GÃ¼nther H J Peters

List of Publications by Year
in descending order

153 papers	5,368 citations	87723 38 h-index	98622 67 g-index
159 all docs	159 docs citations	159 times ranked	6307 citing authors

#	Article	IF	Citations
1	Structural and Evolutionary Relationships among Protein Tyrosine Phosphatase Domains. Molecular and Cellular Biology, 2001, 21, 7117-7136.	1.1	660
2	Crystal Structure of Glucagon-like Peptide-1 in Complex with the Extracellular Domain of the Glucagon-like Peptide-1 Receptor. Journal of Biological Chemistry, 2010, 285, 723-730.	1.6	239
3	Water in Contact with Extended Hydrophobic Surfaces: Direct Evidence of Weak Dewetting. Physical Review Letters, 2003, 90, 086101.	2.9	224
4	Structure-based Design of a Low Molecular Weight, Nonphosphorus, Nonpeptide, and Highly Selective Inhibitor of Protein-tyrosine Phosphatase 1B. Journal of Biological Chemistry, 2000, 275, 10300-10307.	1.6	158
5	Structure Determination of T Cell Protein-tyrosine Phosphatase. Journal of Biological Chemistry, 2002, 277, 19982-19990.	1.6	152
6	Reconciliation of opposing views on membraneâ€“sugar interactions. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 1874-1878.	3.3	126
7	The effect of calcium on the properties of charged phospholipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2006, 1758, 573-582.	1.4	123
8	Methodological problems in pressure profile calculations for lipid bilayers. Journal of Chemical Physics, 2005, 122, 124903.	1.2	114
9	The Importance of Magnesium in the Human Body. Advances in Clinical Chemistry, 2016, 73, 169-193.	1.8	114
10	Electrostatic Evaluation of the Signature Motif (H/V)CX5R(S/T) in Proteinâ˜Tyrosine Phosphatases. Biochemistry, 1998, 37, 5383-5393.	1.2	107
11	The hydrophobic effect: Molecular dynamics simulations of water confined between extended hydrophobic and hydrophilic surfaces. Journal of Chemical Physics, 2004, 120, 9729-9744.	1.2	104
12	Reparameterization of All-Atom Dipalmitoylphosphatidylcholine Lipid Parameters Enables Simulation of Fluid Bilayers at Zero Tension. Biophysical Journal, 2007, 92, 4157-4167.	0.2	83
13	Ligand-Induced Conformational Changes: Improved Predictions of Ligand Binding Conformations and Affinities. Biophysical Journal, 2003, 84, 2273-2281.	0.2	82
14	Steric Hindrance as a Basis for Structure-Based Design of Selective Inhibitors of Protein-Tyrosine Phosphatasesâ€. Biochemistry, 2001, 40, 14812-14820.	1.2	79
15	Liposomal Formulation of Retinoids Designed for Enzyme Triggered Release. Journal of Medicinal Chemistry, 2010, 53, 3782-3792.	2.9	77
16	Domain-Induced Activation of Human Phospholipase A2 Type IIA: Local versus Global Lipid Composition. Biophysical Journal, 2006, 90, 3165-3175.	0.2	70
17	Protein Dynamics in Organic Media at Varying Water Activity Studied by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2012, 116, 2575-2585.	1.2	68
18	Drug Delivery by an Enzymeâ€Mediated Cyclization of a Lipid Prodrug with Unique Bilayerâ€Formation Properties. Angewandte Chemie - International Edition, 2009, 48, 1823-1826.	7.2	67

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19	Simulations of a Membrane-Anchored Peptide: Structure, Dynamics, and Influence on Bilayer Properties. Biophysical Journal, 2004, 86, 3556-3575.	0.2	66
20	Binding of Serotonin to Lipid Membranes. Journal of the American Chemical Society, 2013, 135, 2164-2171.	6.6	65
21	Activation of interfacial enzymes at membrane surfaces. Journal of Physics Condensed Matter, 2006, 18, S1293-S1304.	0.7	64
22	Water-molecule network and active-site flexibility of apo protein tyrosine phosphatase 1B. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1527-1534.	2.5	60
