.	О
111	Efficient seawater desalination in lamellar nanochannel-based boridene filtration membrane.	O
110	Molecular Mechanisms of Na+-driven Bile Acid Transport in Human NTCP.	0
109	IFITM3 blocks influenza virus entry by sorting lipids and stabilizing hemifusion. <b>2023</b> , 31, 616-633.e20	O
108	Large-scale Annotation of Biochemically Relevant Pockets and Tunnels in Cognate Enzyme-Ligand Complexes.	О
107	Partial Denaturation of Double-Stranded DNA on Pristine Graphene under Physiological-like Conditions. <b>2023</b> , 3, 168-186	Ο

106	Mutation in glutamate transporter homologue GltTk provides insights into pathologic mechanism of episodic ataxia 6. <b>2023</b> , 14,	0
105	ZIF-8 thin films by a vapor-phase process: limits to growth. <b>2023</b> , 15, 7115-7125	O
104	How SGLT2 inhibitors interact with metformin? A molecular dynamics study. 1-10	O
103	In silico and in vitro Identification of Compounds with Dual Pharmacological Activity against Metionyl-tRNA Synthetase and Isoleucyl-tRNA Synthetase of Staphylococcus aureus. <b>2023</b> , 8,	o
102	Dynamics of the personalities of PCSK9 on missense variants (rs505151 and rs562556) from elderly cohort studies in Brazil. 1-9	O
101	Identification of novel peptide inhibitors for oncogenic KRAS G12D as therapeutic options using mutagenesis-based remodeling and MD simulations. 1-13	O
100	Structural and molecular insights into tacrine-benzofuran hybrid induced inhibition of amyloid- peptide aggregation and BACE1 activity. 1-17	О
99	WrappingII rapping versus Extraction Mechanism of Bactericidal Activity of MoS2 Nanosheets against Staphylococcus aureus Bacterial Membrane. <b>2023</b> , 39, 5440-5453	О
98	Single-molecule fingerprinting of protein-drug interaction using a funneled biological nanopore. <b>2023</b> , 14,	0
97	Molecular Dynamic Simulation Studies on Cyclophilin- a Missing Cord in HIV-1 Capsid Assembly.	O
96	A Computational Biology Study on the Structure and Dynamics Determinants of Thermal Stability of the Chitosanase from Aspergillus fumigatus. <b>2023</b> , 24, 6671	0
95	Machine annealing-guided navigation of antihypertensive food peptide selectivity between human ACE N- and C-domains in structurally interacting diversity space.	O
94	Influence of Core Topologies on Poly-l-lysine Dendrimer Structures. <b>2023</b> , 127, 3364-3371	O
93	The Role of C2 Domains in Two Different Phosphatases: PTEN and SHIP2. <b>2023</b> , 13, 408	O
92	X-ray Structure Characterization of the Selective Recognition of AT Base Pair Sequences.	O
91	Deep Eutectic Solvents for the Enzymatic Synthesis of Sugar Esters: A Generalizable Strategy?. <b>2023</b> , 11, 5926-5936	O
90	Resolution of Maximum Entropy Method-Derived Posterior Conformational Ensembles of a Flexible System Probed by FRET and Molecular Dynamics Simulations.	0
89	Carbon nanotube recognition by human Siglec-14 provokes inflammation.	O

88	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	O
87	Dynamics and rheological properties of suspensions of paramagnetic spherical particles under constant magnetic fields. <b>2023</b> , 8,	O
86	In Silico Investigation on the Selective Nanotoxicity of Two-Dimensional Materials to Hen Egg White Lysozyme Protein.	0
85	Identification of a 1, 8-naphthyridine-containing compound endowed with the inhibition of p53-MDM2/X interaction signaling: a computational perspective.	O
84	Continuous millisecond conformational cycle of a DEAH box helicase reveals control of domain motions by atomic-scale transitions. <b>2023</b> , 6,	0
83	Influence of hydrostatic pressure during gelation on physicochemical properties of cellulose hydrogels prepared from ionic liquid/DMSO solution. <b>2023</b> , 381, 121810	O
82	Novel hits for autosomal dominated polycystic kidney disease (ADPKD) targeting derived by in silico screening on ZINC-15 natural product database. 1-18	0
81	G∃ slow conformational transition upon GTP binding and a novel G∃ regulator. <b>2023</b> , 26, 106603	O
80	Performance efficient macromolecular mechanics via sub-nanometer shape based coarse graining. <b>2023</b> , 14,	0
79	Interfacial properties of protein nanofibrils with different morphology prepared using aqueous solvent with ethanol: Part I. preparation and characterization. <b>2023</b> , 142, 108754	O
78	Molecular Recognition of Methacryllysine and Crotonyllysine by the AF9 YEATS Domain. 2023, 24, 7002	0
77	Ion Conduction Mechanisms in Potassium Channels Revealed by Permeation Cycles.	O
76	Improving the activity of horseradish peroxidase in betaine-based natural deep eutectic systems.	O
75	Computational and structural insights into the pre- and post-hydrolysis states of bovine multidrug resistance-associated protein 1.	O
74	Molecular insights into the effects of lignin on methane hydrate formation in clay nanopores. <b>2023</b> , 276, 127496	O
73	Magnetic Polaron States in Photoluminescent Carbon Dots Enable Hydrogen Peroxide Photoproduction.	O
72	Direct monitoring of the thermodynamics and kinetics of DNA and RNA dinucleotide dehybridization from gaps and overhangs.	O
71	Predictive mutagenesis of prolyl endopeptidase from non-pathogenic acidophilic bacteria for gliadin catalysis.	O

70	A Unified Description of the Liquid Structure, Static and Dynamic Anomalies, and Criticality of TIP4P/2005 Water by a Hierarchical Two-State Model. <b>2023</b> , 127, 3452-3462	O
69	Design of 2-amino-6-methyl-pyrimidine benzoic acids as ATP competitive casein kinase-2 (CK2) inhibitors using structure- and fragment-based design, docking and molecular dynamic simulation studies. 1-20	O
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