23	Ammonium Recruitment and Ammonia Transport by E. coli Ammonia Channel AmtB. Biophysical Journal, 2006, 91, 4401-4412.	0.2	58
24	Mechanistic Study of the sPLA₂-Mediated Hydrolysis of a Thio-ester Pro Anticancer Ether Lipid. Journal of the American Chemical Society, 2009, 131, 12193-12200.	6.6	57
25	Computer simulation of the rheology of grafted chains under shear. Physical Review E, 1995, 52, 1882-1890.	0.8	54
26	Essential dynamics of lipase binding sites: the effect of inhibitors of different chain length. Protein Engineering, Design and Selection, 1997, 10, 149-158.	1.0	54
27	Simulation of the Coupling between Nucleotide Binding and Transmembrane Domains in the ATP Binding Cassette Transporter BtuCD. Biophysical Journal, 2007, 92, 2727-2734.	0.2	53
28	Evolution of a Rippled Membrane during Phospholipase A2 Hydrolysis Studied by Time-Resolved AFM. Biophysical Journal, 2004, 87, 408-418.	0.2	52
29	Molecular Dynamics Simulations of Protein-Tyrosine Phosphatase 1B. II. Substrate-Enzyme Interactions and Dynamics. Biophysical Journal, 2000, 78, 2191-2200.	0.2	48
30	Application of interpretable artificial neural networks to early monoclonal antibodies development. European Journal of Pharmaceutics and Biopharmaceutics, 2019, 141, 81-89.	2.0	48
31	A Theoretical Study of the Separation Principle in Size Exclusion Chromatography. Macromolecules, 2010, 43, 1651-1659.	2.2	47
32	Homology Modeling of the Serotonin Transporter: Insights into the Primary Escitalopram-binding Site. ChemMedChem, 2007, 2, 815-826.	1.6	45
33	A Correlation between the Activity of Candida antarctica Lipase B and Differences in Binding Free Energies of Organic Solvent and Substrate. ACS Catalysis, 2016, 6, 6350-6361.	5.5	45
34	Active Serine Involved in the Stabilization of the Active Site Loop in theHumicolalanuginosaLipaseâ€. Biochemistry, 1998, 37, 12375-12383.	1.2	43
35	Residue 259 Is a Key Determinant of Substrate Specificity of Protein-tyrosine Phosphatases 1B and Î±. Journal of Biological Chemistry, 2000, 275, 18201-18209.	1.6	43
36	Mapping of Epitopes for Autoantibodies to the Type 1 Diabetes Autoantigen IA-2 by Peptide Phage Display and Molecular Modeling: Overlap of Antibody and T Cell Determinants. Journal of Immunology, 2004, 172, 4084-4090.	0.4	43

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37	Molecular Dynamics Simulations of Protein-Tyrosine Phosphatase 1B. I. Ligand-Induced Changes in the Protein Motions. Biophysical Journal, 1999, 77, 505-515.	0.2	42
38	Orientation and Conformation of a Lipase at an Interface Studied by Molecular Dynamics Simulations. Biophysical Journal, 2002, 83, 98-111.	0.2	41
39	Molecular Basis of Phospholipase A2 Activity toward Phospholipids with sn-1 Substitutions. Biophysical Journal, 2008, 94, 14-26.	0.2	40
40	Affinity of Four Polar Neurotransmitters for Lipid Bilayer Membranes. Journal of Physical Chemistry B, 2011, 115, 196-203.	1.2	40
41	Structural and functional aspects of mannuronic acidâ€“specific PL6 alginate lyase from the human gut microbe Bacteroides cellulosilyticus. Journal of Biological Chemistry, 2019, 294, 17915-17930.	1.6	40
42	Computational analysis of chain flexibility and fluctuations in Rhizomucor miehei lipase. Protein Engineering, Design and Selection, 1999, 12, 747-754.	1.0	38
43	Computational studies of the activation of lipases and the effect of a hydrophobic environment. Protein Engineering, Design and Selection, 1997, 10, 137-147.	1.0	36
44	Structure and dynamics of lipid monolayers: implications for enzyme catalysed lipolysis. Nature Structural and Molecular Biology, 1995, 2, 395-401.	3.6	35
45	Molecular Dynamics Simulations of Na+/Clâ¯-Dependent Neurotransmitter Transporters in a Membrane-Aqueous System. ChemMedChem, 2007, 2, 827-840.	1.6	35
46	Oligomerization of a Glucagon-like Peptide 1 Analog: Bridging Experiment and Simulations. Biophysical Journal, 2015, 109, 1202-1213.	0.2	35
47	Influence of a Lipid Interface on Protein Dynamics in a Fungal Lipase. Biophysical Journal, 2001, 81, 3052-3065.	0.2	34
48	Molecular Dynamics Simulations of the Melting of a Hexane Monolayer:â€‰ Isotropic versus Anisotropic Force Fields. Langmuir, 1996, 12, 1557-1565.	1.6	33
49	Residue 182 influences the second step of protein-tyrosine phosphatase-mediated catalysis. Biochemical Journal, 2004, 378, 421-433.	1.7	32
50	Molecular packing in 1-hexanolâ€“DMPC bilayers studied by molecular dynamics simulation. Biophysical Chemistry, 2007, 125, 104-111.	1.5	32
51	Diffusion of water and selected atoms in DMPC lipid bilayer membranes. Journal of Chemical Physics, 2012, 137, 204910.	1.2	32
52	Soluble 1:1 complexes and insoluble 3:2 complexes â€“ Understanding the phase-solubility diagram of hydrocortisone and Î³-cyclodextrin. International Journal of Pharmaceutics, 2017, 531, 504-511.	2.6	30
53	Influence of Surface Properties of Mixed Monolayers on Lipolytic Hydrolysis. Langmuir, 2000, 16, 2779-2788.	1.6	29
54	Modeling of complex biological systems. I. Molecular dynamics studies of diglyceride monolayers. Journal of Chemical Physics, 1994, 100, 5996-6010.	1.2	28

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55	Interaction of neurotransmitters with a phospholipid bilayer: A molecular dynamics study. Chemistry and Physics of Lipids, 2014, 184, 7-17.	1.5	28
56	Mean Span Dimensions of Ideal Polymer Chains Containing Branches and Rings. Macromolecules, 2011, 44, 403-412.	2.2	27
57	Secretory Phospholipase A2Hydrolysis of Phospholipid Analogues Is Dependent on Water Accessibility to the Active Site. Journal of the American Chemical Society, 2007, 129, 5451-5461.	6.6	25
58	Advancing Therapeutic Protein Discovery and Development through Comprehensive Computational and Biophysical Characterization. Molecular Pharmaceutics, 2020, 17, 426-440.	2.3	25
59	Enzyme kinetic characterization of protein tyrosine phosphatases. Biochimie, 2003, 85, 527-534.	1.3	24
60	Equilibrium partitioning of macromolecules in confining geometries: Improved universality with a new molecular size parameter. Journal of Chemical Physics, 2008, 128, 124904.	1.2	24
61	Accurate Kirkwoodâ€“Buff integrals from molecular simulations. Molecular Simulation, 2010, 36, 1243-1252.	0.9	24
62	Self-Interaction of Human Serum Albumin: A Formulation Perspective. ACS Omega, 2018, 3, 16105-16117.	1.6	24
63	Effects of Fatty Acid Inclusion in a DMPC Bilayer Membrane. Journal of Physical Chemistry B, 2009, 113, 92-102.	1.2	21
64	Synthesis and serotonin transporter activity of 1,3-bis(aryl)-2-nitro-1-propenes as a new class of anticancer agents. Bioorganic and Medicinal Chemistry, 2011, 19, 1328-1348.	1.4	21
65	Physical constraints and functional plasticity of cellulases. Nature Communications, 2021, 12, 3847.	5.8	21
66	Computer simulation of the rheology of grafted chains under shear. II. Depletion of chains at the wall. Physical Review E, 1996, 54, 5493-5501.	0.8	20
67	Synthesis and serotonin transporter activity of sulphur-substituted Î±-alkyl phenethylamines as a new class of anticancer agents. European Journal of Medicinal Chemistry, 2009, 44, 4862-4888.	2.6	20
68	Membrane Interaction of the Factor VIIIa Discoidin Domains in Atomistic Detail. Biochemistry, 2015, 54, 6123-6131.	1.2	20
69	Effect of Water Clustering on the Activity of Candida antarctica Lipase B in Organic Medium. Catalysts, 2017, 7, 227.	1.6	20
70	The molecular dynamics simulations of the melting of a hexane bilayer. Surface Science, 1996, 347, 169-181.	0.8	19
71	A novel strategy for the development of selective active-site inhibitors of the protein tyrosine phosphatase-like proteins islet-cell antigen 512 (IA-2) and phogrin (IA-2beta). Biochemical Journal, 2003, 373, 393-401.	1.7	19
72	Membrane Restructuring by Phospholipase A2 Is Regulated by the Presence of Lipid Domains. Biophysical Journal, 2011, 101, 90-99.	0.2	19

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73	Extending the hydrophobic cavity of Î²-cyclodextrin results in more negative heat capacity changes but reduced binding affinities. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2014, 78, 351-361.	0.9	19
74	The influence of different linker modifications on the catalytic activity and cellulose affinity of cellobiohydrolase Cel7A from Hypocrea jecorina. Protein Engineering, Design and Selection, 2017, 30, 495-501.	1.0	19
75	Effect of substrate potential strength on the melting temperature of a hexane monolayer adsorbed on graphite. Journal of Chemical Physics, 1995, 102, 1098-1099.	1.2	18
76	Glucagon-like Peptide 1 Conjugated to Recombinant Human Serum Albumin Variants with Modified Neonatal Fc Receptor Binding Properties. Impact on Molecular Structure and Half-Life. Biochemistry, 2017, 56, 4860-4870.	1.2	18
77	State conditions transferability of vaporâ€“liquid equilibria via fluctuation solution theory with correlation function integrals from molecular dynamics simulation. Fluid Phase Equilibria, 2007, 260, 169-176.	1.4	17
78	Determination of stability constants of tauro- and glyco-conjugated bile salts with the negatively charged sulfobutylether-Î²-cyclodextrin: comparison of affinity capillary electrophoresis and isothermal titration calorimetry and thermodynamic analysis of the interaction. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2014, 78, 185-194.	0.9	17
79	Computational Investigation of Enthalpyâ€“Entropy Compensation in Complexation of Glycoconjugated Bile Salts with Î²-Cyclodextrin and Analogs. Journal of Physical Chemistry B, 2014, 118, 10889-10897.	1.2	17
80	Small-Angle X-ray Scattering Data in Combination with RosettaDock Improves the Docking Energy Landscape. Journal of Chemical Information and Modeling, 2017, 57, 2463-2475.	2.5	17
81	Generation of thermodynamic data for organic liquid mixtures from molecular simulations. Molecular Simulation, 2007, 33, 449-457.	0.9	16
82	Total and direct correlation function integrals from molecular simulation of binary systems. Fluid Phase Equilibria, 2011, 302, 32-42.	1.4	16
83	Dual Nicotinic Acetylcholine Receptor Î±4Î²2 Antagonists/Î±7 Agonists: Synthesis, Docking Studies, and Pharmacological Evaluation of Tetrahydroisoquinolines and Tetrahydroisoquinolinium Salts. Journal of Medicinal Chemistry, 2018, 61, 1719-1729.	2.9	16
84	Modeling of Complex Biological Systems. 2. Effect of Chain Length on the Phase Transitions Observed in Diglyceride Monolayers. Langmuir, 1995, 11, 4072-4081.	1.6	15
85	Essential motions in a fungal lipase with bound substrate, covalently attached inhibitor and product. Journal of Molecular Recognition, 2002, 15, 393-404.	1.1	15
86	Synthesis of sn-1 functionalized phospholipids as substrates for secretory phospholipase A2. Chemistry and Physics of Lipids, 2007, 146, 54-66.	1.5	15
87	Correlated Volumeâ^'Energy Fluctuations of Phospholipid Membranes: A Simulation Study. Journal of Physical Chemistry B, 2010, 114, 2124-2130.	1.2	15
88	Removal of N-linked glycans in cellobiohydrolase Cel7A from Trichoderma reesei reveals higher activity and binding affinity on crystalline cellulose. Biotechnology for Biofuels, 2020, 13, 136.	6.2	15
89	The Catalytic Acidâ€“Base in GH109 Resides in a Conserved GGHGG Loop and Allows for Comparable Î±-Retaining and Î²-Inverting Activity in an N-Acetylgalactosaminidase from Akkermansia muciniphila. ACS Catalysis, 2020, 10, 3809-3819.	5.5	15
90	Isoform-Specific Substrate Inhibition Mechanism of Human Tryptophan Hydroxylase. Biochemistry, 2017, 56, 6155-6164.	1.2	14

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91	Conformational Stability Study of a Therapeutic Peptide Plectasin Using Molecular Dynamics Simulations in Combination with NMR. Journal of Physical Chemistry B, 2019, 123, 4867-4877.	1.2	14
92	Evaluation of a concerted vs. sequential oxygen activation mechanism in Î±-ketoglutarateâ€“dependent nonheme ferrous enzymes. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5152-5159.	3.3	14
93	Structure and thermodynamics of vapor condensate in a finite system. The Journal of Physical Chemistry, 1991, 95, 909-920.	2.9	13
94	Pair correlation function integrals: Computation and use. Journal of Chemical Physics, 2011, 135, 084113.	1.2	13
95	Glycosylation of Thermomyces lanuginosa lipase enhances surface binding towards phospholipids, but does not significantly influence the catalytic activity. Colloids and Surfaces B: Biointerfaces, 2002, 26, 125-134.	2.5	12
96	Residue 259 in Protein-Tyrosine Phosphatase PTP1B and PTPÎ± Determines the Flexibility of Glutamine 262. Biochemistry, 2004, 43, 8418-8428.	1.2	12
97	Substrate Recognition in the Escherichia coli Ammonia Channel AmtB: A QM/MM Investigation. Journal of Physical Chemistry B, 2010, 114, 11859-11865.	1.2	12
98	The dynamic response of a fungal lipase in the presence of charged surfactants. Colloids and Surfaces B: Biointerfaces, 2002, 26, 84-101.	2.5	11
99	Total correlation function integrals and isothermal compressibilities from molecular simulations. Fluid Phase Equilibria, 2008, 273, 1-10.	1.4	11
100	Revealing the Compact Structure of Lactic Acid Bacterial Heteroexopolysaccharides by SAXS and DLS. Biomacromolecules, 2017, 18, 747-756.	2.6	11
101	Virtual Bioprospecting of Interfacial Enzymes: Relating Sequence and Kinetics. ACS Catalysis, 2022, 12, 7427-7435.	5.5	11
102	Thermodynamic models from fluctuation solution theory analysis of molecular simulations. Fluid Phase Equilibria, 2007, 261, 185-190.	1.4	10
103	Proof of the identity between the depletion layer thickness and half the average span for an arbitrary polymer chain. Journal of Chemical Physics, 2008, 129, 074904.	1.2	10
104	Solution structures of long-acting insulin analogues and their complexes with albumin. Acta Crystallographica Section D: Structural Biology, 2019, 75, 272-282.	1.1	10
105	Multipolar electrolyte solution models. II. Monte Carlo convergence and size dependence. Journal of Chemical Physics, 1993, 98, 1539-1545.	1.2	9
106	X-ray diffraction and molecular-dynamics studies: Structural analysis of phases in diglyceride monolayers. Physical Review E, 1998, 57, 3153-3163.	0.8	9
107	Secretory Phospholipase A₂ Activity toward Diverse Substrates. Journal of Physical Chemistry B, 2011, 115, 6853-6861.	1.2	9
108	Transmembrane Î±-Helix 2 and 7 Are Important for Small Molecule-Mediated Activation of the GLP-1 Receptor. Pharmacology, 2011, 88, 340-348.	0.9	9

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109	Exploring the Local Elastic Properties of Bilayer Membranes Using Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2014, 118, 12883-12891.	1.2	9
110	Structure and dynamics of water and lipid molecules in charged anionic DMPG lipid bilayer membranes. Journal of Chemical Physics, 2016, 144, 144904.	1.2	9
111	Small angle X-ray scattering and molecular dynamic simulations provide molecular insight for stability of recombinant human transferrin. Journal of Structural Biology: X, 2020, 4, 100017.	0.7	9
112	The Effect of Point Mutations on the Biophysical Properties of an Antimicrobial Peptide: Development of a Screening Protocol for Peptide Stability Screening. Molecular Pharmaceutics, 2020, 17, 3298-3313.	2.3	9
113	pH- and concentration-dependent supramolecular assembly of a fungal defensin plectasin variant into helical non-amyloid fibrils. Nature Communications, 2022, 13, .	5.8	9
114	Stabilization of tryptophan hydroxylase 2 by <scp>l</scp>â€phenylalanineâ€induced dimerization. FEBS Open Bio, 2016, 6, 987-999.	1.0	8
115	Investigations of Albuminâ€“Insulin Detemir Complexes Using Molecular Dynamics Simulations and Free Energy Calculations. Molecular Pharmaceutics, 2020, 17, 132-144.	2.3	8
116	Albumin-neprilysin fusion protein: understanding stability using small angle X-ray scattering and molecular dynamic simulations. Scientific Reports, 2020, 10, 10089.	1.6	8
117	Direct coordination of pterin to Fe ^{II} enables neurotransmitter biosynthesis in the pterin-dependent hydroxylases. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	8
118	Influence of surface and torsion potentials on the melting properties of a hexane monolayer on a graphite substrate. Molecular Physics, 1995, 84, 1039-1047.	0.8	7
119	Analysis of the Dynamics ofRhizomucor mieheiLipase at Different Temperatures. Journal of Biomolecular Structure and Dynamics, 1999, 16, 1003-1018.	2.0	7
120	Development of a cysteine-deprived and C-terminally truncated GLP-1 receptor. Peptides, 2013, 49, 100-108.	1.2	7
121	Synthesis and crystal structures of 2-methyl-4-aryl-5-oxo-5H-indeno [1,2-b] pyridine carboxylate derivatives. Chemistry Central Journal, 2014, 8, .	2.6	7
122	Chemoenzymatic synthesis of fluorogenic phospholipids and evaluation in assays of phospholipases A, C and D. Chemistry and Physics of Lipids, 2017, 202, 49-54.	1.5	7
123	Computing Cellulase Kinetics with a Two-Domain Linear Interaction Energy Approach. ACS Omega, 2021, 6, 1547-1555.	1.6	7
124	Binding Sites for Oligosaccharide Repeats from Lactic Acid Bacteria Exopolysaccharides on Bovine Î²-Lactoglobulin Identified by NMR Spectroscopy. ACS Omega, 2021, 6, 9039-9052.	1.6	7
125	Structure-based discovery of a new protein-aggregation breaking excipient. European Journal of Pharmaceutics and Biopharmaceutics, 2019, 144, 207-216.	2.0	6
126	Water Distribution and Clustering on the Lyophilized IgG1 Surface: Insight from Molecular Dynamics Simulations. Molecular Pharmaceutics, 2020, 17, 900-908.	2.3	6

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127	Effects of Mannose, Fructose, and Fucose on the Structure, Stability, and Hydration of Lysozyme in Aqueous Solution. Current Physical Chemistry, 2013, 3, 113-125.	0.1	5
128	In silico study of amphiphilic nanotubes based on cyclic peptides in polar and non-polar solvent. Journal of Molecular Modeling, 2016, 22, 264.	0.8	5
129	Development of a fast screening method for selecting excipients in formulations using MD simulations, NMR and microscale thermophoresis. European Journal of Pharmaceutics and Biopharmaceutics, 2021, 158, 11-20.	2.0	5
130	Combination of high throughput and structural screening to assess protein stability â€“ A screening perspective. European Journal of Pharmaceutics and Biopharmaceutics, 2022, 171, 1-10.	2.0	5
131	Electrostatics Drive Oligomerization and Aggregation of Human Interferon Alpha-2a. Journal of Physical Chemistry B, 2021, 125, 13657-13669.	1.2	5
132	Phase transitions in diglyceride monolayers studied by computer simulations, pressure-area isotherms and X-ray diffraction. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1994, 16, 1479-1485.	0.4	4
133	Assignment of sideâ€chain conformation using adiabatic energy mapping, free energy perturbation, and molecular dynamic simulations. Protein Science, 1999, 8, 25-34.	3.1	4
134	The effect of Asp54 phosphorylation on the energetics and dynamics in the response regulator protein Spo0F studied by molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2009, 75, 648-658.	1.5	4
135	Theoretical Assessment of Fluorinated Phospholipids in the Design of Liposomal Drug-Delivery Systems. Journal of Physical Chemistry B, 2016, 120, 9661-9671.	1.2	4
136	Interaction between structurally different heteroexopolysaccharides and Î²-lactoglobulin studied by solution scattering and analytical ultracentrifugation. International Journal of Biological Macromolecules, 2018, 111, 746-754.	3.6	4
137	Investigation of the pH-dependent aggregation mechanisms of GCSF using low resolution protein characterization techniques and advanced molecular dynamics simulations. Computational and Structural Biotechnology Journal, 2022, 20, 1439-1455.	1.9	4
138	Multipolar electrolyte solution models. III. Free energy of the charged and dipolar hard sphere mixture. Journal of Chemical Physics, 1993, 98, 1546-1551.	1.2	3
139	Observation of Droplet Growth and Coalescence in Phase-Separating Lennard-Jones Fluids. The Journal of Physical Chemistry, 1995, 99, 12335-12340.	2.9	3
140	Dynamics of the Substrate Binding Pocket in the Presence of an Inhibitor Covalently Attached to a Fungal Lipase. Journal of Biomolecular Structure and Dynamics, 2001, 19, 1-14.	2.0	3
141	Volume-Energy Correlations in the Slow Degrees of Freedom of Computer-Simulated Phospholipid Membranes. AIP Conference Proceedings, 2008, , .	0.3	3
142	Concentrated protein solutions investigated using acoustic levitation and small-angle X-ray scattering. Journal of Synchrotron Radiation, 2020, 27, 396-404.	1.0	3
143	Self-Interactions of Two Monoclonal Antibodies: Small-Angle X-ray Scattering, Light Scattering, and Coarse-Grained Modeling. Molecular Pharmaceutics, 2022, 19, 508-519.	2.3	3
144	Pyrazole Based Inhibitors against Enzymes of Staphylococcus aureus: A Computational Study. Journal of Proteomics and Bioinformatics, 2015, 08, .	0.4	2

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145	Studies of the oligomerisation mechanism of a cystatin-based engineered protein scaffold. Scientific Reports, 2019, 9, 9067.	1.6	2
146	Water-Intake and Water-Molecule Paths to the Active Site of Secretory Phospholipase A₂ Studied Using MD Simulations and the Tracking Tool AQUA-DUCT. Journal of Physical Chemistry B, 2020, 124, 1881-1891.	1.2	2
147	In-silicostudy of the interactions between acylated glucagon like-peptide-1 analogues and the native receptor. Journal of Biomolecular Structure and Dynamics, 0, , 1-15.	2.0	2
148	Computing at different levels of approximation: examples in molecular biology. IEEE Computational Science and Engineering, 1995, 2, 43-54.	0.6	1
149	Dipolar and chain-linking effects on the rheology of grafted chains in a nanopore under shear at different grafting densities. Physical Review E, 2001, 64, 011507.	0.8	1
150	Dynamics of Human Serum Transferrin in Varying Physicochemical Conditions Explored by Using Molecular Dynamics Simulations. Molecular Pharmaceutics, 2022, 19, 2795-2806.	2.3	1
151	Integral Equation Analysis of Homogeneous Nucleation. ACS Symposium Series, 1990, , 16-34.	0.5	0
152	Methyl 1-ethyl-3â€²-[hydroxy(naphthalen-1-yl)methyl]-1â€²-methyl-2-oxospiro[indoline-3,2â€²-pyrrolidine]-3â€²-carboxylate. Acta Crystallographica Section E: Structure Reports Online, 2014, 70, o540-o540.	0.2	0
153	Water Distribution on Protein Surface of the Lyophilized Proteins With Different Topography Studied by Molecular Dynamics Simulations. Journal of Pharmaceutical Sciences, 2022, 111, 2299-2311.	1.6	0